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Online
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Welcome to the 2021 Virtual International Symposium on Molecular Spectroscopy

On behalf of the Executive Committee, I extend a heartfelt welcome to all the attendees of the 2021 Virtual Symposium.

The Symposium presents research in fundamental molecular spectroscopy and a wide variety of related fields and applications. The continued vitality and significance of spectroscopy is annually re-affirmed by the number of talks, their variety, and the fact that many are given by students. These presentations are the heart of the meeting and are documented by this Abstract Book. Equally important is the information flowing from informal exchanges and discussions. As organizers, we strive to provide an environment that facilitates both kinds of interactions.

The essence of the meeting lies in the scientific discussions and your personal experiences this week independent of the number of times that you have attended this meeting. It is our sincere hope that you will find this meeting informative and enjoyable both scientifically and personally, whether it is your first or 50th meeting. If we can help to enhance your experience, please do not hesitate to ask the Symposium staff or the Executive Committee.

Ben McCall and Josh Vura-Weis
Symposium Co-Chairs

SCHEDULE OF TALKS

ABSTRACTS

MA. Plenary

Monday, June 21, 2021 – 8:0 AM

Room: 2021 Online Everywhere

Chair: Cathy Murphy, University of Illinois at Urbana-Champaign, Urbana, IL, USA

Welcome **8:00**

Susan Martinis, Vice Chancellor for Research and Innovation
University of Illinois at Urbana-Champaign

MA01 **8:10 – 8:50**
PREBIOTIC ASTROCHEMISTRY IN THE "THz-GAP", Susanna L. Widicus Weaver

RAO AWARDS **8:55**
Presentation of Awards by Jennifer van Wijngaarden, University of Manitoba

2019 Rao Award Winners
Mark Babin, University of California Berkeley
Lidor Foguel, Yale University
Sommer Johansen, University of California Davis

MILLER PRIZE **9:05**
Introduction by Michael Heaven, Emory University

MA02 ***Miller Prize Lecture*** **9:50 – 10:05**
ENHANCING NONLINEAR OPTICAL RESPONSE IN ARTIFICIAL STACKED 2D MATERIALS, Fang Liu

COBLENTZ AWARD **10:10**
Presentation of Award by Ellen Miseo, Coblentz Society

MA03 **10:15 – 10:55**
PARA-ORTHO HYDROGEN CONVERSION; SOLVING A 90-YEAR OLD MYSTERY, Ad van der Avoird

TA. Mini-symposium: Large Amplitude Motions

Tuesday, June 22, 2021 – 8:0 AM

Room: 2021 Online Everywhere

Chair: Sonia Melandri, University of Bologna, Bologna, Italy

TA01 ***INVITED TALK*** **8:00 – 8:02**
MOLECULES' ROTATION SIGNALS (AND THEIR OBSERVATION): TORSION, INVERSION, FLEXIBILITY, CHIRALITY, PHASE, Jens-Uwe Grabow

TA02 **8:08 – 8:09**
BROADBAND MICROWAVE AND COMPUTATIONAL STUDY OF HEXAFLUORO-O-XYLENE: HIGHLY COUPLED CF3 ROTORS, Sven Herbers, Sean Fritz, Piyush Mishra, Yongbin Kim, Lyudmila V Slipchenko, Timothy S. Zwier

TA03 **8:12 – 8:13**
2-PROPIONYLTHIOPHENE: PLANAR, OR NOT PLANAR, THAT IS THE QUESTION, Christina Dindić, Wolfgang Stahl, Ha Vinh Lam Nguyen

TA04 **8:16 – 8:17**
Ka BAND MICROWAVE SPECTRUM OF METHYL TERT-BUTYL ETHER, J. H. Westerfield, Kelly S. Meyer, Sommer L. Johansen, Kyle N. Crabtree

TA05 **8:20 – 8:21**
MENTHYL ACETATE. A NEW LINK IN THE CHAIN OF ACETATES STUDIED WITH ROTATIONAL SPECTROSCOPY, Anna Krin, Pablo Pinacho, Cristobal Perez, Melanie Schnell

TA06 **8:24 – 8:25**
MICROWAVE SPECTRA OF A POTENTIAL FOUR-FOLD INTERNAL ROTOR, PHENYLSULFUR PENTAFLUORIDE, Joshua A. Signore, Christopher Falls, Susanna L. Stephens, Daniel A. Obenchain, Carlos A Jimenez-Hoyos, S. A. Cooke, Stewart E. Novick

TA07 **8:28 – 8:29**
LOWERING THE TORSIONAL BARRIERS BY STERICAL HINDRANCE: MICROWAVE SPECTRUM OF THE THREE-TOP MOLECULE 2,6-DIMETHYLANISOLE, Lynn Ferres, Joshua Spautz, Wolfgang Stahl, Ha Vinh Lam Nguyen

TA08 **8:32 – 8:33**
LOCAL AND GLOBAL APPROACHES TO TREAT THE TORSIONAL BARRIERS OF 4-METHYL-ACETOPHENONE USING MICROWAVE SPECTROSCOPY, Sven Herbers, Sean Fritz, Piyush Mishra, Ha Vinh Lam Nguyen, Timothy S. Zwier

TA09 **8:36 – 8:37**
STERIC EFFECTS ON TWO METHYL INTERNAL ROTATIONS OF 2,6- AND 3,4-DIMETHYLFLUOROBENZENE, Safa Khemissi, Julie Melan, Ha Vinh Lam Nguyen

TA10 **8:40 – 8:41**
INTERNAL ROTATIONS OF METHYL PIVALATE BY ROTATIONAL SPECTROSCOPY, Nobuhiko Kuze, Yoshiyuki Kawashima

TA11 **8:44 – 8:45**
CHARACTERIZATION OF *SEC*-BUTOXYTRIMETHYLSILANE BY CHIRPED-PULSE FOURIER TRANSFORM MICROWAVE SPECTROSCOPY, Freya E. L. Berggötz, Himanshi Singh, Melanie Schnell

TB. Instrument/Technique Demonstration

Tuesday, June 22, 2021 – 8:0 AM

Room: 2021 Online Everywhere

Chair: Anna C. Wannenmacher, University of California, Davis, Davis, CA, USA

TB01 **8:00 – 8:01**
MIXING SYNCHROTRON RADIATION AND LASER SOURCES: DUAL-COMB SPECTROSCOPY IN THE SUBMILLIMETER-WAVE REGION, Francis Hindle, Gaël Mouret, Thomas Sandow Hearne, Olivier Pirali, Marie-Aline Martin-Drumel, Zachary Buchanan, Sophie Eliet, Jean-François Lampin

TB02 **8:04 – 8:05**
HIGH-RESOLUTION MICROSECOND-TIME-RESOLVED DUAL-COMB SPECTROSCOPY OF TRANSIENT INTERMEDIATES, Pei-Ling Luo

TB03 **8:08 – 8:09**
DIRECT FREQUENCY COMB CAVITY ENHANCED SPECTROSCOPY FOR TRACE GAS DETECTION USING MID-INFRARED INTERBAND CASCADE LASERS, Charles R. Markus, TzuLing Chen, Douglas Ober, Lukasz A. Sterczewski, Mahmood Bagheri, Mitchio Okumura

TB04 **8:12 – 8:13**
HIGH-RESOLUTION SPECTROSCOPY OF COLD SAMPLES IN SUPERSONIC BEAMS USING A QCL DUAL-COMB SPECTROMETER, Josef A. Agner, Pitt Allmendinger, Urs Hollenstein, Andreas Hugi, Karen Keppler, Markus Mangold, Frédéric Merkt, Martin Quack

TB05 **8:16 – 8:17**
HIGH-RESOLUTION COMB-BASED FOURIER TRANSFORM SPECTROSCOPY IN THE 3.3 μm AND 7.8 μm RANGE, Adrian Hjältén, Matthias Germann, Chuang Lu, Francisco Senna Vieira, Aleksandra Foltynowicz, Ibrahim Sadiek, Michael Stuhr, Karol Krzempek, Arkadiusz Hudzikowski, Aleksander Gluszek, Dorota Tomaszewska, Grzegorz Soboń

TB06 **8:20 – 8:21**
HIGH-PRECISION MID-INFRARED SPECTROSCOPY WITH A WIDELY TUNEABLE SI-TRACEABLE FREQUENCY-COMB-STABILISED QCL , Nicolas Cahuzac, Mathieu Manceau, Dang Bao An Tran, Rosa Santagata, Etienne Cantin, Olivier Lopez, Dan Xu, Michel Abgrall, Yann Le Coq, Paul-Eric Pottie, Rodolphe Le Targat, Anne Amy-Klein, Benoit Darquie

TB07 **8:24 – 8:25**
TOWARDS REAL-TIME PROCESSING OF DUAL-COMB SPECTROSCOPY DATA WITH QUANTUM CASCADE LASERS, Michele Gianella, Simon Vogel, Béla Tuzson, Akshay Nataraj, Kenichi Komagata, Stéphane Schilt, Thomas Südmeyer, Andreas Hugi, Markus Mangold, Pierre Jouy, Filippos Kapsalidis, Johannes Hillbrand, Mattias Beck, Jérôme Faist, Lukas Emmenegger

TB08 **8:28 – 8:29**
TWO-COLOR, INTRACAVITY PUMP-PROBE, CAVITY RINGDOWN SPECTROSCOPY, Jun Jiang, A. Daniel McCartt

TB09 **8:32 – 8:33**
MEASURING ROTATIONAL SPECTRA IN EXCITED VIBRATIONAL MODES: A NEW TECHNIQUE BASED ON A QUANTUM CASCADE LASER-PUMPED MOLECULAR LASER, Paul Chevalier, Arman Amirzhan, Marco Piccardo, Federico Capasso, Henry O. Everitt

TB10 **8:36 – 8:37**
DEVELOPMENT OF A CBGB SOURCE AND A QCL LASER SYSTEM FOR STUDYING THE IR SPECTROSCOPY OF CLUSTERS, Gregory T. Pullen, Gary E. Douberly, Heather Lewandowski

TB11 **8:40 – 8:41**
HIGH-TEMPERATURE HYPERSONIC LAVAL NOZZLE FOR NON-LTE CAVITY RINGDOWN SPECTROSCOPY, Eszter DUDÁS, Robert Georges, Abdessamad Benidar, Shuvayan Brahmachary, Vinayak Kulkarni, Samir Kassi, Christine Charles, Nicolas Suas-David

TB12 **8:44 – 8:45**
INTRACAVITY LASER SPECTROSCOPY INTEGRATED WITH FOURIER TRANSFORM DETECTION, Jack C Harms, James J O'Brien, Leah C O'Brien

TB13 **8:48 – 8:49**
CHARACTERISATION OF A 17 μm QUANTUM CASCADE LASER AND SPECTROSCOPY OF THE ν_2 FUNDAMENTAL MODE OF N_2O, Mathieu Manceau, Thomas Wall, Hadrien Philippe, Alexei Baranov, Michael Tarbutt, Roland Teissier, Benoit Darquie

TC. Dynamics and kinetics

Tuesday, June 22, 2021 – 8:0 AM

Room: 2021 Online Everywhere

Chair: Elsa Yan, Yale University, New Haven, CT, USA

TC01 ***Coblentz Society Award Lecture*** **8:00 – 8:02**
NONCOVALENT INTERACTIONS OF HYDRATED DNA AND RNA MAPPED BY 2D-IR SPECTROSCOPY, Benjamin P Fingerhut

TC02 **8:08 – 8:09**
UREA-WATER DYNAMICS IN PROTEINS: AN ULTRAFAST SPECTROSCOPIC STUDY, Sneha Banerjee, Rapti Goswami, Pankaj Mandal

TC03 **8:12 – 8:13**
STRUCTURAL FLUCTUATIONS IN AN AZEOTROPE: UNDERSTANDING THE BENZENE-METHANOL AZEOTROPE, Sneha Banerjee, Sohini Sarkar, Pankaj Mandal

TC04 **8:16 – 8:17**
ACOUSTIC STUDIES OF RELAXATION PROCESSES DUE TO CONFORMATIONAL TRANSITIONS OF FURFURAL MOLECULES, Farkhad Akhmedzhanov, Sirojiddin Zainievich Mirzaev, Kamoliddin Egamberdiev

TC05 **8:20 – 8:21**
DYNAMICS OF COPPER PHTHALOCYANINE MOLECULES INSIDE AN OPTICAL CAVITY REVEALED BY TWO-DIMENSIONAL ELECTRONIC SPECTROSCOPY (2DES), Tuphan Devkota, Kenneth L. Knappenberger, Jr.

TC06 **8:24 – 8:25**
ULTRAFAST PUMP-PROBE PHOTODISSOCIATION DYNAMICS OF CO_2 FOR THE PRODUCTION OF MOLECULAR OXYGEN, Jacob M Garcia, Scott G Sayres

TC07 **8:28 – 8:29**
USING COMPUTATIONAL CHEMISTRY TO DESIGN A PUMP-PROBE SCHEME FOR MEASURING NITROBENZENE RADICAL CATION DYNAMICS, Hugo A. López Peña, Derrick Ampadu Boateng, Shane L. McPherson, Katharine Moore Tibbetts

TC08 **8:32 – 8:33**
ULTRAFAST COULOMB EXPLOSION OF FORMIC ACID CLUSTERS AND PRODUCTION OF TRIPLY CHARGED CARBON MONOXIDE, Shaun Sutton, Scott G Sayres, tarakeshwar pilarisetty, Dane Miller

TC09 **8:36 – 8:37**
SITE-SPECIFIC CHARACTERIZATION OF P450CAM SUBSTRATE RECOGNITION *VIA* 2D IR SPECTROSCOPY, Sashary Ramos, Claire C Mammoser, Megan Thielges

TC10 **8:40 – 8:41**
THE RISE OF THE EXCITON IN SOLID AMMONIA, Andrew Cassidy, Rachel James, Anita Dawes, David Field

TC11 **8:44 – 8:45**
REIMAGINING OF OPTICAL KERR EFFECT SPECTROSCOPY: DEVELOPMENT OF A NEW SPECTROSCOPIC TECHNIQUE, Matthew M Brister, Richard Thurston, Liang Z. Tan, Thorsten Weber, Niranjan Shivaram, Daniel S. Slaughter

TC12 **8:48 – 8:49**
HIGH SENSITIVITY BROADBAND TRANSIENT ABSORPTION SPECTROSCOPY OF MOLECULAR BEAMS, Myles C Silfies, Grzegorz Kowzan, Neomi Lewis, Thomas K Allison

TD. Fundamental interest

Tuesday, June 22, 2021 – 8:0 AM

Room: 2021 Online Everywhere

Chair: Trevor Sears, Stony Brook University, Stony Brook, NY, USA

TD01 **8:00 – 8:01**
PERTURBATIONS OF THE A'$^1\Pi$ AND C$^1\Sigma^+$ STATES OF CaO, Sean Michael Bresler, Joel R Schmitz, Robert W Field, Michael Heaven

TD02 **8:04 – 8:05**
THE MOLECULAR CONSTANTS OF THE X2Σ+, A2Π, B2Σ+, AND C2Π ELECTRONIC STATES OF THE CALCIUM MONOHALIDE RADICALS, Robert W Field, Guy Taieb, Chiheb Bahrini

TD03 **8:08 – 8:09**
A LIGAND FIELD THEORY VIEW OF THE ELECTRONIC STRUCTURE OF CaX (X=F, Cl, Br, I, AND O), Robert W Field, Christopher Cummins, Michael Heaven, Guy Taieb

TD04 **8:12 – 8:13**
THE MOLECULAR CONSTANTS OF THE X$^2\Sigma^+$, A$^2\Pi$, B$^2\Sigma^+$, AND C$^2\Pi$ ELECTRONIC STATES OF THE CALCIUM MONOHALIDE RADICALS, Chiheb Bahrini, Robert W Field, Guy Taieb

TD05 **8:16 – 8:17**
THE DIATOMIC MOLECULAR SPECTROSCOPY DATABASE: DATA-SCIENCE DRIVEN APPLICATIONS, Xiangyue Liu, Stefan Truppe, Gerard Meijer, Jesús Pérez-Ríos

TD07 **8:24 – 8:25**
NONLINEAR FOURIER-TRANSFORM SPECTROSCOPY OF SINGLE GOLD NANOPARTICLES, Megan A. Steves, Kenneth L. Knappenberger, Jr.

TD08 **8:28 – 8:29**
A GENERALIZED BADGER'S RULE QUANTIFYING THE STRUCTURE-SPECTRA RELATIONSHIP FOR HYDROGEN-BONDED SYSTEMS, Mark A. Boyer, Ondrej Marsalek, Joseph P Heindel, Thomas E Markland, Anne B McCoy, Sotiris Xantheas

TD09 **8:32 – 8:33**
HIGH-SENSITIVITY FRANCK-CONDON FACTOR MEASUREMENTS ENABLED BY OPTICAL CYCLING, Benjamin Augenbraun, Zack Lasner, Nathaniel Vilas, Timothy Steimle, John M. Doyle

TD10 **8:36 – 8:37**
HIGH-RESOLUTION AND HIGH-PRECISION LASER SPECTROSCOPY OF A-BENZANTHRACENE, Masaaki Baba, Sho Yamasaki, Akiko Nishiyama, Masatoshi Misono

TD11 **8:40 – 8:41**
HIGH-RESOLUTION LASER SPECTROSCOPY OF TRANS-STILBENE : NONPLANAR STRUCTURE IN THE GROUND STATE , Akira Shimizu, Kosuke Nakajima, Shunji Kasahara, Masatoshi Misono, Masaaki Baba

TE. Comparing theory and experiment

Tuesday, June 22, 2021 – 8:0 AM

Room: 2021 Online Everywhere

Chair: Edwin Sibert, University of Wisconsin–Madison, Madison, WI, USA

TE01 **8:00 – 8:01**
ANALYSIS OF THE CORIOLIS- AND FERMI-COUPLED TRIAD NEAR 315 cm^{-1} OF BENZONITRILE ($\mathrm{C_6H_5CN}$), Maria Zdanovskaia, Brian J. Esselman, R. Claude Woods, Robert J. McMahon, Zbigniew Kisiel

TE02 **8:04 – 8:05**
BRIEF SUMMARY OF THE MILLIMETER-WAVE ROTATIONAL SPECTRA OF 2-, 3-, AND 4-CYANOPYRIDINE: THEIR VIBRATIONAL GROUND STATES AND THE CORIOLIS-COUPLED DYADS OF THEIR LOWEST-ENERGY VIBRATIONALLY EXCITED STATES , P. Matisha Dorman, Brian J. Esselman, R. Claude Woods, Robert J. McMahon

TE03 **8:08 – 8:09**
HIGH-RESOLUTION FTIR SPECTROSCOPY OF BENZALDEHYDE IN THE FAR-INFRARED REGION: PROBING THE ROTATIONAL BARRIER , Yue Liang, Yichi Zhang, Csaba Fábri, Jiarui Ma, Jianbao Zhao, Brant E. Billinghurst, Ziqiu Chen

TE04 **8:12 – 8:13**
IMPROVED SEMI-EXPERIMENTAL EQUILIBRIUM STRUCTURE DETERMINATION AND THEORETICAL PREDICTION OF HYDRAZOIC ACID ($\mathrm{HN_3}$), Andrew N. Owen, Nitai P Sahoo, Brian J. Esselman, John F. Stanton, R. Claude Woods, Robert J. McMahon

TE05 **8:16 – 8:17**
UPDATES TO AUTOFIT: PROGRESS AND PROSPECTS, Arianna T Rodriguez, Steven Shipman

TE06 **8:20 – 8:21**
MOLECULES PROBED WITH A SLOW CHIRPED-PULSE EXCITATION: ANALYTICAL MODEL OF THE FREE-INDUCTION-DECAY SIGNAL, Guillaume Dhont, Daniele Fontanari, Cédric Bray, Gaël Mouret, Arnaud Cuisset, Francis Hindle, Robin Bocquet, Kevin Hickson

TE07 **8:24 – 8:25**
FREQUENCY COMB ASSISTED, CAVITY RING-DOWN, LAMB-DIP SPECTROSCOPY OF ACETYLENE AT 1.39 μm., Antonio Castrillo, Eugenio Fasci, Stefania Gravina, Giuseppe Porzio, Livio Gianfrani

TE08 **8:28 – 8:29**
THEORY OF INTRACAVITY NEAR-RESONANT TWO-PHOTON ABSORPTION, Kevin Lehmann

TE09 **8:32 – 8:33**
CAVITY RING-DOWN SPECTROSCOPY MEASUREMENTS OF RESONANCE-ENHANCED TWO-PHOTON ABSORPTION BY $\mathrm{N_2O}$, Gang Zhao, Adam J. Fleisher, D. Michelle Bailey, Joseph T. Hodges, Kevin Lehmann

TE10 **8:36 – 8:37**
AN EDGE-SPECIFIC SCHEME FOR EQUATION-OF-MOTION COUPLED-CLUSTER CALCULATIONS OF X-RAY ABSORPTION SPECTRA, Xuechen Zheng, Chaoqun Zhang, Lan Cheng

TE11 **8:40 – 8:41**
DENSITY DEPENDENCE OF SPECTRAL DETAIL IN PRESSURIZED AND SUPERCRITICAL CARBON DIOXIDE ELECTRONIC ABSORPTION SPECTRA, Timothy W Marin, Ireneusz Janik

TE12 **8:44 – 8:45**
DYNAMICS OF NITRO-NITRITE REARRANGMENT IN NITROMETHANE RADICAL CATION, Mi'Kayla D Word, Hugo A. López Peña, Derrick Ampadu Boateng, Katharine Moore Tibbetts

TE13 **8:48 – 8:49**
TRAJECTORY-BASED SIMULATION OF FAR-INFRARED CIA PROFILES OF $\mathrm{CH_4-N_2}$ FOR MODELING TITAN'S ATMOSPHERE, Artem Finenko, Iouli E Gordon, Eamon K Conway, Bruno Bézard, Yulia N Kalugina, Daniil Chistikov, Sergei E Lokshtanov, Sergey V Petrov, Andrei Vigasin

TF. Linelists

Tuesday, June 22, 2021 – 8:0 AM

Room: 2021 Online Everywhere

Chair: Frances M Skinner, Harvard-Smithsonian Center for Astrophysics, Malden, MA, USA

TF01 **8:00 – 8:01**
HITRAN2020: ACT (ACCURACY, COMPLETENESS, TRACEABILITY), Iouli E Gordon, Laurence S. Rothman, Robert J. Hargreaves, Robab Hashemi, Ekaterina Karlovets, Frances M Skinner, Artem Finenko, Eamon K Conway, Kyle Nelson, Tijs Karman, Yan Tan, Roman Kochanov, Christian Hill

TF02 **8:04 – 8:05**
A URANIUM ATLAS IN ASCII FORMAT, 20000 – 27000 cm^{-1} , Amanda J. Ross, Patrick Crozet, Dennis W. Tokaryk, Allan G. Adam

TF03 **8:08 – 8:09**
THE ELECTRIC QUADRUPOLE SPECTRA OF DIATOMIC MOLECULES, Wilfrid Somogyi, Sergei N. Yurchenko

TF04 **8:12 – 8:13**
EXOMOL ROVIBRATIONAL LINELIST FOR NaO, Georgi B Mitev, Jonathan Tennyson, Sergei N. Yurchenko, Alexei Buchachenko, Andrey Stolyarov, Steven Taylor

TF05 **8:16 – 8:17**
AN *AB INITIO* STUDY OF ELECTRONICALLY EXCITED STATES OF SiN AND SO, Gap-Sue Kim, Ryan Brady, Nicholas Clark, Wilfrid Somogyi, Mikhail Semenov, Sergei N. Yurchenko

TF06 **8:20 – 8:21**
AB INITIO AND EMPIRICAL STUDIES OF ELECTRONICALLY EXCITED STATES OF PHOSPHOROUS MONONITRIDE (PN) AND ITS ROVIBRONIC SPECTROSCOPY , Mikhail Semenov, Nayla El-Kork, Sergei N. Yurchenko, Jonathan Tennyson

TF07 **8:24 – 8:25**
SPEED-DEPENDENT VOIGT LINESHAPE PARAMETER DATABASE USING DUAL FREQUENCY COMB LASER ABSORPTION MEASUREMENTS OF PURE AND AIR-BROADENED H_2O FROM 6656-7540 CM^{-1} UP TO 1100 K, Scott C Egbert, Nathan A Malarich, David Yun, Keeyoon Sung, Sean Coburn, Brian Drouin, Gregory B Rieker

TF08 **8:28 – 8:29**
A THEORETICAL RO-VIBRATIONAL LINE LIST OF H2CS USING A NEW APPROACH TO CONSTRUCT THE EXACT KINETIC ENERGY OPERATOR, Thomas Mellor, Sergei N. Yurchenko

TF10 **8:36 – 8:37**
MEASUREMENTS OF NEW LINE POSITIONS AND EFFECTIVE LINE INTENSITIES OF CIS-HONO OF THE ν_2 BAND AROUND 1660 cm^{-1}USING QUANTUM CASCADE LASER ABSORPTION SPECTROSCOPY , Nhut Minh Ngo, Qian Gou, Nicolas Houzel, Tong Nguyen-Ba, Cécile Coeur, Weidong Chen

TF11 **8:40 – 8:41**
SHOCKGAS-IR: A HIGH-TEMPERATURE AND HIGH-PRESSURE ABSORPTION CROSS-SECTION DATABASE, Christopher L Strand, Yiming Ding, Sarah E Johnson, Wey-Wey Su, Ronald K Hanson

TF12 **8:44 – 8:45**
A NEW STRATEGY FOR COLLECTION OF HIGH-TEMPERATURE BROAD-BAND ABSORPTION SPECTRA FOR GAS-PHASE MOLECULES IN THE MID-INFRARED, Yiming Ding, Sarah E Johnson, Christopher L Strand, Ronald K Hanson

TG. Plenary

Tuesday, June 22, 2021 – 9:0 AM

Room: 2021 Online Everywhere

Chair: Robert W Field, MIT, Cambridge, MA, USA

TG02 **9:03 – 9:43**

IMAGING ROTATIONAL WAVE PACKETS IN MOLECULES AND CLUSTERS, Yasuhiro Ohshima

TH. Mini-symposium: Large Amplitude Motions

Tuesday, June 22, 2021 – 10:0 AM

Room: 2021 Online Everywhere

Chair: Kaori Kobayashi, University of Toyama, Toyama, Japan

TH01 ***INVITED TALK*** **10:00 – 10:02**
THE EXCEL-ERATION OF METHANOL SPECTROSCOPY: ISOTOPIC TUNING OF TORSION-VIBRATION INTERACTIONS, Ronald M. Lees

TH03 **10:12 – 10:13**
A NEW PROGRAM FOR RADICALS WITH INTERNAL ROTATION, J. H. Westerfield, Kyle N. Crabtree

TH04 **10:16 – 10:17**
1- AND 2-DIMENSIONAL POTENTAL FUNCTIONS WHEN V_3 IS NOT THE BARRIER , Peter Groner

TH05 **10:20 – 10:21**
GLOBAL ANALYSIS OF THE CD_2HOH MOLECULE ROTATION-TORSION SPECTRUM, L. Margulès, R. A. Motiyenko, F. Kwabia Tchana, L. H. Coudert

TH06 **10:24 – 10:25**
NEW MEASUREMENTS AND ASSIGNMENTS IN THE v_t = 0, 1, 2 TORSIONAL STATES OF CD_3OH AND CH_3OD: FROM MILLIMETER-WAVE TO FIR SPECTRA, V. Ilyushin, Yan Bakhmat, E. A. Alekseev, Olga Dorovskaya, Holger S. P. Müller, Frank Lewen, Stephan Schlemmer, Sigurd Bauerecker, Christof Maul, K. Berezkin, Ronald M. Lees, Li-Hong Xu

TH07 **10:28 – 10:29**
A SIMULTANEOUS FIT OF THE TORSION-WAGGING-ROTATIONAL LEVELS FROM THE EXCITED (V_t = 0, 1 and 2) STATES OF METHYLAMINE USING A HYBRID (TUNNELING AND NON-TUNNELING) HAMILTONIAN FORMALISM, Isabelle Kleiner, Iwona Gulaczyk, Marek Kreglewski, R. A. Motiyenko, Prakash Gyawali, V. Ilyushin

TH08 **10:32 – 10:33**
ULTRAHIGH-RESOLUTION LASER SPECTROSCOPY OF ACETALDEHYDE : TORSION-INVERSION-ROTATION INTERACTION IN THE EXCITED STATE, Kosuke Nakajima, Akira Shimizu, Shunji Kasahara, Masatoshi Misono, Masaaki Baba

TH09 **10:36 – 10:37**
MULTI-DIMENSIONAL PROTON TUNNELING IN 2-METHYLMALONALDEHYDE, Iwona Gulaczyk, Marek Kreglewski

TH10 **10:40 – 10:41**
A UBIQUITOUS KINETIC COUPLING BETWEEN TORSION AND IN- AND OUT-OF-PLANE XH_3 WAGGING VIBRATIONS FOR AN -XH_3 GROUP ATTACHED TO A PLANAR FRAME, Jason R. Gascooke, Warren D. Lawrance

TH11 **10:44 – 10:45**
ROTATIONALLY RESOLVED $S_1 \leftarrow S_0$ ORIGIN BANDS OF DIFFERENT METHYLINDOLES AND THEIR INTERNAL ROTATION EFFECTS , Marie-Luise Hebestreit, Hilda Lartian , Hajo Böschen, W. Leo Meerts, Michael Schmitt

TH12 **10:48 – 10:49**
STUDY OF LARGE AMPLITUDE MOTIONS OF METHYL GROUP IN 9-METHYLANTHRACENE BY HIGH-RESOLUTION SPECTROSCOPY, Masatoshi Misono, Sho Yamasaki, Shunji Kasahara, Akiko Nishiyama, Masaaki Baba

TI. Instrument/Technique Demonstration

Tuesday, June 22, 2021 – 10:0 AM

Room: 2021 Online Everywhere

Chair: Brant E. Billinghurst, Canadian Light Source Inc., Saskatoon, SK, Canada

TI01 **10:00 – 10:01**
THE HEROES OF TERAHERTZ SYNCHROTRON SPECTROSCOPY, Thomas Sandow Hearne, Olivier Pirali, Marie-Aline Martin-Drumel, P. Roy, Jean-François Lampin, Marie-Hélène Mammez, Dominique Mammez, Francis Hindle, Gaël Mouret

TI02 **10:04 – 10:05**
CHARACTERIZATION OF A THZ ELECTRIC FIELD BY MOLECULAR ION SPECTROSCOPY, Florin Lucian Constantin

TI03 **10:08 – 10:09**
AN HETERODYNE SPECTROMETER FOR TERAHERTZ SPECTROSCOPY, Dominique Mammez, Marie-Hélène Mammez, Francis Hindle, Gaël Mouret, Thomas Sandow Hearne, Marie-Aline Martin-Drumel, Olivier Pirali, Sophie Eliet, Jean-François Lampin

TI04 **10:12 – 10:13**
THZ FABRY-PEROT SPECTROMETER, Francis Hindle, Coralie Elmaleh, Fabien Simon, A. Pienkina, Robin Bocquet, Arnaud Cuisset, Gaël Mouret

TI05 **10:16 – 10:17**
TECHNICAL ENHANCEMENTS OF A SUBMILLIMETER-WAVE SPECTROMETER: LABORATORY DETECTION OF NEW LINES OF METHANOL RADICAL DERIVATIVES, Jean-Thibaut Spaniol, Olivia Chitarra, Thomas Sandow Hearne, Marie-Aline Martin-Drumel, Olivier Pirali

TI06 **10:20 – 10:21**
OPTICALLY-PUMPED AMMONIA TERAHERTZ LASER UP TO 5.5 THz, Marie-Hélène Mammez, Francis Hindle, Gaël Mouret, Jean-François Lampin, Sophie Eliet, Stefano Barbieri, Marie-Aline Martin-Drumel, Olivier Pirali, P. Roy

TI07 **10:24 – 10:25**
CONSTRUCTION AND DEMONSTRATION OF A MICROWAVE THREE-WAVE MIXING SPECTROMETER AT THE MISSOURI UNIVERSITY OF SCIENCE AND TECHNOLOGY, Nicole Moon, Amanda Duerden, Joshua E. Isert, G. S. Grubbs II

TI08 **10:28 – 10:29**
TWO INSTRUMENTS IN ONE: A NEW CP-FTMW EXPERIMENTAL SETUP TO MEASURE MULTIPLE FREQUENCY BANDS SIMULTANEOUSLY , Cristobal Perez, Amanda Steber, Melanie Schnell

TI09 **10:32 – 10:33**
IMPROVING THE SENSITIVITY OF CHIRPED-PULSE FOURIER TRANSFORM MM-WAVE DETECTION IN UNIFORM SUPERSONIC FLOWS, Omar Abdelkader Khedaoui, Brian M Hays, Ilsa Rose Cooke, Thomas Sandow Hearne, Theo Guillaume, Divita Gupta, Myriam Drissi, Ian R. Sims

TI10 **10:36 – 10:37**
A CHIRP PULSE FOURIER TRANSFORM MICROWAVE SPECTROMETER WITH MULTI-ANTENNA DETECTION (MAD-CP-FTMW), Amanda Duerden, Nicole Moon, Christian Swanson, Frank E Marshall, Joshua E. Isert, Kristen Donnell, G. S. Grubbs II

TI11 **10:40 – 10:41**
A HEIGHT ADJUSTABLE LASER ABLATION SOURCE FOR A CP-FTMW SPECTROMETER AT THE MISSOURI UNIVERSITY OF SCIENCE AND TECHNOLOGY, Joshua E. Isert, Josie Glenn, Amanda Duerden, Nicole Moon, Frank E Marshall, G. S. Grubbs II

TI12 **10:44 – 10:45**
MICROWAVE SPECTROSCOPY: LINESHAPE APPROXIMATION FOR SQUARE-WAVE FREQUENCY MODULATION, E. A. Alekseev, V. Ilyushin

TI13 **10:48 – 10:49**
MILLIMETER-MILLIMETER-WAVE DOUBLE-MODULATION DOUBLE-RESONANCE SPECTROSCOPY, Oliver Zingsheim, Luis Bonah, Holger S. P. Müller, Frank Lewen, Sven Thorwirth, Stephan Schlemmer

TI14 **10:52 – 10:53**
MILLIMETER-WAVE DETECTIONS OF LASER-ABLATED SALTS WITH A MINIATURE SPECTROMETER, Alexander W Raymond, Kelvin Lee, Michael C McCarthy, Eric Mazur, Brian Drouin

TJ. Astronomy

Tuesday, June 22, 2021 – 10:0 AM

Room: 2021 Online Everywhere

Chair: Brett A. McGuire, Massachusetts Institute of Technology, Cambridge, MA, USA

TJ01 **10:00 – 10:01**
METHYL-CARBON CHAIN CHEMISTRY IN TMC-1: THE FIRST INTERSTELLAR DETECTION OF METHYL-CYANOTRIACETYLENE (CH_3C_7N), Mark A. Siebert, Anthony Remijan, Kelvin Lee, Andrew M Burkhardt, Michael C McCarthy, Brett A. McGuire

TJ02 **10:04 – 10:05**
DETECTION OF CH_3NCO IN THE GALACTIC CENTER STAR-FORMING REGION SAGITTARIUS B2(M) BY RADIO ASTRONOMICAL OBSERVATIONS, Yuki Ohno, Mitsunori Araki, Yoshiaki Minami, Takahiro Oyama, Shuro Takano, Nobuhiko Kuze, Yoshihiro Sumiyoshi, Koichi Tsukiyama

TJ03 **10:08 – 10:09**
FIRST INTERSTELLAR DETECTION OF ISOCYANODIACETYLENE (HC_4NC), THE LARGEST ISOCYANIDE MOLECULE IN THE ISM, Ci Xue, Eric R. Willis, Eric Herbst, Anthony Remijan, Ryan A Loomis, Andrew M Burkhardt, Kelvin Lee, Brett A. McGuire

TJ04 **10:12 – 10:13**
INDIVIDUAL DETECTIONS OF POLYCYCLIC AROMATIC HYDROCARBONS IN TMC-1, Andrew M Burkhardt, Kelvin Lee, Bryan Changala, Christopher N Shingledecker, Ilsa Rose Cooke, Ryan A Loomis, Hongji Wei, Steven B Charnley, Eric Herbst, Michael C McCarthy, Brett A. McGuire

TJ05 **10:16 – 10:17**
A SENSITIVE LINE SURVEY OF TMC-1: THE CHEMICAL COMPLEXITY OF A COLD DARK CLOUD, Jose Cernicharo, Carlos Cabezas, Marcelino Agúndez, Belén Tercero, Pablo de Vicente, Nuria Marcelino, Juan R. Pardo

TJ06 **10:20 – 10:21**
IDENTIFICATION OF PHOSPHORUS MONOXIDE ($X^2\Pi_r$) IN THE ORION MOLECULAR CLOUD: FURTHER EVIDENCE FOR THE UBIQUITOUS P-O BOND, Jacob Bernal, Lucy M. Ziurys, Lilia Koelemay

TJ08 **10:28 – 10:29**
RADIAL LOCATION OF SGR B2 MEASURED FROM H_3^+ AND H_2O^+ ABSORPTION SPECTRA, Takeshi Oka, Thomas R. Geballe

TJ09 **10:32 – 10:33**
METHANOL AT THE EDGE OF THE GALAXY: NEW OBSERVATIONS TO CONSTRAIN THE GALACTIC HABITABLE ZONE, Jacob Bernal, Lucy M. Ziurys, Cathryn Sephus

TJ10 **10:36 – 10:37**
PUSHING THE LIMITS OF MOLECULAR COMPLEXITY IN THE OUTER GALAXY - THE SEARCH FOR FORMAMIDE (NH_2CHO) AT VARIOUS GALACTOCENTRIC DISTANCES, Maryam Hami, Anthony Remijan

TJ11 **10:40 – 10:41**
COMPLEX ENVELOPE CHEMISTRY AND DYNAMICS OF NML CYGNUS, Ambesh Pratik Singh, Jessica L Edwards, Lucy M. Ziurys

TJ12 **10:44 – 10:45**
RESOLVING THE NEW CHEMICALLY-ACTIVE OUTFLOW HH114, Aditya Pothanaboyina, Andrew M Burkhardt, Qizhou Zhang

TJ13 **10:48 – 10:49**
MOLECULES IN OUTFLOW OF HIGH-MASS PROTOSTAR IRAS 20126-4104, Bore Gao, Andrew M Burkhardt, Qizhou Zhang

TJ14 **10:52 – 10:53**
ALMA CN ZEEMAN OBSERVATIONS OF AS 209: LIMITS ON MAGNETIC FIELD STRENGTH AND MAGNETICALLY DRIVEN ACCRETION RATE, Rachel E. Harrison, Leslie Looney, Ian Stephens, Zhi-Yun Li, Richard Teague, Richard Crutcher, Haifeng Yang, Erin Guilfoil Cox, Manuel Fernandez-Lopez, Hiroko Shinnaga

TJ15 **10:56 – 10:57**
A SEARCH FOR LIGHT HYDRIDES IN THE ENVELOPES OF EVOLVED STARS, Mark A. Siebert, Anthony Remijan, Brett A. McGuire, Christopher N Shingledecker, Andrew M Burkhardt

TK. Comparing theory and experiment

Tuesday, June 22, 2021 – 10:0 AM

Room: 2021 Online Everywhere

Chair: Karl K. Irikura, National Institute of Standards and Technology, Gaithersburg, MD, USA

TK01 **10:00 – 10:01**
VAPOR-PHASE INFRARED AND RAMAN SPECTRA AND THEORETICAL INVESTIGATIONS OF π-TYPE INTRAMOLECULAR HYDROGEN BONDING IN 3-CYCLOPENTEN-1-OL AND 3-CYCLOPENTEN-1-AMINE, Esther Juliana Ocola, Jaan Laane

TK02 **10:04 – 10:05**
VIBRATIONAL SPECIFICITY OF PROTON-TRANSFER DYNAMICS IN ELECTRONICALLY EXCITED 6-HYDROXY-2-FORMYLFULVENE, Lidor Foguel, Zachary Vealey, Patrick Vaccaro

TK03 **10:08 – 10:09**
THE MYSTERIOUS CASE OF THE MISSING NH STRETCH TRANSITION, Karl N. Blodgett, Timothy S. Zwier, Edwin Sibert

TK04 **10:12 – 10:13**
ABNORMAL RAMAN BANDS OF AROMATICAL AMINES AND BENZYL RADICALS ADSORBED ON METAL SURFACES, De-Yin Wu, Zhong-Qun Tian

TK06 **10:20 – 10:21**
CONFORMATIONAL ISOMERS OF NICOTINE, NORNICOTINE AND THEIR HYDRATED CLUSTERS , Garrett D Santis, Naoya Takeda, Shun-ichi Ishiuchi, Kazuya Tsuruta, Masaaki Fujii, Sotiris Xantheas

TK07 **10:24 – 10:25**
TOWARD 0.1% UNCERTAINTY FOR CO_2 THEORETICAL IR INTENSTIES, Xinchuan Huang, David Schwenke, Timothy J. Lee

TK08 **10:28 – 10:29**
ACCURATE PREDICTION OF VIBRONIC LEVELS AND BRANCHING RATIOS FOR LASER-COOLABLE LINEAR POLYATOMIC MOLECULES: APPLICATIONS TO CAOH, SROH, AND YBOH, Chaoqun Zhang, Lan Cheng

TK09 **10:32 – 10:33**
SPECTROSCOPIC-NETWORK-ASSISTED PRECISION SPECTROSCOPY AND ITS APPLICATION TO WATER: THE EXPERIMENT, Roland Tóbiás, Tibor Furtenbacher, Attila Császár, Irén Simkó, Meissa Diouf, Frank M.J. Cozijn, Edcel John Salumbides, Wim Ubachs

TK10 **10:36 – 10:37**
SPECTROSCOPIC-NETWORK-ASSISTED PRECISION SPECTROSCOPY AND ITS APPLICATION TO WATER: THEORETICAL FRAMEWORK, Roland Tóbiás, Tibor Furtenbacher, Attila Császár, Irén Simkó, Meissa Diouf, Frank M.J. Cozijn, Edcel John Salumbides, Wim Ubachs

TK11 **10:40 – 10:41**
VIBRATIONAL LAMB-DIP SPECTROSCOPY OF WATER ISOTOPOLOGUES: HYPERFINE STRUCTURE IN $H_2{}^{17}O$ AND PERTURBATIONS IN $HD^{16}O$, Meissa Diouf, Frank M.J. Cozijn, Edcel John Salumbides, Wim Ubachs, Mattia Melosso, Cristina Puzzarini, Roland Tóbiás, Attila Császár

TK12 **10:44 – 10:45**
COUPLED-CLUSTER APPROACHES TO ELECTRIC POLARIZABILITIES FOR LONG-RANGE FORCE FIELDS, Stephen L Coy, Timothy J Barnum, Robert W Field, John F. Stanton

TK13 **10:48 – 10:49**
LONG-RANGE POLARIZATION MODEL OF VIBRATIONAL AUTOIONIZATION IN RYDBERG STATES OF NITRIC OXIDE, Timothy J Barnum, Gloria Clausen, Stephen L Coy, Robert W Field

TL. Ions

Tuesday, June 22, 2021 – 10:0 AM

Room: 2021 Online Everywhere

Chair: Stephan Schlemmer, I. Physikalisches Institut, Köln, Germany

TL01 **10:00 – 10:01**
VIBRATIONAL SPECTROSCOPY OF H_2He^+ and D_2He^+, Oskar Asvany, Stephan Schlemmer, Ad van der Avoird, Tamás Szidarovszky, Attila Császár

TL02 **10:04 – 10:05**
KINETIC AND SPECTROSCOPIC STUDIES OF C_2^- IN A CRYOGENIC WIRE TRAP, Markus Nötzold, Robert Wild, Christine Lochmann, Roland Wester

TL03 **10:08 – 10:09**
THE SPECTRUM OF ν_3 BAND OF CH_3^+ IN HELIUM NANODROPLETS, Swetha Erukala, Deepak Verma, Andrey Vilesov

TL04 **10:12 – 10:13**
HIGH-RESOLUTION DOUBLE RESONANCE ACTION SPECTROSCOPY IN ION TRAPS: VIBRATIONAL AND ROTATIONAL FINGERPRINTS OF $CH_2NH_2^+$, Charles R. Markus, Sven Thorwirth, Oskar Asvany, Stephan Schlemmer

TL05 **10:16 – 10:17**
THE ν_1 VIBRATIONAL MODE OF HC_3O^+ OBSERVED AT HIGH SPECTRAL RESOLUTION, Oskar Asvany, Michael E. Harding, Stephan Schlemmer, Sven Thorwirth

TL06 **10:20 – 10:21**
NITROUS OXIDE IS NOTHING TO LAUGH ABOUT: $Au_2N_2O^+$, Kai Pollow, Marko Förstel, Taarna Studemund, Robert G. Radloff, Otto Dopfer

TL07 **10:24 – 10:25**
INFRARED SPECTROSCOPY OF SINGLE-TURN AND DOUBLE-TURN TETHERED ALPHA-HELICES IN THE GAS PHASE: DON'T LET YOUR LEFT HAND KNOW WHAT YOUR RIGHT HAND IS DOING., John T Lawler, Timothy S. Zwier

TL08 **10:28 – 10:29**
PROBING THE CONFORMATIONAL LANDSCAPE AND THERMOCHEMISTRY OF DINUCLEOTIDE ANIONS VIA HELIUM NANODROPLET INFRARED ACTION SPECTROSCOPY, Daniel A Thomas, Rayoon Chang, Eike Mucha, Maike Lettow, Kim Greis, Gerard Meijer, Gert von Helden

TL09 **10:32 – 10:33**
DOUBLE-RESONANCE SPECTROSCOPY WITH A CONTINUUM: APPLICATION TO THE Mg($3d_\delta$)Ar^+ $^2\Delta$ STATE OF $MgAr^+$, Matthieu Génévriez, Dominik Wehrli, Thomas Berglitsch, Frédéric Merkt

TL10 **10:36 – 10:37**
VIBRONIC SPECTRA OF GROUP 13 METAL-PIPERIDINE COMPLEXES, Micheal Okeke, Dong-Sheng Yang

TL11 ***Post-Deadline Abstract*** **10:40 – 10:41**
INFRARED SPECTROSCOPIC OBSERVATION OF THE MCLAFFERTY REARRANGEMENT IN IONIZED 2-PENTANONE, Yoshiyuki Matsuda, RYO YASUMOTO, Asuka Fujii

TM. Lineshapes, collisional effects

Tuesday, June 22, 2021 – 10:0 AM

Room: 2021 Online Everywhere

Chair: Keeyoon Sung, Jet Propulsion Laboratory/Caltech, Pasadena, CA, USA

TM01 **10:00 – 10:01**
INVESTIGATION OF ZEEMAN STATE-TO-STATE COLLISION-INDUCED TRANSITIONS IN NITRIC OXIDE USING TWO-COLOR POLARIZATION SPECTROSCOPY, Ziqiao Chang, Aman Satija, Robert P. Lucht

TM02 **10:04 – 10:05**
LINE MIXING STUDY ON THE NITRIC OXIDE FUNDAMENTAL BAND NEAR 5.3 MICRONS, Wey-Wey Su, Christopher Almodovar, Yiming Ding, Christopher L Strand, Ronald K Hanson

TM03 **10:08 – 10:09**
AIR-BROADENING IN NEAR-INFRARED CARBON DIOXIDE LINE SHAPES: QUANTIFYING CONTRIBUTIONS FROM O_2, N_2, AND Ar, Erin M. Adkins, David A. Long, Joseph T. Hodges

TM04 **10:12 – 10:13**
REVISING THE LINESHAPE PARAMETERS FOR AIR- AND SELF- BROADENED CO_2 LINES AT A SUB-PERCENT LEVEL, Robab Hashemi, Iouli E Gordon, Thi Ngoc Ha Tran, Roman V Kochanov, Julien Lamouroux, Yan Tan, Laurence S. Rothman

TM05 **10:16 – 10:17**
DUAL FREQUENCY COMB ABSORPTION SPECTROSCOPY OF CO_2 AT HIGH PRESSURE AND TEMPERATURE, Ryan K. Cole, Nazanin Hoghooghi, Gregory B Rieker

TM06 **10:20 – 10:21**
ADAPTATION TO HIGH RESOLUTION OF AN ALGORITHM TO RETRIEVE THE INSTRUMENT LINE SHAPE OF A FOURIER TRANSFORM SPECTROMETER, Thibault Bertin, Jean Vander Auwera

TM07 **10:24 – 10:25**
A POTASSIUM LINE SHAPE STUDY AT STELLAR ATMOSPHERIC TEMPERATURES OF BROWN DWARFS, Yiming Ding, Joshua A Vandervort, Christopher L Strand, Ronald K Hanson

TM08 **10:28 – 10:29**
CONTINUING INVESTIGATIONS OF ORTHO-PARA-DEPENDENT PRESSURE BROADENING IN THE $\nu_1 + \nu_3$ BAND OF ACETYLENE , Eisen C. Gross, Kimberly A Tsang, Trevor Sears

TM09 **10:32 – 10:33**
CO_2 COLLISION-INDUCED LINE PARAMETERS IN THE ν_3 BAND OF CH_4, Thibault Bertin, Jean Vander Auwera

TM11 **10:40 – 10:41**
COMB-ANCHORED, CAVITY RING-DOWN SPECTROSCOPY OF THE 1.27 μm BAND OF O_2, Helene Fleurbaey, Zachary Reed, Erin M. Adkins, David A. Long, Joseph T. Hodges

TM12 **10:44 – 10:45**
AB INITIO CALCULATIONS OF QUANTUM SCATTERING AND LINE-SHAPE PARAMETERS IN O_2 PERTURBED BY N_2, Maciej Grzegorz Gancewski, Hubert Jóźwiak, Franck Thibault, Ernesto Quintas Sánchez, Richard Dawes, Piotr Wcislo

TM13 **10:48 – 10:49**
SUBPERCENT AGREEMENT BETWEEN AB INITIO AND EXPERIMENTAL COLLISION-INDUCED LINE SHAPES OF CARBON MONOXIDE PERTURBED BY ARGON, Grzegorz Kowzan, Hubert Cybulski, Piotr Wcislo, Michał Słowiński, Piotr Maslowski, Alexandra Viel, Franck Thibault

TM14 ***Post-Deadline Abstract*** **10:52 – 10:53**
PREDICTION OF LINE-SHAPE PARAMETERS AND THEIR TEMPERATURE DEPENDENCES BY REQUANTIZED CLASSICAL MOLECULAR DYNAMICS SIMULATIONS, Ha Tran, Ngoc Hoa NGO, Huyen Trang NGUYEN

WA. Mini-symposium: Large Amplitude Motions

Wednesday, June 23, 2021 – 8:0 AM

Room: 2021 Online Everywhere

Chair: R. A. Motiyenko, Université de Lille, Villeneuve d'Ascq, France

WA01 ***INVITED TALK*** **8:00 – 8:02**
AB INITIO CALCULATION APPLIED TO THE STUDY OF ORGANIC NON-RIGID MOLECULES WITH (AT LEAST) THREE TORSIONAL MODES, Maria Luisa S Senent

WA02 **8:08 – 8:09**
CHALLENGES IN CONFORMATIONAL ANALYSIS OF FLEXIBLE MOLECULES, Malgorzata Biczysko

WA03 **8:12 – 8:13**
INTERNAL ROTATION AND CHLORINE NUCLEAR QUADRUPOLE COUPLING IN 2-CHLORO-4-FLUOROTOLUENE EXPLORED BY MICROWAVE SPECTROSCOPY AND QUANTUM CHEMISTRY, K.P. Rajappan Nair, Sven Herbers, Daniel A. Obenchain, Jens-Uwe Grabow, William C. Bailey, Alberto Lesarri, Ha Vinh Lam Nguyen

WA04 **8:16 – 8:17**
GUIDED DIFFUSION MONTE CARLO APPROACHES FOR STUDIES OF WATER CLUSTERS: APPLICATIONS TO WATER HEXAMER, Victor G M Lee, Mark A. Boyer, Anne B McCoy

WA05 **8:20 – 8:21**
GUIDED DIFFUSION MONTE CARLO BASED ON BONDING ENVIRONMENT: AN EFFICIENT APPROACH FOR STUDYING MOLECULAR VIBRATIONS IN PATHOLOGICAL SYSTEMS, Jacob M Finney, Anne B McCoy

WA06 **8:24 – 8:25**
LARGE AMPLITUDE MOTIONS AND π-HYDROGEN BONDING IN THE THIOPHENE–WATER COMPLEX CHARACTERIZED BY ROTATIONAL SPECTROSCOPY AND QUANTUM CHEMICAL CALCULATIONS, Weslley G. D. P. Silva, Jennifer van Wijngaarden

WA07 **8:28 – 8:29**
VIBRATIONALLY AVERAGED STRUCTURE AND FREQUENCIES OF $(XeHXe)^+$: COMPUTATIONAL MOLECULAR SPECTROSCOPY STUDY, Tsuneo Hirano, Umpei Nagashima, Masaaki Baba

WA08 **8:32 – 8:33**
LARGE AMPLITUDE MOTIONS IN THE 1,1,1,3,3,3-HEXAFLUORO-2-PROPANOL BINARY WATER COMPLEX, Bowei Wu, Nathan A. Seifert, Soenke Oswald, Yunjie Xu

WA09 **8:36 – 8:37**
LARGE AMPLITUDE MOTIONS IN 2,2,3,3,3-PENTAFLUOROPROPANOL AND ITS BINARY WATER COMPLEX, Bowei Wu, Nathan A. Seifert, Soenke Oswald, Wolfgang Jäger, Yunjie Xu

WA10 **8:40 – 8:41**
COUPLING OF TORSION AND OH-STRETCHING IN *TERT*-BUTYL HYDROPEROXIDE AND ITS RADICAL ANALOG, QOOH, Rachel M. Huchmala, Mark A. Boyer, Anne B McCoy

WB. Instrument/Technique Demonstration

Wednesday, June 23, 2021 – 8:0 AM

Room: 2021 Online Everywhere

Chair: Marie-Aline Martin-Drumel, Université Paris Saclay, CNRS , Orsay Cedex, France

WB01 **8:00 – 8:01**
ENTANGLED PHOTON SPECTROSCOPY OF MOLECULES, Scott Kevin Cushing

WB02 **8:04 – 8:05**
A NANOSECOND-RESOLVED ULTRAHIGH-DENSITY SPIN-POLARIZED HYDROGEN MAGNETOMETER, Alexandros Spiliotis, Michalis Xygkis, Konstantinos Tazes, George E. Katsoprinakis, Giorgos Vasilakis, T. Peter Rakitzis

WB03 **8:08 – 8:09**
POLARIZATION CONTROL OF ROTATIONALLY RESOLVED 2DIR SPECTROSCOPY, Grzegorz Kowzan, Myles C Silfies, Neomi Lewis, Thomas K Allison

WB04 **8:12 – 8:13**
HIGH RESOLUTION COHERENT MULTIDIMENSIONAL SPECTROSCOPY FOR OVERCOMING SEVERE SPECTRAL CONGESTION, Peter Chen

WB05 **8:16 – 8:17**
NOISE IMMUNE CAVITY ENHANCED OPTICAL HETERODYNE ZEEMAN MODULATION SPECTROSCOPY, Anna C. Wannenmacher, Charles R. Markus, Kyle N. Crabtree

WB06 ***Post-Deadline Abstract*** **8:20 – 8:21**
QUANTITY DETERMINTATION AND TRACEABILITY FOR SUPER-RESOLUTION MID-INFRARED LASER ABSORPTION SPECTROSCOPY, Zhenhui Du

WB07 **8:24 – 8:25**
THE FAR-INFRARED BEAMLINE AT THE CANADIAN LIGHT SOURCE, Brant E. Billinghurst

WB08 **8:28 – 8:29**
NEAR-FOURIER-TRANSFORM-LIMITED LONG-PULSE YAG-PUMPED DYE LASER SYSTEM, Holger Herburger, Urs Hollenstein, Frédéric Merkt

WB09 **8:32 – 8:33**
DEVELOPING PROBABLISTIC MACHINE LEARNING MODELS FOR ION IMAGING ANALYSIS, G. Stephen Kocheril, Kelvin Lee

WB10 **8:36 – 8:37**
SPECTROSCOPICALLY IDENTIFYING FROM GAS-PHASE REACTIONS OF DISTONIC BENZONITRILEH^+ RADICAL IONS IN AN ION-TRAP MASS SPECTROMETER, Oisin J. Shiels, Samuel Marlton, P. D. Kelly, Gabriel da Silva, Stephen J. Blanksby, Adam J. Trevitt

WB11 **8:40 – 8:41**
A MODULAR DESIGN FOR REACTION TRAPS IN CRYOGENIC ION TRAP MASS SPECTROMETERS, Gina Roesch, Etienne Garand

WB12 **8:44 – 8:45**
SOFTWARE IMPLEMENTATION OF A MULTI-CHANNEL, MULTI-FREQUENCY LOCK-IN AMPLIFIER , Amrut Nadgir, Daniel S. Slaughter, Richard Thurston, Matthew M Brister, Niranjan Shivaram

WB13 **8:48 – 8:49**
LLWP - A NEW LOOMIS-WOOD SOFTWARE AT THE EXAMPLE OF PROPANONE-$^{13}C_1$, Luis Bonah, Oliver Zingsheim, Sven Thorwirth, Holger S. P. Müller, Frank Lewen, J.-C. Guillemin, Stephan Schlemmer

WB14 **8:52 – 8:53**
SPATIALLY ENHANCED ELECTRIC FIELD INDUCED SECOND HARMONIC (SEEFISH) GENERATION FOR MEASUREMENTS OF ELECTRIC FIELD DISTRIBUTIONS IN GASES AND PLASMAS , Sai Raskar, Keegan Orr, Igor V. Adamovich

WC. Dynamics and kinetics

Wednesday, June 23, 2021 – 8:0 AM

Room: 2021 Online Everywhere

Chair: Scott G Sayres, Arizona State University, Tempe, AZ, USA

WC01 **8:00 – 8:01**
TIME-RESOLVED CAVITY RINGDOWN MEASUREMENTS OF HO_2 RADICAL IN A HEATED PLASMA FLOW REACTOR , Elijah R Jans, Ian Jones, Xin Yang, Anam C. Paul, Terry A. Miller, Igor V. Adamovich

WC02 **8:04 – 8:05**
MEASURING TIME-RESOLVED CONCENTRATIONS OF FREE RADICALS IN CHEMICAL REACTIONS WITH CAVITY RINGDOWN SPECTROSCOPY, Ian Jones, Elijah R Jans, Terry A. Miller, Igor V. Adamovich, John F. Stanton

WC03 **8:08 – 8:09**
SINGLE SUBSTITUTION KINETIC ISOTOPE EFFECT MEASUREMENTS FOR CH_4 + O(^{1}D) USING CAVITY RINGDOWN SPECTROSCOPY, Douglas Ober, TzuLing Chen, LINHAN SHEN, THINH Bui, Mitchio Okumura

WC04 **8:12 – 8:13**
PREDICTING FLUORESCENCE QUANTUMN YIELD of NO $A^2\Sigma^+$ VIA STATE-TO-STATE COLLISIONAL ENERGY TRANSFER MODEL, Zeyu Yan, Shengkai Wang

WC05 **8:16 – 8:17**
OBSERVING CHEMICAL REACTIONS IN LOW-TEMPERATURE SUPERSONIC FLOWS USING CHIRPED PULSE FOURIER TRANSFORM MILLIMETER WAVE SPECTROSCOPY, Theo Guillaume, Divita Gupta, Brian M Hays, Ilsa Rose Cooke, Omar Abdelkader Khedaoui, Thomas Sandow Hearne, Myriam Drissi, Ian R. Sims

WC06 **8:20 – 8:21**
SIGNATURES OF HYDROGEN ATOM QUANTUM DIFFUSION: H + N_2O REACTION IN SOLID PARAHYDROGEN, Kelly M. Olenyik, Fredrick M. Mutunga, Aaron I. Strom, David T. Anderson

WC07 **8:24 – 8:25**
N AND H TALIF MEASUREMENTS, $N_2(A^3\Sigma_u^+)$ TDLAS MEASUREMENTS, AND KINETIC MODELING OF NANOSECOND PULSE DISCHARGE PLASMAS IN N_2-H_2 MIXTURES , Xin Yang, caleb richards, Elijah R Jans, Sai Raskar, Dirk van den Bekerom, Igor V. Adamovich

WC08 **8:28 – 8:29**
CHARACTERIZATION OF HYBRID NS PULSE/RF PLASMAS AND ATMOSPHERIC PRESSURE PLASMA JETS, caleb richards, Elijah R Jans, Dirk van den Bekerom, David Kyle Mignogna, Igor V. Adamovich

WC09 **8:32 – 8:33**
KINETICS OF $N_2(A^3\Sigma_u^+$,v) GENERATION AND DECAY IN REACTING GAS MIXTURES EXCITED BY NANOSECOND PULSE DISCHARGE PLASMAS , David Kyle Mignogna, Elijah R Jans, Igor V. Adamovich

WC10 **8:36 – 8:37**
THERMAL DECOMPOSITION OF CYCLOHEXANE BY FLASH PYROLYSIS VACUUM ULTRAVIOLET PHOTOIONIZATION TIME-OF-FLIGHT MASS SPECTROMETRY: A STUDY ON THE INITIAL UNIMOLECULAR DECOMPOSITION MECHANISM, Kuanliang Shao, Xinghua Liu, Paul Jones, Ge Sun, Mariah Gomez, Blake Riser, Jingsong Zhang

WC11 **8:40 – 8:41**
THE STUDY OF DIRECT D ATOM INCORPORATION IN RADICALS AT LOW TEMPERATURE PROBED BY CHIRPED PULSE mm-WAVE SPECTROSCOPY , Nureshan Dias, Ranil Gurusinghe, Bernadette M. Broderick, Arthur Suits

WC12 **8:44 – 8:45**
REACTION DYNAMICS OF PROPARGYL + NH_2 PROBED USING CHIRPED PULSE ROTATIONAL SPECTROSCOPY IN A PULSED QUASI-UNIFORM FLOW (CPUF), Ranil Gurusinghe, Nureshan Dias, Alexander M Mebel, Arthur Suits

WC13 **8:48 – 8:49**
LASER INDUCED FLUORESCENCE MEASUREMENTS OF VIBRATIONALLY EXCITED OXYGEN PRODUCED BY RECOMBINATION OF O ATOMS, Dirk van den Bekerom, Keegan Orr, Elijah R Jans, Xin Yang, Anam C. Paul, Igor V. Adamovich

WD. Non-covalent interactions

Wednesday, June 23, 2021 – 8:0 AM

Room: 2021 Online Everywhere

Chair: Gang Feng, Chongqing University, Chongqing, China

WD01 **8:00 – 8:01**
MICROWAVE SPECTRUM OF TRIFLIC ACID DIHYDRATE AND TRIHYDRATE: EVIDENCE FOR COMPLETE PROTON TRANSFER IN A MICROSOLVATED SUPERACID , Anna Huff, Nathan Love, Kenneth R. Leopold

WD02 **8:04 – 8:05**
EVIDENCE FOR SPONTANEOUS PROTON TRANSFER IN THE COMPLEX FORMED FROM TRIFLIC ACID AND TRIMETHYLAMINE: MICROWAVE SPECTRUM AND COMPUTATIONAL ANALYSIS OF THE TRIMETHYLAMMONIUM TRIFLATE ION PAIR, Nathan Love, Anna Huff, Kenneth R. Leopold

WD03 **8:08 – 8:09**
HOW INTERMOLECULAR INTERACTIONS EFFECT ESTERIFICATION REACTIONS? A MICROWAVE STUDY OF THE GAS-PHASE COMPLEXES OF FORMIC ACID WITH TWO METHANOL DERIVATIVES AND THEIR ESTERIFICATION PRODUCTS., Wenhao Sun, Melanie Schnell

WD04 **8:12 – 8:13**
CONFORMATIONAL EQUILIBRIA BETWEEN ALDEHYDES AND ALCOHOLS: ROTATIONAL SPECTRA OF ACROLEIN-METHANOL AND ACROLEIN-ETHANOL COMPLEXES, Dingding Lv, Wentao Song, Luca Evangelisti, Assimo Maris, Sonia Melandri

WD05 **8:16 – 8:17**
ROTATIONAL SPECTROSCOPY AND CONFORMATIONAL SPACE OF GLYCEROL DIMERS, Jiarui Ma, FAN XIE, Nathan A. Seifert, Yunjie Xu

WD06 **8:20 – 8:21**
INVESTIGATING INTERMOLECULAR INTERACTIONS WITHIN NAPHTHOL DIMERS USING BROADBAND ROTATIONAL SPECTROSCOPY, Arsh Singh Hazrah, Nathan A. Seifert, Wolfgang Jäger

WD07 **8:24 – 8:25**
OBSERVATION OF 2-NAPHTHALENETHIOL HOMODIMER USING ROTATIONAL SPECTROSCOPY, Rizalina Tama Saragi, Marcos Juanes, Alberto Lesarri, Lourdes Enriquez, Martin Jaraiz

WD08 **8:28 – 8:29**
INVESTIGATING SUBSTITUENT EFFECTS IN DISPERSION-CONTROLLED ACETOPHENONE-PHENOL BALANCES, C. Zimmermann, Martin A. Suhm

WD09 **8:32 – 8:33**
BINDING SITES SWITECHED BY ALKYL SUBSTITUENTS: ROTATIONAL SIGNATURES OF $C_6H_5(CH_2)_nOH$-CO_2 (n = 0-2), Hao Wang, Junha Chen, Qian Gou

WD10 **8:36 – 8:37**
P...N PNICOGEN BONDING INTERACTION IN PHOSPHORYL CHLORIDE...NITROGEN BASES: EVIDENCE FROM MATRIX ISOLATION INFRARED SPCTROSCOPY AND QUANTUM CHEMICAL CALCULATIONS, P K Sruthi, Nagarajan Ramanathan, K Sundararajan

WE. Theory and Computation

Wednesday, June 23, 2021 – 8:0 AM

Room: 2021 Online Everywhere

Chair: Inga Ulusoy, Heidelberg University, Heidelberg, Germany

WE01 **8:00 – 8:01**
STACKED ENSEMBLE LEARNING FOR RANGE-SEPARATION PARAMETERS, Cheng-Wei Ju, Ethan French, Nadav Geva, Alexander W. Kohn, Zhou Lin

WE02 **8:04 – 8:05**
TOO MANY UNKNOWN MOLECULES IN THE LABORATORY ITSELF , Krishnan Thirumoorthy, Amir Karton, Nisha Job, Inga Ulusoy, Andrew L. Cooksy, Venkatesan S. Thimmakondu

WE03 **8:08 – 8:09**
IMPROVING SPECTRAL SYNTHESIS PERFORMANCE BY UP TO 5 ORDERS OF MAGNITUDE WITH THE DISCRETE INTEGRAL TRANSFORM APPROACH, Dirk van den Bekerom, Pankaj Mishra, Erwan Pannier

WE04 **8:12 – 8:13**
PARTICIPATION RATIO AND QUANTUM FIDELITY SUSCEPTIBILITY AS TOOLS TO CHARACTERIZE BENT-TO-LINEAR SHAPE TRANSITIONS, Jamil Khalouf-Rivera, Miguel Carvajal, Francisco Curro Pérez-Bernal

WE05 **8:16 – 8:17**
ASSIGNING THE COMPLICATED DISPERSED FLUORESCENCE SPECTRUM OF PhCCCN, James H. Thorpe, Khadija M. Jawad, Timothy S. Zwier, John F. Stanton

WE06 **8:20 – 8:21**
SUB-EV ACCURACY DELTA-COUPLED-CLUSTER CALCULATIONS FOR HETERO-SITE DOUBLE CORE-IONIZED STATES, Xuechen Zheng, Junzi Liu, Lan Cheng, Gilles Doumy, Linda Young

WE07 **8:24 – 8:25**
MODELLING THE DIPOLE MOMENT FUNCTION OF CARBON MONOXIDE CAPABLE OF PREDICTING THE ROTATIONAL DISTRIBUTION IN THE 7-0 BAND, Emile S. Medvedev, Vladimir G. Ushakov

WE08 **8:28 – 8:29**
GLOBAL ROVIBRATIONAL ANALYSIS FOR THE 20 LOWEST VIBRATIONAL BANDS OF HYDROGEN SULFIDE ($H_2^{32}S$), Miguel Carvajal, Jamil Khalouf-Rivera, Francisco Curro Pérez-Bernal, Renato Lemus

WE09 **8:32 – 8:33**
COMPUTATIONAL NMR STUDY OF ION PAIRING OF 1-DECYL-3-METHYL-IMIDAZOLIUM CHLORIDE IN MOLECULAR SOLVENTS, Dovile Lengvinaite, Vytautas Klimavicius, Vytautas Balevicius , Kestutis Aidas

WE10 **8:36 – 8:37**
XANES SPECTRA OF VANADIUM COMPLEXES CALCULATED BY TWO TDDFT METHODS, Jun Yi, Zhou Lin

WE11 **8:40 – 8:41**
COMPUTATIONAL INFRARED SPECTROSCOPY OF PHOSPHORUS-CONTAINING POTENTIAL BIOSIGNATURES, Juan C. Zapata Trujillo, Anna-Maree Syme, Keiran N. Rowell, Clara Sousa-Silva, Laura K McKemmish

WE12 **8:44 – 8:45**
MOLECULAR FRAGMENT MACHINE LEARNING TRAINING TECHNIQUES TO PREDICT CLUSTER ENERGETICS AND FREQUENCIES IN BROWN CARBON AEROSOL CLUSTERS, Emily E. Chappie, Daniel P. Tabor, Nathanael M. Kidwell

WE13 **8:48 – 8:49**
IMPROVING THE ROTATION VIBRATIONAL LINE LISTS FOR OZONE, Apoorva Upadhyay, Oleg L. Polyansky, Jonathan Tennyson, Alec Owens, Nikolay F. Zobov, Eamon K Conway

WE14 **8:52 – 8:53**
NON-ADIABATIC CALCULATIONS OF SPECTRA OF OPEN-SHELL DIATOMIC MOLECULES, Sergei N. Yurchenko

WF. Linelists

Wednesday, June 23, 2021 – 8:0 AM

Room: 2021 Online Everywhere

Chair: Amanda J. Ross, Universite de Lyon, Villeurbanne, France

WF01 **8:00 – 8:01**
LINE LISTS FOR HIGH RESOLUTION STUDIES OF EXOPLANETS, Jonathan Tennyson, Sergei N. Yurchenko

WF02 **8:04 – 8:05**
EXPANSION OF THE HITEMP DATABASE, Robert J. Hargreaves, Eamon K Conway, Iouli E Gordon, Laurence S. Rothman

WF03 **8:08 – 8:09**
THE NON-LTE SPECTROSCOPY OF MOLECULAR REACTIONS USING THE EXOMOL DATABASE, Victoria H.J. Clark, Sergei N. Yurchenko, Jonathan Tennyson

WF04 **8:12 – 8:13**
EXOPLINES: MOLECULAR ABSORPTION CROSS-SECTION DATABASE FOR BROWN DWARF AND GIANT EXOPLANET ATMOSPHERES, Ehsan Gharib-Nezhad, Aishwarya Iyer, Michael R Line, Richard S Freedman, Mark S Marley, Natasha E Batalha

WF05 **8:16 – 8:17**
MODELING PLANETARY OPACITIES WITH HITRAN AND HAPI: TEST CASE OF AMMONIA MICROWAVE ABSORPTION SPECTRA UNDER JOVIAN CONDITION, Frances M Skinner, Robert J. Hargreaves, Iouli E Gordon

WF06 **8:20 – 8:21**
MOLECULAR LINE LISTS FOR HOT ROCKY SUPER-EARTHS, Alec Owens, Sergei N. Yurchenko, Jonathan Tennyson

WF07 **8:24 – 8:25**
BUILDING A HIGH RESOLUTION LINE LIST FOR ALUMINIUM MONOXIDE, Charles A Bowesman

WF08 **8:28 – 8:29**
LINE LIST FOR THE LOWEST FOUR STATES OF NO, Qianwei Qu, Sergei N. Yurchenko, Jonathan Tennyson

WF09 **8:32 – 8:33**
UPDATING CH_4 SPECTROSCOPIC MODELS FROM 6770-7630 CM^{-1} WITH DUAL FREQUENCY COMB ABSORPTION SPECTROSCOPY UP TO 1000 K, Nathan A Malarich, David Yun, Keeyoon Sung, Scott C Egbert, Sean Coburn, Brian Drouin, Gregory B Rieker

WF10 **8:36 – 8:37**
THE SECOND RESONANCE SYSTEM OF HC_3N. NEW RO-VIBRATIONAL GLOBAL ANALYSIS FOR ALL THE EXCITED STATES BELOW 1300 cm^{-1}., Luca Bizzocchi, Mattia Melosso, Cristina Puzzarini, Filippo Tamassia, Andrea Pietropolli Charmet, Marie-Aline Martin-Drumel, Olivier Pirali, Barbara Michela Giuliano, Paola Caselli, J.-C. Guillemin

WF11 **8:40 – 8:41**
A RE-EXAMINATION OF THE QUANTITATIVE INFRARED ABSORPTION CROSS-SECTIONS OF ISOBUTANE, Kendall D. Hughey, Steven W. Sharpe, Robert L. Sams, Timothy J. Johnson, Tanya L. Myers, Thomas A. Blake

WF12 **8:44 – 8:45**
INFRARED ABSORPTION CROSS SECTIONS OF NEOPENTANE AND ETHANE, Randika Dodangodage, Peter F. Bernath, Andy Wong, Brant E. Billinghurst, Jianbao Zhao

WF13 **8:48 – 8:49**
MEASUREMENT OF CROSS-SECTIONS AND PSEUDOLINE GENERATION FOR TOLUENE(C_7H_8) IN THE 7-15 μM REGION AT 240 – 298 K, Keeyoon Sung, Deacon J Nemchick, Geoffrey C. Toon, Conor A Nixon

WG. Plenary

Wednesday, June 23, 2021 – 9:0 AM

Room: 2021 Online Everywhere

Chair: Melanie Schnell, Deutsches Elektronen-Synchrotron (DESY), Hamburg, Germany

WG02 **9:03 – 9:43**

MOLECULAR COMPLEXES ON THE BRINK OF CHEMICAL CHANGE, Kenneth R. Leopold

WH. Mini-symposium: Large Amplitude Motions

Wednesday, June 23, 2021 – 10:0 AM

Room: 2021 Online Everywhere

Chair: Miguel Carvajal, Universidad de Huelva, Huelva, Spain

WH01 **10:00 – 10:01**
EXCITED TORSIONAL STATES OF DIMETHYLETHER $(CH_3)_2O$, V. Ilyushin, Yan Bakhmat, E. A. Alekseev, Olga Dorovskaya, Brian Drouin, Stephan Schlemmer, Christian Endres

WH02 **10:04 – 10:05**
FAR-INFRARED AND MICROWAVE SPECTROSCOPY OF $HCOOCH_3$ II., Kaori Kobayashi, AKIO ITOH, Masaharu Fujitake, Nobukimi Ohashi, Dennis W. Tokaryk, Brant E. Billinghurst

WH03 **10:08 – 10:09**
MICROWAVE SPECTRUM OF ACETIC ACID: THE THIRD AND FOURTH EXCITED TORSIONAL STATES, V. Ilyushin, Yan Bakhmat, Olga Dorovskaya, E. A. Alekseev

WH04 **10:12 – 10:13**
EXTENDING THE MILLIMETER/SUBMILLIMETER ROTATIONAL SPECTRUM OF GROUND STATE PYRUVIC ACID, Connor J. Wright, Jay A Kroll, Susanna L. Widicus Weaver

WH05 **10:16 – 10:17**
LARGE AMPLITUDE TORSIONS IN NITROTOLUENE ISOMERS STUDIED BY ROTATIONAL SPECTROSCOPY AND QUANTUM CHEMISTRY CALCULATIONS, Anthony Roucou, Manuel Goubet, Sabath Bteich, Isabelle Kleiner, Arnaud Cuisset

WH06 **10:20 – 10:21**
NEXT LEVEL ACHIEVEMENT OF THE *XIAM* CODE IN MODELING MICROWAVE SPECTRA OF MOLECULES WITH VERY LOW TORSIONAL BARRIERS, Ha Vinh Lam Nguyen, Sven Herbers, K.P. Rajappan Nair, Jens-Uwe Grabow

WH07 **10:24 – 10:25**
INTERNAL ROTATION OF THE ACETYL METHYL GROUP IN METHYL ALKYL KETONES: THE MICROWAVE SPECTRUM OF OCTAN-2-ONE, Maike Andresen, Damian Schoengen, Isabelle Kleiner, Martin SCHWELL, Wolfgang Stahl, Ha Vinh Lam Nguyen

WH08 **10:28 – 10:29**
COMBINATION OF IODINE QUADRUPOLE COUPLING AND ESSENTIALLY FREE METHYL INTERNAL ROTATION IN 3-IODOTOLUENE, Joshua A. Signore, Ha Vinh Lam Nguyen, Wallace C. Pringle, S. A. Cooke, Stewart E. Novick

WH09 **10:32 – 10:33**
STRUCTURE AND DYNAMICS OF METHACRYLAMIDE, Assimo Maris, Sonia Melandri, Luca Evangelisti, Camilla Calabrese

WH10 **10:36 – 10:37**
THE EFFECTS OF PROTON TUNNELLING, ^{14}N QUADRUPOLE COUPLING, AND METHYL INTERNAL ROTATIONS OF PLANAR SECONDARY AMINES, Kenneth J Koziol, Wolfgang Stahl, Ha Vinh Lam Nguyen

WH11 **10:40 – 10:41**
ACCURATE TORSIONAL BARRIER HEIGHT OF TRIFLUROACETIC ACID, Luyao Zou, R. A. Motiyenko, L. Margulès

WI. Mini-symposium: Precision Spectroscopy for Fundamental Physics

Wednesday, June 23, 2021 – 10:0 AM

Room: 2021 Online Everywhere

Chair: Benoit Darquie, Laboratoire de Physique des Lasers, Villetaneuse, France

WI01 ***INVITED TALK*** **10:00 – 10:02**
PRECISION MEASUREMENTS IN FEW-ELECTRON ATOMS AND MOLECULES, Frederic Merkt

WI02 **10:08 – 10:09**
MEASUREMENTS OF np–2s TRANSITIONS IN THE HYDROGEN ATOM, Simon Scheidegger, Josef A. Agner, Hansjürg Schmutz, Frédéric Merkt

WI03 **10:12 – 10:13**
DETERMINATION OF THE IONIZATION ENERGY OF THE METASTABLE 2 $^1S_0$ STATE OF ^{4}He THROUGH RYDBERG-SERIES EXTRAPOLATION, Gloria Clausen, Paul Jansen, Josef A. Agner, Hansjürg Schmutz, Frédéric Merkt

WI04 **10:16 – 10:17**
PHOTOLYSIS PRODUCTION AND PRECISION MEASUREMENT OF THE HIGHEST VIBRATIONAL STATES ($v = 14$) AND QUASI-BOUND RESONANCES IN $X^1\Sigma_g^+$ H_2, Kin Fung Lai, Maximilian Beyer, Edcel John Salumbides, Wim Ubachs

WI05 **10:20 – 10:21**
IONIZATION ENERGIES OF PARA-H_2 FROM ZERO-QUANTUM-DEFECT POSITIONS, Nicolas Hölsch, Frédéric Merkt

WI06 **10:24 – 10:25**
PRECISION MEASUREMENT OF THE IONIZATION AND DISSOCIATION ENERGIES OF THE DEUTERIUM MOLECULE, Joël Hussels, Nicolas Hölsch, Maximilian Beyer, Edcel John Salumbides, Christian Jungen, Frédéric Merkt, Wim Ubachs

WI07 **10:28 – 10:29**
PRECISE MEASUREMENT OF A FUNDAMENTAL VIBRATIONAL TRANSITION FREQUENCY IN HD, Arthur Fast, Samuel Meek

WI08 **10:32 – 10:33**
SUB-DOPPLER FREQUENCY METROLOGY IN HD FOR TESTS OF FUNDAMENTAL PHYSICS, Frank M.J. Cozijn, Meissa Diouf, Edcel John Salumbides, Wim Ubachs

WI09 **10:36 – 10:37**
COMB-CALIBRATED NONLINEAR SPECTROSCOPY OF THE Q(1) 1-0 LINE OF MOLECULAR HYDROGEN , Marco Lamperti, Lucile Rutkowski, Daniele Ronchetti, Davide Gatti, Riccardo Gotti, Giulio Cerullo, Franck Thibault, Hubert Jóźwiak, Szymon Wojtewicz, Piotr Maslowski, Piotr Wcislo, Dario Polli, Marco Marangoni

WI10 **10:40 – 10:41**
A WIDELY TUNABLE HIGH-POWER CONTINUOUS-WAVE OPTICAL PARAMETRIC OSCILLATOR (CW-OPO) SYSTEM FOR MID-INFRARED SPECTROSCOPY AND FREQUENCY METROLOGY, Hamzeh Telfah, S M Shah Riyadh, Jinjun Liu, David B. Foote, Walter Hurlbut, Matthew J. Cich, Ulrich Eismann, Adam Heiniger, Chris Haimberger

WI11 **10:44 – 10:45**
NARROW LINEWIDTH OPO LIGHT SOURCE FOR PRECISION SPECTROSCOPY, Zitan Zhang, Cunfeng Cheng, Yu Robert Sun, Shui-Ming Hu

WI12 **10:48 – 10:49**
PRECISE FREQUENCY MEASUREMENTS OF THE $2\nu_3$ A_1 - ν_3 BAND TRANSITIONS OF METHANE WITH COMB-REFERENCED INFRARED-INFRARED DOUBLE-RESONANCE , Hiroyuki Sasada, Sho Okubo, Hajime Inaba, Shoko Okuda

WI13 **10:52 – 10:53**
COMB-LOCKED CAVITY RING-DOWN SPECTROSCOPY FOR MOLECULAR TRANSITION FREQUENCY MEASUREMENTS BELOW 10^{-12} RELATIVE UNCERTAINTY, Zachary Reed, David A. Long, Helene Fleurbaey, Joseph T. Hodges

WI14 **10:56 – 10:57**
COMB-LOCKED CAVITY-ASSISTED DOUBLE RESONANCE (COCA-DR) SPECTROSCOPY OF MOLECULES WITH kHz ACCURACY, Changle Hu, Valery Perevalov, Cunfeng Cheng, Tian-Peng Hua, An-Wen Liu, Yu Robert Sun, Jin Wang, Yan Tan, Shui-Ming Hu

WJ. Astronomy

Wednesday, June 23, 2021 – 10:0 AM

Room: 2021 Online Everywhere

Chair: Harshal Gupta, National Science Foundation, Alexandria, VA, USA

WJ01 **10:00 – 10:01**
HIGH-RESOLUTION GIGAHERTZ AND TERAHERTZ SPECTROSCOPY OF THE ISOTOPICALLY CHIRAL MOLECULE TRANS-2,3-DIDEUTERO-OXIRANE(c-CHD-CHDO) , Ziqiu Chen, Sieghard Albert, Karen Keppler, Martin Quack, Volker Schurig, Oliver Trapp

WJ02 **10:04 – 10:05**
MICROWAVE AND MILLIMETER WAVE SPECTRUM OF STYRENE OXIDE $C_6H_5C_2H_3O$, Pascal Stahl, Benjamin E Arenas, Sergio R Domingos, Guido W Fuchs, Melanie Schnell, Thomas Giesen

WJ03 **10:08 – 10:09**
THE PURE ROTATIONAL SPECTRUM OF THE HYDROXYMETHYL RADICAL REINVESTIGATED TO ENABLE ITS INTERSTELLAR DETECTION, Olivia Chitarra, Marie-Aline Martin-Drumel, Bérenger Gans, Olivier Pirali, Silvia Spezzano, Valerio Lattanzi, Holger S. P. Müller, J.-C. Loison

WJ04 **10:12 – 10:13**
SUBMILLIMETER WAVE INVESTIGATION OF TWO FORMAMIDE ISOMERS: FORMALDOXIME (CH_2NOH) AND NITROSOMETHANE (CH_3NO), Luyao Zou, L. Margulès, R. A. Motiyenko, J.-C. Guillemin

WJ05 **10:16 – 10:17**
A ROTATIONAL STUDY OF INTERSTELLAR ACETOHYDROXAMIC ACID, A GLYCINE ISOMER , Miguel Sanz Novo, Iker León, Santiago Mata, José L. Alonso

WJ06 **10:20 – 10:21**
MICROWAVE AND MILLIMETER WAVE SPECTRUM OF FIVE CONFORMERS OF CYSTEAMINE AND SEARCH IN SAGITTARIUS B2(N), Wentao Song, Assimo Maris, Luca Evangelisti, Dingding Lv, Sonia Melandri

WJ07 **10:24 – 10:25**
MILLIMETER-WAVE SPECTRA OF 5-METHYL HYDANTOIN IN ITS VIBRATIONALLY EXCITED STATES, Minami Awadu, Hiroyuki Ozeki, Kaori Kobayashi, Soichiro Watanabe

WJ08 **10:28 – 10:29**
LABORATORY SPECTROSCOPY OF ALLYLIMINE AND ITS TENTATIVE DETECTION IN THE INTERSTELLAR MEDIUM, Mattia Melosso, Luca Bizzocchi, Ningjing Jiang, Davide Alberton, Paola Caselli, Victor Manuel Rivilla, Andrea Pietropolli Charmet, Luca Dore, Cristina Puzzarini

WJ09 **10:32 – 10:33**
HIGH TEMPERATURE FOURIER TRANSFORM SPECTROSCOPY OF THE B $^1\Pi$ - X $^1\Sigma^+$ TRANSITION OF ZrO, Jason J Sorensen, Peter F. Bernath

WJ10 **10:36 – 10:37**
THE PURE ROTATIONAL SPECTRUM OF THE SiP RADICAL ($X^2\Pi_i$), Mark Burton, Phillip M. Sheridan, Lucy M. Ziurys

WJ11 **10:40 – 10:41**
HIGH RESOLUTION INFRARED SPECTROSCOPY OF CYANO-OXIRANE (c-C_2H_3OCN) , Sieghard Albert, Ziqiu Chen, Karen Keppler, Philippe Lerch, Carine Manca Tanner, Martin Quack, Jürgen Stohner

WJ12 **10:44 – 10:45**
HIGH-RESOLUTION INFRARED SPECTROSCOPY OF DC_3N IN THE STRETCHING REGION, Ningjing Jiang, Mattia Melosso, Filippo Tamassia, Luca Bizzocchi, Luca Dore, Elisabetta Canè, Davide Fedele, J.-C. Guillemin, Cristina Puzzarini

WJ13 **10:48 – 10:49**
STUDIES OF IRON MONODEUTERIDE, FeD, VIA LASER EXCITATION SPECTROSCOPY AND DISPERSED FLUORESCENCE SPECTROSCOPY, Dennis W. Tokaryk, Allan G. Adam, Ryan A. R. Harvey

WJ14 **10:52 – 10:53**
IMPROVED CENTRIFUGAL AND HYPERFINE ANALYSIS OF ND_2H AND NH_2D AND ITSAPPLICATION TO THE SPECTRAL LINE SURVEY OF L1544, Mattia Melosso, Luca Bizzocchi, Luca Dore, Zbigniew Kisiel, Ningjing Jiang, Jürgen Gauss, Cristina Puzzarini

WK. Theory and Computation

Wednesday, June 23, 2021 – 10:0 AM

Room: 2021 Online Everywhere

Chair: John F. Stanton, University of Florida, Gainesville, FL, USA

WK01 **10:00 – 10:01**
UTILIZATION OF NEURAL NETWORKS FOR GPU-ACCELERATED DIFFUSION MONTE CARLO FOR VIBRATIONAL PROBLEMS, Fenris Lu, Ryan J. DiRisio, Anne B McCoy

WK02 **10:04 – 10:05**
DIFFUSION MONTE CARLO USING MACHINE LEARNING POTENTIAL ENERGY SURFACES, Ryan J. DiRisio, Mark A. Boyer, Jacob M Finney, Fenris Lu, Anne B McCoy

WK03 **10:08 – 10:09**
PHYSICS-GUIDED CURVE FITTING FOR POTENTIAL-ENERGY FUNCTIONS OF DIATOMIC MOLECULES, Karl K. Irikura

WK04 **10:12 – 10:13**
JIM WATSON AND THE THEORY OF VIBRATION-ROTATION INTERACTION, Takeshi Oka

WK05 **10:16 – 10:17**
A SPARSE LINEAR ALGEBRAIC APPROACH TO ARBITRARY-ORDER VIBRATIONAL PERTURBATION THEORY, Mark A. Boyer, Anne B McCoy

WK06 ***Post-Deadline Abstract*** **10:20 – 10:21**
RECONSTRUCTION OF TERM DIAGRAMS WITHOUT USING A MODEL HAMILTONIAN, Stefan Brackertz, Sven Kristkeitz, Oskar Asvany, Stephan Schlemmer

WK07 **10:24 – 10:25**
A DISCRETE VARIABLE APPROACH FOR INVESTIGATING TUNNELING SPLITTINGS AND VIBRATIONAL WAVE FUNCTIONS IN RARE GAS-ASYMMETRIC TOP HETERODIMERS, Ezra Arumi Alexander, Mark D. Marshall, Helen O. Leung

WK08 **10:28 – 10:29**
VARIATIONAL ROVIBRATIONAL CALCULATION FOR LINEAR TETRAATOMIC MOLECULES: I. THE C8V4 APPROACH, Benjamin Schröder

WK09 **10:32 – 10:33**
VARIATIONAL ROVIBRATIONAL CALCULATION FOR LINEAR TETRAATOMIC MOLECULES: II. THE B11244 STORY RETOLD, Benjamin Schröder, Peter Sebald

WK11 ***Post-Deadline Abstract*** **10:40 – 10:41**
SIMULATION OF THE ABSORPTION SPECTRUM OF CHLORINE PEROXIDE (ClOOCl), Megan R Bentley, John F. Stanton

WK12 **10:44 – 10:45**
VIBRONICALLY COUPLED STATES: COMPUTATION AND CHARACTERIZATION OF VIBRONIC AND ROVIBRONIC SPECTROSCOPIC PARAMETERS, Ketan Sharma, Terry A. Miller, John F. Stanton

WK13 **10:48 – 10:49**
VIBRONIC AND SPIN ANGULAR MOMENTUM IN ROTATIONALLY RESOLVED SPECTRA OF JAHN-TELLER ACTIVE MOLECULES, Ketan Sharma, Terry A. Miller, John F. Stanton

WK14 **10:52 – 10:53**
ACCURATE PREDICTION OF VIBRONIC LEVELS AND BRANCHING RATIOS FOR LASER-COOLABLE LINEAR POLYATOMIC MOLECULES: THE CONSTRUCTION OF THE QUASIDIABATIC HAMILTONIAN, Chaoqun Zhang, Lan Cheng

WL. Large molecules

Wednesday, June 23, 2021 – 10:0 AM

Room: 2021 Online Everywhere

Chair: Etienne Garand, University of Wisconsin-Madison, Madison, WI, USA

WL01 **10:00 – 10:01**
ELECTRONIC AND INFRARED PHOTODISSOCIATION SPECTROSCOPY OF THE GREEN FLUORESCENT PROTEIN CHROMOPHORE IN VACUO, Wyatt Zagorec-Marks, Madison M. Foreman, J. Mathias Weber

WL02 **10:04 – 10:05**
MICROSOLVATION OF THE GREEN FLUORESCENT PROTEIN CHROMOPHORE ONE WATER MOLECULE AT A TIME, Wyatt Zagorec-Marks, Madison M. Foreman, J. Mathias Weber

WL03 **10:08 – 10:09**
LOST AND BOUND: UNDERSTANDING THE ELECTRON DETACHMENT PATHWAYS OF THE TETRACENYL ANION ISOMERS, Cole R Sagan, Etienne Garand

WL04 **10:12 – 10:13**
LABORATORY IR SPECTRA OF PROTONATED FULLERENES, Julianna Palotás, Jonathan K Martens, Giel Berden, Jos Oomens

WL05 **10:16 – 10:17**
ELECTRONIC AND INFRARED PHOTODISSOCIATION SPECTROSCOPY OF PROTOPORPHYRIN IN VACUO, Wyatt Zagorec-Marks, Madison M. Foreman, J. Mathias Weber

WL06 **10:20 – 10:21**
STRUCTURAL CHARACTERIZATION OF METAL BIPYRIDINE COMPLEXES VIA CRYOGENIC ION SPECTROSCOPY, Madison M. Foreman, Wyatt Zagorec-Marks, J. Mathias Weber

WL07 **10:24 – 10:25**
THE ROTATIONAL SPECTRA OF FLAVONE AND FLAVANONE: LASER ABLATION AND HEATING METHODS FOR VAPORIZATION., Susana Blanco, Alberto Macario, Juan Carlos Lopez

WL09 **10:32 – 10:33**
A ROTATIONAL STUDY OF 1-SUBSTITUTED BARBARALONES, Mauro Mato, Miguel Sanz Novo, Iker León, Elena R. Alonso, Antonio M Echavarren, José L. Alonso

WL10 **10:36 – 10:37**
DAPPERS: A NEW PROGRAM FOR THE RAPID ASSIGNMENT AND FITTING OF DENSE ROTATIONAL SPECTRA BASED ON SPECTRAL PROGRESSIONS , Nathan Love, Anna Huff, Kenneth R. Leopold

WL11 **10:40 – 10:41**
A MICROWAVE AND COMPUTATIONAL STUDY OF CARBOXYLIC ACID ANHYDRIDES, Nathan Love, Anna Huff, Kenneth R. Leopold

WL12 **10:44 – 10:45**
MICROWAVE AND COMPUTATIONAL STUDIES OF HYDRATED ACID ANHYDRIDES: CAPTURING A LOCAL POTENTIAL ENERGY MINIMUM AND EXPLORING THE EFFECT OF $C(CH_3)_3$ AND CF_3 SUBSTITUENTS, Nathan Love, Anna Huff, Kenneth R. Leopold

WL13 ***Post-Deadline Abstract*** **10:48 – 10:49**
CHEMO-DYNAMICAL MODELING OF CHA-MMS1 TO PREDICT NEW SOLID-PHASE SPECIES FOR DETECTION WITH JWST , Miwha Jin, Kaho Lam, Jeroen Terwisscha van Scheltinga, Robin T. Garrod, Zhi-Yun Li, Melissa K McClure, Adwin Boogert, Eric Herbst

WM. Radicals

Wednesday, June 23, 2021 – 10:0 AM

Room: 2021 Online Everywhere

Chair: Mitchio Okumura, California Institute of Technology, Pasadena, CA, USA

WM01 **10:00 – 10:01**
MEASUREMENT OF THE $\tilde{A}\leftarrow\tilde{X}$ BAND OF 1- AND 2-METHYLALLYL RADICALS USING CAVITY RINGDOWN SPECTROSCOPY, Charles R. Markus, Wen Chao, Gregory H Jones, Mitchio Okumura

WM02 **10:04 – 10:05**
HIGH-RESOLUTION INFRARED SPECTROSCOPY OF JET COOLED HCBr SINGLET BROMOCARBENE DIRADICAL, Ya-Chu Chan, Andrew Kortyna, David Nesbitt

WM03 **10:08 – 10:09**
INFRARED SPECTRUM OF THE 1-IODOPROPYL RADICAL PRODUCED FROM REACTION OF I + PROPENE IN SOLID PARA-HYDROGEN , Wei Lin, Huei-Ru Tsai, Yu-Hsuan Chen, Yuan-Pern Lee

WM04 **10:12 – 10:13**
INFRARED SPECTRA OF GASEOUS (Z)-3-IODO-BUT-2-EN-1-YL [$C_2H_3C(CH_3)I$] RADICAL, METHYL VINYL KETONE OXIDE [$C_2H_3C(CH_3)OO$] CRIEGEE INTERMEDIATE, AND $C_2H_3CI(CH_3)OO$ PEROXY RADICAL PRODUCED UPON PHOTODISSOCIATION OF (Z)-1,3-DIIODO-BUT-2-ENE [$(CH_2I)HC=C(CH_3)I$] IN OXYGEN , Yuan-Pern Lee, Chen-An Chung

WM05 **10:16 – 10:17**
PRODUCTION OF $HOCH_2CO$, HOCHCHO, AND HOCHCO IN THE REACTION H + GLYCOLALDEHYDE ($HOCH_2CHO$) IN SOLID *p*-H_2 AND ITS IMPLICATION IN ASTROCHEMISTRY , Prasad Ramesh Joshi, Yuan-Pern Lee

WM06 **10:20 – 10:21**
AB INITIO SPECTROSCOPIC PARAMETERS OF PYRIDYL RADICALS, Kelly S. Meyer, Sommer L. Johansen, J. H. Westerfield, Anahut Sandhu, Jasmine Keane, Kyle N. Crabtree

WM07 **10:24 – 10:25**
COUPLED CLUSTER CHARACTERIZATION OF 1-, 2-, AND 3-PYRROLYL FOR VIBRATIONAL AND ROTATIONAL SPECTROSCOPY, Sommer L. Johansen, Zhongxing Xu, J. H. Westerfield, Anna C. Wannenmacher, Kyle N. Crabtree

WM08 **10:28 – 10:29**
ELECTRONIC SPECTROSCOPY OF *CIS*- AND *TRANS-META*-VINYLBENZYL RADICALS , Sederra D. Ross, Jonathan Flores, Daniel M. Hewett, Neil J. Reilly

WM09 **10:32 – 10:33**
THE GROUND AND EXCITED STATES OF AROMATIC OXIDE RADICALS VIA ANION PHOTOELECTRON SPECTROSCOPY, Steven J. Kregel, Etienne Garand

WM10 **10:36 – 10:37**
VIBRATIONAL ANALYSIS OF DF SPECTRUM OF THE NO_3 $\tilde{B}\ ^2E' - {}^2A_2'$ SYSTEM (II): COMBINED ANALYSIS WITH CRYO-SEVI PE SPECTRUM OF NO_3^- , Masaru Fukushima

WM11 **10:40 – 10:41**
GATEWAY STATES OF THE $1^2\Delta$ STATE OF CaH., Shota Yaguramaki, Jin Furuta, Kaori Kobayashi, Yoshiki Moriwaki, Stephen Cary Ross

WM12 **10:44 – 10:45**
ELECTRONIC STRUCTURE AND VIBRATIONAL SIGNATURES OF THE DELOCALIZED RADICAL IN HYDRATED CLUSTERS OF COPPER (”II”) HYDROXIDE, CUOH+(H2O)0-2, Elizabeth G. Christensen, Kevin T Lutz, Ryan P Steele

WM13 **10:48 – 10:49**
CHIRPED-PULSE MILLIMETER-WAVE SPECTROSCOPY OF ASTROPHYSICAL RADICALS IN A PULSE JET DISCHARGE EXPERIMENT, Olivia Chitarra, Bérenger Gans, Olivier Pirali, Marie-Aline Martin-Drumel

WM14 ***Post-Deadline Abstract*** **10:52 – 10:53**
HIGH RESOLUTION ANION PHOTOELECTRON SPECTRA OF CRYOGENICALLY COOLED SILICON CARBIDES, Mark C Babin, Martin DeWitt, Marissa L. Weichman, Jessalyn A. DeVine, Daniel Neumark

RA. Rotational structure/frequencies

Thursday, June 24, 2021 – 8:0 AM

Room: 2021 Online Everywhere

Chair: G. S. Grubbs II, Missouri University of Science and Technology, Rolla, MO, USA

RA01 **8:00 – 8:01**
THE 130-360 GHZ ROTATIONAL SPECTRUM OF THE CHLORINE ISOTOPOLOGUES OF CHLOROBENZENE AND ITS EXCITED VIBRATIONAL STATES, P. Matisha Dorman, Brian J. Esselman, R. Claude Woods, Robert J. McMahon

RA02 **8:04 – 8:05**
MILLIMETER-WAVE SPECTROSCOPY OF THE EXCITED VIBRATIONAL STATES OF THIOPHENE (C_4H_4S) , Vanessa L. Orr, Brian J. Esselman, Yotaro Ichikawa, Kaori Kobayashi, R. Claude Woods, Robert J. McMahon

RA03 **8:08 – 8:09**
THE ROTATIONAL ANALYSES OF 2-CYANOPYRIMIDINE ($C_5H_3N_3$) AND 2-CYANOPYRAZINE ($C_5H_3N_3$): VIBRATIONAL GROUND STATES AND DYAD OF LOWEST-ENERGY VIBRATIONALLY EXCITED STATES, Houston H. Smith, Brian J. Esselman, R. Claude Woods, Robert J. McMahon

RA04 **8:12 – 8:13**
ANALYTICAL QUARTIC CENTRIFUGAL DISTORTION CONSTANTS BY FOURTH-ORDER RAYLEIGH SCHRÖDINGER PERTURBATION THEORY, Peter R. Franke, John F. Stanton

RA05 **8:16 – 8:17**
PHASE DETERMINATION IN MULTI-ANTENNA DETECTION CHIRPED-PULSE MICROWAVE SPECTROSCOPY, Christian Swanson, Nicole Moon, Amanda Duerden, Joshua E. Isert, G. S. Grubbs II

RA06 **8:20 – 8:21**
MICROWAVE STUDY COMPLEMENTED WITH COMPUTATIONAL DATA OF MONO-CHLOROBENZALDEHYDES, Maria Dohmen, Sean Arnold, Pablo Pinacho, Gordon G Brown, Melanie Schnell, Daniel A. Obenchain

RA07 **8:24 – 8:25**
CYCLOHEXANE VIBRATIONS: HIGH RESOLUTION SPECTRA AND ANHARMONIC LOCAL MODE CALCULATIONS, Peter F. Bernath, Edwin Sibert

RA08 **8:28 – 8:29**
SPECTROSCOPIC CHARACTERIZATION OF *E*- AND *Z*-PHENYLMETHANIMINE, Alessio Melli, Lorenzo Spada, Vincenzo Barone, Sven Herbers, Kevin G. Lengsfeld, Jens-Uwe Grabow, Mattia Melosso, Luca Dore, Cristina Puzzarini

RA09 **8:32 – 8:33**
THE MILLIMETER/SUBMILLIMETER SPECTRUM OF 2-CHLOROETHANOL, Hayley Bunn, Susanna L. Widicus Weaver

RA10 **8:36 – 8:37**
ROTATIONAL SPECTRUM OF 2-CYCLOPROPYLIDENEACETONITRILE - A NEW ISOMER OF PYRIDINE, Brian J. Esselman, Samuel M. Kougias, R. Claude Woods, Robert J. McMahon

RA11 ***Post-Deadline Abstract*** **8:40 – 8:41**
CHEMICAL DISTRIBUTION OF ACETALDEHYDE IN ORION KL , Miwha Jin, Anthony Remijan, Robin T. Garrod

RA12 **8:44 – 8:45**
THE MILLIMETER- AND SUBMILLIMETER-WAVE SPECTROSCOPY OF ISOPRENE., Daniel J Tyree, Ivan Medvedev

RA13 **8:48 – 8:49**
THE MILLIMETER/SUBMILLIMETER SPECTRUM OF DIACETYL, Jonathan Rebelsky, Chase P Schultz, Susanna L. Widicus Weaver

RA14 **8:52 – 8:53**
INVESTIGATION OF PURE ROTATIONAL SPECTROSCOPY OF ETHYNYLBENZONITRILE ISOMERS USING CHIRPED-PULSE W-BAND SPECTROSCOPY, Jean-Thibaut Spaniol, Kelvin Lee, Olivier Pirali, Marie-Aline Martin-Drumel

RB. Mini-symposium: Precision Spectroscopy for Fundamental Physics

Thursday, June 24, 2021 – 8:0 AM

Room: 2021 Online Everywhere

Chair: Andrew Jayich, University of California, Santa Barbara, , USA

RB01 ***INVITED TALK*** **8:00 – 8:02**
SPECTROSCOPY OF SHORT-LIVED RADIOACTIVE MOLECULES, Ronald Fernando Garcia Ruiz

RB02 **8:08 – 8:09**
THEORETICAL STUDY OF PROPERTIES OF RADIUM MONOFLUORIDE , Aleksandra A. Kyuberis, Anastasia Borschevsky, Lukáš Félix Pašteka

RB03 **8:12 – 8:13**
INFLUENCE OF VIBRATIONS ON THE SENSITIVITY OF RAOH AND YBOH MOLECULES TO THE P, T-VIOLATION, Anna Zakharova, Alexander Petrov

RB04 ***Post-Deadline Abstract*** **8:16 – 8:17**
CALCULATION OF THE CORRECTION ON THE MAGNETIZATION DISTRIBUTION IN THE NUCLEUS TO THE HYPERFINE STRUCTURE OF HEAVY ATOMS, Sergey Prosnyak, Leonid V. Skripnikov, Daniel E. Maison

RB05 **8:20 – 8:21**
SEARCH FOR PARITY VIOLATION USING $^{177,179}HFF^{+}$ CATIONS, Igor Kurchavov, Alexander Petrov

RB06 **8:24 – 8:25**
TANTALUM OXIDE SPECTROSCOPY TO FACILITATE EXPLORING NEW PHYSICS BEYOND THE STANDARD MODEL, Timothy Chung, Matthew Charles Cooper, Yan Zhou

RB07 **8:28 – 8:29**
TAO^{+} CATION FOR THE STUDY OF QUADRUPLE NEUTRON DISTRIBUTION IN NUCLEI, Gleb Olegovich Penyazkov, Leonid V. Skripnikov

RB08 **8:32 – 8:33**
ACCURATE PREDICTION OF CLOCK TRANSITIONS IN A HIGHLY CHARGED ION WITH COMPLEX ELECTRONIC STRUCTURE, Charles Cheung, Marianna Safronova, Sergey Porsev, Mikhail Kozlov, Ilya Tupitsyn, Andrey Bondarev

RB09 **8:36 – 8:37**
QUANTUM LOGIC CONTROL AND SPECTROSCOPY OF A SINGLE MOLECULAR ION, Alejandra Collopy, David Leibrandt, Dietrich Leibfried, Chin-wen Chou

RB10 **8:40 – 8:41**
SPECTROSCOPIC CHARACTERIZATION OF A THERMODYNAMICALLY STABLE DOUBLY CHARGED DIATOMIC MOLECULE: $MgAr^{2+}$, Dominik Wehrli, Matthieu Génévriez, Frédéric Merkt

RB11 **8:44 – 8:45**
HYBRID LINE LIST AND SPECTROSCOPIC MODEL FOR CN, Anna-Maree Syme, Laura K McKemmish

RB12 **8:48 – 8:49**
VIBRATIONAL BENDING MODES METROLOGY IN THE 670-720 cm^{-1}RANGE, Marco Lamperti, Riccardo Gotti, Davide Gatti, Mohammad Khaled Shakfa, Elisabetta Canè, Filippo Tamassia, Paolo Laporta, P. G. Schunemann, Aamir Farooq, Marco Marangoni

RB13 **8:52 – 8:53**
MULTISPECTRUM ROTATIONAL STATES DISTRIBUTION THERMOMETRY, Riccardo Gotti, Marco Lamperti, Davide Gatti, Szymon Wojtewicz, Thomas Puppe, Yuriy Mayzlin, Bidoor Alsaif, Julian Robinson-Tait, Felix Rohde, Rafal Wilk, Patrick Leisching, Wilhelm Kaenders, Paolo Laporta, Marco Marangoni

RC. Astronomy

Thursday, June 24, 2021 – 8:0 AM

Room: 2021 Online Everywhere

Chair: Mitsunori Araki, Tokyo University of Science, Shinjuku-ku, Tokyo, Japan

RC01 **8:00 – 8:01**
A STATUS REPORT ON THE COLOGNE DATABASE FOR MOLECULAR SPECTROSCOPY, CDMS, Holger S. P. Müller, P. Schilke, Stephan Schlemmer

RC03 **8:08 – 8:09**
ASTROCHEMICAL FORECASTING WITH MACHINE LEARNING, Kelvin Lee, Andrew M Burkhardt, Michael C McCarthy, Brett A. McGuire

RC04 **8:12 – 8:13**
LABORATORY ICE ASTROCHEMISTRY AT LARGE FACILITIES, SERGIO IOPPOLO

RC05 **8:16 – 8:17**
SPECTROMETER USING SUPERCONDUCTOR MIXER RECEIVER (SUMIRE) FOR MICROWAVE SPECTROSCOPY OF MOLECULES IN ASTRONOMICAL INTERESTS , Yoshimasa Watanabe, Akemi Tamanai, Nami Sakai

RC06 **8:20 – 8:21**
THE 2021 CENSUS OF INTERSTELLAR, CIRCUMSTELLAR, EXTRAGALACTIC, PROTOPLANETARY DISK, AND EXOPLANETARY MOLECULES: WHAT ARE THE PRESSING SPECTROSCOPIC NEEDS FROM THE LABORATORY?, Brett A. McGuire

RC07 **8:24 – 8:25**
A RIGOROUS K/KA-BAND HUNT FOR AROMATIC MOLECULES (ARKHAM): UBIQUITOUS AROMATIC CARBON CHEMISTRY AT THE EARLIEST STAGES OF STAR FORMATION, Andrew M Burkhardt, Ryan A Loomis, Christopher N Shingledecker, Kelvin Lee, Anthony Remijan, Michael C McCarthy, Brett A. McGuire

RC08 **8:28 – 8:29**
SPECTRAL STACKING AND MATCHED FILTERING AS A RIGOROUS DETECTION TECHNIQUE FOR INTERSTELLAR MOLECULES, Ryan A Loomis, Kelvin Lee, Ci Xue, Andrew M Burkhardt, Christopher N Shingledecker, Steven B Charnley, Martin Cordiner, Eric Herbst, Sergei Kalenskii, Brett A. McGuire, Michael C McCarthy, Anthony Remijan

RC09 **8:32 – 8:33**
LABORATORY SPECTROSCOPY FOR ASTROCHEMISTRY: A ROTATIONAL INVESTIGATION OF 3-AMINO-2-PROPENENITRILE, Davide Alberton, Valerio Lattanzi, Christian Endres, Paola Caselli, Luca Bizzocchi

RC10 **8:36 – 8:37**
HIGH-RESOLUTION, ROTATIONALLY-RESOLVED FTIR SPECTRUM OF THE 3300 cm^{-1} TRANSITION OF ASTROPHYSICALLY-RELEVANT HCN, Jessica Palko, Thomas Howard, Leah G Dodson

RC11 **8:40 – 8:41**
COMPREHENSIVE ROTATIONAL SPECTROSCOPY OF METHYL CYANOACETATE FOR ASTRONOMICAL SEARCHES, Gayatri Batra, Pablo Pinacho, Amanda Steber, Melanie Schnell

RC12 **8:44 – 8:45**
LINE LISTS FOR THE $b^1\Sigma^+ - X^3\Sigma^-$ AND $a^1\Delta - X^3\Sigma^-$ TRANSITIONS OF SO , Peter F. Bernath, Ryan Johnson, Jacques Liévin

RC13 **8:48 – 8:49**
HIGH-TEMPERATURE SPECTROSCOPIC DATA FOR EXO-PLANETARY STUDIES: THE e-PYTHEAS PROJECT, Vincent Boudon, Athena Coustenis, Alain Campargue, Robert Georges, Vladimir Tyuterev

RD. Non-covalent interactions

Thursday, June 24, 2021 – 8:0 AM

Room: 2021 Online Everywhere

Chair: Malgorzata Biczysko, Shanghai University, Shanghai, China

RD01 **8:00 – 8:01**
IMAGING THE NONREACTIVE COLLISIONAL QUENCHING DYNAMICS OF NO ($A^2\Sigma^+$) RADICALS WITH O_2 ($X^3\Sigma_g{}^-$), K. Jacob Blackshaw, Naa-Kwarley Quartey, David J. Hood, Christian D. Hettwer, Nathanael M. Kidwell

RD02 **8:04 – 8:05**
N_2O-AR AND N_2O-KR: SYMMETRY BREAKING OF INTRAMOLECULAR BENDING MODE OF N_2O IN THE PRESENCE OF A RARE GAS , Chris Gergess, M. Dehghany, A. J. Barclay, A.R.W. McKellar, Nasser Moazzen-Ahmadi

RD03 **8:08 – 8:09**
THE 4.2 MICRON SPECTRA OF CO_2-CO DIMER FOR BOTH THE C- AND O-BONDED ISOMERS, INCLUDING SPLITTING OF THE DEGENERATE ν_2 BEND IN THE PRESENCE OF CO, Praveen Wakwella, A. J. Barclay, Bob McKellar, Nasser Moazzen-Ahmadi

RD04 **8:12 – 8:13**
INFRARED SPECTROSCOPY OF TITANIUM CATION ACETYLENE COMPLEXES: CATION-π COMPLEXES VS REACTED STRUCTURES, Anna G Batchelor, Joshua H Marks, Michael A Duncan

RD05 **8:16 – 8:17**
SPECTROSCOPIC CHARACTERIZATION OF PSEUDOCARBYNES: INTERACTION BETWEEN –C≡C– CHAINS AND METAL CLUSTERS, Hyunsub Kim, Scott G Sayres

RD06 **8:20 – 8:21**
INFRARED SPECTRA OF THE METHYLAMINE DIMER AND METHYLAMINE-WATER COMPLEXES IN SOLID NEON BETWEEN 80 AND 5500 cm^{-1}, Pascale Soulard, Benoît Tremblay

RD07 **8:24 – 8:25**
WETTING TRIACETONE TRIPEROXIDE ALLOWS ITS DETECTION BY MICROWAVE SPECTROSCOPY, Susana Blanco, Alberto Macario, José García-Calvo, Andrea Revilla-Cuesta, Tomás Torroba , Juan Carlos Lopez

RD08 **8:28 – 8:29**
A BROADBAND MICROWAVE STUDY OF ISOLATED α-METHOXY PHENYLACETIC ACID: STRUCTURE, INTERNAL ROTATION, AND MICRO-SOLVATION, Himanshi Singh, Pablo Pinacho, Daniel A. Obenchain, María Mar Quesada-Moreno, Melanie Schnell

RD09 **8:32 – 8:33**
EXPLOITING F LONE PAIR$\cdots\pi_{AROMATIC}$-HOLE INTERACTION BETWEEN BENZALDEHYDE AND TETRAFLUOROMETHANE, Hao Wang, Junha Chen, Qian Gou

RD10 ***Post-Deadline Abstract*** **8:36 – 8:37**
STRUCTURE AND NON-COVALENT INTERACTIONS OF THE BENZOFURAN-FORMALDEHYDE COMPLEX EXPLORED BY MICROWAVE SPECTROSCOPY AND QUANTUM-CHEMICAL CALCULATIONS, Xiaolong Li, Silvia Alessandrini, Yang Zheng, Lorenzo Spada, Kevin G. Lengsfeld, Jens-Uwe Grabow, Cristina Puzzarini, Gang Feng, Vincenzo Barone

RD11 **8:40 – 8:41**
COLD ION SPECTROSCOPY OF B_{12} DERIVATIVES: STRETCHING THE LIMITS OF THEORETICAL INTERPRETATION, Alexandra Tsybizova, Larisa Miloglyadova, Peter Chen

RE. Atmospheric science

Thursday, June 24, 2021 – 8:0 AM

Room: 2021 Online Everywhere

Chair: Christopher J. Johnson, Stony Brook University, Stony Brook, NY, USA

RE01 **8:00 – 8:01**
WATER VAPOR NEAR-UV ABSORPTION: LABORATORY SPECTRUM, FIELD EVIDENCE, AND ATMOSPHERIC IMPACTS, Lei Zhu, Linsen Pei, Qilong Min, Yuyi Du, Zhe-Chen Wang, Bangsheng Yin, Kai Yang, Patrick Disterhoft, Thomas J Pongetti

RE02 **8:04 – 8:05**
TRENDS IN ATMOSPHERIC COMPOSITION FROM THE ATMOSPHERIC CHEMISTRY EXPERIMENT (ACE) SATELLITE, Peter F. Bernath, Chris Boone, Jeff Crouse

RE03 **8:08 – 8:09**
SULFUR DIOXIDE FROM THE ATMOSPHERIC CHEMISTRY EXPERIMENT (ACE) SATELLITE, William D Cameron, Peter F. Bernath, Chris Boone

RE04 **8:12 – 8:13**
ABSORPTION COEFFICIENT (ABSCO) TABLES FOR THE ORBITING CARBON OBSERVATORIES, Vivienne H Payne, Brian Drouin, Fabiano Oyafuso, Le Kuai, Brendan M Fisher, Keeyoon Sung, Deacon J Nemchick, Timothy J. Crawford, Mike Smyth, David Crisp, Erin M. Adkins, Joseph T. Hodges, David A. Long, Eli J Mlawer, Aronne Merrelli, Elizabeth M Lunny

RE05 **8:16 – 8:17**
THE MICROWAVE SPECTRUM OF 2-CHLOROETHYL RADICAL, CH_2ClCH_2, Michael J. Carrillo, Wei Lin, Yasuki Endo

RE06 **8:20 – 8:21**
DETAILED ANALYSIS OF THE INFRARED SPECTRUM OF SiF_4: AN UPDATE, Vincent Boudon, Laurent Manceron

RE07 **8:24 – 8:25**
MICROWAVE SPECTROSCOPY STUDY SUPPORTED BY QUANTUM CHEMISTRY CALCULATIONS OF LIMONA KETONE, A KEY OXIDATION PRODUCT OF LIMONENE, Noureddin OSSEIRAN, Annunziata Savoia, Pascal Dréan, Manuel Goubet, Therese R. Huet

RE08 **8:28 – 8:29**
REVEALING LONG-RANGE SUBSTITUENT EFFECTS IN THE LASER-INDUCED FLUORESCENCE AND DISPERSED FLUORESCENCE SPECTRA OF JET-COOLED $CH_XF_{3-X}CH_2O$ (X = 1, 2, 3) RADICALS, Benedek Koncz, Gabor Bazso, Md Asmaul Reza, Hamzeh Telfah, Kristof Hegedus, Jinjun Liu, Gyorgy Tarczay

RE09 **8:32 – 8:33**
SENSITIVE INFRARED SPECTROSCOPY OF ISOPRENE AT THE PART PER BILLION LEVEL, Jacob Stewart, Jacob Beloin, Melanie Jean Fournier, Grace Kovic

RE10 **8:36 – 8:37**
A COLLISIONAL TRANSFER MECHANISM FOR SULFUR MASS INDEPENDENT FRACTIONATION IN WEAKLY INTERACTING EXCITED ELECTRONIC STATES OF S_2, Alexander W Hull, Shuhei Ono, Robert W Field

RF. Spectroscopy as an analytical tool

Thursday, June 24, 2021 – 8:0 AM

Room: 2021 Online Everywhere

Chair: David A. Long, National Institute of Standards and Technology, Gaithersburg, MD, USA

RF01 ***Post-Deadline Abstract*** **8:00 – 8:01**
MICRO-PARTICLES IMMUNOASSAYS FOR EARLY DETECTION OF OVARIAN CANCER USING LASER INDUCED BREAKDOWN SPECTROSCOPY., Robinson Karunanithy, P Sivakumar, Torrey E. Holland

RF02 ***Post-Deadline Abstract*** **8:04 – 8:05**
LASER INDUCED BREAKDOWN SPECTROSCOPY FOR DETECTION OF HEAVY METALS IN CANCEROUS AND HEALTHY COLON TISSUES , Mohammed A Gondal

RF03 **8:08 – 8:09**
STUDY OF MOLECULAR BAND PRESENT IN THE LASER-INDUCED PLASMA OF CHOLESTEROL GALLSTONE, Zainab Gazali, PRADEEP KUMAR RAI, Surya Narayan Thakur, A. K. Rai

RF04 **8:12 – 8:13**
COMPOSITIONAL ANALYSIS OF GREEN TEA LEAVES USING LASER INDUCED BREAKDOWN SPECTROSCOPY (LIBS) , Tejmani Kumar, Abhishek Dwivedi, Zainab Gazali, Abhishek Rai, A. K. Rai

RF05 **8:16 – 8:17**
COMPOSITIONAL ANALYSIS OF AYURVEDIC MEDICINE USING LIBS ALONG WITH PAS TECHNIQUES, Reshu Kumari, Zainab Gazali, Abhishek Dwivedi, A. K. Rai

RF06 **8:20 – 8:21**
LOOKING FOR CACAO IN ALL THE WRONG PLACES: AN ANALYSIS OF MAYA POTTERY WITH 2-PHOTON RESONANCE SPECTROSCOPY, Ann Williams , Mattanjah DE VRIES

RF07 **8:24 – 8:25**
DEVELOPMENT OF A SUPERSONIC WIND TUNNEL FOR A CAVITY RINGDOWN SPECTROMETER, Elijah R Jans, Terry A. Miller, Igor V. Adamovich

RF08 **8:28 – 8:29**
OPTICALLY-SWITCHED DUAL-WAVELENGTH CAVITY RING-DOWN SPECTROMETER FOR HIGH-PRECISION ISOTOPIC RATIO MEASUREMENTS OF METHANE δD and ^{13}C IN THE NEAR-INFRARED, TzuLing Chen, Douglas Ober, ROBIN MIRI, THINH Bui, LINHAN SHEN, Mitchio Okumura

RF09 **8:32 – 8:33**
HIGH RESOLUTION INFRARED CAVITY ENHANCED ABSORPTION AT LOW TEMPERATURES , Carlos Manzanares, Suresh Sunuwar

RF10 **8:36 – 8:37**
SPECTROSCOPIC DETECTION OF METHANE AT A PPT SENSITIVITY LEVEL IN MID-IR WITH A LONG-PATH MULTIPASS CELL, Hans A Schuessler, Jinbao Xia, carlos Rodriguez, James R Bounds, Alexandre Kolomenskii

RF11 **8:40 – 8:41**
A PHOTONIC GAS SENSOR FOR THE MID-INFRARED, Travis A Gartner, Paul Barclay, Nasser Moazzen-Ahmadi

RF12 **8:44 – 8:45**
MEASURING ACCURATE STIMULATED RAMAN SCATTERING CROSS-SECTIONS OF LIQUIDS, Prasenjit Srivastava, Kristen H. Burns, Christopher G. Elles

RG. Plenary

Thursday, June 24, 2021 – 9:0 AM

Room: 2021 Online Everywhere

Chair: Martin Gruebele, University of Illinois at Urbana-Champaign, Urbana, IL, USA

RG02 **9:03 – 9:43**

INFLUENCE OF NATURALLY-OCCURRING AND SYNTHETIC MODIFICATIONS ON THE STRUCTURES AND GLYCOSIDIC BOND STABILITIES OF DNA AND RNA NUCLEOSIDES, M T Rodgers, Ranran Wu, Yanlong Zhu, Lucas Hamlow, Chenchen He, Zachary J Devereaux, Harrison Roy, Erik O Soley, Chase Leslie, Giel Berden, Jos Oomens

RH. Mini-symposium: Large Amplitude Motions

Thursday, June 24, 2021 – 10:0 AM

Room: 2021 Online Everywhere

Chair: Arnaud Cuisset, Université du Littoral Côte d'Opale, Dunkerque, France

RH01 **10:00 – 10:01**
MOLECULAR ROTATION IN FLOPPY MOLECULES: HE-H_3^+, Thomas Salomon, Oskar Asvany, Dieter Gerlich, Igor Savic, Ad van der Avoird, Michael E. Harding, Filippo Lipparini, Jürgen Gauss, Stephan Schlemmer

RH02 ***Post-Deadline Abstract*** **10:04 – 10:05**
SYMMETRIES of CH_5^+, Stefan Brackertz, Benjamin Nukic, Per Jensen, Stephan Schlemmer

RH03 **10:08 – 10:09**
$^{14}NH_3$ ROVIBRATIONAL IR ANALYSIS AT 6000 CM^{-1}, Xinchuan Huang, Keeyoon Sung, Timothy J. Lee, David Schwenke, Geoffrey C. Toon

RH04 **10:12 – 10:13**
THE BENDING-ROTATION APPROACH APPLIED TO THE METHYLENE RADICAL CH_2, L. H. Coudert

RH05 **10:16 – 10:17**
TUNNELING AND RING OPENING IN THE CYCLOPROPYL RADICAL AND CATION , Nadav Genossar, Bryan Changala, Marie-Aline Martin-Drumel, Bérenger Gans, J.-C. Loison, Joshua H Baraban

RH06 **10:20 – 10:21**
STATE-DISTRIBUTION CONTROL OF LARGE AMPLITUDE VIBRATION IN SUBSTITUTED BIPHENYLS WITH INTENSE LASER PULSES, Makoto Nikaido, Kenta Mizuse, Yasuhiro Ohshima

RH07 **10:24 – 10:25**
NUCLEAR DYNAMICS OF FLEXIBLE CYCLIC MOLECULES: CONFORMATIONAL SPACE, PSEUDOROTATIONAL AND ROTATIONAL MOTIONS OF DIOXOLANES, DITHIOLANES AND OXATHIOLANES, Lorenzo Paoloni, Sergio Rampino, Assimo Maris

RH08 **10:28 – 10:29**
ROTATIONAL AND VIBRATIONAL WAVE PACKET IMAGING SPECTROSCOPY: BROAD BANDWIDTH, HIGH-RESOLUTION SPECTRA AND DYNAMICS OF WEAKLY BOUND MOLECULAR DIMERS, Ar_2, $(N_2)_2$, AND $(CH_4)_2$, Kenta Mizuse, Hikaru Sato, Haruki Ishikawa, Yuhei Oyagi, Tomomi Murai, Genki Ishibashi, Yuya Tobata, Yasuhiro Ohshima

RH09 **10:32 – 10:33**
HIGH-RESOLUTION GAS PHASE THz SPECTROSCOPY OF THE CATECHOL LOW FREQUENCY MODES INVOLVING AN INTRAMOLECULAR HYDROGEN BOND , Jonas Bruckhuisen, Guillaume Dhont, Anthony Roucou, Atef Jabri, Hamdi Bayoudh, Thi Thanh Tran, Manuel Goubet, Marie-Aline Martin-Drumel, Arnaud Cuisset

RH10 **10:36 – 10:37**
HIGH RESOLUTION INFRARED SPECTROSCOPY OF OC-HOH TRAPPED IN SOLID PARAHYDROGEN: COHERENT TUNNELING IN A QUANTUM SOLID, Morgan E. Balabanoff, Aaron I. Strom, Kelly M. Olenyik, David T. Anderson

RH11 **10:40 – 10:41**
IN SEARCH OF VIBRATIONALLY EXCITED STATE MONODROMY IN NCNCS, Dennis W. Tokaryk, Stephen Cary Ross, Manfred Winnewisser, Brenda P. Winnewisser, Frank C. De Lucia, Brant E. Billinghurst

RI. Mini-symposium: Precision Spectroscopy for Fundamental Physics

Thursday, June 24, 2021 – 10:0 AM

Room: 2021 Online Everywhere

Chair: Alejandra Collopy, National Institute of Standards and Technology, Boulder, CO, USA

RI02 ***Journal of Molecular Spectroscopy Review Lecture*** **10:06 – 10:08**
SEARCHING FOR FUNDAMENTAL SYMMETRY VIOLATIONS WITH POLYATOMIC MOLECULES, Nicholas R Hutzler

RI03 **10:14 – 10:15**
USE OF MOLECULES TO SEARCH FOR NEW PHYSICS AND STUDY PROPERTIES OF THE NUCLEUS., Leonid V. Skripnikov

RI04 **10:18 – 10:19**
CALCULATION AND UNCERTAINTY EVALUATION OF THE P,T-ODD ENHANCEMENT FACTORS OF POLYATOMIC MOLECULES , Aleksandra A. Kyuberis, Anastasia Borschevsky, Lukáš Félix Pašteka

RI05 **10:22 – 10:23**
ANALYTIC RELATIVISTIC COUPLED-CLUSTER CALCULATIONS OF TIME-REVERSAL VIOLATING PARAMETERS, Chaoqun Zhang, Xuechen Zheng, Lan Cheng

RI06 **10:26 – 10:27**
ELECTRONIC STRUCTURE OF TRIATOMIC MOLECULES FOR SEARCH OF AXIONLIKE PARTICLES, Daniel E. Maison

RI07 **10:30 – 10:31**
A NEW EXPERIMENT TO TEST PARITY SYMMETRY IN COLD CHIRAL MOLECULES USING PRECISE MID-INFRARED SPECTROSCOPY, Mathieu Manceau, Louis Lecordier, Anne Cournol, Nicolas Cahuzac, Dang Bao An Tran, Rosa Santagata, Matthieu Pierens, Alexander Shelkovnikov, Andrei Goncharov, Olivier Lopez, Anne Amy-Klein, Sean Tokunaga, Benoit Darquie

RI08 **10:34 – 10:35**
SPECTROSCOPY ON ALUMINUM MONOCHLORIDE (ALCL) FOR LASER COOLING AND TRAPPING, John Daniel, Kayla Rodriguez, Taylor Lewis, Alexander Teplukhin, Chen Wang, Madhav Dhital, Brian K Kendrick, Christopher Bardeen, Shan-Wen Tsai, Boerge Hemmerling

RI09 **10:38 – 10:39**
OBSERVATION AND LASER SPECTROSCOPY OF YTTERBIUM MONOMETHOXIDE, $YbOCH_3$, Benjamin Augenbraun, Timothy Steimle, Zack Lasner, Alexander Frenett, Hiromitsu Sawaoka, Anh T. Le, John M. Doyle

RI10 **10:42 – 10:43**
SPECTROSCOPIC STUDIES OF ALUMINUM MONOFLUORIDE WITH RELEVANCE FOR LASER COOLING AND TRAPPING, Stefan Truppe, Silvio Marx, Sebastian Kray, Maximilian Doppelbauer, Simon Hofsäss, Christian Schewe, Nicole Walter, Jesús Pérez-Ríos, Boris Sartakov, Gerard Meijer

RI11 **10:46 – 10:47**
INVESTIGATION OF THE $b^3\Sigma^+, v = 0$ STATE IN ALUMINIUM MONOFLUORIDE, Maximilian Doppelbauer, Nicole Walter, Simon Hofsäss, Silvio Marx, Christian Schewe, Sebastian Kray, Jesús Pérez-Ríos, Boris Sartakov, Stefan Truppe, Gerard Meijer

RI12 **10:50 – 10:51**
SPECTROSCOPIC CHARACTERIZATION OF THE $A^1\Pi, v = 6 \leftrightarrow b^3\Sigma^+, v = 5$ INTERACTION OF ALUMINUM MONOFLUORIDE IN VIEW OF LASER COOLING AND TRAPPING EXPERIMENTS, Nicole Walter, Silvio Marx, Johannes Seifert, Boris Sartakov, Stefan Truppe, Gerard Meijer

RI13 **10:54 – 10:55**
FINE AND HYPERFINE INTERACTIONS IN ^{171}YbOH AND ^{173}YbOH, Nickolas H Pilgram, Arian Jadababaie, Yi Zeng, Nicholas R Hutzler, Timothy Steimle

RI14 **10:58 – 10:59**
$\mathcal{P}, \mathcal{T}$-ODD FARADAY EFFECT: A NEW APPROACH TO IMPROVE THE SENSITIVITY OF THE SEARCH FOR TIME-REFLECTION-NONINVARIANT INTERACTIONS IN NATURE, Dmitry Chubukov

RI15 **11:02 – 11:03**
ISOTOPE SHIFT IN OPTICAL SPECTRA OF MoO MOLECULE, Lei Zhang, Yao Yu, Jie Yang

RJ. Dynamics and kinetics

Thursday, June 24, 2021 – 10:0 AM

Room: 2021 Online Everywhere

Chair: Scott Kevin Cushing, Caltech, Pasadena, CA, USA

RJ01 **10:00 – 10:01**
ULTRAFAST EXCITED STATE DYNAMICS OF TWISTED AROMATICS, Mahesh Hariharan

RJ02 **10:04 – 10:05**
TRACKING THE REACTION COORDINATE OF ULTRAFAST SPIN-CROSSOVER IN Fe(II) COMPLEXES WITH FEMTOSECOND M-EDGE XANES, Ryan T Ash, Kaili Zhang, Josh Vura-Weis

RJ03 **10:08 – 10:09**
FEMTOSECOND PUMP-PROBE SPECTROSCOPY OF NEUTRAL Ni AND Cr OXIDE CLUSTERS , Jacob M Garcia, Scott G Sayres

RJ04 **10:12 – 10:13**
ELECTRONIC STATE-RESOLVED RELAXATION DYNAMICS IN METAL CLUSTERS STUDIED USING TWO-DIMENSIONAL ELECTRONIC SPECTROSCOPY, William R. Jeffries, Jordan Wallace, Kenneth L. Knappenberger, Jr.

RJ05 **10:16 – 10:17**
SIZE EFFECTS ON EXCITED STATE LIFETIMES OF TITANIUM OXIDE CLUSTERS, Lauren F Heald, Jacob M Garcia, Scott G Sayres

RJ06 **10:20 – 10:21**
ULTRAFAST REACTION DYNAMICS OF NEUTRAL ALUMINUM OXIDE CLUSTERS USING TWO COLOR FEMTOSECOND SPECTROSCOPY, Ananya Sen, Scott G Sayres

RJ07 **10:24 – 10:25**
PHOTOPHYSICS OF EXCITED STATES IN THE Co_4O_4 CUBANE CATALYST FOLLOWED VIA FEMTOSECOND $M_{2,3}$-EDGE ABSORPTION SPECTROSCOPY, Yusef A. Shari'ati, Josh Vura-Weis

RJ08 **10:28 – 10:29**
OPTICALLY PUMPED RESTSTRAHLEN BAND TUNING OF WIDE BANDGAP SEMICONDUCTORS, Elizabeth S Ryland, Vanessa M Breslin, Daniel C Ratchford, Jeff Owrutsky, Adam Dunkelberger

RJ09 **10:32 – 10:33**
MEASUREMENT AND EXCITED STATE PREDICTION OF PHOTOEXCITED ELECTRON AND HOLE DYNAMICS IN ZnTe WITH TRANSIENT ULTRAVIOLET REFLECTION SPECTROSCOPY, Hanzhe Liu, Jonathan M Michelsen, Isabel M Klein, Scott Kevin Cushing

RJ10 **10:36 – 10:37**
ULTRAFAST CARRIER SPECIFIC DYNAMICS AND BAND GAP RENORMALIZATION IN $CH_3NH_3PbBr_3$ UNDERSTOOD BY FEMTOSECOND TABLETOP EXTREME ULTRAVIOLET SPECTROSCOPY, Aastha Sharma, Josh Leveillee, Max A Verkamp, André Schleife, Josh Vura-Weis

RJ11 **10:40 – 10:41**
MONITORING PHOTOINDUCED AND PHOTOCATALYTIC SURFACE REACTIONS WITH TIME, MASS, AND ENERGY RESOLUTION, Mihai E Vaida

RJ12 **10:44 – 10:45**
X-RAY TRANSIENT ABSORPTION REVEALS THE ^1A_u ($n\pi^*$) STATE OF PYRAZINE IN ELECTRONIC RELAXATION, Valeriu Scutelnic, Shota Tsuru, Mátyás Pápai, Zheyue Yang, Michael Epshtein, Tian Xue, Eric Haugen, Yuki Kobayashi, Anna Krylov, Klaus Møller, Sonia Coriani, Stephen R. Leone

RJ13 **10:48 – 10:49**
CHARACTERIZATION OF THE $N_{6,7}$-EDGE AND $O_{2,3}$-EDGE OF Pt AND Ir COMPLEXES BY EXTREME ULTRAVIOLET SPECTROSCOPY, Clare Leahy, Josh Vura-Weis

RK. Structure determination

Thursday, June 24, 2021 – 10:0 AM

Room: 2021 Online Everywhere

Chair: Ha Vinh Lam Nguyen, Université Paris-Est Créteil, Créteil, France

RK01 **10:00 – 10:01**
MICROWAVE SPECTRA AND MOLECULAR STRUCTURES OF THE GAS-PHASE HOMOCHIRAL HOMODIMERS OF 3,3-DIFLUORO-1,2-EPOXYPROPANE AND 3-FLUORO-1,2-EPOXYPROPANE, Mark D. Marshall, Helen O. Leung

RK02 **10:04 – 10:05**
THE MICROWAVE SPECTRUM AND MOLECULAR STRUCTURE OF *TRANS*-2-FLUORO-3-(TRIFLUOROMETHYL)OXIRANE AND ITS COMPLEX WITH THE ARGON ATOM, Jordan M. Aucoin, Helen O. Leung, Mark D. Marshall

RK03 **10:08 – 10:09**
STRUCTURE AND INTERNAL MOTIONS OF THE PROPARGYL ALCOHOL-WATER COMPLEX, Sharon Priya Gnanasekar, Elangannan Arunan

RK04 **10:12 – 10:13**
ROTATIONAL SPECTRUM OF 2-AMINOACETOPHENONE AND ITS 1:1 WATER COMPLEX, Giovanna Salvitti, Assimo Maris, Susana Blanco, Juan Carlos Lopez

RK05 **10:16 – 10:17**
CHARACTERIZING HYDROGEN-BONDED SYSTEMS BY COLD-ION INFRARED ACTION SPECTROSCOPY: THE FORMIC ACID TRIMER CASE, Martín Taccone, Daniel A Thomas, Katja Ober, Gert von Helden, Gerard Meijer

RK06 **10:20 – 10:21**
IRMPD SPECTROSCOPY OF $CO_3^-(H_2O)_{1,2}$ AND $CO_4^-(H_2O)_{1,2}$, Maximilian G Münst, Milan Oncak, Martin K Beyer, Christian van der Linde

RK07 **10:24 – 10:25**
ROTATIONAL SPECTROSCOPY OF IMINE-BASED MOLECULAR SWITCHES: ISOLATED AND MICRO-SOLVATED, Nuno Campos, Pablo Pinacho, Corina H. Pollok, Christian Merten, Manuela Ramos Silva, Melanie Schnell, Sergio R. Domingos

RK08 **10:28 – 10:29**
INTRAMOLECULAR INTERACTIONS WITHIN 1- AND 2-NAPHTHOL: A ROTATIONAL SPECTROSCOPIC AND THEORETICAL STUDY, Arsh Singh Hazrah, Sadisha Nanayakkara, Nathan A. Seifert, Elfi Kraka, Wolfgang Jäger

RK09 **10:32 – 10:33**
MULTI-AGENT CONSENSUS EQUILIBRIUM (MACE) IN MOLECULAR AND ELECTRONIC STRUCTURE DETERMINATION, Jiayue Rong

RK10 **10:36 – 10:37**
THE SHAPES OF SULFONAMIDES: ROTATIONAL SPECTRA OF BENZENESULFONAMIDE, *ortho*-TOLUENSULFONAMIDE, *para*-TOLUENSULFONAMIDE AND SULFANILAMIDE, Sonia Melandri, Annalisa Vigorito, Assimo Maris, Camilla Calabrese, M. Eugenia Sanz, Donatella Loru, Isabel Peña

RK11 **10:40 – 10:41**
NEW INVESTIGATION OF THE ROTATIONAL SPECTRUM OF SABINENE, Mhamad Chrayteh, Therese R. Huet, Pascal Dréan

RK12 **10:44 – 10:45**
THE SHAPE OF LEVODOPA: A LASER ABALATION ROTATIONAL STUDY, Miguel Sanz Novo, Elena R. Alonso, Iker León, José L. Alonso

RK14 **10:52 – 10:53**
CONFORMERS OF VANILLIC ACID: A ROTATIONAL SPECTROSCOPIC AND THEORETICAL STUDY, Mohamad Al-Jabiri, Wolfgang Jäger

RK15 **10:56 – 10:57**
PROGRESS MADE TOWARDS CONTEXT-FREE MOLECULAR STRUCTURE DETERMINATION FROM ISOTOPOLOGUE ROTATIONAL SPECTROSCOPY, Lia Yeh, Dylan Finestone, Lincoln Satterthwaite, Jieyu Yan, David Patterson

RL. Electronic structure, potential energy surfaces

Thursday, June 24, 2021 – 10:0 AM

Room: 2021 Online Everywhere

Chair: Mallory Green, Fritz Haber Institute of the Max Planck Society, Berlin, Germany

RL01 **10:00 – 10:01**
LASER-INDUCED FLUORESCENCE (LIF) OF JET-COOLED SmO, Joel R Schmitz, Arianna Rodriguez, Michael Heaven

RL02 **10:04 – 10:05**
LASER-INDUCED FLUORESCENCE (LIF) OF JET-COOLED NdO AND NdO^+ , Joel R Schmitz, Arianna Rodriguez, Michael Heaven

RL03 ***Post-Deadline Abstract*** **10:08 – 10:09**
ELECTRONIC STRUCTURE OF THE GROUND AND EXCITED STATES OF RhO^{2+}: ITS ROLE IN THE C-H BOND ACTIVATION OF METHANE, Shahriar N Khan, Evangelos Miliordos

RL04 **10:12 – 10:13**
ELECTRONIC STRUCTURE ANALYSIS OF GROUND AND EXCITED STATES OF $MO^{2+/+/0/-}$ (M = Mo, Ru) AND THEIR WATER ACTIVATION STRENGTHS, Isuru R. Ariyarathna, Evangelos Miliordos

RL05 **10:16 – 10:17**
ADIABATIC MOLECULAR ORBITAL TRACKING IN AB INITIO MOLECULAR DYNAMICS, Asylbek A Zhanserkeev, Ryan P Steele

RL06 **10:20 – 10:21**
PROBING THE WAVELENGTH-DEPENDENT EXCITED-STATE DYNAMICS OF A PHOTOCHROMIC MOLECULAR SWITCH USING RESONANCE RAMAN SPECTROSCOPY, Kristen H. Burns, Christopher G. Elles

RL07 **10:24 – 10:25**
THE EFFECT OF THE SADDLE POINT POSITION AND THE OH-BONDING FORCE CONSTANT ON THE TRANSITION FREQUENCIES OF H-BOND OF NAPHTHAZARIN, Fatemeh Afshar Ghahremani, Mansoureh Zahedi-Tabrizi, Sayyed Faramarz Tayyari

RL08 **10:28 – 10:29**
VALENCE-HOLE ELECTRON CONFIGURATIONS: A NEW GLOBAL ELECTRONIC STRUCTURE PARADIGM FOR C_2 AND BEYOND , Jun Jiang, Timothy Schmidt, Klaas Nauta, Robert W Field

RL09 **10:32 – 10:33**
EXAMINING HYPERMETALLIC OXIDE MgOMg WITH LASER INDUCED FLUORESCENCE AND PHOTOIONIZATION SPECTROSCOPY , Thomas D. Persinger, Michael Heaven

RL10 **10:36 – 10:37**
STUDY OF LiMg AND $LiMg^+$ USING LASER INDUCED FLUORESCENCE AND TWO-PHOTON IONIZATION, Thomas D. Persinger, Jiande Han, Michael Heaven

RL11 **10:40 – 10:41**
INTERPRETING THE ELECTRONIC STRUCTURE OF SUPERATOMIC $AU_8(PPH_3)_7^{2+}$, Jonathan Wood Fagan, Christopher J. Johnson

RL12 **10:44 – 10:45**
SPECTROSCOPIC STUDIES OF SMALL POLYATOMIC MOLECULES NEAR ION-PAIR DISSOCIATION THRESHOLDS, Carla Kreis, Urs Hollenstein, Frédéric Merkt

RL14 **10:52 – 10:53**
DETAILED VIEW INTO THE Au_2^+ POTENTIAL ENERGY SURFACES, Marko Förstel, Kai Pollow, Taarna Studemund, Robert G. Radloff, Roland Mitric, Otto Dopfer

RM. Action spectroscopy (incl. PE, PD, PI, LIR)

Thursday, June 24, 2021 – 10:0 AM

Room: 2021 Online Everywhere

Chair: Michael D. Morse, University of Utah, Salt Lake City, UT, USA

RM01 **10:00 – 10:01**
OBSERVATION OF A DIPOLE-BOUND STATE IN THRESHOLD PHOTODETACHMENT SPECTROSCOPY OF THE INTERSTELLAR ANION C_3N^-, Malcolm James Simpson, Markus Nötzold, Tim Michaelsen, Robert Wild, Franco A. Gianturco, Roland Wester

RM02 ***Post-Deadline Abstract*** **10:04 – 10:05**
A GENERAL PATH TO INFRARED SPECTROSCOPY OF SINGLE MOLECULAR IONS , David Patterson

RM03 **10:08 – 10:09**
THE ZEEMAN EFFECT IN CO^+ OBSERVED WITH ROTATIONAL ACTION SPECTROSCOPY, Aravindh Nivas Marimuthu, Kim Steenbakkers, Britta Redlich, Sandra Brünken

RM04 **10:12 – 10:13**
STRUCTURE AND OPTICAL PROPERTIES OF THE $Si_4C_2^+$ CATION, Robert G. Radloff, Marko Förstel, Kai Pollow, Taarna Studemund, Otto Dopfer

RM05 **10:16 – 10:17**
PHOTODEPLETION SPECTROSCOPY OF IO^- WITHIN THE ACTINIC RANGE, Benjamin McKinnon, Samuel Marlton, Boris Ucur, Berwyck Poad, Stephen J. Blanksby, Evan Bieske, Adam J. Trevitt

RM06 **10:20 – 10:21**
HIGH-RESOLUTION PHOTODISSOCIATION SPECTROSCOPY OF N_2O^+, Anthony Roucou, Xavier Urbain, Clément Lauzin

RM07 **10:24 – 10:25**
ROVIBRATIONAL SPECTROSCOPY OF THE CH^+-He AND CH^+-He_4 COMPLEXES, Thomas Salomon, José Luis Doménech, Philipp C Schmid, Ernest A Michael, Stephan Schlemmer, Oskar Asvany

RM08 **10:28 – 10:29**
INFRARED SPECTROSCOPY OF THE $Co^+(H_2O)$ COMPLEX WITH He, Ne, AND Ar TAGGING., Joshua H Marks, Evangelos Miliordos, Michael A Duncan

RM09 **10:32 – 10:33**
AN ION MOBILITY MASS SPECTROMETRY CRYOGENIC ION TRAP INSTRUMENT COUPLED TO THE FRITZ HABER INSTITUTE INFRARED FREE ELECTRON LASER, Maike Lettow, Eike Mucha, Jan Horlebein, Gerard Meijer, Gert von Helden

RM10 **10:36 – 10:37**
CIVP SPECTROSCOPY OF PYRIDINIUM IONS: SURPRISING PERTURBATION BY TAG MOLECULES, Alexandra Tsybizova, Eno Paenurk, Vladimir Gorbachev, Peter Chen

RM11 **10:40 – 10:41**
OPTICAL SPECTRUM OF THE ADAMANTANE RADICAL CATION, Parker B. Crandall, David Müller, Marko Förstel, Otto Dopfer

RM12 **10:44 – 10:45**
DETERMINATION OF SPECTROSCOPICALLY-STRUCTURAL CONNECTION IN THE PYRIDINIUM SERIES TO PROBE LONDON DISPERSION FORCES, Vladimir Gorbachev, Alexandra Tsybizova, Larisa Miloglyadova, Peter Chen

RM13 **10:48 – 10:49**
TEMPERATURE DEPENDENCE IN RELATIVE POPULATIONS BETWEEN ISOMERS HAVING DISTINCT HYDROGEN BOND STRUCTURES OF PHENOL-METHANOL CLUSTER CATIONS, Masataka Orito, Masayoshi Ozeki, Haruki Ishikawa

RM14 **10:52 – 10:53**
DIRECT OBSERVATION OF IR INDUCED ISOMERIZATIONS OF HYDROGEN-BONDED PHENOL CLUSTER CATIONS, Masayoshi Ozeki, Masataka Orito, Kenta Mizuse, Haruki Ishikawa

RM15 ***Post-Deadline Abstract*** **10:56 – 10:57**
HIGH RESOLUTION ANION PHOTOELECTRON SPECTRA OF NDO^-, Mark C Babin, Martin DeWitt, Jessalyn A. DeVine, David C McDonald II, Nicholas S. Shuman, Albert Viggiano, Lan Cheng, Daniel Neumark

FA. Mini-symposium: Spectroscopy with Undergraduates

Friday, June 25, 2021 – 8:0 AM

Room: 2021 Online Everywhere

Chair: AnGayle (AJ) Vasiliou, Middlebury College , Middlebury , VT, USA

FA01 ***INVITED TALK*** **8:00 – 8:02**
RESEARCH WITH UNDERGRADUATES: SPECTROSCOPY IS JUST THE BEGINNING, Laura R. McCunn

FA02 **8:08 – 8:09**
OBSERVATION OF THE C_6H_7 RADICAL IN AN ARGON MATRIX USING MATRIX ISOLATION INFRARED SPECTROSCOPY, Jay C. Amicangelo, Lia Totleben, Jacob Oslosky, Yen Jui Su, Nicole Orwat

FA03 **8:12 – 8:13**
HELIUM NANODROPLETS AND LIQUID HOT NAGMA: WHAT STUDENTS CAN LEARN ABOUT THERMODYNAMICS FROM INFRARED SPECTROSCOPY AND A MODEL DIPEPTIDE, Alaina R. Gunn

FA04 **8:16 – 8:17**
WEAK HYDROGEN BONDING IN COMPLEXES OF SELENOPHENE AND WATER: A MATRIX ISOLATION FTIR AND COMPUTATIONAL STUDY, Josh Newby, Tiara Sivells

FA05 **8:20 – 8:21**
HELIUM NANODROPLET ISOLATION SPECTROSCOPY IN AN UNDERGRADUATE TEACHING LABORATORY, Paul Raston

FA06 **8:24 – 8:25**
COMPOSITIONAL ANALYSIS OF TITAN'S ATMOSPHERE USING SPITZER INFRARED SPECTROGRAPH DATA, Brandon Park Coy, Conor A Nixon, Naomi Rowe-Gurney

FA07 **8:28 – 8:29**
A BROADBAND ROTATIONAL SPECTROSCOPIC STUDY OF DIETHYL PHTHALATE, Raiden Speelman, Arsh Singh Hazrah, Nathan A. Seifert, Wolfgang Jäger

FA08 **8:32 – 8:33**
FABRICATION AND CHARACTERIZATION OF HIGHLY EFFICIENT DYE-SENSITIZED SOLAR CELL WITH COMPOSITED DYES, Garris H.C. Radloff, Feven M Naba, Dorothy B Ocran-Sarsah, Makenzie E Bennett, Kathryn M Sterzinger, Abigail T Armstrong, Nahom Zewde, Cameron Gray, Mahesh B. Dawadi

FA09 **8:36 – 8:37**
EFFICIENT COMPRESSION OF MOLECULAR LINE LISTS: APPLICATION OF 'SUPER-ENERGIES' TO THE EXOMOL DATABASE, Xudong Ke Lin, Samuel Wright, Alec Owens, Jonathan Tennyson, Sergei N. Yurchenko

FA10 **8:40 – 8:41**
INVOLVING HIGH-SCHOOL STUDENTS IN COMPUTATIONAL CHEMISTRY MOLECULAR DATA GENERATION FOR EXOPLANET SPECTROSCOPY, Laura K McKemmish, Anna-Maree Syme, Clara Sousa-Silva

FA11 **8:44 – 8:45**
EPR SPECTROSCOPY OF RUBY IN THE UNDERGRADUATE PHYSICAL CHEMISTRY TEACHING LABORATORY, Bryan Lynch

FA12 **8:48 – 8:49**
GUIDED-INQUIRY SPECTROSCOPIC PROJECTS IN THE PHYSICAL CHEMISTRY LAB, Steven Shipman

FA13 **8:52 – 8:53**
BUILDING A RESEARCH PROGRAM AT A PRIMARILY UNDERGRADUATE INSTITUTION, Jacob Stewart

FB. Clusters/Complexes

Friday, June 25, 2021 – 8:0 AM

Room: 2021 Online Everywhere

Chair: Daniel A. Obenchain, Georg-August-Universität Göttingen, Göttingen, Germany

FB01 **8:00 – 8:01**
HOW SOLVENTS CHANGE THE CONFORMATIONAL LANDSCAPE IN MOLECULES WITH WEAK INTRAMOLECULAR INTERACTIONS: METHYL 2-METHOXYBENZOATE, Alberto Macario, Juan Carlos Lopez, Susana Blanco

FB02 **8:04 – 8:05**
PROBING AZULENE-WATER INTERACTIONS AND AZULENE AGGREGATION BY BROADBAND ROTATIONAL SPECTROSCOPY, Shefali Saxena, Ecaterina Burevschi, Yang Zheng, Qian Gou, M. Eugenia Sanz

FB03 **8:08 – 8:09**
UNRAVELLING THE MICROSOLVATION FRAMEWORK AROUND PROTOTYPE POLYCYCLIC AROMATIC HYDROCARBON, NAPHTHALENE, BY HIGH-RESOLUTION INFRARED SPECTROSCOPY, Kuntal Chatterjee, Tarun Kumar Roy, Jai Khatri, Martina Havenith

FB04 **8:12 – 8:13**
MICROWAVE SPECTROSCOPY OF THE 2-METHYLAMINOETHANOL-WATER COMPLEX, DYLAN S VALENTE, Dinesh Marasinghe, Michael Tubergen

FB05 **8:16 – 8:17**
MICROWAVE SPECTRUM AND LARGE AMPLITUDE MOTION OF METHANESULFONIC ACID , Anna Huff, Nathan Love, Kenneth R. Leopold

FB06 **8:20 – 8:21**
MICROWAVE SPECTRUM OF THE METHANESULFONIC ACID – WATER COMPLEX, Anna Huff, Nathan Love, Kenneth R. Leopold

FB07 **8:24 – 8:25**
ATTENUATED STABILITY OF DEUTERIUM-BOUND COMPLEXES AT ROOM TEMPERATURE, Alexander Kjærsgaard, Emil Vogt, Henrik G. Kjaergaard

FB08 **8:28 – 8:29**
ROTATIONAL SPECTRA OF THE CH_3CN-CO_2 COMPLEX: OBSERVING A CARBON 'TETREL BOND', Sharon Priya Gnanasekar, Elangannan Arunan

FB09 **8:32 – 8:33**
BOUND STATE CALCULATIONS OF THE VAN DER WAALS NH_3-Ne COMPLEX AND FIRST MICROWAVE DETECTION OF THE MISSING ($para$)-NH_3-Ne NUCLEAR SPIN ISOMER, Leonid Surin, Ivan Tarabukin, Cristobal Perez, Melanie Schnell, Jerome Loreau, Ad van der Avoird

FB10 **8:36 – 8:37**
ETHANOL TRIMER CONFIGURATIONS REVEALED BY CP-FTMW SPECTROSCOPY AND COMPUTATIONAL CALCULATIONS, S. Indira Murugachandran, Isabel Peña, Al Mokhtar Lamsabhi, Manuel Yáñez, M. Eugenia Sanz

FB11 **8:40 – 8:41**
CONFORMATIONAL LANDSCAPES OF 2-FUROIC ACID MONOMERS AND DIMERS BY ROTATIONAL SPECTROSCOPY AND DFT CALCULATIONS, Qian Yang, FAN XIE, Wolfgang Jäger, Yunjie Xu

FB12 **8:44 – 8:45**
ROOM TEMPERATURE GAS-PHASE GIBBS ENERGIES OF WATER AMINE COMPLEXES, Emil Vogt, Alexander Kjærsgaard, Henrik G. Kjaergaard

FB13 **8:48 – 8:49**
MICROSOLVATION OF CARBENES IN SUPERFLUID HELIUM NANODROPLETS, Jai Khatri, Tarun Kumar Roy, Stefan Henkel, Kuntal Chatterjee, Gerhard Schwaab, Martina Havenith

FC. Astronomy

Friday, June 25, 2021 – 8:0 AM

Room: 2021 Online Everywhere

Chair: SERGIO IOPPOLO, Queen Mary University of London (QMUL), London, United Kingdom

FC01 **8:00 – 8:01**
SUBLIMATION OF LABORATORY ICES MILLIMETER/SUBMILLIMETER EXPERIMENT (SubLIME): IDENTIFICATION AND QUANTIFICATION OF ORGANIC SPECIES FROM A UV PHOTOLYZED METHANOL ICE, Katarina Yocum, Stefanie N Milam, Perry A. Gerakines, Susanna L. Widicus Weaver

FC02 **8:04 – 8:05**
REVEALING THE CHEMISTRY OF POLYCYCLIC AROMATIC HYDROCARBONS BY PLASMA SOURCES, Donatella Loru, Daniel Rap, Sébastien Gruet, Amanda Steber, Melanie Schnell

FC03 **8:08 – 8:09**
IR ABSORPTION AND CALCULATED FREQUENCIES OF FORMALDEHYDE DISSOLVED IN LIQUID Kr, Suresh Sunuwar, Carlos Manzanares

FC04 **8:12 – 8:13**
FORMATION OF PYRUVIC ACID AND 1,2-ETHENEDIOL IN INTERSTELLAR ANALOG ICES, N. Fabian Kleimeier, André K. Eckhardt, Peter R. Schreiner, Ralf Ingo Kaiser

FC05 **8:16 – 8:17**
SPECTROSCOPIC STUDIES OF METHYL FORMATE AND ITS FORMATION PATHWAYS IN SPACE UPON ION IRRADIATION, Alejandra Traspas Muiña , SERGIO IOPPOLO, Peter Herczku, Zoltan Juhász, Sándor T. S. Kovács, Duncan Mifsud, Zuzana Kaňuchová, Nigel Mason, Robert w McCullough, Béla Sulik

FC06 **8:20 – 8:21**
DISCOVERING NOVEL GAS-PHASE NITROGEN-HETEROCYCLE FORMATION PATHWAYS WITH AN AB INITIO NANOREACTOR, Sommer L. Johansen, Lisa Oh, Lee-Ping Wang, Kyle N. Crabtree

FC07 **8:24 – 8:25**
MEASURING THE DIFFERENCE IN COLLISIONAL INTERACTION OF HCN/HNC WITH He AT LOW TEMPERATURES USING THE CPUF TECHNIQUE, Brian M Hays, Theo Guillaume, Divita Gupta, Franck Thibault, François Lique, Ian R. Sims

FC08 **8:28 – 8:29**
LOW-TEMPERATURE KINETICS MEASUREMENTS OF THE GAS-PHASE REACTIONS BETWEEN AROMATIC SPECIES AND THE CN RADICAL , Divita Gupta, Ilsa Rose Cooke, Joseph P. Messinger, Mitchio Okumura, Ian R. Sims

FC09 **8:32 – 8:33**
REACTION RATE MODELING TO OPTIMIZE O(^{1}D) INSERTION INTO METHYLAMINE FOR THE DETECTION OF AMINOMETHANOL , Hayley Bunn, Chase P Schultz, Christopher M Jernigan, Susanna L. Widicus Weaver

FC10 **8:36 – 8:37**
TESTING DUST-SURFACE FORMATION MODEL OF PREBIOTIC MOLECULE CH_3NCO IN STAR-FORMING CORE SAGITTARIUS B2(N1) BY ALMA, Kyoichi Izuoka, Mitsunori Araki, Yuki Ohno, Takahiro Oyama, Shuro Takano, Nobuhiko Kuze, Koichi Tsukiyama

FC11 **8:40 – 8:41**
REEVALUATION OF THE C_4H ABUNDANCE BASED ON THE REVISED DIPOLE MOMENT, Takahiro Oyama, Yoshihiro Sumiyoshi, Mitsunori Araki, Shuro Takano, Nobuhiko Kuze, Koichi Tsukiyama

FC12 **8:44 – 8:45**
ANALYSIS OF THE CH_2OH RADICAL SPECTRUM WITH AN IAM TUNNELING APPROACH, L. H. Coudert, Olivia Chitarra, Jean-Thibaut Spaniol, Marie-Aline Martin-Drumel, Olivier Pirali, J.-C. Loison

FC13 **8:48 – 8:49**
HIGH-LEVEL ROVIBRATIONAL CALCULATIONS ON KETENIMINE, Martin Tschöpe, Benjamin Schröder, Sebastian Erfort, Guntram Rauhut

FD. Small molecules

Friday, June 25, 2021 – 8:0 AM

Room: 2021 Online Everywhere

Chair: Qian Gou, Chongqing University, Chongqing , China

FD01 **8:00 – 8:01**
IN SEARCH OF PHOSPHORUS IN ASTRONOMICAL ENVIRONMENTS: THE REACTION BETWEEN THE CP RADICAL ($X^2\Sigma^+$) AND METHANIMINE, Silvia Alessandrini, Francesca Tonolo, Cristina Puzzarini

FD02 **8:04 – 8:05**
THE STRUCTURE OF ScC_2 ($\tilde{X}^2A_1$): A COMBINED FOURIER TRANSFORM MICROWAVE/MILLIMETER-WAVE SPECTROSCOPY AND COMPUTATIONAL STUDY, Mark Burton, Qianyi Cheng, DeWayne T Halfen, J. Hayden Lane, Nathan DeYonker, Lucy M. Ziurys

FD03 **8:08 – 8:09**
THE MILLIMETER WAVE SPECTRUM OF RARE IRON MONOXIDE ISOTOPOLOGUES: A MASS INDEPENDENT ANALYSIS, Björn Waßmuth, Alexander A. Breier, Guido W Fuchs, Thomas Giesen

FD04 **8:12 – 8:13**
HYPERFINE STRUCTURE OF NITROSYL IODIDE (INO), Akiko Nishitsunoi, Hiroyuki Ozeki, Kaori Kobayashi, Stephane Bailleux

FD06 **8:20 – 8:21**
HIGH-RESOLUTION ANALYSIS OF THE 83.3 μm TORSIONAL BANDS OF THE $ClONO_2$ MOLECULE, F. Kwabia Tchana, Anusanth Anantharajah, Jean-Marie Flaud, Laurent Manceron, Johannes Orphal

FD07 **8:24 – 8:25**
HIGH-RESOLUTION FAR INFRARED SPECTROSCOPY AND ANALYSES OF TRIOXANE, Cyril Richard, Vincent Boudon, Olivier Pirali, Pierre Asselin

FD08 **8:28 – 8:29**
HIGH RESOLUTION INFRARED SPECTRA OF THE LINEAR DIALUMINUM MONOXIDE Al-O-Al, Daniel Witsch, Eileen Döring, Jürgen Gauss, Thomas Giesen, Guido W Fuchs

FD09 **8:32 – 8:33**
SUB-DOPPLER DOUBLE-RESONANCE SPECTROSCOPY OF METHANE USING A FREQUENCY COMB PROBE, Vinicius Silva de Oliveira, Isak Silander, Alexandra C Johanssson, Ove Axner, Aleksandra Foltynowicz, Lucile Rutkowski, Grzegorz Soboń, Kevin Lehmann

FD10 **8:36 – 8:37**
NEW LINE POSITIONS ANALYSIS OF THE ν_3 BANDS OF $^{35}ClNO_2$ AND $^{37}ClNO_2$ AROUND 370 cm^{-1}, Anusanth Anantharajah, F. Kwabia Tchana, Jean-Marie Flaud, Laurent Manceron, Johannes Orphal

FD11 **8:40 – 8:41**
ISOTOPIC RELATIONS FOR TETRAHEDRAL AND OCTAHEDRAL MOLECULES, Michel Loete, Cyril Richard, Vincent Boudon

FD12 **8:44 – 8:45**
ROTATIONAL ANALYSIS OF A NEW [15.05] Ω=0^+ – $X\ ^3\Sigma(0^+)$ ELECTRONIC TRANSITION OF TUNGSTEN SULFIDE (WS) IN THE 14,900 - 16,100 cm^{-1} REGION OBSERVED USING ILS-FTS, Kristin N Bales, Jack C Harms, James J O'Brien, Leah C O'Brien

FD13 **8:48 – 8:49**
CHARACTERIZATION OF THE $A^2\Sigma^+$ STATE OF SH/SD RADICALS BY PHOTODISSOCIATION SPECTROSCOPY, Yuan Qin, Xianfeng Zheng, Yu Song, Ge Sun, Jingsong Zhang

FE. Atmospheric science

Friday, June 25, 2021 – 8:0 AM

Room: 2021 Online Everywhere

Chair: Hamzeh Telfah, University of Louisville, LOUISVILLE, KY, USA

FE01 **8:00 – 8:01**
COMPUTATIONAL KINETICS STUDY OF ATMOSPHERIC RING-CLOSURE AND DEHYDRATION REACTIONS OF 1,4-HYDROXYCARBONYLS IN THE GAS PHASE, Parandaman Arathala, Chanin B. Tangtartharakul, Amitabha Sinha

FE03 **8:08 – 8:09**
TEMPERATURE-DEPENDENT WATER UPTAKE BEHAVIOR OF CLUSTERS RELEVANT TO NEW PARTICLE FORMATION, John J. Kreinbihl, Nicoline C. Frederiks, Christopher J. Johnson

FE04 **8:12 – 8:13**
A SPECTROSCOPIC AND COMPUTATIONAL PEEK INTO THE STRUCTURE OF ATMOSPHERICALLY RELEVANT DRY AND HYDRATED AMMONIUM BISULFATE CLUSTERS, Nicoline C. Frederiks, John J. Kreinbihl, Christopher J. Johnson

FE05 **8:16 – 8:17**
LOW-PRESSURE YIELDS OF STABILIZED CRIEGEE INTERMEDIATES PRODUCED FROM OZONOLYSIS OF A SERIES OF ALKENES, Lei Yang, Mixtli Campos-Pineda, Jingsong Zhang

FE06 **8:20 – 8:21**
LONG-OPEN-PATH MONITORING OF GREENHOUSE GASES BY NEAR-IR SPECTROSCOPY, Hans A Schuessler, Jinbao Xia, carlos Rodriguez, Alexandre Kolomenskii

FE07 **8:24 – 8:25**
MULTICHARME : A NEW CHERNIN TYPE MULTIPASS CELL FOR LONG PATHLENGTH TERAHERTZ SPECTROSCOPY EXPERIMENTS IN AN ATMOSPHERIC SIMULATION CHAMBER., Jean Decker, Jonas Bruckhuisen, Eirc Fertein, Nicolas Houzel, Pierre Kulinski, Robin Bocquet, Francis Hindle, Guillaume Dhont, Gaël Mouret, Cécile Coeur, Arnaud Cuisset

FE08 **8:28 – 8:29**
MOLECULAR TRANSITION FREQUENCES OF CO_2 NEAR 1.6 μ WITH KHZ-LEVEL UNCERTAINTIES, Zachary Reed, Brian Drouin, David A. Long, Joseph T. Hodges

FE09 **8:32 – 8:33**
HIGH ACCURACY NEAR-INFRARED CARBON DIOXIDE INTENSITY MEASUREMENTS TO SUPPORT REMOTE SENSING, David A. Long, Zachary Reed, Adam J. Fleisher, Joseph Mendonca, Sebastien Roche, Joseph T. Hodges

FE10 **8:36 – 8:37**
DOPPLER-FREE SATURATED ABSORPTION SPECTROSCOPY OF CH_4 IN THE MID-INFRARED REGION USING A CONTINUOUS-WAVE OPTICAL PARAMETRIC OSCILLATOR, S M Shah Riyadh, Hamzeh Telfah, Meagan Nicole Haase, Brianna Paige Haase, Jinjun Liu, Cunfeng Cheng

FF. Spectroscopy as an analytical tool

Friday, June 25, 2021 – 8:0 AM

Room: 2021 Online Everywhere

Chair: Carlos Manzanares, Baylor University, Waco, TX, USA

FF01 **8:00 – 8:01**
GENERATIVE ADVERSARIAL LINEAR DISCRIMINANT ANALYSIS FOR DISTINGUISHING API POLYMORPHS BY RAMAN SPECTROSCOPY, Ziyi Cao, Casey J Smith, Youlin Liu, Alex M Sherman, Garth Simpson

FF02 **8:04 – 8:05**
IDENTIFYING UNKNOWN MOLECULES WITH PROBABILISTIC DEEP LEARNING AND ROTATIONAL SPECTROSCOPY, Kelvin Lee, Michael C McCarthy

FF03 ***Post-Deadline Abstract*** **8:08 – 8:09**
EXHAUSTIVE PRODUCT ANALYSIS OF THREE BENZENE DISCHARGES BY MICROWAVE SPECTROSCOPY, Michael C McCarthy, Kelvin Lee, Brandon Carroll, Jessie P Porterfield, Bryan Changala, James H. Thorpe, John F. Stanton

FF04 **8:12 – 8:13**
IS IT CHIRAL?TOWARDS IDENTIFYING CHIRALITY IN UNKNOWN SAMPLES WITHOUT PRIOR SPECTRAL ASSIGNMENT., Greta Koumarianou, Lincoln Satterthwaite, Irene Wang, David Patterson

FF05 **8:16 – 8:17**
TIME-RESOLVED ROTATIONAL SPECTROSCOPY OF CARBOXYLIC ACIDS. IDENTIFICATION AND QUANTIFICATION OF THE COMPONENTS FROM HEATING ADIPIC ACID., Pablo Pinacho, Wenhao Sun, Daniel A. Obenchain, Melanie Schnell

FF06 **8:20 – 8:21**
CHIRPED PULSE MILLIMETER WAVE SPECTROSCOPY OF COMPLEX MOLECULES, Marius Hermanns, Nadine Wehres, Bettina Heyne, Frank Lewen, Stephan Schlemmer

FF08 **8:28 – 8:29**
LASER SYNTHESIS AND SPECTROSCOPY OF PYRENE DIMERS, Ian Webster, Michael A Duncan

FF09 **8:32 – 8:33**
DEEP REPRESENTATION LEARNING OF SPECTROSCOPIC GRAPHS, Kelvin Lee, Christine Li, Brett A. McGuire, Kyle N. Crabtree

FF10 **8:36 – 8:37**
COMBINED ROTATIONAL AND VIBRATIONAL CARS SPECTRA OF O_2 FOR SIMULTAENOUS TEMPERATURE AND PRESSURE MEASUREMENTS, Aman Satija, Robert P. Lucht

FF11 **8:40 – 8:41**
USING ULTRAVIOLET LASER ABSORPTION SPECTROSCOPY TO MEASURE VIBRATIONAL TEMPERATURE TIME HISTORIES OF SHOCK-HEATED OXYGEN, Ajay Krish, Jesse William Streicher, Ron K Hanson

FF12 **8:44 – 8:45**
BROADBAND FREQUENCY COMB VERNIER SPECTROSCOPY IN THE MID-IR WITH VIDEO-RECORDING RETRIEVAL OF ABSORPTION SPECTRUM, Hans A Schuessler, James R Bounds, Alexandre Kolomenskii

FG. Plenary

Friday, June 25, 2021 – 9:0 AM

Room: 2021 Online Everywhere

Chair: Anthony Remijan, NRAO, Charlottesville, VA, USA

FG02 **9:03 – 9:43**

CHIRALITY RECOGNITION/TRANSFER/AMPLIFICATION: ROTATIONAL SPECTROSCOPIC AND CHIROPTICAL SPECTROSCOPIC STUDIES, Yunjie Xu

FH. Mini-symposium: Spectroscopy with Undergraduates

Friday, June 25, 2021 – 10:0 AM

Room: 2021 Online Everywhere

Chair: Jacob Stewart, Connecticut College, New London, CT, USA

FH01 ***INVITED TALK*** **10:00 – 10:02**
UNDERGRADUATE MOLECULAR SPECTROSCOPY APPROACHES IN RESEARCH AND TEACHING AS AN EXPERIENTIAL LEARNING ENTERPRISE AT MISSOURI S&T, G. S. Grubbs II

FH02 **10:08 – 10:09**
OODLES OF UNDERGRADS UNDERGROUND: CLASSROOM UNDERGRADUATE RESEARCH AT WIND CAVE NATIONAL PARK, Joshua A Sebree

FH03 **10:12 – 10:13**
USING COMPUTATIONAL TOOLS TO ENHANCE LEARNING IN AN UNDERGRADUATE MOLECULAR SPECTROSCOPY COURSE, M. Reza Poopari, Shyam Parshotam, Yunjie Xu

FH04 **10:16 – 10:17**
BIOMOLECULAR STRUCTURE OF TROPINE DETERMINED FROM QUANTUM CHEMISTRY SIMULATIONS OF VIBRATIONAL SPECTROSCOPY, Emily Lyn Yang, Ryan P Steele

FH05 **10:20 – 10:21**
AN EXOMOL LINE LIST FOR SO: ROVIBRONIC SPECTRUM OF SULFUR MONOXIDE, Ryan Brady, Gap-Sue Kim, Wilfrid Somogyi, Jonathan Tennyson, Sergei N. Yurchenko

FH07 **10:28 – 10:29**
COMPUTATIONAL SPECTROSCOPIC SIGNATURES OF PROTEINOGENIC GLUTAMIC ACID AND ITS ISOMERIC SPECIES OF ASTROPHYSICAL IMPORTANCE , Namrata Rani, Vikas

FH08 **10:32 – 10:33**
NARROWING DOWN THE POSSIBLE GEOMETRIES OF A MOLECULE FROM ISOTOPOLOGUE ROTATIONAL CONSTANTS WITH STRUCTURAL FILTERS, Jieyu Yan, David Patterson

FH09 **10:36 – 10:37**
USE OF STUDENT-SPECIFIC MOLECULES AND THEIR SPECTROSCOPIC PROPERTIES IN PHYSICAL CHEMISTRY COURSES, David E. Woon

FH10 ***Post-Deadline Abstract*** **10:40 – 10:41**
THE CHIRPED-PULSE CLUB: MICROWAVE SPECTROSCOPY RESEARCH IN HIGH SCHOOL, Josue Cervantes, Emily Geraghty, Anish Kanthamneni, Ziwei Liu, Shamitha Nandi, Elic Weeks, Garrett Youngblood, Gordon G Brown

FH11 **10:44 – 10:45**
EXPLAINER: EFFECTS OF NUCLEAR QUADRUPOLE COUPLING TENSOR MAGNITUDE, ASYMMETRY, AND ORIENTATION ON THE APPEARANCE OF ROTATIONAL HYPERFINE STRUCTURE, S. A. Cooke

FH12 **10:48 – 10:49**
IMPLEMENTING EXTENDED CROSS CORRELATION AS A TOOL FOR SEMI-AUTOMATED MICROWAVE SPECTROSCOPIC ANALYSIS OF WEAKLY BOUND CLUSTER SPECTRA, Hannah Fino, Rebecca A. Peebles, Sean A. Peebles, Channing West, Brooks Pate

FH13 **10:52 – 10:53**
ENGAGING UNDERGRADUATE STUDENTS IN SPECTROSCOPY RESEARCH VIA DEVELOPMENT AND INCORPORATION OF ADVANCED DATA ANALYSIS TECHNIQUES, Rebecca A. Peebles, Sean A. Peebles, Prashansa Kannangara, Hannah Fino

FI. Clusters/Complexes

Friday, June 25, 2021 – 10:0 AM

Room: 2021 Online Everywhere

Chair: Wenhao Sun, DESY, Hamburg, Germany

FI01 **10:00 – 10:01**
INFRARED SPECTRA OF $(CO_2)_n$ - (RARE GAS)$_m$ TRIMERS AND TETRAMER, (n, m) = (1,2), (1,3), (2,1), A. J. Barclay, A.R.W. McKellar, Andrea Pietropolli Charmet, Nasser Moazzen-Ahmadi

FI02 **10:04 – 10:05**
INFRARED SPECTROSCOPY OF $[H_2O\text{-}(Kr)_n]^+$ (n=1-3): HEMIBOND FORMATION WITH WATER, Tomoki Nishigori, Toshihiko Maeyama, Marusu Katada, Asuka Fujii, Jing-Min Liu, Jer-Lai Kuo

FI03 ***Post-Deadline Abstract*** **10:08 – 10:09**
NEUTRAL IRON (III) SPECIES OBSERVED BY SECOND HARMONIC GENERATION SPECTROSCOPY AT THE AQUEOUS INTERFACE, Ka Chon Ng, Heather C. Allen

FI04 **10:12 – 10:13**
A CLOSE COMPETITION BETWEEN OH-O AND OH-π HYDROGEN BONDING: IR SPECTROSCOPY OF ANISOLE-METHANOL COMPLEX IN HELIUM NANODROPLETS , Tarun Kumar Roy, Devendra Mani, Gerhard Schwaab, Martina Havenith

FI05 **10:16 – 10:17**
HIGH-RESOLUTION INFRARED STUDY OF THE C_3Te AND TeC_3Te CLUSTERS, Sven Thorwirth, Thomas Salomon, Sophia Burger, Jürgen Gauss, Stephan Schlemmer, John B Dudek

FI06 **10:20 – 10:21**
STRUCTURE AND INFRARED SPECTRA OF NEW AEROSOL PARTICLE FORMATION SEED CLUSTERS, Daniel P. Tabor, Jezrielle R. Annis, Nathanael M. Kidwell

FI07 **10:24 – 10:25**
AB INITIO STUDY ON THE VIBRATIONAL SIGNATURES OF Ar_nH^+ (n=2–3), Jake A. Tan, Jer-Lai Kuo

FI09 **10:32 – 10:33**
NEW INFRARED SPECTRA OF CO_2-Xe: MODELING Xe ISOTOPE EFFECTS, INTERMOLECULAR BEND AND STRETCH, AND SYMMETRY BREAKING OF THE CO_2 BEnd, A. J. Barclay, A.R.W. McKellar, Colin Western, Nasser Moazzen-Ahmadi

FI10 **10:36 – 10:37**
$Si_nO_m^+$ – OPTICAL ABSORPTION AND PHOTODISSOCIATION PROPERTIES, Taarna Studemund, Marko Förstel, Lars Dahllöf, Kai Pollow, Robert G. Radloff, Otto Dopfer

FI11 **10:40 – 10:41**
INFRARED SPECTRA OF $(CO_2)_2$-X, CO_2-X_2, AND CO_2-X_3, X = CO OR N_2, A. J. Barclay, A.R.W. McKellar, Andrea Pietropolli Charmet, Nasser Moazzen-Ahmadi

FI12 **10:44 – 10:45**
THE INFRARED SPECTRUM OF CO_2-Kr, INCLUDING THE INTERMOLECULAR BENDING MODE AND SYMMETRY BREAKING OF THE CO_2 BEND, Sye Ghebretnsae, A. J. Barclay, Nasser Moazzen-Ahmadi

FI13 **10:48 – 10:49**
TUNNELING DYNAMICS IN $N_2 - D_2O$ OBSERVED IN THE OD STRETCHING REGION, R. Glorieux, Clément Lauzin, A. J. Barclay, Michel Herman, Nasser Moazzen-Ahmadi

FJ. Photodissociation and photochemistry

Friday, June 25, 2021 – 10:0 AM

Room: 2021 Online Everywhere

Chair: Katharine Moore Tibbetts, Virginia Commonwealth University, Richmond, VA, USA

FJ01 **10:00 – 10:01**
DYNAMICAL SIGNATURES FROM COMPETING, NONADIABATIC FRAGMENTATION PATHWAYS OF S-NITROSOTHIOPHENOL, K. Jacob Blackshaw, Marcus Marracci, Andrew S. Petit, Nathanael M. Kidwell

FJ02 ***Post-Deadline Abstract*** **10:04 – 10:05**
THE PHOTOCHEMICAL PATHWAYS FOR THE NONREACTIVE ELECTRONIC QUENCHING OF NO ($A^2\Sigma^+$) BY CO AND H_2O, Jose Guardado Sandoval, Nathanael M. Kidwell, Andrew S. Petit

FJ03 **10:08 – 10:09**
UNIMOLECULAR DISSOCIATION OF PEROXYFORMIC ACID INITIATED BY VIBRATIONAL OVERTONE EXCITATION TO THE 6νOH STATE, Josue Emmanuel Perez, Madhusudan Roy, Amitabha Sinha

FJ04 **10:12 – 10:13**
ROTATIONAL COOLING DYNAMICS OF HOT TRAPPED OH^- IONS PROBED BY VMI PHOTOELECTRON SPECTROSCOPY, Abhishek Shahi, Saurabh Mishra, Dhanoj Gupta, Oded Heber, Daniel Zajfman

FJ05 **10:16 – 10:17**
BOND DISSOCIATION DYNAMICS AND THERMODYNAMICS OF NiO^+ AND NiS^+, Schuyler P Lockwood, Ricardo B. Metz

FJ06 **10:20 – 10:21**
SPECTROSCOPIC STUDIES OF TRANSITION METAL AND LANTHANIDE BORIDES WITH RESONANT TWO-PHOTON IONIZATION SPECTROSCOPY, Dakota M. Merriles, Kimberly H. Tomchak, Christopher Nielson, Erick Tieu, Michael D. Morse

FJ07 **10:24 – 10:25**
BOND DISSOCIATION ENERGIES OF DIATOMIC LANTHANIDE SULFIDES AND SELENIDES, Jason J Sorensen, Erick Tieu, Michael D. Morse

FJ08 **10:28 – 10:29**
EXOMOLHD: PHOTODISSOCIATION OF DIATOMIC MOLECULES, Marco Pezzella, Sergei N. Yurchenko, Jonathan Tennyson

FJ09 **10:32 – 10:33**
AB INITIO STUDY OF THE HIGHLY EXCITED ELECTRONIC STATES OF C_2 AND ITS PHOTODISSOCIATION, Zhongxing Xu, Lee-Ping Wang, Steven Federman, William M. Jackson, Cheuk-Yiu Ng, Kyle N. Crabtree

FJ10 **10:36 – 10:37**
PHOTOINDUCED CHARGE TRANSFER PROCESSES, Ethan M Cunningham, Christian van der Linde, Milan Oncak, Martin K Beyer

FJ11 **10:40 – 10:41**
PROTOMERS OF FLAVIN RADICAL ANIONS PROBED WITH PD ACTION SPECTROSCOPY, Samuel Marlton, Benjamin McKinnon, Boris Ucur, James P Bezzina, Stephen J. Blanksby, Adam J. Trevitt

FJ12 **10:44 – 10:45**
DELIBERATE FUNCTIONALIZATION AND THE CONSEQUENTIAL ELECTRONIC RELAXATION PATHWAYS OF THE PYRIMIDINE CHROMOPHORE, Sean J. Hoehn, Sarah E. Krul, Carlos E. Crespo-Hernández

FJ13 **10:48 – 10:49**
ELECTRONIC RELAXATION MECHANISM OF GUANINE DERIVATIVES IN SOLUTION, Sarah E. Krul, Sean J. Hoehn, Carlos E. Crespo-Hernández

FJ14 **10:52 – 10:53**
POTENTIAL DEPENDENT PLASMONIC CATALYZED CLEAVAGE OF C-BR BOND OF 8-BROMOADENINE ON SILVER ELECTRODES OF NANOSTRUCTURE, De-Yin Wu, Zhong-Qun Tian

FK. Structure determination

Friday, June 25, 2021 – 10:0 AM

Room: 2021 Online Everywhere

Chair: Helen O. Leung, Amherst College, Amherst, MA, USA

FK01 **10:00 – 10:01**
SEMI-EXPERIMENTAL EQUILIBRIUM STRUCTURE (r_e^{SE}) OF METHACRYLONITRILE(C_4H_5N), Houston H. Smith, Samuel M. Kougias, Danny J Lee, Brian J. Esselman, R. Claude Woods, Robert J. McMahon

FK02 **10:04 – 10:05**
SEMI-EXPERIMENTAL EQUILIBRIUM STRUCTURE OF 1H- AND 2H-1,2,3-TRIAZOLES ($C_2H_3N_3$), Maria Zdanovskaia, Brian J. Esselman, Samuel M. Kougias, John F. Stanton, R. Claude Woods, Robert J. McMahon

FK03 **10:08 – 10:09**
DETERMINATION OF SUBSTITUTION EFFECTS ON THE STRUCTURES OF 2-, 3-, AND 4-PICOLYLAMINE USING FOURIER TRANSFORM MICROWAVE SPECTROSCOPY, Ryan G Bird, Caleb B Shiery, Kaylee X Shook

FK04 **10:12 – 10:13**
OXAZOLE: PRECISE SEMI-EXPERIMENTAL EQUILIBRIUM STRUCTURE DETERMINATION BY ROTATIONAL SPECTROSCOPY, Taylor K. Adkins, Maria Zdanovskaia, Kaori Kobayashi, Shozo Tsunekawa, Brian J. Esselman, R. Claude Woods, Robert J. McMahon

FK05 **10:16 – 10:17**
PRECISE SEMI-EXPERIMENTAL EQUILIBRIUM STRUCTURE OF THIAZOLE (C_3H_3NS), Brian J. Esselman, Maria Zdanovskaia, John F. Stanton, R. Claude Woods, Robert J. McMahon

FK06 **10:20 – 10:21**
PROPANE ISOTOPOLOGUES: HIGH RESOLUTION SYNCHROTRON FAR-IR SPECTRA OF THE SYMMETRICALLY DEUTERATED SPECIES $CH_3CH_2CD_3$, $CD_3CH_2CD_3$ AND C_3D_8. FIRST EXPERIMENTALLY DETERMINED GROUND STATE CONSTANTS FOR THESE SPECIES, Stephen J. Daunt, Robert Grzywacz, Colin Western, Brant E. Billinghurst, Jianbao Zhao

FK07 **10:24 – 10:25**
SEMI-EXPERIMENTAL EQUILIBRIUM STRUCTURE DETERMINATION OF THIOPHENE (C_4H_4S), Vanessa L. Orr, Yotaro Ichikawa, Brian J. Esselman, Aatmik R. Patel, Samuel M. Kougias, Andrew N. Owen, Kaori Kobayashi, John F. Stanton, R. Claude Woods, Robert J. McMahon

FK08 **10:28 – 10:29**
IMPROVED SEMI-EXPERIMENTAL EQUILIBRIUM STRUCTURE DETERMINATION AND THEORETICAL PREDICTION OF PYRIDAZINE (*o*-$C_4H_4N_2$), AND THE IMPACT OF THE ISOTOPOLOGUE DATA SET, Andrew N. Owen, Maria Zdanovskaia, Brian J. Esselman, John F. Stanton, R. Claude Woods, Robert J. McMahon

FK09 **10:32 – 10:33**
MICROWAVE SPECTRUM AND IODINE NUCLEAR QUADRUPOLE COUPLING CONSTANTS OF 1,1-DIIODOETHANE, Michael J. Carrillo, Wei Lin, Yasuki Endo

FK10 **10:36 – 10:37**
A MICROWAVE STUDY OF THREE BROMINE-CONTAINING MOLECULES: CBr_2F_2, AgBr, and H_2-AgBr, Joshua A. Signore, Christopher Falls, Corey J Evans, Wallace C. Pringle, S. A. Cooke, Stewart E. Novick, Daniel A. Obenchain

FK11 **10:40 – 10:41**
STRUCTURE OF THE MODEL GRIGNARD-TYPE REAGENT $ClZnCH_3$ ($\tilde{X}^1A_1$) BY MILLIMETER-WAVE SPECTROSCOPY , Mark Burton, Nazifa Tabassum, Lucy M. Ziurys

FK12 **10:44 – 10:45**
RO-VIBRATIONALLY AVERAGED MOLECULAR STRUCTURE OF BENZENE I. ALMOST THE SAME BOND LENGTHS FOR THE C–H AND C–D BONDS., Masaaki Baba, Umpei Nagashima, Tsuneo Hirano

FK13 **10:48 – 10:49**
RO-VIBRATIONALLY AVERAGED MOLECULAR STRUCTURE OF BENZENE II. COMPUTATIONAL MOLECULAR SPECTROSCOPY STUDY., Tsuneo Hirano, Umpei Nagashima, Masaaki Baba

FK14 **10:52 – 10:53**
THE EQUILIBRIUM STRUCTURE OF SMALL RADICALS: THE SEMI-EXPERIMENTAL APPROACH AT WORK, Silvia Alessandrini, Mattia Melosso, Cristina Puzzarini

FL. Small molecules

Friday, June 25, 2021 – 10:0 AM

Room: 2021 Online Everywhere

Chair: Kyle N. Crabtree, University of California, Davis, CA, USA

FL01 **10:00 – 10:01**
THE (1,0) BAND OF THE [13.10] Ω=1 – X $^3\Sigma^-(0^+)$ TRANSITION OF TUNGSTEN SULFIDE, WS, OBSERVED BY ILS-FTS, Jack C Harms, Brendan M. Ratay, Kristin N Bales, James J O'Brien, Leah C O'Brien

FL02 **10:04 – 10:05**
DETECTION AND IDENTIFICATION OF PLATINUM FLUORIDE, PTF: ANALYSIS OF THE (0,0) BAND OF THE [15.3]Ω=3/2 – $X\ ^2\Pi_{3/2}$ TRANSITION USING INTRACAVITY LASER SPECTROSCOPY, Caroline A Welch, Jack C Harms, James J O'Brien, Leah C O'Brien

FL03 **10:08 – 10:09**
OBSERVATION AND SPECTRAL ANALYSIS OF THE A Ω=1 – X $\Omega=0^+$ ELECTRONIC TRANSITION OF DIATOMIC PLATINUM SULFIDE, PtS, BY INTRACAVITY LASER ABSORPTION SPECTROSCOPY WITH FOURIER TRANSFORM DETECTION (ILS-FTS), Leah C O'Brien, Jack C Harms, James J O'Brien, Wenli Zou

FL04 **10:12 – 10:13**
DISPERSED LASER INDUCED FLUORESCENCE STUDY OF $CaNH_2$ AND CaSH , Timothy Steimle, Anh T. Le, Chaoqun Zhang, Lan Cheng, Benjamin Augenbraun, John M. Doyle

FL05 **10:16 – 10:17**
HIGH RESOLUTION LASER INDUCED FLUORESCENCE AND ZEEMAN EFFECT IN THE [18.6]1.5-$X^2\Sigma^+$ TRANSITION OF YbOH , Colan Linton, Timothy Steimle, Ephriem Tadesse Mengesha, Allan G. Adam, Anh T. Le

FL06 **10:20 – 10:21**
A COUPLED-CHANNELS POTENTIAL FIT DESCRIBING THE LOW-LYING $X^2\Delta$, $^2\Pi$ AND $^2\Sigma^+$ STATES OF NiH TO EXPERIMENTAL ACCURACY , Ilvie Havalyova, Ivayla BOZHINOVA, Asen Pashov, Amanda J. Ross, Patrick Crozet

FL07 **10:24 – 10:25**
PHOTOELECTRON VELOCITY MAP IMAGING SPECTROSCOPY OF THE BERYLLIUM TETRAMER ANION Be_4^- , Noah B Jaffe, Michael Heaven

FL08 **10:28 – 10:29**
HIGH-RESOLUTION LASER SPECTROSCOPY OF LEAD OXIDE (PbO) IN 400-450 NM, Katsunari Enomoto, Takehiro Suzuki, Masaaki Baba

FL09 **10:32 – 10:33**
EVOLUTION OF IRON AND CALCIUM MONOOXIDES' BANDS IN LASER PLASMA UNDEL LOW PRESSURE, Aleksandr Zakuskin, Babken Beglaryan, Timur A. Labutin

FL10 **10:36 – 10:37**
FREQUENCY COMB REFERENCED SPECTRA OF $A - X$ TRANSITIONS IN SH, Arthur Fast, Samuel Meek

FL11 **10:40 – 10:41**
REVIEW OF DIATOMIC SPECTROSCOPIC DATA, Laura K McKemmish

FL12 **10:44 – 10:45**
IR, VISIBLE, AND UV LINE LIST OF SILICON MONOXIDE (SiO) – A HACKATHON PROJECT, Ahmad Y. Adam, Victoria H.J. Clark, Bridgette Cooper, Pria Dobney, Shaun T. E. Donnelly, Maire N. Gorman, Anthony E. Lynas-Gray, Thomas Meltzer, Alec Owens, Qianwei Qu, Mikhail Semenov, Wilfrid Somogyi, Anna-Maree Syme, Jonathan Tennyson, Apoorva Upadhyay, Samuel Wright, Sergei N. Yurchenko, Juan C. Zapata Trujillo

FL13 **10:48 – 10:49**
HIGH RESOLUTION LASER SPECTROSCOPY OF RUTHENIUM MONOXIDE, Allan G. Adam, Geoffrey M. Chenard, Colan Linton, Dennis W. Tokaryk

FL14 **10:52 – 10:53**
EXPERIMENTAL AND THEORETICAL ANALYSIS OF THE INTER- AND INTRA-MOLECULAR DYNAMICS OF FORMYL RADICAL TRAPPED IN SOLID CO, Yurij Dmitriev, Aatto Laaksonen, Nikolas Ploutarch Benetis

FM. Chirality and stereochemistry

Friday, June 25, 2021 – 10:0 AM

Room: 2021 Online Everywhere

Chair: Guojie Li, University of Alberta, Edmonton, Canada

FM01 **10:00 – 10:01**
ASSESSING THE PERFORMANCE OF ROTATIONAL SPECTROSCOPY IN CHIRAL ANALYSIS, Sergio R. Domingos, Cristobal Perez, Mark D. Marshall, Helen O. Leung, Melanie Schnell

FM02 **10:04 – 10:05**
CHIRALITY RECOGNITION IN THE TERNARY AGGREGATES OF PROPYLENE OXIDE: EXPERIMENTALLY GUIDED THEORETICAL CONFORMATIONAL SEARCHES , Fan Xie, Marco Fusè, Arsh Singh Hazrah, Wolfgang Jäger, Vincenzo Barone, Yunjie Xu

FM03 **10:08 – 10:09**
CHIRAL TAG ROTATIONAL SPECTROSCOPY FOR CHIRAL ANALYSIS OF CARBOXYLIC ACIDS, Haley N. Scolati, Kevin J Mayer, Brooks Pate

FM04 **10:12 – 10:13**
REACTION CHEMISTRY OF EPOXIDES WITH FLUORINATED CARBOXYLIC ACIDS, Kevin J Mayer, Brooks Pate, Haley N. Scolati, Martin S. Holdren, Reilly E. Sonstrom, Channing West

FM05 **10:16 – 10:17**
A BROADBAND ROTATIONAL SPECTROSCOPIC AND THEORETICAL STUDY OF CIS AND TRANS (-)-CARVEOL, Arsh Singh Hazrah, Mohamad Al-Jabiri, Raiden Speelman, Wolfgang Jäger

FM06 **10:20 – 10:21**
CHIRAL MOLECULAR RECOGNITION TRENDS IN AROMATIC AND HELICAL SYSTEMS REVEALED WITH ROTATIONAL SPECTROSCOPY, Sergio R. Domingos, Cristobal Perez, Narcis Avarvari, Melanie Schnell

FM07 **10:24 – 10:25**
CHIRAL TAG ROTATIONAL SPECTROSCOPY FOR STRUCUTRE ANALYSIS OF CHIRAL METHYLPHENYL OXIRANE, Haley N. Scolati, Kevin J Mayer, Martin S. Holdren, Brooks Pate

FM08 **10:28 – 10:29**
MANIPULATION OF COLD CHIRAL MOLECULES USING ELECTRONIC AND ROTATIONAL SPECTROSCOPY, A. O. Hernandez-Castillo, Johannes Bischoff, Ju Hyeon Lee, Gerard Meijer, Sandra Eibenberger-Arias

FM09 **10:32 – 10:33**
EXPLORING CONFORMATIONAL SPACES AND AGGREGATION PREFERENCES OF SERINE-ASPARAGINE AND VALINE-ASPARAGINE DIMERS BY IRMPD SPECTROSCOPY AND QUANTUM CHEMISTRY , Matthias Heger, Haolu Wang, Mohamad Al-Jabiri, Yunjie Xu

FM10 **10:36 – 10:37**
CAN PHOTOELECTRON CIRCULAR DICHROISM WORK FOR CHIRAL ANIONS?, Mallory Green, Jenny Triptow, Gerard Meijer

FM11 **10:40 – 10:41**
MATRIX ISOLATION-VIBRATIONAL CIRCULAR DICHROISM SPECTROSCOPIC STUDY OF TETRAHYDRO-2-FUROIC ACID AND ITS AGGREGATES , Yanqing Yang, Joseph Cheramy, Yunjie Xu

FM12 **10:44 – 10:45**
COMPUTATIONAL INSIGHTS INTO THE CHIRAL SUM FREQUENCY GENERATION RESPONSE OF WATER SUPERSTRUCTURES SURROUNDING AN ANTIPARALLEL β-SHEET, Daniel Konstantinovsky, Ethan Alexander Perets, Sharon Hammes-Schiffer, Elsa Yan

FM13 **10:48 – 10:49**
CHIRAL SUM FREQUENCY GENERATION SPECTROSCOPY REVEALS HOW MIRROR-IMAGE β-SHEETS ORGANIZE WATER SUPERSTRUCTURES WITH OPPOSITE CHIRALITY, Ethan Alexander Perets, Daniel Konstantinovsky, Ty Santiago, Luis Velarde, Sharon Hammes-Schiffer, Elsa Yan