

TALKS

(150 talks)

TA. Plenary
Tuesday, Sept. 2, 2014 – 9:00
Room A – Belmeloro 14

Chair: Jon T. Hougen, Sensor Science Division, NIST, USA

- Welcome and Opening talks** **9:00**
Prof. Dario Braga, Vice Rector for Research, University of Bologna
Prof. Francesco Zerbetto, Director of the Department of Chemistry
Prof. Vincenzo Barone, Past President of the Italian Chemical Society
Prof. Eizi Hirota, Representative of IUPAC
Prof. Sonia Melandri, dep-chair Local Organizing Committee
- TA01** **10:00 – 10:50**
TOWARD A ROBUST AND USER FRIENDLY MULTI-FREQUENCY VIRTUAL SPECTROMETER, Vincenzo Barone
- Intermission**
- TA02** **11:20 – 12:10**
SENSITIVE CHIRAL ANALYSIS VIA MICROWAVE SPECTROSCOPY, David Patterson
- TA03** **12:10 – 13:00**
STRUCTURE AND DYNAMICS OF THE HYDRATION SHELL OF BIOLOGICAL IONS AT THE MOLECULAR LEVEL PROBED BY IR SPECTROSCOPY, Otto Dopfer
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TB. MW & Chemistry
Tuesday, Sept. 2, 2014 – 15:00
Room 1, Chemistry

Chair: Yoshiyuki Kawashima, Kanagawa Inst. Tech., Atsugi 243-0292, Japan

- TB01** **15:00 – 15:17**
MOLECULAR CHIRALITY: ENANTIOMER DIFFERENTIATION BY HIGH-RESOLUTION SPECTROSCOPY, Eizi Hirota
- TB02** **15:17 – 15:32**
CHIRALITY SYNCHRONIZATION IN TRIFLUOROETHANOL DIMER REVISITED: THE MISSING HETEROCHIRAL DIMER, Javix Thomas, Yunjie Xu
- TB03** **15:32 – 15:49**
OBSERVATION BY CHIRPED-PULSE ROTATIONAL SPECTROSCOPY AND PROPERTIES OF THE (H₂O)₃HCL AND (H₂O)₂(HCL)₂ HYDROGEN-BONDED CLUSTERS, Zbigniew Kisiel, Cristóbal Pérez, Justin L.Neill, Matt T.Muckle, Luca Evangelisti, Simon Lobsiger, Brooks H.Pate
- TB04** **15:49 – 16:06**
ROTATIONAL SPECTRUM AND STRUCTURE OF THE FORMIC ACID•••CARBON DIOXIDE MOLECULAR COMPLEX, Annalisa Vigorito, Camilla Calabrese, Qian Gou, Sonia Melandri, Walther Caminati, Assimo Maris
- TB05** **16:06 – 16:23**

FOURIER-TRANSFORM MICROWAVE AND MILLIMETERWAVE SPECTROSCOPY OF THE H₂-HCN MOLECULAR COMPLEX, Keiichi Tanaka, M. Ishiguro, K. Harada, Y. Sumiyoshi, M. Nakashima, Y. Endo.

TB06 **16:23 – 16:40**
THE ROTATIONAL SPECTRA OF AMINOISOBUTYRIC AND ITS MONOHYDRATE, Juan C. López, Vanesa Vaquero, Elena R. Alonso, Isabel Peña, José L. Alonso

TB07 **16:40 – 16:57**
MILLIMETER-WAVE DETECTION OF THE NH₃-H₂ VAN DER WAALS COMPLEX, Ivan Tarabukin, Victor Panfilov, Leonid Surin, Stephan Schlemmer

TC. IR & Chemistry
Tuesday, Sept. 2, 2014 – 15:00
Room 4, Chemistry

Chair: Ben M. Elliott, NASA Jet Propulsion Laboratory, Pasadena, USA

TC01 **15:00 – 15:17**
JET-COOLED HIGH RESOLUTION INFRARED SPECTROSCOPY OF MOLECULAR COMPLEXES, P. Asselin, Y. Berger, P. Soulard, M. Goubet, T.R. Huet, R. Georges, O. Pirali, P. Roy

TC02 **15:17 – 15:32**
VIBRATIONAL SPECTRA AND STRUCTURES OF SILICON HYDRIDE CLUSTER CATIONS, Martin Andreas Robert George, Marco Savoca, Judith Langer, Truong Nguyen, Otto Dopfer

TC03 **15:32 – 15:49**
TRANSITION STATE SPECTROSCOPY OF THE [H,C,N] MOLECULAR SYSTEM, Georg Mellau, Robert W. Field

TC04 **15:49 – 16:06**
HYDRATION STATE AND NUMBERS OF HIGHLY POLAR COMPOUNDS IN AQUEOUS SOLUTION, Toshiyuki Shikata, Naoya Sagawa

TC05 **16:06 – 16:23**
HIGH-RESOLUTION INFRARED SPECTROSCOPIC INVESTIGATION OF AMMONIA-CONTAINING MOLECULAR COMPLEXES AROUND 1.5 MICRON, Thomas Vanfleteren, Tomas Foldes, Michel Herman

TC06 **16:23 – 16:40**
EXPERIMENTAL STUDY OF PHASE TRANSFORMATIONS IN METHANOL, Valeriy Pogorelov, Iryna Doroshenko, Yelizaveta Chernolevskaya, Yevhenii Vaskivskyi¹, Vytautas Balevicius, Valdas Sablinskas, Justinas Ceponkus

TC07 **16:40 – 16:57**
IR SPECTROSCOPY OF LIMONENE AND ITS OXYDATION PRODUCTS COMPLEMENTED BY QUANTUM CHEMICAL CALCULATIONS, Juan-Ramon Aviles Moreno, Thérèse R. Huet

TD. Electronic & Chemistry
Tuesday, Sept. 2, 2014 – 15:00
Room 2, Chemistry

Chair: John Furneaux, Department of Physics & Astronomy, Norman, OK, USA

- TD01** **15:00 – 15:17**
N \rightarrow π^* INTERACTION: TOO WEAK BUT CAN COMPETE WITH STRONG HYDROGEN BONDING INTERACTION, Santosh K. Singh, Sumit Kumar, Jamuna Vaishnav, Aloke Das
- TD02** **15:17 – 15:32**
VIBRONIC EMISSION SPECTROSCOPY OF BENZYL-TYPE RADICALS GENERATED BY CORONA DISCHARGE, Eun Hye Yi, Young Wook Yoon, Sang Kuk Lee
- TD03** **15:32 – 15:49**
REMPE SPECTROSCOPY OF HALOGEN CONTAINING REAGENTS: ENERGETICS, STATE INTERACTION AND PHOTOFRAGMENTATION OF RYDBERG AND ION-PAIR STATES, Helgi Rafn Hróðmarsson, Arnar Hafliðason, Huasheng Wang, Ágúst Kvaran
- TD04** **15:49 – 16:06**
FRANCK-CONDON FACTORS CALCULATION FOR VIBRATIONAL PROGRESSION IN PAH MOLECULES, P.M Mishra, L Avaldi, P Bolognesi, K C Prince, R Richter, S Vig, U Kadhane
- TD05** **16:06 – 16:23**
SPECTROSCOPIC AND DFT STUDY OF DIPOL MOMENTS OF D0 ORGANOMETALLICS IN S0 AND T1 STATES EXEMPLIFIED FOR ZR COMPLEX, Galina Loukova, Alexey Milov, Vladimir Vasilyev.
- TD06** **16:23 – 16:40**
ENERGY TRANSFER: IMPACT OF WEAK INTERACTIONS UNRAVELLED BY PHOTOPHYSICAL AND THEORETICAL METHODS, Galina Loukova, Alexey Milov
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WA. MW – Conformation & Structure
Wednesday, Sept. 3, 2014 – 9:00
Room 1, Chemistry

Chair: Yunjie Xu, University of Alberta, Edmonton, Alberta, Canada

- WA01** **9:00 – 9:17**
CONFORMATIONAL ANALYSIS OF WHISKY LACTONE USING FOURIER TRANSFORM MICROWAVE SPECTROSCOPY AND QUANTUM CHEMICAL CALCULATIONS, Yoshiyuki Kawashima, Ryusuke Katsuragi, Jun Utsugi, Eizi Hirota
- WA02** **9:17 – 9:32**
ROTATIONAL SPECTRA OF SUGARS: RING-PUCKERING IN RIBOFURANOSE, Patricia Écija, Iciar Uriarte, Lorenzo Spada, Emilio Cocinero, Alberto Lesarri, José A. Fernández, Walther Caminati
- WA03** **9:32 – 9:49**
SECOND (PLANAR) MOMENTS AND THEIR APPLICATION IN SPECTROSCOPY, Robert K. Bohn, John A. Montgomery, Jr., H. Harvey Michels
- WA04** **9:49 – 10:06**
A BROAD VIEW RESOLVING THE DETAILS: IMPACT-FT-MW INVESTIGATION OF MOLECULES WITH CONFORMATIONAL FREEDOM, Dennis Wachsmuth, Jan-Hendrik Borter, Jens-Uwe Grabow, Alberto Lesarri
- WA05** **10:06 – 10:23**
HALOGEN SUBSTITUTION EFFECTS ON THE TAUTOMERIC AND CONFORMATIONAL EQUILIBRIA OF MOLECULES AND MOLECULAR

COMPLEXES: A ROTATIONAL STUDY, Qian Gou, Lorenzo Spada, Montserrat Vallejo-López, Assimo Maris, Sonia Melandri, Walther Caminati, Camilla Calabrese.

WA06 **10:23 – 10:40**
STRUCTURE DETERMINATION OF CINNAMALDEHYDE USING BROADBAND MICROWAVE SPECTROSCOPY, Sabrina Zinn, Thomas Betz, Melanie Schnell

Intermission

WA07 **11:10 – 11:27**
ROTATIONAL SPECTRUM OF ZINGERONE: CHECKING THE AB INITIO AND DFT CALCULATION METHODS, P. Écija, I. Uriarte, A. Lesarri, F. Basterretxea, E.J. Cocinero

WA08 **11:27 – 11:44**
IBUPROFEN: CONFORMERS AND THERMAL DECOMPOSITION PRODUCTS, T. Betz, S. Zinn, M. Schnell

WA09 **11:44 – 12:01**
THE STRUCTURE OF THE ANESTHETIC FLUOROXENE BY BROADBAND ROTATIONAL SPECTROSCOPY, I. Uriarte, P. Écija, L. Spada, A. Lesarri, J. A. Fernández, F. Castaño, W. Caminati, E. J. Cocinero

WA10 **12:01 – 12:18**
INTRAMOLECULAR INTERACTIONS IN THE POLAR HEAD OF SPHINGOSINE, D. Loru, M. E. Sanz, I. Peña, J. L. Alonso

WA11 **12:18 – 12:35**
CONFORMATIONAL LANDSCAPE OF AROMATIC MOLECULES: A ROTATIONAL STUDY OF MEPHENESIN AND ISOBUTAMBEN, Montserrat Vallejo-López, Patricia Écija, Luca Evangelisti, Francisco J. Basterretxea, Emilio J. Cocinero, Alberto Lesarri, Fernando Castaño, Walther Caminati

WB. IR – Astrophysics & Atmosphere

Wednesday, Sept. 3, 2014 – 9:00

Room 4, Chemistry

Chair: Agnes Perrin, LISA, CNRS, Univ Paris-Est Creteil & Paris Diderot

WB01 **9:00 – 9:17**
SYNCHROTRON HIGH-RESOLUTION FTIR SPECTROSCOPY SORTS OUT THE GROUND STATE AND LOW WAVENUMBER MODES OF KETENIMINE, D. McNaughton, M. K. Bane, C. D. Thompson, E. G. Robertson, D. R. T. Appadoo, C. Medcraft

WB02 **9:17 – 9:32**
TEN-STATE FIT TO ACROLEIN LEVELS BETWEEN 850 AND 1020 cm^{-1} : LOCATION OF THE ELUSIVE ν_{15} VIBRATION, A.R.W. McKellar, B.E. Billinghurst, Li-Hong Xu, R.M. Lees

WB03 **9:32 – 9:49**
HIGH-RESOLUTION MOLECULAR BEAM SPECTROSCOPY OF POLYCYCLIC AROMATIC HYDROCARBONS IN THE 3 μM REGION, Elena Maltseva, Annemieke Petrigani, Alessandra Candian, Xander Tielens, Jos Oomens, Wybren Jan Buma

WB04 **9:49 – 10:06**

FREQUENCY COMB ASSISTED MIR SPECTROSCOPY OF H_3^+ and CD_2H^+ , Oskar Asvany, Pavol Jusko, Sandra Brünken, Stephan Schlemmer

WB05 **10:06 – 10:23**
CRDS OF ACETYLENE NEAR 1.6 μ M, O. M. Lyulin, D. Mondelain, S. Kassi, J. Vander Auwera, A. Campargue

WB06 **10:23 – 10:40**
ACCURATE HIGH RESOLUTION FTIR MEASUREMENTS OF THE SELF- AND AIR-BROADENING COEFFICIENTS IN THE $2N_3$ -BAND OF N_2O , Viktor Werwein, Jens Brunzendorf, Olav Werhahn, Volker Ebert

Intermission

WB07 **11:10 – 11:27**
FTS STUDIES OF THE ISOTOPOLOGUES OF CO_2 TOWARD CREATING A COMPLETE AND HIGHLY ACCURATE REFERENCE STANDARD, Ben M. Elliott, Keeyoon Sung, Charles E. Miller

WB08 **11:27 – 11:44**
THE WATER SELF CONTINUUM NEAR 1.6 μ M, D. Mondelain, S. Kassi, A. Campargue

WB09 **11:44 – 12:01**
AN ACCURATE AND COMPLETE EMPIRICAL LINE LIST FOR WATER VAPOR BETWEEN 5850 AND 7920 CM^{-1} , A. Campargue, S. N. Mikhailenko, D. Mondelain, S. Kassi

WB10 **12:01 – 12:18**
SPECTROSCOPY OF $^{14}NH_3$ AND $^{15}NH_3$ IN THE RANGE 6369 TO 6578 CM^{-1} . DETERMINATION OF LOWER STATE ENERGY TRANSITIONS USING TEMPERATURE DEPENDENCE FROM 134K TO 296K, J. EL Romh, P.Cacciani, J.Cosléou, M. Khelkhal, F.Taher

WB11 **12:18 – 12:35**
INFRARED SPECTROSCOPY OF ^{17}O -ENRICHED CARBON DIOXIDE IN THE 3200-5340 CM^{-1} RANGE. IMPROVEMENT OF THE GLOBAL MODELING OF THE LINE POSITIONS AND INTENSITIES OF RARE CO_2 ISOTOPOLOGUES, Yu.G. Borkov, D. Jacquemart, O.M. Lyulin, S.A. Tashkun, V.I. Perevalov

WC. Theory
Wednesday, Sept. 3, 2014 – 9:00
Room 2, Chemistry

Chair: Isabelle Kleiner, LISA, CNRS, Univ Paris-Est Creteil & Paris Diderot

WC01 **9:00 – 9:17**
A HYBRID FITTING PROGRAM FOR METHYLAMINE-LIKE MOLECULES WITH TWO LARGE-AMPLITUDE MOTIONS, Jon T. Hougen, Isabelle Kleiner

WC02 **9:17 – 9:32**
MULTICHANNEL QUANTUM DEFECT THEORY FOR POLAR MOLECULE, Sergei V. Elfimov, Dmitrii L. Dorofeev, Boris A. Zon

WC03 **9:32 – 9:49**
A NEW HOT LINE LIST FOR FORMALDEHYDE, A. F. Al-Refaaie, S. N. Yurchenko, A. Yachmenev, J. Tennyson

WC04 **9:49 – 10:06**

NON-EMPIRICAL CONSTRUCTION OF THE EFFECTIVE DIPOLE MOMENT OF METHANE BY CONTACT TRANSFORMATIONS, Thibault Delahaye, Michaël Rey, Sergei Tashkun, Vladimir Tyuterev

WC05 **10:06 – 10:23**
THE ROVIBRATIONAL SPECTROSCOPY OF H_5^+ , János Sarka, Csaba Fábri, Attila Császár

WB06 **10:23 – 10:40**
DEPOPULATION OF METASTABLE HELIUM BY RADIATIVE ASSOCIATION IN INTERSTELLAR ENVIRONMENT, Lucie Augustovičová, Wolfgang. P. Kraemer, Vladimír Špirko, Pavel Soldán

Intermission

WC07 **11:10 – 11:27**
EXPERIMENTAL AND THEORETICAL COLLISIONAL PARAMETERS OF CH_3D-N_2 LINES FOR REMOTE SENSING OF PLANETARY ATMOSPHERES: J- AND K-DEPENDENCES AND TEMPERATURE EXPONENTS, T. Sinyakova, J. Buldyreva, V.M. Devi, D.C. Benner, K. Sung, A. Predoi-Cross, M.A.H. Smith, A. Mantz

WC08 **11:27 – 11:44**
AB INITIO MODEL OF ANOMALOUSLY BROADENED H_2 Q(1) LINE PERTURBED BY AR, P. Wcisło, F. Thibault, H. Cybulski, R. Ciuryło

WC09 **11:44 – 12:01**
GLOBAL MODELING OF NO_2 HIGH RESOLUTION SPECTRA, A.A. Lukasheskaya, O.M. Lyulin, A. Perrin, V.I. Perevalov

WC10 **12:01 – 12:13**
THE EQUIVALENCE OF THE METHYL GROUPS IN PUCKERED 3,3-DIMETHYL OXETANE, Alberto Macario, Susana Blanco, Juan C. López

WC11 **12:13 – 12:30**
TRAJECTORY ANALYSIS OF RO-VIBRATIONAL PROBLEM, Sergey V. Petrov, Sergei E. Lokshtanov

WC12 **12:30 – 12:47**
INFLUENCE OF THE ISOTOPIC SUBSTITUTION ON THE EFFECTIVE DIPOLE MOMENT PARAMETERS OF CARBON DIOXIDE MOLECULE, V.I. Perevalov, E.V. Karlovets

WD. MW & Internal Dynamics

Wednesday, Sept. 3, 2014 – 15:00

Room 1, Chemistry

Chair: Luca Evangelisti, University of Virginia, Charlottesville, Virginia, USA

WD01 **15:00 – 15:17**
STUDIES ON THE CONFORMATIONAL LANDSCAPE OF TERT-BUTYL ACETATE USING MICROWAVE SPECTROSCOPY AND QUANTUM CHEMICAL CALCULATIONS, Y. Zhao, H. Mouhib, G. Li, W. Stahl, I. Kleiner

WD02 **15:17 – 15:32**
THE EFFECTS OF INTERNAL ROTATION AND ^{14}N QUADRUPOLE COUPLING IN N,N-DIETHYLACETAMIDE, Raphaela Kannengießer, Ha Vinh Lam Nguyen, Wolfgang Stahl

- WD03** **15:32 – 15:49**
MICROWAVE SPECTRUM OF METHYL ARSINE, Roman A. Motiyenko, Jean Demaison, Laurent Margulès, Harald Møllendal, Jean-Claude Guillemin, Vadim V. Ilyushin
- WD04** **15:49 – 16:06**
MICROWAVE AND FAR-INFRARED SPECTRUM OF DIMETHYL SULFIDE, A. Jabri, V. Van, H. V. L. Nguyen, F. Kwabia Tchana, L. Manceron, I. Kleiner, W. Stahl, B. Tercero, J. Cernicharo
- WD05** **16:06 – 16:18**
INTRA- AND INTERMOLECULAR HYDROGEN BONDING INTERACTIONS IN THE TRIFLUOROETHANOL-AMMONIA DIMER, Javix Thomas, Yisi Yang, Wolfgang Jäger, Yunjie Xu
- WD06** **16:18 – 16:35**
GAS PHASE STRUCTURES OF 2-METHYLTETRAHYDROTHIOPHENE INVESTIGATED BY ROTATIONAL SPECTROSCOPY, Vinh Van, Ha Vinh Lam Nguyen, Wolfgang Stahl
- WD07** **16:35 – 16:52**
TWO ASPECTS OF PARTIALLY DEUTERATED METHYL GROUP INTERNAL ROTATION: CD₂HOH AND CH₂DCOH, L. H. Coudert, M. Ndao, F. Kwabia Tchana, L. Margulès, R. Motiyenko, J.-C. Guillemin, J. Barros, L. Manceron, P. Roy
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WE. Fundamental Physics
Wednesday, Sept. 3, 2014 – 15:00
Room 4, Chemistry

Chair: Vladimir Spirko, Academy of Sciences of the Czech Republic, Prague

- WE01** **15:00 – 15:17**
MANIPULATION OF TRANSLATIONAL MOTION OF POLAR MOLECULES BY STRONG RESONANT MICROWAVE FIELDS, Wei Zhong, Manish Vashishta, Pavle Djuricanin, and Takamasa Momose
- WE02** **15:17 – 15:34**
A VERSATILE METHOD FOR PRODUCTION OF COLD POLYATOMIC POLAR MOLECULES, Sotir Chervenkov, Xing Wu, Thomas Gantner, Rosa Glöckner, Alexander Prehn, Martin Zeppenfeld, and Gerhard Rempe
- WE03** **15:34 – 15:51**
TOWARDS MEASURING PARITY VIOLATION IN CHIRAL MOLECULES USING VIBRATIONAL SPECTROSCOPY, Sean K. Tokunaga, Alexander Shelkovnikov, Papa Lat Tabara Sow, Sinda Mejri, Olivier Lopez, Andrey Goncharov, Bérengère Argence, Christophe Daussy, Anne Amy-Klein, Christian Chardonnet, Benoît Darquié
- WE04** **15:51 – 16:08**
QUANTUM INTERFERENCE ASSISTED MEASUREMENT OF ABSOLUTE ABSORPTION CROSS SECTIONS, Sandra Eibenberger, Joseph Cotter, Xiaxi Cheng, Lukas Mairhofer, and Markus Arndt
- WE05** **16:08 – 16:25**
HIGH-RESOLUTION ROTATIONAL SPECTROSCOPY IN A CRYOGENIC 22-POLE ION TRAP, Sandra Brünken, Lars Kluge, Alexander Stoffels, Oskar Asvany, Stephan Schlemmer
- WE06** **16:25 – 16:37**

USING MOLECULAR ALIGNMENT TO TRACK THE COLLISIONAL RELAXATION OF A GAS SAMPLE, G. Karras, F. Billard, J. Houzet, E. Hertz, B. Lavorel, J.M. Hartmann, O. Faucher

WE07

16:37 – 16:54

TWO PHOTON ROTATIONAL ACTION SPECTROSCOPY OF COLD OH- IN A 22-POLE TRAP, Pavol Jusko, Oskar Asvany, Ann-Christin Wallerstein, Sandra Brünken, Stephan Schlemmer

WF. Applied Spectroscopy
Wednesday, Sept. 3, 2014 – 15:00
Room 2, Chemistry

Chair: Pierre Asselin, Sorbonne Universités, UPMC Univ Paris 06, Paris

WF01

15:00 – 15:17

HIGH-SENSITIVITY DETECTION OF TRACE MOISTURE IN GAS USING CAVITY RING-DOWN SPECTROSCOPY, H. Abe, D. Lisak, A. Cygan, R. Ciuryło

WF02

15:17 – 15:32

GAS TEMPERATURE DETERMINATION IN CO₂-CONTAINING DISCHARGES BASED ON ROTATIONAL SPECTRAL ANALYSIS, Nikolay Britun, Tiago Silva, Thomas Godfroid, Rony Snyders

WF03

15:32 – 15:49

INFRARED CROSS-SECTIONS OF NITRO-DERIVATIVES VAPORS: NEW SPECTROSCOPIC SIGNATURES OF EXPLOSIVE TAGGANTS AND DEGRADATION PRODUCTS, Arnaud Cuisset, Clara Stoeffler, Sébastien Gruet, Olivier Pirali, Gaël Mouret

WF04

15:49 – 16:06

SYNTHESIS, SPECTROSCOPIC AND THERMAL BEHAVIOR ON SOME BINUCLEAR TRANSITION METAL COMPLEXES OF HYDRAZONES, ANTIMICROBIAL AND CYTOTOXIC STUDIES WITH MOLECULAR ORBITAL CALCULATIONS, Badr A. ElSayed, Salah M. Shaaban

WF05

16:06 – 16:18

MODELLING AND SPECTROSCOPIC ANALYSES OF WATER HYACINTH, Medhat Ibrahim, Hanan Ibrahim, Hanan Elhaes

WF06

16:18 – 16:30

PHOTOACOUSTIC MEASUREMENT OF THE AIR QUALITY WITHIN URBAN POLLUTED SITES, I. R. Ivascu, C. E. Matei, M. Patachia, A. M. Bratu and D. C. Dumitras

WF07

16:30 – 16:47

DETERMINATION OF FLUORINE IN TURKISH WINES BY MOLECULAR ABSORBANCE OF CAF USING A HIGH-RESOLUTION CONTINUUM SOURCE ATOMIC ABSORPTION SPECTROMETER, Nil Ozbek, Suleyman Akman

WF08

16:47– 17:02

A PRACTICAL METHOD FOR THE DETERMINATION OF SULPHUR IN COAL SAMPLES BY HIGH-RESOLUTION CONTINUUM SOURCE FLAME ATOMIC ABSORPTION SPECTROMETRY, A. Baysal, S. Akman

GA. Plenary
Thursday, Sept. 4, 2014 – 9:00

Room A – Belmeloro 14

Chair: P. R. Bunker, National Research Council of Canada, Ottawa, Canada

GA01 **9:00 – 9:50**
MICROWAVE SPECTROSCOPY OF INTERSTELLAR MOLECULES WITH LARGE AMPLITUDE MOTIONS, Kaori Kobayashi

GA02 **9:50 – 10:40**
PRECISION SPECTROSCOPY DIRECTED TOWARDS THE POSSIBLE MEASUREMENT OF AN ELECTRON ELECTRIC DIPOLE MOMENT, Aaron E. Leanhardt

Intermission

GA03 **11:10 – 11:50**
HIGH-PRECISION AND HIGH-ACCURACY ROVIBRATIONAL SPECTROSCOPY OF MOLECULAR IONS, James N. Hodges, Adam J. Perry, Charles R. Markus, G. Stephen Kocheril, Paul A. Jenkins II, Benjamin J. McCall

GA04 **11:50 – 12:40**
ACCURATE BROADBAND MILLIMETER-WAVE SPECTROSCOPY OF ATMOSPHERIC GASES, M.Yu. Tret'yakov

FA. Plenary

Friday, Sept. 5, 2014 – 9:00
Room A – Belmeloro 14

Chair: A.R.W. McKellar, National Research Council, Ottawa, Canada

FA01 **9:00 – 9:50**
HIGH-RESOLUTION OVERTONE SPECTROSCOPY AND DYNAMICS OF STRONGLY AND WEAKLY BOUND SPECIES, M. Herman

FA02 **9:50 – 10:40**
PRECISE MOLECULAR SPECTROSCOPY AND THEORY OF SPECTRAL LINE SHAPES, Roman Ciuryło

Intermission

FA03 **11:10 – 11:50**
NEW LIFE FOR AN OLD TOPIC: CONFORMATIONAL STUDIES OF BIOMOLECULES BY MICROWAVE SPECTROSCOPY, Alberto Lesarri

FA04: An intriguing talk **11:50 – 12:07**
ARE YOUR SPECTROSCOPIC DATA BEING USED? Iouli E. Gordon, Laurence S. Rothman, Jonas S. Wilzewski

Pliva award **12:07 – 12:20**
Qian Gou communicates the results, and Jens-Uwe Grabow awards the winner

The next meeting **12:20 – 12:40**
Jens-Uwe Grabow announces the news

FB. Theory
Friday, Sept. 5, 2014 – 15:00
Room 1, Chemistry

Chair: Cristina Puzzarini, University of Bologna, Italy

- FB01** **15:00 – 15:17**
ULTRA-SENSITIVE AMMONIA PROBES OF A VARIABLE PROTON-TO-ELECTRON MASS RATIO, Vladimir Spirko
- FB02** **15:17 – 15:32**
DYNAMICS OF ETHYL RADICAL, Marek Kreglewski, Iwona Gulaczyk
- FB03** **15:32 – 15:49**
THE SPECTRUM OF HOT METHANE IN ASTRONOMICAL OBJECTS USING A COMPREHENSIVE COMPUTED LINE LIST, S. N. Yurchenko, J. Tennyson, J. Bailey, M. D. J. Hollis, G. Tinetti
- FB04** **15:49 – 16:06**
N-MODE REPRESENTATION OF THE ROTATIONAL-VIBRATIONAL HAMILTONIAN USING CURVILINEAR COORDINATES AND AN ECKART AXES SYSTEM, Andrey Yachmenev, Sergei Yurchenko, Jonathan Tennyson
- FB05** **16:06 – 16:23**
NEW INSIGHT ON THE OZONE TRANSITION STATE NEAR THE DISSOCIATION THRESHOLD FROM *AB INITIO* CALCULATIONS AND HIGHLY SENSITIVE SPECTROSCOPIC EXPERIMENTS, V. Tyuterev, R. Kochanov, A. Campargue, S. Kassi, D. Mondelain, A. Barbe, E. Starikova, M-R. De Backer, P. Szalay, S. Tashkun.
- FB06** **16:23 – 16:40**
STUDY OF IR SPECTRA OF THE ISOTOPIC SPECIES OF NITROSYL HALIDES USING THE U(4) ALGEBRAIC MODEL, Nirmal Kumar Sarkar, Rupam Sen, Ashim Kalyan, Raghunandan Das, Subha Gaurab Roy, Joydeep Choudhury, Srinivasa Rao Karumuri
- FB07** **16:40 – 16:57**
THE FIRST LOW-LYING ELECTRONIC STATES OF STRONTIUM MONOXIDE, Fadia Taher, A.R. Allouche, W. Anil, J. AlHout

FC. IR
Friday, Sept. 5, 2014 – 15:00
Room 4, Chemistry

Chair: Valeri I. Perevalov, Russian Academy of Sciences, Tomsk, Russia

- FC01** **15:00 – 15:17**
SIMULTANEOUS ABSORPTIVE AND DISPERSIVE MEASUREMENTS WITH CAVITY-ENHANCED SPECTROSCOPY, A. Cygan, P. Wcisło, S. Wójtewicz, P. Masłowski, R. S. Trawiński, R. Ciuryło, D. Lisak
- FC02** **15:17 – 15:32**
INELASTIC COLLISIONS IN O₂+HE SUPERSONIC JETS BY HIGH-RESOLUTION RAMAN SPECTROSCOPY, F. Gámez, E. Moreno, G. Tejada, M. Bartolomei, M. I. Hernández, J. Campos-Martínez, J. M. Fernández, and S. Montero
- FC03** **15:32 – 15:49**
H₂O NUCLEAR-SPIN CONSERVATION/RELAXATION IN SUPERSONIC JET EXPANSION PROBED BY QUANTITATIVE DIRECT ABSORPTION SPECTROSCOPIC DETECTION, Ondřej Votava, Veronika Horká-Zelenková, Jozef Rakovský, Vít Svoboda, Michal Fárník
- FC04** **15:49 – 16:06**

REINVESTIGATION OF THE FIRST TORSIONAL BAND OF METHYLAMINE, Iwona Gulaczyk, Marek Kręglewski, Veli-Matti Horneman

FC05

16:06 – 16:23

MICROWAVE AND INFRARED SPECTROSCOPES OF α - AND β -PINENE COMPLEMENTED BY QUANTUM CHEMICAL CALCULATIONS, Juan-Ramon Aviles Moreno, Thérèse R. Huet, Manuel Goubet, Pascale Soulard, Pierre Asselin, Robert Georges, Olivier Pirali, Pascale Roy

FC06

16:23 – 16:40

QUANTUM MONODROMY IN NCNCs: TOWARDS A FULLY EXPERIMENTAL ENERGY-MOMENTUM MAP OF THE LARGE-AMPLITUDE BENDING MODE, Dennis W. Tokaryk, Manfred Winniwisser, Brenda P. Winniwisser, Frank C. De Lucia, Stephen C. Ross, Brant E. Billingham

FD. Electronic – Small molecules

Friday, Sept. 5, 2014 – 15:00

Room 2, Chemistry

Chair: <u>Ágúst Kvaran</u>, University of Iceland, Reykjavik, Iceland
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FD01

15:00 – 15:17

PRECISION SATURATED ABSORPTION SPECTROSCOPY OF $^{130}\text{TE}_2$ FROM 22100 – 22600 CM^{-1} , J. E. Furneaux, James Coker, D. LaMantia, and Jeffrey Gillian

FD02

15:17 – 15:32

SPECTROSCOPIC OBSERVATION AND DEPERTURBATION TREATMENT OF THE $A^1\Sigma^+$ AND $b^3\Pi_0$ STATES IN LiCs MOLECULE, A.Grochola, J. Szczepkowski, W. Jastrzebski, P. Kowalczyk

FD03

15:32 – 15:49

OPTICAL POPULATION OF IODINE MOLECULE UNGRADE STATES CORRELATING WITH $I(^2P_{1/2}) + I(^2P_{1/2})$ DISSOCIATING LIMIT FROM UNGRADE BO_v^+ STATE, M.E. Akopyan, V.V. Baturó, S.S. Lukashov, L.D. Mikheev, S.A. Poretsky, A.M. Privilov, O.S. Vasyutinskii

FD04

15:49 – 16:06

TWO-COLOUR POLARISATION SPECTROSCOPY IN Rb_2 : THE $5^1\Sigma_u^+$ AND $5^1\Pi_u$ STATES, W. Jastrzebski, J. Szczepkowski, P. Kowalczyk, A.J. Ross, P. Crozet

FD05

16:06 – 16:23

THE USE OF LASER EXCITED RO-VIBRATIONAL SPECTRA OF OH RADICALS AS A PROBE OF A GAS PHASE COMPOSITION, A. Nikiforov, L. Li, N. Britun, R. Snyders, Ch. Leys.

FD06

16:23 – 16:35

FT HIGH ROTATIONAL SPECTRUM OF THE $A^3\Pi_0-X^1\Sigma^+$ AND $B^3\Pi_1-X^1\Sigma^+$ TRANSITIONS OF THE InBr MOLECULE, Renu Singh, M. D. Saksena, M.N. Deo, K. Sunanda, K. N. Uttam

FD07

16:35 – 16:52

ELECTRONIC STRUCTURE AND SPECTROSCOPY OF O_2 AND O_2^+ , G. J. Vázquez, H. P. Liebermann, H. Lefebvre-Brion

SA. MW

Saturday, Sept. 6, 2014 – 9:00

Room 1, Chemistry

Chair: Juan C. López, Universidad de Valladolid, Valladolid, Spain

- SA01** **9:00 – 9:16**
SUBMILLIMETER-WAVE SPECTROSCOPY OF NITROGEN CONTAINING MOLECULES OF ASTROPHYSIC INTEREST, L. Margulès, R.A. Motiyenko, J.C. Guillemin
- SA02** **9:16 – 9:32**
MILLIMETER AND SUB-MILLIMETER WAVE ROTATIONAL SPECTRUM OF METHYL NITRATE, Jessica Thomas, Douglas Petkie, Ivan Medvedev, David Dolson
- SA03** **9:32 – 9:48**
LINE-SHAPES AND BROADENINGS OF ROTATIONAL LINES OF CH₃³⁵CL IN COLLISION WITH HE, AR AND KR, V. Gupta, F. Rohart, L. Margulès, R.A. Motiyenko, J.V. Buldyreva
- SA04** **9:48 – 9:59**
MILLIMETER-WAVE SPECTRUM OF THE MONO-DEUTERATED ISOTOPOLOGUES OF ETHANOL FOR RADIO-ASTRONOMY, Adam Walters, Mirko Schäfer, Holger S.P. Müller, Matthias H. Ordu, Frank Lewen, Stephan Schlemmer
- SA05** **9:59 – 10:15**
COMPREHENSIVE ANALYSIS OF THE MOLECULAR OXYGEN 60 GHZ BAND: EXPERIMENT AND MODELLING, Maksim Koshelev, Ilya Vilkov, Dmitrii Makarov, Evgeny Serov, Vladimir Parshin and Mikhail Tretyakov.
- SA06** **10:15 – 10:31**
THE EFFECTS OF TWO INTERNAL ROTATIONS IN THE MICROWAVE SPECTRUM OF ETHYL METHYL KETONE, Ha Vinh Lam Nguyen, Vinh Van, Wolfgang Stahl, Isabelle Kleiner
- SA07** **10:31 – 10:42**
TERAHERTZ LABORATORY EMISSION SPECTROMETER (TELM): ROTATIONAL SPECTRUM AND PRESSURE BROADENING OF METHANOL NEAR 800 GHZ, Alexey Potapov, Silvia Spezzano, Frank Lewen, Matthias H. Ordu, Ronan Higgins, Karl Jacobs, Stephan Schlemmer, Urs U. Graf
- Intermission**
- SA08** **11:12 – 11:23**
ACCURATE REST FREQUENCIES OF HC₃N AND ITS ISOTOPOLOGUES, Alexander V. Lapinov, German Yu. Golubiatnikov, Alexander P. Velmuzhov, Jens-Uwe Grabow, Antonio Guarnieri
- SA09** **11:23 – 11:34**
DIPOLE MOMENTS OF CH₃F IN THE N₃ AND N₆ VIBRATIONAL EXCITED STATES FROM THE STARK EFFECT, Jindřich Koubek, Patrik Kania, Štěpán Urban
- SA10** **11:34 – 11:50**
HIGH-RESOLUTION ROTATIONAL MOLECULAR SPECTROSCOPY: A POWERFUL TOOL TO UNVEIL THE UNIVERSE, Valerio Lattanzi, Cristina Puzzarini
- SA11** **11:50 – 12:06**
SUB-DOPPLER RESOLUTION IN THE THZ FREQUENCY DOMAIN, Gabriele Cazzoli, Cristina Puzzarini
- SA12** **12:06 – 12:22**
FREE JET MILLIMETER WAVE SPECTROSCOPY OF OXAZOLIDONE COMPOUNDS, Assimo Maris, Sonia Melandri, Camilla Calabrese, Annalisa Vigorito, Laura B. Favero

- SA13** **12:22 – 12:33**
DEUTERATED WATER HEXAMER FROM BROADBAND ROTATIONAL SPECTROSCOPY, Luca Evangelisti, Cristobal Perez, Simon Lobsiger, Nathan A. Seifert, Daniel P. Zaleski, Brooks H. Pate, Zbigniew Kisiel, Berhame Temelso, George C. Shields
- SA14** **12:33 – 12:44**
LONE PAIR... π INTERACTION: A ROTATIONAL STUDY OF THE CHLOROTRIFLUOROETHYLENE-AMMONIA ADDUCT, Qian Gou, Lorenzo Spada, Yannick Geboes, Sonia Melandri, Wouter A. Herrebout, Walther Caminati
- SA15** **12:44 – 12:50**
HALOGEN BOND FEATURES REVEALED IN THE GAS PHASE BY ROTATIONAL SPECTROSCOPY, Lorenzo Spada, Qian Gou, Montserrat Vallejo-Lopez, Andrea Staffolani, Alberto Lesarri, Emilio Josè Cocinero, Walther Caminati
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SB. Theory
Saturday, Sept. 6, 2014 – 9:00
Room 4, Chemistry

Chair: Iwona Gulaczyk, Adam Mickiewicz University, Poznań, Poland

- SB01** **9:00 – 9:17**
AB INITIO CALCULATIONS FOR THE GROUP 2 M₂O HYPERMETALLIC OXIDES, B. Ostojić, Per Jensen, P. A. Schwerdtfeger, and P. R. Bunker
- SB02** **9:17 – 9:32**
APPLICATION OF GENERALIZED EULER SERIES TRANSFORMATION (GET) TO CALCULATIONS OF ROTATION ENERGY LEVELS OF H₂ MOLECULE, A.N. Duchko, T.V. Kruglova, K.V. Kalinin, A.D. Bykov
- SB03** **9:32 – 9:49**
TOWARDS A COMPREHENSIVE LINE LIST FOR HOT CHROMIUM HYDRIDE, M.N. Gorman, S.N. Yurchenko, L. Lodi, Jonathan Tennyson
- SB04** **9:49 – 10:01**
THEORETICAL INVESTIGATION OF THE LOW-LYING ELECTRONIC STRUCTURE OF LACL MOLECULE BY AB-INITIO METHODS, Yaman Hamade, Ahmad Sobhahi, Fadia Taher
- SB05** **10:01 – 10:18**
DETECTABLE ORGANOSULFUR COMPOUNDS, M.L. Senent, C. Puzzarini, R. Domínguez-Gómez, M. Carvajal, M. Hochlaf.
- SB06** **10:18 – 10:35**
AN UPDATE OF THE CO₂ LINE-MIXING DATABASE AND SOFTWARE AND ITS TESTS IN THE 2.1 AND 4.3 MM REGIONS, Julien Lamouroux, Laurence Régalia, Jean Vander Auwera, Robert R. Gamache, Jean-Michel Hartmann
- SB07** **10:35 – 10:52**
HOW TO FILL SPECTROSCOPIC DATABASES WITH ACCURATE LINE SHAPE PARAMETERS? THE EXAMPLES OF H₂O AND CO₂, Julien Lamouroux, Robert R. Gamache
- Intermission**
- SB08** **11:22 – 11:39**
AB INITIO/FCF SIMULATIONS OF VIBRATIONALLY RESOLVED PHOTODETACHMENT AND PHOTOELECTRON SPECTRA OF REACTIVE SPECIES INCLUDING SOME CRIEGEE INTERMEDIATES, Edmond P. F. Lee, Daniel K. W. Mok, John M. Dyke

SB09 **11:39 – 12:51**
COMPUTATION OF VIBRATIONAL ENERGY LEVELS OF TRIATOMIC MOLECULES BY SUMMING DIVERGENT SERIES OF THE RAYLEIGH-SCHRÖDINGER PERTURBATION THEORY, A.D. Bykov, K.W. Kalinin, A.N. Duchko

SB10 **12:51 – 12:03**
AB INITIO CALCULATIONS OF H_2F^+ , A. A. Kuyberis, N. F. Zobov, L. Lodi, R.I. Ovsyannikov, O. L. Polyansky

SB11 **12:03 – 12:20**
THE STATIONARY POINTS ON THE POTENTIAL ENERGY SURFACES OF $(SO_2)_2$ AND $(CH_2F)_2$ DIMERS STUDIED BY COUPLING DISPERSION-CORRECTED DFT-D3 THEORY AND COLLISION-INDUCED BROADENING OF RO-VIBRATIONAL LINES, Nicola Tassinato, Stefan Grimme

SB12 **12:20 – 12:37**
THEORETICAL VIBRATIONAL FINGER-PRINTS FOR MEDIUM-SIZED MOLECULES: THE ROLE OF BAND POSITION AND INTENSITIES, Malgorzata Biczysko, Julien Bloino

SC. IR
Saturday, Sept. 6, 2014 – 9:00
Room 2, Chemistry

Chair: Veronika Zelenkova, Heyrovsky Institute of Physical Chemistry, Prague

SC01 **9:00 – 9:17**
MEASUREMENT AND VALIDATION OF WATER VAPOR LINE STRENGTHS IN THE 1.4-2.7 μ M RANGE BY HIGH SENSITIVITY TDLAS, Andrea Pogány, Alexander Klein, Bernhard Buchholz, Volker Ebert

SC02 **9:17 – 9:32**
UNDERSTANDING THE INTERNAL TORSION AND BENDING MOTION OF DIMETHYL ETHER VIA ISOTOPIC STUDIES, P. Kutzer, O. Pirali, P. Roy, T. F. Giesen

SC03 **9:32 – 9:49**
SELF-, N_2 -, O_2 - AND AIR- BROADENING COEFFICIENTS OF HFC-32 RO-VIBRATIONAL- AND ROTATIONAL- TRANSITIONS FOR ATMOSPHERIC APPLICATIONS, Nicola Tassinato, Arianna Turchetto, Cristina Puzzarini, Paolo Stoppa, Andrea Pietropoli Charmet, Santi Giorgianni

SC04 **9:49 – 10:01**
RECENT LINE-SHAPE AND DOPPLER THERMOMETRY STUDIES INVOLVING TRANSITIONS IN THE $\nu_1+\nu_3$ BAND OF ACETYLENE, Robab Hashemi, Haimonti Rozario, Chad Povey, Jolene Garber, Mark Derksen, Adriana Predoi-Cross

SC05 **10:01 – 10:18**
FOUR-WAVE MIXING SPECTROSCOPY OF THE $NO_3 \tilde{B}^2E' - \tilde{X}^2A_2'$ SYSTEM, Masaru Fukushima, Takashi Ishiwata.

SC06 **10:18 – 10:30**
A STUDY OF THE MOLECULAR STRUCTURE AND SPECTROSCOPIC PROPERTIES OF 2-FORMYLPHENYLBORONIC ACID PINACOL ESTER BY EXPERIMENTAL METHODS AND QUANTUM CHEMICAL CALCULATIONS, M. Kurt, E. Babur Sas

SC07 **10:30 – 10:42**

MEASUREMENTS OF CO₂ LINE PARAMETERS IN THE 9250-9500 CM⁻¹ AND 10700-10800 CM⁻¹ REGIONS, T.M. Petrova, A.M. Solodov, A.A. Solodov, O.M. Lyulin, Yu.G. Borkov, S.A. Tashkun, V.I. Perevalov

Intermission

SC08

11:12 – 11:24

FOURIER TRANSFORM OPTICAL FREQUENCY COMB SPECTROSCOPY IN THE MID-INFRARED BASED ON DOUBLY RESONANT OPO, P. Maslowski, K. F. Lee, A. Mills, C. Mohr, J. Jiang, M. E. Fermann

SC09

11:24 – 11:31

NH₃ SPECTRA IN THE 2.3 MICRONS REGION, P. Čermák, J. Hovorka, P. Cacciani, J. El Romh, J. Cosléou, M. Khelkhal

POSTERS

(152 posters)

Poster Session TP
Tuesday, Sept. 2, 2014 – 17:30
Palazzo Poggi – Largo Trombetti 4

TP01

RUBIDIUM D₁ AND D₂ ATOMIC LINES PRESSURE-BROADENED BY GROUND HELIUM ATOMS, K. Alioua, F. Bouhadjar, M.T. Bouazza, and M. Bouledroua

TP02

HIGH SENSITIVITY CAVITY RING DOWN SPECTROSCOPY OF CARBON DIOXIDE IN THE 1.19-1.26 μm REGION, E.V. Karlovets, S. Kassi, S.A.Tashkun, V.I. Perevalov, A. Campargue

TP03

ANALYSIS AND THEORETICAL MODELING OF THE SPECTRA OF ¹⁷O ISOTOPOLOGUES OF CARBON DIOXIDE BETWEEN 5850 AND 7000 cm^{-1} , E.V. Karlovets, A. Campargue, D. Mondelain, S. Kassi, S.A. Tashkun, V.I. Perevalov

TP04

ZEEMAN EFFECTS IN OPEN-SHELL VAN DER WAALS COMPLEXES: THE ARNO CASE, Sarantos Marinakis, Brian J. Howard

TP05

FIRST-PRINCIPLE CALCULATION OF CH₃D AND PH₃ SPECTRA IN THE INFRARED, Michaël Rey, Andrei Nikitin, Vladimir Tyuterev

TP06

METASTABLE VIBRATIONAL STATES OF OZONE ABOVE THE DISSOCIATION THRESHOLD: LIFETIME CALCULATIONS, IMPACT ON THE DYNAMICS, V. Kokoouline, D. Lapierre, R. V. Kochanov, A. Alijah, V.G.Tyuterev

TP07

IR SPECTRA OF 1-CHLORO-1-FLUOROETHENE INVESTIGATED BY A COMBINED EXPERIMENTAL AND COMPUTATIONAL STUDY, Andrea Pietropolli Charmet, Paolo Stoppa, Nicola Tasinato, Santi Giorgianni, Alberto Gambi

TP08

A JOINT EXPERIMENTAL AND COMPUTATIONAL STUDY ON THE VIBRATIONAL SPECTRA OF R1122, Andrea Pietropolli Charmet, Paolo Stoppa, Nicola Tasinato, Santi Giorgianni

TP09

HIGH RESOLUTION ANALYSIS OF THE N₃ BAND OF ³⁶SF₆ AND NEW GLOBAL FIT OF ³²SF₆ PARAMETERS INCLUDING NEW 3N₃ BAND DATA, Mbaye Faye, Vincent Boudon, Laurent Manceron, Fridolin Kwabia Tchana

TP10

AB INITIO STRUCTURAL AND SPECTROSCOPIC STUDY OF HPS^X AND HSP^X (X = 0,+1,-1) IN THE GAS PHASE, Saida ben Yaghlane, C. Eric Cotton and Joseph S. Francisco, Roberto Linguerra and Majdi Hochlaf

TP11 HIGH RESOLUTION SPECTROSCOPY OF NAPHTHALENE WITH AN OPTICAL FREQUENCY COMB, Akiko Nishiyama, Ayumi Matsuba, and Masatoshi Misono

TP12

HIGH RESOLUTION INVESTIGATION OF THE ν_3 BAND OF TRIFLUORIMETHYL IODIDE (CF₃I) AT SYNCHROTRON SOLEIL, F.Willaert, P. Roy, O. Pirali, L. Manceron, C. Medcraft, D. Appadoo, R. Plathe, D. McNaughton, J.Demaison, A.Perrin, F. Kwabia-Tchana

TP13

DETECTION OF ATMOSPHERIC $^{15}\text{NO}_2$ ENABLED BY NEW ν_3 LINELIST, Agnès Perrin, Geoffrey Toon, Johannes Orphal

TP14

ROVIBRATIONAL SPECTRUM OF DEUTERATED FLUOROFORM IN THE 1900 CM^{-1} REGION: HIGH-RESOLUTION STUDY OF THE $\nu_3+\nu_4/2\nu_3+\nu_6$ FERMI-INTERACTING BANDS, Adina-Adriana Ceausu-Velcescu, Petr Pracna

TP15

ROVIBRATIONAL SPECTRA OF DCF_3 IN THE 2000 CM^{-1} REGION: HIGH-RESOLUTION STUDY OF THE $V_5=2$ AND $V_2=V_5=1$ LEVELS, Adina-Adriana Ceausu-Velcescu, Petr Pracna, Adriana Predoi-Cross

TP16

ON THE "EXPANDED LOCAL MODE" APPROACH APPLIED TO THE ETHYLENE MOLECULE, O. N. Ulenikov, E. S. Bekhtereva, A. L. Fomchenko, O. V. Gromova, C. Leroy

TP17

ANALYSIS OF NEW BANDS OF $^{16}\text{O}_3$ AND $^{18}\text{O}_3$ BY CRDS CLOSE TO THE DISSOCIATION ENERGY, D. Mondelain, A. Campargue, S. Kassi, E. Starikova, A. Barbe, M.-R. De Backer, VI.G. Tyuterev

TP18

CRDS OF THE $^{18}\text{O}^{16}\text{O}^{18}\text{O}$ AND $^{16}\text{O}^{18}\text{O}^{18}\text{O}$ ISOTOPOLOGUES OF OZONE BETWEEN 6340 AND 6800 cm^{-1} , E. Starikova, A. Barbe, M.-R. De Backer, VI.G. Tyuterev, D. Mondelain, S. Kassi, A. Campargue

TP19

EXACT FORM OF THE VIBRATIONAL HAMILTONIAN AND SYMMETRY COORDINATES, G.A. Pitsevich

TP20

MODELING THE 10 MM REGION OF THE ETHYLENE SPECTRUM USING THE D_{2H} TOP DATA SYSTEM: FREQUENCY AND INTENSITY ANALYSIS, M.-T. Bourgeois, A. Alkadrou, M. Rotger, M. Tudorie, J. Vander Auwera, V. Boudon

TP21

TEMPERATURE DEPENDENCE OF CO-SELF-BROADENING COEFFICIENTS, Anton Serdyukov, Jens Brunzendorf, Volker Ebert

TP22

SULFUR DETERMINATION IN SOME NUTS AND DRIED FRUITS SOLD IN TURKEY BY HIGH RESOLUTION GRAPHITE FURNACE MOLECULAR ABSORPTION SPECTROMETRY, Sema Gunduz, Suleyman Akman

TP23

PHOTOFRAGMENTATIONS AND ENERGETICS OF RYDBERG AND ION-PAIR STATES IN THE (2+N) REMPI SPECTRA OF HI, Helgi Rafn Hróðmarsson, Huasheng Wang, Ágúst Kvaran

TP24

LINE-SHAPES AND BROADENINGS OF ROTATIONAL LINES OF $\text{CH}_3^{35}\text{Cl}$ IN COLLISION WITH He, Ar AND Kr, V. Gupta, F. Rohart, L. Margulès, R.A. Motiyenko, J.V. Buldyreva

TP25

SPECTROSCOPIC INVESTIGATION OF THE $V_1 + V_2$ VIBRATIONAL BAND OF THE TRANS-FORMIC ACID AT ROOM TEMPERATURE AND IN A FREE JET EXPANSION, Dariusz Golebiowski, Thomas Vanfleteren, Tomas Földes, Michel Herman

TP26

OSCILLATOR STRENGTHS FOR RYDBERG STATES IN ARH CALCULATED IN MQDT, Sergei V. Elfimov, Dmitrii L. Dorofeev, Boris A. Zon

TP27

SELF BROADENING COEFFICIENTS AND IMPROVED LINE INTENSITIES FOR THE ν_7 BAND OF C_2H_4 NEAR $10.5 \mu m$, AND IMPACT ON ETHYLENE RETRIEVALS FROM JUNGFRAUJOCH SOLAR SPECTRA, J. Vander Auwera, A. Fayt, M. Tudorie, M. Rotger, V. Boudon, B. Franco, E. Mahieu

TP28

MB-FTMW SPECTROSCOPY OF THE CAMPHOR HYDRATES, P. Dréan, J.R. Avilès Moreno, T. R. Huet, A. Hamieh

TP29

DIODE-LASER SPECTROSCOPY: TEMPERATURE DEPENDENCE OF THE CO_2 -BROADENING COEFFICIENTS IN THE ν_4 BAND OF METHANE, Félix Maldague, Laurent Fissiaux, Miguël Dhyne, Jean-Claude Populaire, Nicolas Hespel, Séverine Robert, Ann Carine Vandaele, Muriel Lepère

TP30

CO_2 -BROADENING COEFFICIENTS IN THE ν_3 FUNDAMENTAL BAND OF METHANE AT ROOM TEMPERATURE, Laurent Fissiaux, Muriel Lepère

TP31

N_2 -BROADENING STUDY IN THE N_2 BAND OF METHYL CHLORIDE, Sylvain Léonis, Muriel Lepère

TP32

O_2 -BROADENING COEFFICIENTS IN THE $\nu_4 + \nu_5$ BAND OF ACETYLENE, Tuong Le Cong, Laurent Fissiaux, Ha Tran, Muriel Lepère

TP33

INTEGRATED EXPERIMENTAL AND COMPUTATIONAL VIBRATIONAL SPECTROSCOPY OF HFC-152A, Nicola Tasinato, Giorgia Ceselin, Giulia Saran, Paolo Stoppa, Andrea Pietropolli Charmet, Santi Giorgianni

TP34

TEMPERATURE DEPENDENCE, PRESSURE SHIFT AND BROADENING COEFFICIENTS OF H_2O AT $1.4 \mu m$ FOR ATMOSPHERIC H_2O MONITORING, Javis. A. Nwaboh, Bernhard Buchholz, Olav Werhahn, Volker Ebert

TP35

MEASUREMENTS AND MULTISPECTRUM FITTING ANALYSIS OF OXYGEN B-BAND SPECTRA, S. Wójtewicz, A. Cygan, P. Masłowski, J. Domysławska, P. Wcisło, M. Zaborowski, D. Lisak, R. S. Trawiński, R. Ciuryło

TP36

FTIR-BASED CO_2 LINE STRENGTH MEASUREMENTS IN THE 20012 – 00001 BAND NEAR $2 \mu m$, Jens Brunzendorf, Anton Serdyukov, Viktor Werwein, Olav Werhahn, Volker Ebert

TP37

VERY HIGH RESOLUTION HETERODYNE DETECTION TECHNIQUE FOR SYNCHROTRON RADIATION IN THE THz RANGE, S. Tammaro, O. Pirali, G. Mouret, J.-F. Lampin, G. Ducournau, A. Cuisset, F. Hindle, P. Roy

TP38

MEASUREMENT OF N_2 -COLLISIONAL SHIFT COEFFICIENTS OF METHANE LINES IN THE ν_3 BAND AT HIGH TEMPERATURES, Bastien Vispoel, Nicolas Hespel, Jean-Claude Populaire, Muriel Lepère

TP39

A HYBRID VARIATION-PERTURBATION METHOD FOR CALCULATING ROVIBRATIONAL ENERGY LEVELS OF POLYATOMIC MOLECULES, A.I. Pavlyuchko, S.N. Yurchenko, Jonathan Tennyson

TP40

MICROWAVE SPECTROSCOPY OF ATMOSPHERIC OXYDATION PRODUCTS OF β -PINENE: THE CASE OF NOPINONE, Elias M. Neeman, Juan-Ramon Aviles-Moreno, Thérèse R. Huet

TP41

MB-FTMW SPECTROSCOPY OF NOPINONE-WATER COMPLEXES, Elias M. Neeman, Juan-Ramon Aviles-Moreno, Thérèse R. Huet

TP42

THE INTERNAL ROTATION OF THE METHYL GROUP IN METHACROLEIN CHARACTERIZED BY MILLIMETER-WAVE SPECTROSCOPY AND QUANTUM CHEMICAL CALCULATIONS, Olena Zakharenko, Juan-Ramon Aviles-Moreno, Roman A. Motiyenko, Thérèse R. Huet

TP43

EXOPLANET ATMOSPHERES: TOWARDS A HOT LINE LIST FOR CH_3Cl , Alec Owens, Sergei N. Yurchenko, Andrey Yachmenev, Walter Thiel

TP44

MW WATER VAPOUR CONTINUUM AT NEAR ROOM TEMPERATURE: HOW THE WATER DIMER EFFECT SHOULD BE TREATED?, A.A. Vigasin, I.A. Buryak, M.Yu. Tretyakov, M.A. Koshelev

TP45

SOLVENT EFFECTS ON THE MOLECULAR STRUCTURE AND VIBRATIONAL SPECTRA OF THEOBROMINE, Özgür Öztürk, Turgay Polat

TP46

INTERMOLECULAR HYDROGEN BONDING INTERACTIONS BETWEEN CAFFEINE AND WATER MOLECULES, Turgay Polat

TP47

THEORETICAL INVESTIGATIONS OF α , α , α -TRIFLUORO-3, -P AND O-NITROTOLUENE BY MEANS OF DENSITY FUNCTIONAL THEORY, G. Yildirim, S. D. Senol, M. Dogruer, O. Ozturk, A. Senol, A. T. Tasci, C. Terzioglu

TP48

THE SPECTRAL LINE CONTOUR SHAPE IN THE LINE WING FOR DIFFERENT BANDS OF H_2O AND CO_2 , Tatiana E. Klimeshina, Olga B. Rodimova

TP49

ROTATIONAL DYNAMICS OF A VIBRATING WATER-LIKE MOLECULE, Sergey V. Petrov, Sergei E. Lokshantov

TP50

CONFORMATIONAL FLEXIBILITY OF LIMONENE OXIDE STUDIED BY MICROWAVE SPECTROSCOPY, María del Mar Quesada-Moreno, Juan Ramón Avilés-Moreno, Juan Jesús López-González, Thérèse R. Huet

TP51

FROM THE GAS TO CONDENSED PHASES: MICROWAVE AND VIBRATIONAL STUDY OF γ -TERPINENE, María del Mar Quesada-Moreno, Juan Ramón Avilés-Moreno, Juan Jesús López-González, Thérèse R. Huet

Poster Session WP
Wednesday, Sept. 3, 2014 – 17:30
Palazzo Poggi, Largo Trombetti, 4

WP01

THE CH(A²Δ) SPECTRA FOLLOWING REMPI OF CH_{4-n}Br_n; n = 1,2,3: LONG-TERM PUZZLE REVISITED, Arnar Hafliðason, Huasheng Wang, Ágúst Kvaran

WP02

HIGH CONTRAST ELECTROMAGNETICALLY INDUCED TRANSPARENCY OF Cs D₁ LINE IN NANOMETRIC-THIN VAPOR CELL, Y. Pashayan-Leroy, A. Sargsyan, C. Leroy, D. Sarkisyan

WP03

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