

# **Program of sessions**

**9:00 Tuesday – 12:00 Saturday**

**Invited Lectures A** **Tuesday, 9:00***chairperson: Jensen P.*A1 **Picqué N.** 9:00*nazev*A2 **Campargue A.,** 9:45Leshchishina O., Wang L., Mondelain D., Kassi S.  
*Ultra sensitive Cavity Ring Down Spectroscopy of methane and hydrogen between 1.26 and 1.71  $\mu\text{m}$* **Contributed Lectures B** **Tuesday, 11:00***chairperson: Puzzarini C.*B1 **Schnell M.,** 11:00Shubert V.A., Schmitz D., Betz T.  
*Chirped-pulse Broadband Rotational Spectroscopy of Large Molecules*B2 **Jäger W.,** 11:15Fahim Amin T.M., Huda Q.M., Ning Y., McKinnon G., Tulip J.  
*Towards a MEMS Based External Cavity Tunable Infrared Laser for Spectroscopic Applications*B3 **Kisiel Z.,** 11:30Pérez C., Muckle M.T., Zaleski D.P., Seifert N.A., Temelso B., Shields G.C., Pate B.H.  
*Chirped-pulse Rotational Spectroscopy and Structures of the Hexamer, Heptamer and Nonamer Water Clusters*B4 **Asvany O.,** 11:45Krieg J., Schlemmer S.  
*Comb-assisted Spectroscopy of Molecular Ions in the MIR*B5 **Strelnikov D.,** 12:00Boettcher A., Kern B., Kappes M.  
*Laboratory and Space Infrared Detection of  $\text{C}_{60}^+$*

- B6 **Yang S.** 12:15  
Ellis A.M., Shepperson B., Boatwright A., Cheng F., Spence D.  
*Depletion Spectroscopy of Water and Water-methane Clusters in Superfluid Helium Nanodroplets*

**Invited Lectures C** **Tuesday, 14:30**

*chairperson: Yamada K.M.T.*

- C1 **Momose T.** 14:30  
*Spectroscopy of Large Hydrogen Clusters in He Droplets*
- C2 **Zehnacker-Rentien A.** 15:15  
*Chiral Recognition in Jet-cooled Complexes: an Electronic and Vibrational Spectroscopy Study*

**Poster session D** **Tuesday, 16:30**

- D1 **Yoon Y.W., Lee S.K.**  
*Spectroscopic Observation of Jet-Cooled 2-Halo-m-Xylyl Radicals*
- D2 **Betz T., Schmitz D., Shubert V.A., Schnell M.**  
*Carbohydrate-Aromatic Complexes Investigated by Broadband Microwave Spectroscopy*
- D3 **Hougen J.T., Xu L.-H., Lees R.M.**  
*Ab-initio Normal-mode Vibrational Displacement Vectors for the Three C-H Stretching Vibrations along the Internal Rotation Path in Methanol*
- D4 **Campargue A., Wang L., Leshchishina O., Mondelain D., Kassi S.**  
*The WKMC Empirical Line Lists (5852–7919  $\text{cm}^{-1}$ ) for Methane between 80 K and 296 K*
- D5 **Cane E., Di Lonardo G., Fusina L., Nivellini G., Tamassia F., Villa M.**  
*The  $\nu_2$  and  $\nu_4$  Bending Fundamental Bands of  $^{15}\text{ND}_3$*

- D6 **Tasinato N., Regini G., Stoppa P., Pietropolli Charmet A., Gambi A.**  
*A Joint Experimental and Computational Study on the Vibrational and Ro-vibrational Spectroscopy of HFC-32*
- D7 **Pietropolli Charmet A., Stoppa P., Tasinato N., Giorgianni S., Puzzarini C., Biczysko M., Bloino J., Cappelli C., Carmineo I.**  
*IR Spectroscopy of HCFC-31 from the FAR up to the NIR Region: a Combined Experimental and Computational Study*
- D8 **Dore L., Degli Esposti C., Fusina L., Tamassia F., Di Lonardo G.**  
*The Rotational Spectrum of  $^{13}\text{C}_2\text{HD}$  and  $^{12}\text{C}_2\text{HD}$  in the Ground and Excited Bending States: a Global Analysis*
- D9 **Fusina L., Di Lonardo G., Villa M., Tamassia F., Cane E.**  
*The Stretching-Bending Bands of  $^{12}\text{C}_2\text{D}_2$*
- D10 **Pracna P., Ceausu-Velcescu A., Horneman V.-M.**  
*The First High-Resolution Analysis of the  $\nu_6$  Fundamental Band of Monoisotopic  $\text{HC}^{35}\text{Cl}_3$*
- D11 **Kasahara S., Kanzawa K., Tada K.**  
*Rotationally-resolved High-resolution Laser Spectroscopy of the  $S_1$ - $S_0$  Electronic Transition of Naphthalene and Cl-naphthalene*
- D12 **Melnikov V.V., Yurchenko S.N.**  
*Rotational States of the Hydrogen Molecule in the Silicon Crystal*
- D13 **Bourgeois M.-T., Rotger M., Boudon V., Vander Auwera J.**  
*Frequency Analysis of the 10 and 3  $\mu\text{m}$  Regions of the Ethylene Spectrum using the  $D_{2h}$  Top Data System*
- D14 **Tudorie M., Di Lauro C., Lattanzi F., Vander Auwera J.**  
*A New Analysis of the  $\nu_7$  Band of Ethane*

- D15 **Civiš S., Ferus M., Kubelík P., Chernov V.E., Zanozina E.M.**  
*High-L atomic Rydberg States of Alkali Metals Studied by High Resolution Time-resolved Fourier-transform Infrared Spectroscopy*
- D16 **Kunimatsu A., Tanabe S., Ogawa S., Kuze N., Nakane A., Okabayashi T., Araki M.**  
*Microwave Spectra of the Linear Carbon-chain Alcohol  $HC_4OH$*
- D17 **Aouididi H., Rotger M., Bermejo D., Martinez R.Z., Boudon V.**  
*High-Resolution Stimulated Raman Spectroscopy and Analysis of the  $\nu_1$  and  $\nu_5$  Bands of  $C_2H_4$*
- D18 **Sahdane T., Badaoui M., Rotger M.**  
*A New Study of  $2\nu_4$  Band of  $PF_3$  Molecule by High Resolution Infrared Spectroscopy*
- D19 **Domysławska J., Wójtewicz S., Lisak D., Cygan A., Ozimek F., Stec K., Bielska K., Masłowski P., Radzewicz Cz., Trawiński R.S., Ciuryło R.**  
*Frequency-comb Assisted Cavity Ring-down Measurements of the Oxygen B-band Transition Frequencies and Pressure Shifts*
- D20 **Brougher G.G., Chen M., Dannenhoffer T.P., Everett R.M., Foelker J.A., Hardwick J.L., Huang J., Huang Z., Kostur L.G., Kovac P.A., O'Brien Johnson, Oh S.H., Robertson S.J., Sitts L.W., Tepfer S.R., Thompson L.T., Wahl K.A., Warrick C.A., Weldon N.C., Westover R.D.**  
*Diode Laser Absorption Spectrum of Cold Bands of  $NH_3$  near  $6500\text{ cm}^{-1}$*
- D21 **Delahaye T., Rey M., Tyuterev V., Nikitin A.**  
*Variational Calculations and Symmetry-adapted Normal Mode Models: Application to Species of Atmospheric Interest*
- D22 **Sousa-Silva C., Polyansky O., Yurchenko S.N., Tennyson J.**  
*Can Anyone Detect Phosphine's Splitting?*

- D23 **Underwood D., Yurchenko S.N., Tennyson J., Fateev A.**  
*Variationally Computed Ro-Vibrational Energies (up to  $J=100$ ) of Sulphur Trioxide*
- D24 **Bray C., Jacquemart D., Lacombe N., Cuisset A., Guinet M., Eliet S., Mouret G., Rohart F., Buldyreva J.**  
*Self-broadening Coefficients of  $CH_3Cl$  Lines*
- D25 **Vogt J., Vogt N., Rudert R.**  
*MOGADOC - A Database with Experimental Structure Information on Small Molecules*
- D26 **Hajigeorgiou P.G.**  
*Accurate Analytical Internuclear Potential for the Ground Electronic State of the Oxygen Molecule*
- D27 **Mladenović M.**  
*Theoretical Investigation of the HOCO radical in the Ground Electronic State*
- D28 **Nikitin A.V., Brown L.R., Rey M., Tyuterev V.G., Sung K., Smith M.A.H., Mantz A.W.**  
*Preliminary Modeling of  $CH_3D$  from 4000 to 4550  $cm^{-1}$*
- D29 **Cacciani P., Čermák P., Cosleau J., Khelkhal M., El Romh J.**  
*Spectroscopy of Ammonia  $^{14}NH_3$  and  $^{15}NH_3$  with VECSEL Laser Source in the Infrared 2.3  $\mu m$  Range*
- D30 **Evangelisti L., Feng G., Gou Q., Caminati W.**  
*Effect of Fluorine Atom Substitutions in Benzyl Alcohol Derivates*
- D31 **Perry A., Martin M.A., Nibler J.W., Maki A., Weber A., Blake T.A.**  
*Coriolis Analysis of Several High Resolution Infrared Bands of Bicyclo[1.1.1]pentane- $d_0$  and - $d_1$*
- D32 **Ulenikov O.N., Bekhtereva E.S., Krivchikova Yu.V., Zamotaeva V.A., Bürger H.**  
*High Resolution Fourier Transform Spectrum of  $PHD_2$  in the Region of 1550 - 1800  $cm^{-1}$*

- D33 **Crogman H., Choi B., Chen H., Harter W.**  
*Symmetric Group and Point Group Analysis of a Coupled Rotor System*
- D34 **Jensen P., Ostojić B., Bunker P.R., Schwerdtfeger P., Gertych A.**  
*The Predicted Infrared Spectrum of the Hypermetallic Molecule CaOCa in its Lowest Two Electronic States  $X^1\Sigma_g^+$  and a  $^3\Sigma_u^+$*
- D35 **Janečková R., May O., Fedor J.**  
*Dissociative Electron Attachment in Molecules from Alkynes Family*
- D36 **Petrov S.V., Lokshtanov S.E.**  
*Classical Dynamic Equations and the Structure of Quantum Rotational Spectra of Molecules*
- D37 **Serdyukov V.I., Sinitza L.N., Vasilchenko S.S., Mikhaleiko S.N.**  
*Absorption Spectra of  $H_2^{18}O$  in the 15150 – 15600  $cm^{-1}$  Spectral Region*
- D38 **Alijah A., Tyuterev V.G., Kokoouline V.**  
*Towards a Dipole Surface and Intensity Calculations for  $H_3^+$  in the Electronic Triplet State*
- D39 **Martin-Drumel M.-A., Pirali O., Loquais Y., Falvo C., Bréchnac P.**  
*Low-energy Vibrational Modes of Some Naphthalene Derivatives*
- D40 **Uhlíková T., Urban Š.**  
*Theoretical Investigation of the Shift of the Degenerate Vibrations in the  $FSO_3$  Radical*
- D41 **Cacciani P., Čermák P., Cosléau J., Khelkhal M., Michaut X., Jeseck P.**  
*New Progress in Spectroscopy of Ammonia in the Infrared 1.5  $\mu m$  Range using Evolution of Spectra from 300 K down to 122 K*
- D42 **Evangelisti L., Maris A., Melandri S., Caminati W.**  
*Internal Dynamics in Phenylacetate*

- D43 **Kirkpatrick R., Masiello T., Martin M., Nibler J.W., Maki A., Weber A., Blake T.A.**  
*High Resolution Infrared Studies of the  $\nu_{10}$ ,  $\nu_{11}$ ,  $\nu_{14}$ , and  $\nu_{18}$  Levels of [1.1.1]propellane*
- D44 **Ulenikov O.N., Bekhtereva E.S., Konov I.A., Raspopova N.I., Litvinovskaya A.G.**  
*Study of Spectroscopic Properties of Di-Atomic Molecules on the Basis of High Order Operator Perturbation Theory*

**Invited Lectures E****Wednesday, 9:00***chairperson: Grabow J.-U.*

- E1 **Plusquellic D.F.,** 9:00  
 Douglass K. O., Maxwell S., Scherschligt J.  
*Chirped Pulse THz and IR Spectroscopy*
- E2 **Stanton J.F.,** 9:45  
 Ichino T., Simmons C.S.  
*Theoretical Insights into the Spectroscopy of  $NO_3$*

**Contributed Lectures F****Wednesday, 11:00***chairperson: Tyuterev V.*

- F1 **Špirko V.,** 11:00  
 Sauer S.P.A., Szalewicz K.  
*On the relation between properties of long-range diatomic bound states*
- F2 **Hirota E.** 11:15  
*Vibrational assignment and vibronic interaction for the nitrate radical  $NO_3$  in the ground electronic state*
- F3 **McKellar A.R.W.,** 11:30  
 Rezaei M., Norooz Oliaee J., Moazzen-Ahmadi N.  
*High Resolution Infrared Spectra of Larger Molecular Clusters:  $(N_2O)_5$ ,  $(CO_2)_3 - (C_2H_2)_2$ , and  $(CO_2)_4 - (C_2H_2)_2$*



- F4 **Puzzarini C.** 11:45  
 Cazzoli G. , Vázquez J., Harding M.E., Gauss J.  
*The rotational spectra of  $D_2^{17}O$  and  $HD^{17}O$ : accurate spectroscopic and hyperfine parameters*
- F5 **Hirano T.** 12:00  
 Nagashima U., Jensen P.  
*Large Amplitude Bending Motion: A Computational Molecular Spectroscopy Approach*
- F6 **Lapinov A.V.,** 12:15  
 Levshakov S.A., Kozlov M.G., Henkel C., Molaro P., Mignano A., Sakai T., Grabow J.-U., Guarnieri A., Lapinova S.A., Golubiatnikov G.Yu., Belov S.P.  
*The Use of Precise Molecular Spectroscopy for a Search of  $m_e/m_p$  Variations*

**Contributed Lectures G****Wednesday, 14:30***chairperson: Lepère M.*

- G1 **Xu Y.,** 14:30  
 Sunahori F.X., Yang G., Kitova E.N., Klassen J.S.  
*Chirality Recognition Study of Protonated Serine Dimer and Octamer by IRMPD Spectroscopy and DFT calculations*
- G2 **Miloglyadov E.,** 14:45  
 Prentner R., Quack M., Seyfang G.  
*Inversion Tunneling and in Chiral  $C_6H_4FNHD$  and  $C_6F_5NHD$  from Infrared Spectroscopy and Quasiadiabatic Channel Reaction Path Hamiltonian Calculations*
- G3 **Čermák P.,** 15:00  
 Cacciani P., Cosléou J., Khelkhal M., Hovorka J., Michaut X., Jeseck P., Coussan S., Pardanaud C., Martin C.  
*Observation of Methane Spin Isomers During Solid Formation by Absorption Spectroscopy at 2.3 microns*
- G4 **Tanaka K.,** 15:15  
 Harada K., Nanbu S., Oka T.  
*Spontaneous Emission between ortho- and para-Levels of Water Ion,  $H_2O^+$*

G5 **Ebert V.** 15:30  
*EUMETRISPEC: Traceability of Spectral Line Data*

G6 **Fissiaux L.,** 15:45  
 Populaire J.-C., Lepère M.  
*High Temperature Infrared Spectroscopy: Determination of Broadening Coefficients of Lines in the  $\nu_4$  Band of  $\text{CH}_4$*

**Poster session H**

**Wednesday, 16:30**

H1 **Abel M., Frommhold L., Li X., Hunt K.L.C**  
*Computation of Collision-Induced Absorption by Simple Molecular Complexes, for Astrophysical Applications*

H2 **Augustovičová L., Špirko V., Kraemer W.P., Soldán P.**  
*Radiative Association of  $\text{LiHe}^+$*

H3 **Tada K., Kasahara S., Baba M., Ishiwata T., Hirota E.**  
*Rotationally-resolved High-resolution Laser Spectroscopy of the B – X Electronic Transition of  $\text{NO}_3$  Radical*

H4 **Dewald D.A., Jahn M.K., Wachsmuth D., Grabow J.-U., Mehrotra S.C.**  
*Rapid Capture of Large Amplitude Motions in 2,6-difluorophenol*

H5 **Economides G., Dyer L., Howard B.J.**  
*The Rotational Spectrum and Quantum Dynamics of the  $\text{Ne-NO}_2$  Van der Waals Complex*

H6 **Wachsmuth D., Dewald D.A., Jahn M.K., Grabow J.-U.**  
*Fourier Transform Microwave IMPACT Spectrometer for Rotational Measurement of Laser Ablated Molecules*

H7 **Furukawa H., Abe K., Araki M., Tsukiyama K.**  
*Laser-Induced Far-Infrared Stimulated Emission from the High Rydberg States of Nitric Oxide*

H8 **Polyak I., Yachmenev A., Thiel W.**  
*Accurate Theoretical Rotation-vibration Spectrum of  $\text{H}_2\text{CS}$*

- H9 **Birzniece I., Docenko O., Nikolayeva O., Tamanis M., Ferber R.**  
*High Resolution Spectroscopy and Description of Low-lying Energy Levels of  $B(1)^1\Pi$  State in  $RbCs$*
- H10 **Aseev O., Koshelev M., Makarov D., Zobov N., Boyarkine O.**  
*Accurate Determination of Energy Levels and Dissociation Threshold of HOD by Multiple Resonance Overtone Spectroscopy*
- H11 **Feng G., Gou Q., Evangelisti L., Caminati W.**  
*Structure, Ubbelohde Effect, Conformational Equilibria and Tunneling Dynamics of Carboxylic acid Bi-molecules*
- H12 **Feng G., Gou Q., Evangelisti L., Caminati W.**  
*Informations on Intermolecular Interaction Between Water and Other Molecules from the Rotational Spectra of the  $^{17}O$  Water Complexes*
- H13 **Jahn M.K., Nair K.P.R., Grabow J.-U., Godfrey P.D., McNaughton D., Lesarri A., Écija P., Méndez E., Basterretxea F.J., Castano F., Cocinero E.J., Vogt N., Vogt J.**  
*From Succinic Acid to Succinic Anhydride: Analysis of the Rotational Spectra*
- H14 **Nguyen H.V.L., Kannengiesser R., Stahl W.**  
*Large Amplitude Motions – a Combination of Nitrogen Inversion Tunneling, Internal Rotation, and  $^{14}N$  Quadrupole Coupling in the Microwave Spectra of Some Amines*
- H15 **Fomchenko A.L., Ulenikov O.N., Bekhtereva E.S., Leroy C.**  
*On the 'Expanded Local Mode' Approach Applied to the Methane Molecule:  $CH_3D/CHD_3$  Isotopic Species*
- H16 **Patrascu A., Yurchenko S.N., Tennyson J.**  
*ExoMol Molecular Line Lists for Astrophysical Applications: A Theoretical Line List for Aluminum Oxide*

- H17 **Koubek J., Kania P., Urban Š.**  
*Hyperfine Splittings in  $CH_3F$  Induced by the Stark Effect*
- H18 **Koucký J., Kania P., Uhlíková T., Beckers H., Willner H., Urban Š.**  
*Microwave Spectra and Molecular Geometry of the Fluoroformyl Radical Isotopologues*
- H19 **Koucký J., Kania P., Uhlíková T., Zeng X., Beckers H., Willner H., Urban Š.**  
*The First Rotational Study of SNP*
- H20 **Pashayan-Leroy Y., Leroy C., Hakhumyan G., Sarkisyan D.**  
*Study of Molecular Transitions of Rb and Cs Dimers in Strong Magnetic Fields up to 7 kG*
- H21 **Louviot M., Boudon V., Manceron L., Bermejo D., Martínez R.Z.**  
*High Resolution Infrared and Raman Spectroscopy of  $^{192}OsO_4$*
- H22 **Herman M., Fusina L., Di Lonardo G., Predoi-Cross A.**  
*The Infrared Spectrum of  $^{13}C_2H_2$ : Bending States up to  $\nu_4 + \nu_5 = 4$*
- H23 **Rezaei M., Rezaei M., Norooz Oliaee J., Moazzen-Ahmadi N., McKellar A.R.W.**  
*Spectroscopy of  $(C_2D_2)_2$ ,  $(C_2D_2)_3$ ,  $C_2D_2-He$ , and  $C_2D_2-Ne$*
- H24 **Ishiwata T., Shimizu N., Fujimori F., Kawaguchi K., Hirota E., Tanaka T.**  
*Analysis of the  $\nu_1 + \nu_4$  Combination Band of  $NO_3$*
- H25 **Martin-Drumel M.-A., Eliet S., Pirali O., Guinet M., Hindle F., Mouret G., Cuisset A.**  
*New Investigation on THz spectra of OH, SH and SO radicals*
- H26 **Cacciani P., Čermák P., Cosléau J., Khelkhal M., Puzzarini C.**  
*Nuclear Spin Conversion in Methane*
- H27 **Degli Esposti C., Dore L., Bizzocchi L.**  
*Submillimetre-wave Spectroscopy of Unstable Imines of Astrophysical Interest:  $CH_2NH$  and  $CH_2CNH$*

- H28 **Cygan A., Lisak D., Wójtewicz S., Domysławska J., Hodges J.T., Trawiński R.S., Ciurylo R.**  
*High Signal-to-noise Ratio Line-shape Measurements of the Oxygen B band by PDH-locked FS-CRDS*
- H29 **Hakalla R., Szajna W., Zachwieja M., Piotrowska I., Ostrowska-Kopeć M., Kolek P., Kepa R.**  
*First Analysis of the Ångström Bands System ( $B\ ^1\Sigma^+ - A\ ^1\Pi$ ) in the Rare  $^{12}\text{C}^{17}\text{O}$  Isotopic Molecule*
- H30 **Tasinato N., Pietropolli Charmet A., Stoppa P., Buffa G.**  
*Experimental and Theoretical Broadening Coefficients of Self-perturbed  $\text{SO}_2$  Ro-vibrational Transitions in the 9 mm Atmospheric Region from Tunable Diode Laser Spectroscopy and Semiclassical Calculations*
- H31 **Boudon V., Bermejo D., Martínez R.Z.**  
*High-Resolution Stimulated Raman Spectroscopy of Carbon Tetrafluoride  $\text{CF}_4$*
- H32 **Ulenikov O.N., Gromova O.V., Bekhtereva E.S., Aslapovskaya Yu.S., Horneman V.-M.**  
*High Resolution Study of  $\text{C}_2\text{H}_4$ : Reanalysis of the Ground and Strongly Interacting  $\nu_4$ ,  $\nu_7$ , and  $\nu_{10}$  Vibrational Bands*
- H33 **Spezzano S., Brünken S., Müller H.S.P., Lewen F., Schlemmer S.**  
*Rotational Spectroscopy of the Isotopic Species of  $\text{CO}^+$  up to 1.3 THz*
- H34 **Yurchenko S.N., Tennyson J., Szabo I., Schmidt T.W., Bacskay G.B., Stolyarov A.V.**  
*High Level Ab Initio Study of the Electronic Interactions between Eight Lowest Electronic States of the  $\text{C}_2$  Radical*
- H35 **Daumont L., Nikitin A., Thomas X., Régalia L., Tyuterev V., Rey M., Boudon V., Wenger Ch., Loëte M., Brown L.R.**  
*New Assignments in the  $2\ \mu\text{m}$  Transparency Window of the  $^{12}\text{CH}_4$  Octad Band System*

- H36 **Vogt N., Vogt J.**  
*Test of Molecular Structure Determination on Some Examples*
- H37 **Azzam A., Yurchenko S.N., Tennyson J.**  
*Hydrogen Sulphide: Dipole Moment Surface and Room Temperature Spectrum*
- H38 **Rakhymzhan A., Chichinin A.**  
*Laser Magnetic Resonance of NO<sub>2</sub> Molecules: Line Positions and Intensities*
- H49 **Dolgov A.A., Potapov A., Panfilov V.A., Surin L.A., Schlemmer S.**  
*New Millimeter-Wave Measurements of the NH<sub>3</sub>-CO and NH<sub>3</sub>-N<sub>2</sub> Molecular Complexes*
- H40 **Asvany O., Brunken S., Potapov A., Kluge L., Gärtner S., Schlemmer S.**  
*High-resolution Spectroscopy of Molecular Ions*
- H41 **Hakalla R., Szajna W., Zachwieja M., Piotrowska I., Ostrowska-Kopeć M., Kolek P., Kepa R.**  
*First Analysis of the 1 - v" Progression of the Ångström System in the Rare <sup>12</sup>C<sup>17</sup>O Isotopic Molecule*
- H42 **Tasinato N., Pietropolli Charmet A., Stoppa P., Giorgianni S.**  
*He-, N<sub>2</sub>- and O<sub>2</sub>- Broadening Coefficients of Sulfur Dioxide Rovibrational Lines in the 9.2 μm Region*
- H43 **Boudon V., Pirali O.**  
*High-Resolution Spectroscopy of Hexamethylenetetramine (HMT) C<sub>6</sub>N<sub>4</sub>H<sub>12</sub>*
- H44 **Ulenikov O.N., Bekhtereva E.S., Bolotova I.B., Albert S., Bauerecker S., Hollenstein H., Quack M.**  
*A High Resolution FTIR Spectroscopic Study of Collisional - Cooled CHF<sub>3</sub>: Re-Analysis of the Strongly Coupled States ν<sub>2</sub>, ν<sub>5</sub>, and ν<sub>3</sub>+ν<sub>6</sub>*

**Invited Lectures I****Thursday, 9:00***chairperson: McKellar R.*

- I1 **McCarthy M.C.** 9:00  
*Reactive and Highly Reactive Species: Characterizing Key Intermediates in Combustion, Atmospheric, and Interstellar Chemistries by Rotational Spectroscopy*
- I2 **Herbst E.** 9:45  
*New Telescopes, New Expectations, Puzzling Results*

**Poster session J****Thursday, 11:00**

- J1 **Elsayed B.A., El-Henawy A.A.**  
*Synthesis, Characterization, Antimicrobial and Cytotoxic Studies on some Novel Transition Metal Complexes of Schiff base Ligand derived from Sulfadiazine with Molecular Orbital calculations*
- J2 **Groner P., Albert S., Quack M.**  
*Effective Rotational Hamiltonian (ERHAM) for High-resolution Infrared Spectra of Molecules with Internal Rotors*
- J3 **Araki M., Takano S., Yamabe H., Tsukiyama K., Kuze N.**  
*Radio Search for H<sub>2</sub>CCC toward HD 183143 as a Candidate for a Diffuse Interstellar Band Carrier*
- J4 **Marinakis S., Howard B.J.**  
*Zeeman Effects in Open-shell van der Waals Complexes*
- J5 **Kongolo Tshikala P., Lepère M.**  
*N<sub>2</sub><sup>-</sup>, O<sub>2</sub><sup>-</sup> and Air-broadening Coefficients of Lines in the ν<sub>2</sub> Band of <sup>13</sup>C<sup>16</sup>O<sub>2</sub> at Room Temperature*
- J6 **Urbanczyk T., Koperski J.**  
*High-temperature Pulsed Source of Cd<sub>2</sub> and CdRg Molecules in Supersonic Beam*
- J7 **Shepherd P.J., Chernov V.E., Dorofeev D.L., Knyazev M.Yu.**  
*Quantum-classical Rydberg Electron Dynamics in a Polar Molecule*

- J8 **Tudorie M., Robert S., Foldes T., Mahieux A., Drummond R., Wilquet V., Vandaele A.C., Vander Auwera J.**  
*CO<sub>2</sub> Broadening and Shift Coefficients for the 2-0 Band of CO and Influence on the Inversion of SOIR Spectra*
- J9 **Makarov D., Boulet C.**  
*On the ECS Formalism Applied to 60-GHz Oxygen Absorption Band Profile*
- J10 **Vallejo M., Écija P., Cocinero E.J., Lesarri A., Basterretxea F.J., Fernández J.A., Castaño F.**  
*Conformational Flexibility of Tropanes: The Rotational Spectrum of Pseudo-Pelletierine*
- J11 **Linton C., Granger A.D., Adam A.G., Frey S.E., Le A., Steimle T.C.**  
*Measurement of Hyperfine Structure and Permanent Electric Dipole Moments in the Electronic Spectrum of Iridium Monohydride and Monodeuteride*
- J12 **Tyuterev V., Tashkun S., Rey M., Delahaye T., Kochanov R., Nikitin A., Lamouroux J.**  
*Non-empirical Spectroscopic Models Derived from Potential and Surfaces via High-order Contact Transformations: Status of the MOL-CT Program Suite*
- J13 **Rothman L.S., Gordon I.E., Li G.**  
*Review of the Recent and Future Extensions of the HITRAN Database to Aid Remote Sensing of Diverse Planetary Atmospheres*
- J14 **Brougher G.G., Cramer R.C., Dannenhoffer T.P., Davis K.E., Everett R.M., Evoniuk C.J., Hardwick J.L., Huang J., O'Brien Johnson G.S., Kostur L.G., Lyubimov I., Robertson S.J., Sidener M.J.**  
*Diode Laser Absorption Spectrum of Hot Bands of C<sub>2</sub>HD near 2ν<sub>1</sub>*
- J15 **Evangelisti L., Feng G., Gou Q., Grabow J.-U., Caminati W.**  
*Halogen Bond and Hindered Motions in Freons by Microwave Spectroscopy*



- J16 **Assaf J., Magnier S., El Haj Hassan F., Taher F.**  
*Theoretical Description of the Lowest-lying Electronic States of LuO*
- J18 **Devi V.M., Benner D.C., Smith M.A.H., Mantz A.W., Sung K., Brown L.R.**  
*Multispectrum Fitting to Determine Line Parameters with Temperature Dependence for the 2←0 Bands of  $^{12}\text{C}^{16}\text{O}$ ,  $^{13}\text{C}^{16}\text{O}$ , and  $^{12}\text{C}^{18}\text{O}$*
- J19 **Vaks V.L., Domracheva E.G., Pripolzin S.I., Sobakinskaya E.A., Chernyaeva M.B.**  
*Applications of the High-Precise THz Nonstationary Spectroscopy*
- J20 **Kalugina Y.N., Lique F.**  
*Potential Energy Surface and Collision Dynamics of  $\text{O}_2(^3\Sigma_g^-) + \text{H}_2$*
- J21 **Civiš S., Ferus M.**  
*A450 TiO<sub>2</sub> Anatase Nanoparticles: Nanomotors Converting CO<sub>2</sub>*
- J22 **Ferus M., Civiš S., Michalčíková R., Španěl P., Sheshtivska V., Kubelík P., Šponerová J.**  
*The Study of Transient Species and Precursors of Biomolecules using Spectroscopic Techniques*
- J23 **Cuisset A., Pirali O., Sadovskii D.A.**  
*Rovibrational Spectroscopy of Bending Modes of DMSO: When THz/FIR Sources Reveal an Unusual Rotational Behaviour*
- J24 **Eliet S., Guinet M., Cuisset A., Hindle F., Bocquet R., Mouret G.**  
*Pollutants Monitoring in the sub THz Frequency Domain*
- J25 **Morino I., Inoue M., Nakamae K., Miyamoto Y., Kikuchi N., Yoshida Y., Yokota T., Uchino O.**  
*Atmospheric Greenhouse Gases Observed with a Fourier Transform Spectrometer onboard GOSAT and Validation of GOSAT Data*

- J26 **Osman O., Mahmoud A.A., Ibrahim M., Refaat A.**  
*Preparation and Characterization of Modified Bio-Polymer as Bio Sensor*
- J27 **Lodi L., Yurchenko S.N., Kerridge A., Tennyson J.**  
*ExoMol: Molecular Line Lists for Astrophysical Applications. A theoretical Line List for Nickel Hydride*
- J28 **Daumont L., Rekik G., Bonhommeau D., Rotger M., Tyuterev V.I.G., Boudon V., Wenger C., Dubernet M.-L.**  
*Databases of Infrared Spectra of Ethylene, Methane and Water for the VAMDC european e-infrastructure*
- J29 **Szajna W., Hakalla R., Zachwieja M., Piotrowska I., Ostrowska-Kopeć M., Kolek P., Kepa R.**  
*New Analysis of the Triplet ( $b^3\Sigma^- - a^3\Pi$ ) System of the AlH*
- J30 **Barbe A., De Backer M.-R., Starikova E., Tashkun S., Thomas X., Tyuterev V.**  
*Ozone FTS Spectrum in the Range 3300–3600  $\text{cm}^{-1}$  Revisited: Half Theoretical / Half Empirical Model for the Polyad of Strongly Coupled (220)/(121)/(022) States*
- J31 **Hezma A., Abdelghany A., Allam M., AbdelRazek E., El-Bahy G.**  
*Physical Studies of Nano-Hydroxapatite-Polyacrylic Acid with Cellulose Acetate*
- J32 **Ulenikov O.N., Bekhtereva E.S., Albert S., Hollenstein H., Quack M.**  
*Joint Ro-Vibrational Analysis of Vibrational States of  $\text{CH}_2\text{D}_2$  up to 9000  $\text{cm}^{-1}$  and Experimental Determination of  $r_e$  and Internal Force Field Methane Parameters*
- J33 **Lavrentieva N.N., Lugovskoy A.A., Sinitza L.N., Sukhov A.**  
*Study of  $\text{D}_2\text{O}$  Absorption Spectrum in Silica Aerogel*
- J34 **Dudaryonok A.S., Lavrentieva N.N., Sinitza L.N., Serdyukov V.I., Vasilchenko S.S.**  
*Water Vapor Line Self-broadening Study in 13400–14000  $\text{cm}^{-1}$  Range*

- J35 **Coudert L.H., Gutle C., Ilyushin V., Grabow J.-U., Levshakov S.A.**  
*Spin-rotation, Spin-torsion, and Spin-spin Coupling in Methanol*
- J36 **Martin-Drumel M.-A., Pirali O., Birk M., Wagner G., Coudert L.H.**  
*Line Position and Line Intensity Analyses of the High-resolution Spectrum of the Water Molecule up to the First Hexad*
- J37 **Gulaczyk I., Kreglewski M.**  
*Theoretical Analysis of the Proton Tunneling and Internal Rotation in 2-methylmalonaldehyde*
- J38 **Zack L.N., Bucchino M.P., Ziurys L.M.**  
*Hyperfine Structure in Transition Metal Nitrides: ScN and YN*
- J39 **Lodyga W., Kreglewski M., Pracna P., Urban Š.**  
*Recent Developments of the Loomis-Wood for Windows Program Package for Interactive Assigning of Vibration-rotation Spectra*
- J43 **Szajna W., Hakalla R., Zachwieja M., Piotrowska I., Ostrowska-Kopeć M., Kolek P., Kepa R.**  
*Rotational Analysis of the  $E^1\Pi - A^1\Pi$  System of AlH*
- J44 **Mondelain D., Kassi S., Campargue A., Barbe A., De Backer M.-R., Starikova E., Tyuterev V.**  
*The CW-CRDS Spectra of the  $^{16}O^{18}O^{16}O$  Ozone Isotope Near  $6200\text{ cm}^{-1}$ : Experiment and Analysis of Three New Bands*
- J45 **Hezma A.M., Abdelghany A.M.**  
*Tissue Bonding Ability of Borate Analogue to Hench's Bioglass Containing Antibacterial Agent*
- J46 **Ulenikov O.N., Bekhtereva E.S., Albert S., Bauerecker S., Niederer H.-M., Quack M.**  
*High Resolution Spectroscopy and Vibrational Dynamics of Methane  $^{12}CH_4$  and  $^{13}CH_4$  up to  $12000\text{ cm}^{-1}$*

**Ioannes Marcus Marci Session K      Thursday, 16:00**

*chairperson: Jäger W.*

**K1 Hougen J.T.** 16:00

*High Resolution Molecular Spectroscopy: A Glance at the Present, two Memories from the Past, and some Hopeful Signs for the Future*

**K2 Cornell E.** 16:45

*A Particle Physics Laboratory Inside a Molecule: Frequency-Comb Molecular Ion Spectroscopy and the Electron's Electric Dipole Moment*

**Invited Lectures L      Friday, 9:00**

*chairperson: Rothman L.*

**L1 Yurchenko S.N.** 9:00

*Theoretical Simulation of Molecular Spectra for Astrophysical and Atmospheric Applications: Cool Stars, Brown Dwarfs and Extrasolar Planets*

**L2 Frommhold L.** 9:45

*Collision-Induced Spectroscopy*

**Contributed Lectures M      Friday, 11:00**

*chairperson: Xu Y.*

**M1 Melandri S.,** 11:00

Calabrese C., Maris A., Evangelisti L., Caminati W.  
*Flexible Molecules: a Challenge for Rotational Spectroscopy and Computational Methods: The Rotational Spectra of 2-fluorobenzylamine, and Methylaminoethanol*

- M2 **Lesarri A.**, 11:15  
Cocinero E.J., Écija P., Basterretxea F.J., Grabow J.-U.,  
Fernández J.A., Castaño F.  
*Rotational Spectra of Sugars: The Six Most-Stable Conformations of Ribose*
- M3 **Doménech J.-L.**, 11:30  
Cueto M.  
*Continuous-wave Stimulated Raman Spectroscopy Inside a Hollow-core Photonic Crystal Fiber*
- M4 **Tyuterev V.**, 11:45  
Kochanov R., Tashkun S., Holka F., Szalay P.  
*New Model for Ab initio Ground Electronic State Potential Energy Surface of the Ozone Molecule and Extended Vibration Predictions*
- M5 **Vaks V.L.**, 12:00  
Pripolzin S.I., Panin A.N., Paveliev D.G.  
*High-precise Spectrometry of the Terahertz Frequency Range: Methods and Devices*
- M6 **Dhyme M.**, 12:15  
Joubert P., Populaire J.-C., Fissiaux L., Lepère M.  
*Infrared Spectroscopy of Gaseous Acetylene Mixtures from Low to High Temperatures*

**Camber Concert Session****Friday, 19:30***chairperson: Di Lonardo G.*

- Melzoch K.**—*The Rector's greeting* 19:35  
**Jensen P.**—*The Pliva's awards* 19:40  
**The String Quartet** 19:55  
*A. Dvořák: Op. 96, F-dur - "American" (The Wihan Quartet)*  
*Allegro ma non troppo - Lento - Molto vivace Finale - Vivace ma non troppo*
- The String Quintet** 20:30  
*F. Schubert: Op. 165, C-dur (The Wihan Quartet + Evžen Rattay (cello))*
- Caminatti W.**—*Stirrup-glass* 21:15

**Contributed Lectures N****Saturday, 9:00***chairperson: Caminati W*

- N1 **Surin L.**, 9:00  
Potapov A., Schlemmer S.  
*Millimeter-wave Spectrum of the OrthoH<sub>2</sub>-CO Molecular Complex: New Measurements and Assignments*
- N2 **Pitsevich G.G.**, 9:15  
Pitsevich G.A.  
*Two-dimension Study of Methanol Internal Rotation in Argon Matrix*
- N3 **Richard C.**, 9:30  
Margules L., Motiyenko R.A., Gröner P., Coudert L.H., Guillemin J.-C.  
*Spectroscopy of a Major Complex Organic Molecule: Mono-Deuterated Dimethyl Ether*
- N4 **Lee S.K.**, 9:45  
Yoon Y.W.  
*Spectroscopic Observation of Benzyl-type Radicals using a Technique of Corona Excited Supersonic Expansion*
- N5 **Du L.**, 10:00  
Kjaergaard H.G.  
*Gas Phase Infrared and Near Infrared Spectroscopy of a Medium Strength Hydrogen Bond Molecular Complex at Room Temperature*
- chairperson: Urban Š.*
- N6 **Hinde R.J.** 10:15  
*Spin-orbit Transitions of Cl and Br Dopants in Solid Parahydrogen: A Quantum Monte Carlo Study*
- N7 **Pogany A.**, 10:30  
Nwaboh J.A., Werhahn O., Ebert V.  
*Towards Traceability in CO<sub>2</sub> Spectroscopic Line Parameter Measurements using Tunable Diode Laser Absorption Spectroscopy*

- N8 **Lewerenz M.**, 10:45  
Jiang J., Mladenović M.  
*Quantum Simulations of Helium Clusters with Open Shell  
and Ionic Dopants*
- N9 **Alijah A.**, 11:00  
Mohallem J.R., Diniz L.G.  
*Core-mass Nonadiabatic Corrections to Molecules:  $H_2$ ,  $H_2^+$   
and Isotopologues*
- N10 **Daneshvar L.**, 11:15  
Buldyreva J.  
*Line Mixing Effects in  $CO_2$  Spectra Modelled by an Energy-  
Corrected Sudden Approach*