The **25th** International Conference on

High Resolution Molecular Spectroscopy

Bilbao 2018 September 3rd–7th

Bizkaia Aretoa – UPV/EHU

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25th International Conference on High Resolution Molecular Spectroscopy – Abstract Book

Bilbao 2018

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Scientific program

Monday, September 3, 2018

Morning Sessions

8:00–9:45	Registration
Main Hall	
9:45–10:30	**Opening Ceremony**
Mitxelena Auditorium	**With the presence of institutions endorsing the conference:** **Prof. Adolfo Morais Ezquerro** Vice Counselor for Research and Universities of the Basque Government **Prof. José Luis Martín González** Vice Rector for Research of the University of the Basque Country **Prof. Fernando Plazaola Muguruza** Dean of the Faculty of Science and Technology of the University of the Basque Country **Prof. Jens-Uwe Grabow** INTERNATIONAL STEERING COMMITTEE Chairman Institut für Physikalische Chemie und Elektrochemie Gottfried Wilhelm Leibniz Universität (LUH) **Prof. Alberto Lesarri** EXECUTIVE COMMITTEE Department of Physical Chemistry and Inorganic Chemistry Faculty of Sciences University of Valladolid (UVa) **Dr. Emilio J. Cocinero** LOCAL ORGANIZING COMMITTEE Department of Physical Chemistry Faculty of Science and Technology – University of the Basque Country (UPV / EHU) and Biofisika Institute (CSIC-UPV / EHU)
10:30–11:10	**Coffee Break**
Main Hall	**Sponsors Stands will be placed at Main Hall**
	Plenary Session
	Chair: **Stepan Urban**, *University of Chemistry & Technology Prague*
11:10–11:55	**Plenary Lecture 1**
Mitxelena Auditorium	PT1. Collision-induced spectra of N_2 and O_2
	Ad Van Der Avoird, *Radboud University*
11:55–12:40	**Plenary Lecture 2**
Mitxelena Auditorium	PT2. Spectroscopy of molecular radicals in Helium droplets
	Gary E. Douberly, *University of Georgia*
13:00–14:30	**Lunch Break**
	Iberdola tower (black tickets) or Deusto Library (white tickets)

Afternoon Sessions

	Oral Sessions 1		
14:30–15:50	**Oral Session A1:**	**Oral Session B1:**	**Oral Session C1:**
	Mitxelena Auditorium	**Baroja Auditorium**	**Oteiza Auditorium**
	Chair: **Vadym Ilyushyn**, *Institute of Radio Astronomy of NASU*	Chair: **Sonia Melandri**, *University of Bologna*	Chair: **Michel Mons**, *CEA Saclay*
	LARGE-AMPLITUDE MOTIONS	WATER CLUSTERS	FREQUENCY COMB AND FAST IR
14:30–14:50	A1.1. Microwave study of internal rotation in para Tolualdehyde: local versus global symmetry at the methyl-rotor site as an indicator of information transfer across the benzene ring	B1.1. Structures and dynamics of acrolein-$(H_2O)_n$ clusters revealed by MW spectroscopy and ab initio calculation	C1.1. Fast scanning IR-spectrometer to measure transient molecules in a pulsed supersonic jet
	Jon Hougen, *NIST*	**Weixing Li,** *University of Bologna*	**Daniel Witsch,** *University of Kassel*
14:50–15:10	A1.2. Effective rotational hamiltonian for two-rotor systems with symmetric and asymmetric internal rotors (like Ethanol) applied to Ethylphosphine, $CH_3CH_2PH_2$	B1.2. Discovering the conformations of formamide complexes and formamide-water clusters by microwave spectroscopy	C1.2. Wide bandwidth mid-IR spectroscopy with comb-referenced EC-QCL: application to the ν_1 fundamental band of $^{14}N_2{}^{16}O$
	Peter Groner, *University of Missouri – Kansas City*	**Susana Blanco,** *Universidad de Valladolid*	**Davide Gatti,** *IFN/CNR & Politecnico di Milano*
15:10–15:30	A1.3. Proton in a double-well potential: Acetylacetone and its derivatives by microwave spectroscopy	B1.3. Does the structure of the polycyclic aromatic hydrocarbon impact the aggregation of water on its surface? fluorene vs acenaphthene	C1.3. Endless frequency-swept comb-calibrated spectrometer
	Luca Evangelisti, *University of Bologna*	**Amanda Steber,** *The Hamburg Centre for Ultrafast Imaging*	**Thomas Puppe,** *TOPTICA Photonics AG*
15:30–15:50	A1.4. Sensing the molecular structures of alkyl methyl ketones by internal rotation in the microwave spectrum	B1.4. Characterization of microsolvated 15C5 crown ether from broadband rotational spectroscopy	C1.4. Broadband complex gas spectroscopy with sub-kHz level resolution comb spectrometer
	Maike Andresen, *IPC RWTH Aachen University*	**Juan Carlos López,** *Universidad de Valladolid*	**Grzegorz Kowzan,** *Nicolaus Copernicus University in Torun*

	Oral Session 2		
16:00–18:00	**Oral Session A2:**	**Oral Session B2:**	**Oral Session C2:**
	Mitxelena Auditorium	**Baroja Auditorium**	**Oteiza Auditorium**
	Chair: **Isabelle Kleiner**, *LISA / CNRS*	Chair: **Wen-Bih Tzeng**, *Academia Sinica*	Chair: **Donald McNaughton**, *Monash University*
	PES AND SPECTRAL INTERPRETATION	RADICALS AND IONS	SMALL MOLECULES: IR
16:00–16:20	A2.1. Empirical potential energy surface and bending angle probability densities for the electronic ground state of HCO^+	B2.1. FTMW spectroscopy of sulfur bearing free radicals, HCSC and CH_3SS	C2.1. The water vapor absorption continuum in the atmospheric windows at 4.0, 2.1, 1.6 and 1.25 μm
	Per Jensen, *University of Wuppertal*	**Yasuki Endo,** *National Chiao Tung University*	**Alain Campargue,** *CNRS/ Université de Grenoble*
16:20–16:40	A2.2. Torsion rotation program for nitromethane CH_3NO_2	B2.2. Millimeter-wave spectroscopy of the HDCCH radical	C2.2. Sub-MHz deuterium spectroscopy and comparison with ab initio calculations of the line-shape effects
	Marek Kręglewski, *Adam Mickiewicz University in Poznań*	**Keiichi Tanaka,** *Kyushu University*	**Mikolaj Zaborowski,** *Nicolaus Copernicus University in Toruń*
16:40–17:00	A2.3. Weak intramolecular interaction effects on the structure and torsional spectra of ethylene glycol isotopologues, an astrophysical species	B2.3. Accurate rotational fingerprints of radioactive radicals by mass-independent studies on AlO, TiO, and FeO	C2.3. The high-resolution spectrum of DC_3N recorded in the infrared and millimeter-wave regions: a global analysis
	María Luisa Senent, *CSIC*	**Alexander Breier,** *Universität Kassel*	**Filippo Tamassia,** *University of Bologna*
17:00–17:20	A2.4. Modelling temperature dependent anharmonic spectra of pyrene ($C_{16}H_{10}$): comparison of computational approaches	B2.4. Accurate sub-millimeter rest-frequencies for HCCO and DCCO radicals	C2.4. Sub-doppler metrology of HD
	Shubhadip Chakraborty, *Institut de Recherche en Astrophysique et Planetologie*	**Johanna Chantzos,** *Max Planck Institut for extraterrestrial Physics*	**Patrick Dupré,** *Laboratoire de Physico-Chimie de l'Atmosphère*
17:20–17:40	A2.5. Non-adiabatic coupling in the ozone molecule	B2.5. Terahertz spectroscopy of isotopologues of amidogen radical	C2.5. IR laser spectroscopy of the deuterated isotopologues of ammonia
	Alexander Alijah, *University of Reims*	**Mattia Melosso,** *Università di Bologna*	**Patrice Cacciani,** *Université Lille /CNRS*
17:40–18:00	A2.6. The long-range behavior of ab initio transition dipole moments and spin-orbit coupling matrix elements between the low-lying electronic states of alkali heterodimers	B2.6. Accurate rotational frequencies of deuterated Ammonium ions (d_1–d_3) measured in a cryogenic ion trap.	C2.6. Photoacoustic spectroscopy of the oxygen a-band in support of OCO-2
	Ekaterina Bormotova, *Moscow State University*	**José Luis Doménech,** *Instituto de Estructura de la Materia CSIC*	**Elizabeth Lunny,** *California Institute of Technology*
18:00–20:00 Menchu Gal Terrace	**Welcome Cocktail With representatives of the City Council of Bilbao**		

Tuesday, September 4, 2018

Morning Sessions

	Plenary Session		
	Chair: **Marek Kręglewski**, *Adam Mickiewicz University in Poznań*		
9:00–9:45	**Plenary Lecture 3**		
Mitxelena Auditorium	PT3. Beryllium bonding probed by anion photodetachment spectroscopy		
	Michael Heaven, *Emory University*		
9:45–10:30	**Plenary Lecture 4**		
Mitxelena Auditorium	PT4. Which spectroscopy to study astro-PAHs?		
	Christine Joblin, *IRAP – Université de Toulouse*		
10:30–11:00	**Coffee Break**		
Main Hall	Sponsors Stands will be placed at Main Hall		
	Oral Sessions 3		
11:00–12:40	**Oral Session A3:**	**Oral Session B3:**	**Oral Session C3:**
	Mitxelena Auditorium	**Baroja Auditorium**	**Oteiza Auditorium**
	Chair: **Per Jensen**, *University of Wuppertal*	Chair: **José A. Fernández,** *Universidad País Vasco UPV/EHU*	Chair: **Robert Gamache**, *University of Massachusetts Lowell*
	LARGE-AMPLITUDE MOTIONS	LIF AND REMPI	INTERMEDIATES, CHIRALITY AND BIOMOLECULES
11:00–11:20	A3.1. Spin-torsion dominated hyperfine splittings in the first excited torsional state ($v_t = 1$) of Methanol	B3.1. High resolution Rydberg spectroscopy of 3d metal sandwich compounds: ultrasensitive probing the electron density changes in organometallic molecules	C3.1. Local interactions of the asparagine and histidine aminoacids in a protein chain: gas phase conformer-selective IR spectroscopy of model molecules
	Li-Hong Xu, *University of New Brunswick*	**Sergey Ketkov,** *G.A. Razuvaev Institute of Organometallic Chemistry RAS*	**Michel Mons,** *CEA Saclay*
11:20–11:40	A3.2. Extension of the normal mode approach to nonrigid polyatomic molecules	B3.2. Two-color REMPI [(1+1')+1] of the singlet oxygen $^1O_2$ arising in UV-photodissociation of van der Waals complex C_5H_8–O_2	C3.2. Water sculpts the distinctive shapes and dynamics of the Tn antigens: implications for their molecular recognition
	Dominika Viglaska, *University of Reims*	**Alexandr Bogomolov,** *Voevodsky Institute of Chemical Kinetics and Combustion*	**Aran Insausti,** *Universidad del País Vasco (UPV/EHU)*
11:40–12:00	A3.3. Essentially free internal rotation of the Propynyl Methyl group investigated by microwave spectroscopy	B3.3. The vibrational structure of the NO_3 X $^2A_2'$ state studied by SVL DF spectrum	C3.3. Testing the parity symmetry in cold chiral molecules using vibrational spectroscopy
	Konrad Eibl, *IPC RWTH Aachen University*	**Masaru Fukushima,** *Hiroshima City University*	**Anne Cournol,** *Université Sorbonne Paris Cité*

12:00–12:20	A3.4. Microwave spectroscopic and quantum chemical studies of the coupled large amplitude motions in S-Phenyl Thioacetate	B3.4. Line shape study of oxygen B-band with CRDS in Dual-Beam configuration	C3.4. Hydrated Lewis antigens in the gas phase: building up the environment or peeling off the solvent?
	Lynn Ferres, *IPC RWTH Aachen University*	**Katarzyna Bielska,** *Nicolaus Copernicus University in Torun*	**Pierre Carçabal,** *Institut des Sciences Moléculaires d'Orsay CNRS*
12:20–12:40	A3.5. Separately fitting the torsional symmetry species of molecules with one or multiple internal rotor(s)	B3.5. LIF Spectrum of a $^1\Sigma$ species containing Si: linear SiOSi ?	C3.5. High-resolution ro-vibrational spectrum of the simplest Criegee intermediate CH_2OO between 880 and 932 cm^{-1}
	Lam Nguyen, *Laboratoire LISA*	**Masaru Fukushima,** *Hiroshima City University*	**Pei-Ling Luo,** *Institute of Atomic and Molecular Sciences Academia Sinica*
13:00–14:30	**Lunch Break**		
	Iberdrola tower (black tickets) or Deusto Library (white tickets)		

Afternoon Sessions

	Oral Session 4		
14:30–15:50	**Oral Session A4:**	**Oral Session B4:**	**Oral Session C4:**
	Mitxelena Auditorium	**Baroja Auditorium**	**Oteiza Auditorium**
	Chair: **Filippo Tamassia**, *University of Bologna*	Chair: **Leonid Surin**, *Institute of Spectroscopy RAS*	Chair: **A. Robert McKellar**, *National Research Council of Canada*
	SMALL MOLECULES: IR	LARGE MOLECULES: MW	LINE SHAPES AND INTENSITIES
14:30–14:50	A4.1. Investigation of the ν_8 and ν_{21} bands of propane $CH_3CH_2CH_3$ at 11.5 and 10.9 µm: evidence of large amplitude tunnelling effects	B4.1. On not yet solved problems concerning some molecular systems investigated by rotational spectroscopy along my research life	C4.1. On the temperature dependence of half-widths and line shifts for molecular transitions in the microwave and infrared regions
	Agnes Perrin, *Laboratoire de Meteorologie Dynamique*	**Walther Caminati,** *University of Bologna*	**Robert Gamache,** *University of Massachusetts Lowell*
14:50–15:10	A4.2. High resolution FTIR study of the ν_6 band of CH_2F_2 in 3 µm spectral region at low temperatures	B4.2. Rotational spectrum and molecular structure of succinic anhydride aided by computational calculations	C4.2. Calculation of half widths and line shifts of H_2O-N_2 collision system using the modified complex Robert-Bonamy formalism
	Chilukoti Ashok, *Homi Bhabha National Institute*	**Donald McNaughton,** *Monash University*	**Bastien Vispoel,** *University of Massachusetts Lowell*
15:10–15:30	A4.3. The NH_2 scissors band of Methylamine	B4.3. Pursuing the rotational spectra of large molecular systems	C4.3. High accuracy ab initio DMS and extra high accuracy PES for sub-percent calculation of line intensities
	Iwona Gulaczyk, *Adam Mickiewicz University in Poznań*	**Iker León,** *Universidad de Valladolid*	**Oleg Polyansky,** *UCL*

15:30–15:50	A4.4. Wrong distance – wrong line strength – wrong concentrations	B4.4. Exploring the generation of new species using laser ablation Fourier transform microwave spectroscopy techniques: the study of N-carbamoyl glycine	C4.4. Line shape parameters from first principles: investigation of the S and O branches in the H_2–He system
	Tom Moses Rubin, *PTB*	**Lucie Kolesniková,** *Universidad de Valladolid*	**Hubert Jóźwiak,** *Nicolaus Copernicus University*
16:00–18:30 Axular Room and Chillida Room	**Poster Session 1 (P1.1. to P1.64.) and Coffee Break**		
18:30–20:30 Meeting point: Main Hall of Bizkaia Aretoa	**City Tour**		

Poster presentations – Session 1

P1.1. DFT and TD DFT modeling of vibrational structures in high resolution MATI and REMPI spectra of chromium bisarene complexes

Sergey Ketkov; Sheng-Yuan Tzeng; Elena Rychagova; Grigory Zhigulin; Wen-Bih Tzeng

P1.2. Vibronic emission spectroscopy of o-Ethynylbenzyl radical generated from corona discharge of o-Ethynyltoluene

Sang Kuk Lee

P1.3. High resolution study of CH_2=CD_2 molecule: line intensities and half-widths

Kirill Berezkin; Elena Bekhtereva; Olga Gromova; Oleg Ulenikov; Claude Leroy; Christian Sydow; Sigurd Bauerecker

P1.4. The classification of lung cancers and their degree of malignancy by FTIR, PCA-LDA analysis, and a physics-based computational model

Joanna Depciuch; Ewa Kaznowska; Kornelia Łach; Magdalena Kołodziej; Anna Koziorowska; Jitraporn Vongsvivut; Izabela Zawlik; Marian Cholewa; Jozef Cebulski

P1.5. Spectroscopy group at the University of the Basque Country

Camilla Calabrese, Aran Insausti; Maider Parra; Cristóbal Pérez; Iciar Uriarte ; Imanol Usabiaga; Emilio J. Cocinero; Francisco J. Basterretxea

P1.6. Spectroscopic characterization of the unsaturated Hydrocabons C_3H and C_5H using highly correlated ab initio methods

Maria Luisa Senent; Sara Cherifa Bennedjai; Dalila Hammoutenne

P1.7. Broadening and shifting coefficients of rovibrational lines of HCl perturbed by He in the fundamental and the first overtone regions

Ruslan Asfin; Alexandra V. Domanskaya; Gang Li; Volker Ebert

P1.8. Predissociation of the B state of S_2: measurements and modeling

Glenn Stark; Brenton Lewis; Stephen Gibson; Hannah Herde; Alan Heays; James Lyons; Nelson de Oliveira; Gillian Nave

P1.9. Resonant two-photon ionization and mass-analyzed threshold Ionization spectroscopy of 2,4-Difluoroanisole

Wen-Bih Tzeng; Shen-Yuan Tzeng

P1.10. High precision spectrum of the second overtone of $^{12}C^{16}O$

Jin Wang; Yu Sun; Anwen Liu; Shuiming Hu

P1.11. CO_2–broadening and shift coefficients in the ν_3 and $\nu_2+(\nu_4+\nu_5)^0$ bands of acetylene

Valerii Perevalov; O.M. Lyulin; T.M. Petrova; A.M. Solodov; A.A. Solodov

P1.12. The ab initio line–shape calculations for purely rotational transitions in the CO–N_2 system

Hubert Jóźwiak; Hubert Cybulski; Franck Thibault; Nikodem Stolarczyk; Piotr Wcisło

P1.13. Spectroscopic study of the $7^1\Pi_u$ and $7^1\Sigma^+_u$ states of Rb_2 molecule

Pawel Kowalczyk; Wlodzimierz Jastrzebski; Anna Grochola; Katarzyna Olkowska; Jacek Szczepkowski

P1.14. The $^{12}CH_4$ and $^{13}CH_4$ absorption spectra at 296 K and 200 K in the range between 6600 and 12000 cm^{-1}

Leonid Sinitsa

P1.15. Study of hydrates of verbenone by microwave Fourier transform spectroscopy and computational chemistry

Pascal Dréan; Mhamad Chrayteh; Annunziata Savoia;Thérèse R. Huet

P1.16. Study of the H_2O–N_2 line broadening and shifting in the region of 16500–17000 cm^{-1}

Leonid Sinitsa; Victor Serdyukov; Nina Lavrentieva; Anna Dudaryonok

P1.17. Rotational–predissociation double resonance spectroscopy of the He–HCO^+ complex

Oskar Asvany; Thomas Salomon; Matthias Töpfer; Phillip Schreier; Stephan Schlemmer; Hiroshi Kohguchi; Leonid Surin

P1.18. Combined PGOPHER analysis of bands in the 1st positive system of N_2, 4500 — 15500 cm^{-1}

Amanda Ross; Patrick Crozet; Jérôme Morville; Colin Western; Dennis Tokaryk

P1.19. Properties of HF@C_{60} endofullerene from first principles

Yulia Kalugina; Pierre–Nicholas Roy

P1.20. High sensitivity Cavity Ring Down Spectroscopy spectroscopy of the $\nu_1+4\nu_3$ band of NO_2 near 1.34 μm

Anastasiia Lukashevskaya; Didier Mondelain; Alain Campargue; Valerii Perevalov

P1.21. Laser absorption spectroscopy of methane at 1000 K between 1.75 and 1.3 μm

Alain Campargue; Semyon Vasilchenko; Mélanie Ghysels; Didier Mondelain; Samir Kassi; Solenne Barry

P1.22. Double resonance rotational spectroscopy of CH_3^+ – He

Matthias Töpfer; Thomas Salomon; Stephan Schlemmer; Oskar Asvany; Otto Dopfer; Hiroshi Kohguch; Koichi M. T.

P1.23. The absorption band of nitrogen dioxide ($^{14}N^{16}O_2$) by CRDS near 6000 cm^{-1}

Anastasiia Lukashevskaya; Olga Naumenko;; Samir Kassi; Alain Campargue

P1.24. Isolated small–amplitude fundamental embedded in a pure torsional bath: assignment and fit of the FIR and microwave spectra of the ν_{10} vibrational state of acetaldehyde

Vadym Ilyushyn; Eugene Alekseev; Olga Dorovskaya; Laurent Margulès; Roman Motiyenko; Manuel Goubet; Olivier Pirali; Sigurd Bauerecker; Christof Maul; Christian Sydow; Georg Mellau; Isabelle Kleiner; Jon T. Hougen

P1.25. The high resolution spectrum of $^{14}ND_3$ in the far–infrared

Elisabetta Cane; Gianfranco Di Lonardo; Luciano Fusina; Adriana Predoi–Cross; Filippo Tamassia

P1.26. Line positions and intensities for the ν_3 band of 5 isotopologues of germane for planetary applications

Vincent Boudon; Tigran Grigoryan; Florian Philipot; Fridolin Kwabia Tchana; Laurent Manceron; Athéna Rizopoulos; Jean Vander Auwera; Thérèse Encrenaz

P1.27. The third and fourth torsional states of acetic acid

Vadym Ilyushyn; Olga Dorovskaya; Eugene Alekseev

P1.28. First detection of $H_2{}^{36}S$ in the infrared region

Valeriya A. Zamotaeva; Elena S. Bekhtereva; Olga V. Gromova; Oleg N. Ulenikov; Claude Leroy; Christian Sydow; Sigurd Bauerecker

P1.29. New electronic states in the spectra of TaH and TaD

Thomas Varberg; Samuel Gleason; Dalir Kellett; Paul Reischmann

P1.30. Accurate first principles global calculations and isotopic effects on infrared spectra for phosphine PH_3 and hydrocarbons (CH_4 ,C_2H_4)

Vladimir Tyuterev; Dominika Viglaska; Michael Rey; Andrey Nikitin; Eveniya Starikova

P1.31. Vibrational dependence and prediction of line shape parameters for the H_2O–H_2 collisional system

Robert Gamache; Bastien Vispoel

P1.32. Ab initio reduced matrix elements for $H_2{}^{16}O$: application to H_2O–H_2 line shape calculations via the modified complex Robert–Bonamy method

Bastien Vispoel; Robert Gamache

P1.33. Classical trajectory simulation of collision–induced absorption spectra

Daniil N. Chistikov; Artem A. Finenko; Yulia N. Kalugina; Sergei E. Lokshtanov; Sergey V. Petrov; Andrey A. Vigasin

P1.34. Atlas of experimental and theoretical high–temperature methane cross–sections from T=296 K to 1000 K in the mid–infrared range

Vladimir Tyuterev; Andy Wong; Peter Bernath; Michael Rey; Andrey Nikitin

P1.35. High–resolution laser spectroscopy of nitrogen dioxide in the region of 14500–16800 cm^{-1}

Shunji Kasahara; Takumi Yoshizawa; Michihiro Hirata; Kohei Tada

P1.36. Modified complex Robert–Bonamy calculations including line coupling on the H_2O–N_2 and CO_2–N_2 molecular systems

Bastien Vispoel; Richard Lynch; Robert Gamache

P1.37. Temperature dependence of line broadening coefficient of chloromethane diluted in carbon dioxide

Sylvain Léonis; Muriel Lepere

P1.38. A room–temperature HCN line list with a new dipole moment surface

Vladimir Makhnev; Aleksandra Kyuberis; Oleg Polyansky; Irina Mizus; Jonathan Tennyson; Nikolay Zobov

P1.39. Quantum chemical characterisation of difluorine peroxide FOOF

Olfa Ferchichi

P1.40. On the consistency of absolute ozone intensities in MW, 10 and 5 micron ranges from ab initio predictions and laboratory observations

Vladimir Tyuterev; Alain Barbe; Semen Mikhailenko; Evgeniya Starikova

P1.41. Rotational and vibrational dependences of line half–widths for CO confined in silica aerogel

Alexander A. Solodov; Tatyana M. Petrova; Yuriy N. Ponomarev; Alexander M. Solodov

P1.42. Measurements and calculations of H_2– broadening and shift parameters of water vapor transitions in 6700—9000 cm^{-1} spectral region

Tatyana M. Petrova; Alexander M. Solodov; Alexander A. Solodov; Vladimir. M. Deichuli; Vitaly. I. Starikov

P1.43. The use of spectral moments to simulate rototranslational collision–induced bandshapes

Sergei Lokshtanov; Daniil Chistikov; Artem Finenko; Yulia Kalugina; Sergey Petrov; Andrey Vigasin

P1.44. The high resolution far infrared spectrum of ^{18}O enriched water vapor at the SOLEIL synchrotron

Mikhail Tretyakov; Semen Mikhailenko; Tatiana Odintsova; Olivier Pirali; Pascale Roy; Alain Campargue

P1.45. Global depetrubation treatment of $5^1\Sigma^+_u$ and $5^1\Pi_u$ states in Rb_2

Asen Pashov; Anna Grochola; Jacek Szczepkowski; Pawel Kowalczyk; Wlodzimierz Jastrzebski

P1.46. Revealing the multiple structures of Glutamine

Iker León; Elena Rita Alonso; Carlos Cabezas; Santiago Mata; José Luis Alonso

P1.47. Linear Rayleigh and Raman scattering to second order

Robert Cameron; Neel Mackinnon

P1.48. The CRDS spectrum of natural and ^{13}C enriched carbon dioxide in the 1.73 μm window

Ekaterina Karlovets; Anna Sidorenko; Peter Čermák; Didier Mondelain; Samir Kassi; Valery Perevalov; Alain Campargue

P1.49. Rotational spectroscopy of organophosphorus chemical agents: Cresyl and Phenyl Saligenin Phosphate

Marcos Juanes San Jose; Rizalina T. Saragi; José L. Abad; Alberto Lesarri; Ruth Pinacho; José E. Rubio

P1.50. FTIR laboratory measurement of O I spectra in the 0.77–12.5 μm spectral range: Rydberg states and oscillator strengths

Vladislav E. Chernov; Svatopluk Civiš; Petr Kubelík; Adam Pastorek; Ekaterina Zanozina; Vladislav Chernov; Alexander Naskidashvili

P1.51. Structural determination of aroma molecules in the gas-phase

Rihab Hakiri

P1.52. High resolution study of the strongly interacting $\nu_3(F_2)/\nu_1(A_1)$ bands of $^{28}SiD_4$

Natalia I. Raspopova; Olga V. Gromova; Elena S. Bekhtereva; Sigurd Bauerecker; Christian Sydow; Oleg N. Ulenikov

P1.53. Molecular spectroscopy using radio-acoustic detection and high power radiation in THz region

Mikhail Tretyakov; German Golubiatnikov; Maxim Koshelev; Alexander Tsvetkov; Andrey Fokin; Mikhail Glyavin

P1.54. Temperature dependence of collisional parameters of water 183-GHz line

Mikhail Tretyakov; Maxim Koshelev; Ilya Vilkov

P1.55. Production of theoretical line lists for polyatomic molecules: SiH_4, C_2H_4, CH_3Cl, CH_3F, C_2H_2, NH_3, OH_3^+, P_2H_2

Sergei N. Yurchenko; Jonathan Tennyson; Barry P. Mant; Alec Owens; Phillip Coles; Andrey Yachmenev; Alexander Fateev; Vladlen Melnikov

P1.56. Indole rotational spectra

Karel Vávra; Kateřina Luková; Jan Koucký; Patrik Kania; Štěpán Urban

P1.57. The visible spectrum of AlD^+: the experimental and theoretical treatment

Rafal Hakalla; Wojciech Szajna; Keith Moore; Ian Lane; Malgorzata Ostrowska-Kopec; Izabela Piotrowska; Przemyslaw Kolek; Miroslaw Zachwieja; Ryszard Kepa

P1.58. High-resolution Fourier-transform spectroscopy of the comet-tail system in the $^{12}C^{17}O^+$ ion

Rafal Hakalla; Izabela Piotrowska; Malgorzata Ostrowska-Kopec; Wojciech Szajna; Przemyslaw Kolek; Marcin Rusznica; Miroslaw Zachwieja; Ryszard Kepa

P1.59. Self-broadening coefficients of rotational transitions of H_2S measured by submillimeter-wave spectroscopy

Meriem Mouelhi; François Rohart; Francis Hindle; Cédric Bray; Gaël Mouret; Robin Bocquet; Hassen Aroui; Arnaud Cuisset

P1.60. Photodissociation dynamics of CF_2I_2 in solution

Manho Lim

P1.61. Influence of the epigenetics marks in the non-covalent interactions between amino acids and DNA

Rodrigo Martínez, José A. Fernández, Judith Millán

P1.62. Investigation on the degree of dissociation of Hydrogen plasma in PIG ion source via optical emission spectroscopy

Seyed Shahab Odin Salimi, Masoud Mahjour Shafiei, Masoomeh Yarmohammadi Satri

P1.63. The optimal origin for computation of wave functions of polar molecules

Anastasiia Chervinskaia, Dmitriy Dorofeev, Sergey Elfimov

P1.64. 300 GHz Laboratory Heterodyne Emission Spectrometer

Jakob Maßen, Nadine Wehres, Bettina Heyne, Kirill Borisov, Katharina von Schoeler, Frank Lewen, Matthias Töpfer, Bernhard Schmidt, Henning Adams, Urs Graf, Netty Honingh, Stephan Schlemmer

Wednesday, September 5, 2018

Morning Sessions

	Plenary Session		
	Chair: **Agnes Perrin**, *Laboratoire de Meteorologie Dynamique*		
9:00–9:45	**Plenary Lecture 5**		
Mitxelena Auditorium	PT5. Spectroscopy for satellite remote sensing of greenhouse gases: recent advances and outstanding challenges		
	Vivienne Payne, *Jet Propulsion Laboratory – NASA*		
9:45–10:30	**Plenary Lecture 6**		
Mitxelena Auditorium	PT6. Odorants and broadband rotational spectroscopy: what can we learn?		
	Maria E. Sainz, *King's College London*		
10:30–11:00	**Coffee Break**		
Main Hall	**Sponsors Stands will be placed at Main Hall**		
	Oral Sessions 5		
11:00–12:40	**Oral Session A5:**	**Oral Session B5:**	**Oral Session C5:**
	Mitxelena Auditorium	**Baroja Auditorium**	**Oteiza Auditorium**
	Chair: **Vladimir Tyuterev**, *University of Reims*	Chair: **Mikhail Tretyakov**, Institute of Applied Physics –RAS	Chair: **Sang Kuk Lee**, *Pusan National University*
	SPECTRAL SIMULATION AND DATABASES	LARGE MOLECULES: MW	NITROGEN AND WATER CLUSTERS
11:00–11:20	A5.1. Spectroscopic databases for the VAMDC and dat@osu portals	B5.1. High-resolution rotational spectroscopy of 3-Methylbutyronitrile – a molecule of astrophysical interest	C5.1. Microwave spectrum and nuclear quadrupole structure analysis of the NH_3–N_2 van der Waals complex
	Vincent Boudon, *Univ. Bourgogne Franche-Comté*	**Nadine Wehres,** *University of Cologne*	**Leonid Surin,** *Institute of Spectroscopy RAS*
11:20–11:40	A5.2. Computing spectra of open-shell diatomic molecules with duo	B5.2. Solving discrepancies between theory and experiment: Methyl Jasmonate and Zingerone	C5.2. New millimeter-wave study of the CO–N_2 van der Waals complex
	Sergey Yurchenko, *University College London*	**Isabelle Kleiner,** *LISA / CNRS*	**Ivan Tarabukin,** *Insitute of Spectroscopy RAS*
11:40–12:00	A5.3. Accurate CO_2 Raman spectral simulation: an algebraic alternative based on anharmonic ladder operators	B5.3. Polyalcohols as artificial sweeteners: signs of a sweetness-structure connection	C5.3. Microsolvation of ethyl carbamate conformers: a rotational spectroscopy study
	Miguel Carvajal, *Universidad de Huelva*	**Elena R. Alonso**, *Universidad de Valladolid*	**Pablo Pinacho,** *Universidad de Valladolid*
12:00–12:20	A5.4. Chiral rotational spectroscopy	B5.4. Microwave spectroscopic and quantum chemical investigations on 2-Acetylthiophene	C5.4. Study of the molecular structure and microsolvation (H_2O N=1-3) of 2-Phenylpyridine by rotational spectroscopy
	Jörg B. Götte, *University of Glasgow*	**Christina Dindic,** *IPC RWTH Aachen University*	**Alberto Macario,** *Universidad de Valladolid*

12:20–12:40	A5.5. Proton transfer tunneling splittings and the imaginary mode Hamiltonian: the beginning of a beautiful friendship	B5.5. Structure and rotational spectral features of N-Butyraldehyde oxime: a study using MB-FTMW	C5.5. Structures of the complexes of Cyclooctanone with water
	Antonio Fernández-Ramos, *Universidade de Santiago de Compostela*	**Nobuhiko Kuze,** *Sophia University*	**Ecaterina Burevschi,** *King's College London*
13:00–14:30	**Lunch Break**		
	Iberdola tower (black tickets) or Deusto Library (white tickets)		

Afternoon Sessions

	Oral Session 6		
14:30–15:50	**Oral Session A6:**	**Oral Session B6:**	**Oral Session C6:**
	Mitxelena Auditorium	**Baroja Auditorium**	**Oteiza Auditorium**
	Chair: **Nobuhiko Kuze**, *Sophia University*	Chair: **Masaru Fukushima**, *Hiroshima City University*	Chair: **Bruno Martínez-Haya**, *Universidad Pablo de Olavide*
	MOLECULAR STRUCTURE	CHIRPED-PULSED, LAMB-DIP AND IMAGING	CLUSTERS: IR
14:30–14:50	A6.1. Microwave spectrum and equilibrium structure of Diphenyl Disulfide	B6.1. Precise lamb-dip studies of monodeuterated Methanol	C6.1. Infrared spectrum and intermolecular potential energy surface of the CO-O_2 dimer
	Jean Demaison, *University of Ulm*	**Alexander Lapinov,** *Institute of Applied Physics of the RAS*	**Andrew R. McKellar,** *National Research Council of Canada*
14:50–15:10	A6.2. Semi-experimental structure of vinyl acetate determined by microwave spectroscopy and ab initio methods	B6.2. State-to-state rotational rate coefficients for NH_3-NH_3 collisions obtained with pump-probe chirped-pulse experiments	C6.2. Production and study of ionic clusters by photodissociation spectroscopy
	Stefanie Genuit, *Leibniz Universität Hannover*	**Christian Endres,** *MPI for Extraterrestrial Physics*	**Raghed Bejjani,** *Université catholique de Louvain*
15:10–15:30	A6.3. Pure rotational spectrum of $^{(15)}ND$ and isotopic-independent Dunham-type analysis of imidogen radical	B6.3. Chirped-pulse millimetre-wave spectrometer for the 140–180 GHz region	C6.3. Unravelling non-covalent interactions in DNA-base ··· Xanthine clusters
	Luca Bizzocchi, *Max-Plank-Institut für extraterrestrische Physik*	**Clément Lauzin,** *Université catholique de Louvain*	**Ander Camiruaga,** *Universidad del País Vasco (UPV/EHU)*
15:30–15:50	A6.4. Rotational spectroscopy of the two higher energy conformers of 2-cyanobutane	B6.4.Wave-packet imaging spectroscopy of the nitrogen dimer	C6.4. High-resolution spectroscopic study of the water-carbon dioxide van der Waals complex in the near-infrared range
	Marius Hermanns, *University of Cologne*	**Yasuhiro Ohshima,** *Tokyo Institute of Technology*	**Clément Lauzin,** *Université catholique de Louvain*
17:00–19:00	**XXV Jubilee Session – Guggenheim Museum** **Joyful Pursuit of Molecular Dynamics and Spectra** **Dudley R. Herschbach,** *Harvard University*		
19:00–20:00	**Optional Guggenheim Museum Visit (reduced admittance fee)**		

Thursday, September 6, 2018

Morning Sessions

	Plenary Session		
	Chair: **Leonid Sinitsa**, Zuev Institute of Atmospheric Optics – RAS		
9:00–9:45	**Plenary Lecture 7**		
Mitxelena Auditorium	PT7. Correlated rotational alignment spectroscopy: high-resolution, absolute frequency spectroscopy in the time domain		
	Thomas Schultz, *Ulsan National Institute Standards and Technology*		
9:45–10:30	**Plenary Lecture 8**		
Mitxelena Auditorium	PT8. Space exploration of Venus, Mars and beyond using (relatively) high resolution spectroscopy		
	Ann Carine Vandaele, *Royal Belgian Institute for Space Aeronomy*		
10:30–11:00	**Coffee Break**		
Main Hall	**Sponsors Stands will be placed at Main Hall**		
	Oral Sessions 7		
11:00–12:40	**Oral Session A7:**	**Oral Session B7:**	**Oral Session C7:**
	Mitxelena Auditorium	**Baroja Auditorium**	**Oteiza Auditorium**
	Chair: **Vincent Boudon**, *ICB Bourgogne – CNRS*	Chair: **Qian Gou**, *Chongqing University*	Chair: **Tom Varberg**, *Macalester College*
	SPECTRAL MODELLING	HOMOCLUSTERS	CALIBRATION, DATABASES AND SOFTWARE
11:00–11:20	A7.1. Universal behaviour of diatomic halo states and mass sensitivities of their properties	B7.1. Observation of two dimers of phenyl ethyl alcohol using rotational spectroscopy	C7.1. Application of molecular spectroscopic databases for certification of calibration gas mixtures
	Vladimir Spirko, *Academy of Sciences of the Czech Republic*	**Rizalina T. Saragi,** *Universidad de Valladolid*	**Vitaly Beloborodov,** *D.I.Mendeleyev Institute for Metrology*
11:20–11:40	A7.2. High energy states of polyatomic molecules: application to hot spectra	B7.2. Self-aggregation process in CH_2F_2: large homoclusters studied by rotational spectroscopy	C7.2. Comb-calibrated coherent Raman spectroscopy of molecular hydrogen
	Vladimir Tyuterev, *University of Reims*	**Camilla Calabrese,** *Universidad del País Vasco (UPV/EHU)*	**Davide Gatti,** *IFN/CNR & Politecnico di Milano*
11:40–12:00	A7.3. Absolute vibrational assignment from fragmentary spectroscopic data in two isotopologues	B7.3. The nitrogen–nitrogen noncovalent interaction in the gas phase	C7.3. Design and fabrication of a high-resolution Fourier-transform spectrometer with a supercontinuum laser source
	Asen Pashov, *Sofia University St. Kliment Ohridski*	**Lorenzo Spada,** *Scuola Normale Superiore*	**Clément Lauzin,** *Université catholique de Louvain*

12:00–12:20	A7.4. Atmospheric oxygen mm-absorption: models review and uncertainties evaluation	B7.4. Understanding structural similarities in the Homodimers of Fluorene, Dibenzofuran and Diphenylether via broadband rotational spectroscopy	C7.4. Line intensities for the ν_6 and $2\nu_3$ bands of Methyl Iodide ($^{12}CH_3I$)
	Dmitriy Makarov, *Institute of Applies Physics*	**Mariyam Fatima,** *Deutsches Elektronen-Sychrotron*	**Agnes Perrin,** *Laboratoire de Meteorologie Dynamique*
12:20–12:40	A7.5. Anharmonic IR spectra of chemical warfare agents from ab initio molecular dynamics simulations	B7.5. Investigation of the products of thermal self-polymerization of Methyl methacrylate by means of microwave spectroscopy – the rotational spectrum of the dimer	C7.5. Automatic assignment and fitting of spectra with PGOPHER
	Pawel Rodziewicz, *University of Bialystok*	**Sven Herbers,** *Leibniz Universität Hannover*	**Colin Western,** *University of Bristol*
13:00–14:30	**Lunch Break**		
	Iberdola tower (black tickets) or Deusto Library (white tickets)		

Afternoon Sessions

	Oral Session 8		
14:30–15:50	**Oral Session A8:**	**Oral Session B8:**	**Oral Session C8:**
	Mitxelena Auditorium	**Baroja Auditorium**	**Oteiza Auditorium**
	Chair: **Pierre Carçabal**, *Institut des Sciences Moléculaires d'Orsay CNRS*	Chair: **Dennis W. Tokaryk**, *University New Brunswick*	Chair: **José Luis Doménech**, *Instituto de Estructura de la Materia CSIC*
	MATRIX AND CONDENSED PHASES	CAVITY RING-DOWN	CLUSTERS: IR
14:30–14:50	A8.1. Does one need a high resolution in matrix isolation studies? the symmetry changes of the $^{28}SiH_4$ molecule in low-temperature matrixes	B8.1. Wavelength-meter controlled cavity ring-down spectroscopy for measurement of trace water vapor at ppt levels	C8.1. High resolution infrared laser jet-cooled spectroscopy of small van der Waals clusters with rare gases
	Ruslan Asfin, *Saint Petersburg State University*	**Hisashi Abe,** *National Metrology Institute of Japan (NMIJ)*	**Pierre Asselin,** *CNRS*
14:50–15:10	A8.2. Gas to solid phase transition of theobromine: crystal vs amorphous structures	B8.2. CRDS of the collision induced absorption (CIA) band of O_2 at 1.27 µm	C8.2. Insights into the binding of protons, cations and anions by azamacrocycles
	Imanol Usabiaga, *Università di Bologna*	**Alain Campargue,** *CNRS/ Université de Grenoble*	**Bruno Martinez-Haya,** *Universidad Pablo de Olavide*
15:10–15:30	A8.3. Seeing more does not necessarily mean seeing clearly	B8.3. Cavity-enhanced dispersion spectroscopy for the highest accuracy applications	C8.3. Infrared spectroscopy and quantum-chemical calculations on diacetylene complexes: a joint experimental study and theoretical investigation on OCS-H_2C_4 and N_2O-H_2C_4 dimers
	Ilya Shenderovich, *University of Regensburg*	**Daniel Lisak,** *Nicolaus Copernicus University*	**Andrea Pietropolli,** Universita' Ca' Foscari Venezia – Dipartimento Scienze Molecolari e Nanosistemi

15:30–15:50	A8.4. Titania– and montmorillonite– photocatalyzed synthesis of methane from carbon dioxide and the subsequent formation of nucleobases on early Mars and Earth	B8.4. H_2–He scattering states observation with cavity ring–down spectroscopy	C8.4. Infrared spectra of the carbon monoxide – water dimer and larger clusters
	Svatopluk Civiš, *J. Heyrovsky Institute of Physical Chemistry*	**Magdalena Konefał,** *Nicolaus Copernicus University in Toruń*	**N. Moazzen–Ahmadi,** *University of Calgary*
16:00–18:30 Axular Room and Chillida Room	**Poster Session 2 (P2.1. a P2.63.) and Coffee Break**		
19:00 –20:00 Meeting point: Maritime Museum, 7 pm	**Boat Tour**		

Poster presentations – Session 2

P2.1. The Rotational study of vitamin B6 form pyridoxine

Elena Rita Alonso; Iker León; Lucie Kolesniková; Santiago Mata; José L. Alonso

P2.2. Rotational spectrum of Methoxy Acetaldehyde: a combined CP–FTMW and millimeter wave study

Lucie Kolesniková; Isabel Peña; Elena R. Alonso; Belén Tercero; José Cernicharo; Santiago Mata; José L. Alonso

P2.3. Conformational study of Cyclooctanone using broadband rotational spectroscopy

Ecaterina Burevschi; Isabel Peña; Maria Eugenia Sanz

P2.4. The monohydrate and dimer of Phenyl Ethyl Mercaptan by rotational spectroscopy

Rizalina Tama Saragi; Marcos Juanes; Alberto Lesarri; Ruth Pinacho; José E. Rubio

P2.5. Spectroscopy group at the University of the Basque Country

Camilla Calabrese, Aran Insausti; Maider Parra, Cristobal Pérez, Iciar Uriarte, Imanol Usabiaga, Emilio J. Cocinero; Francisco J. Basterretxea

P2.6. Nuclear spin conversion of ammonia isolated in noble gas matrices

Haruka Nagamoto; Takeru Sugimoto; Ichiro Arakawa; Koichiro Yamakawa

P2.7. Simulation of rotational energy levels of the ground and first excited vibrational states of H_2S and SO_2 molecules using the effective Hamiltonian approach

Irina Vasilenko; Olga Naumenko; Alexander Bykov

P2.8. Analytical extension of hard–collision model of velocity–changing collisions in the Hartmann–Tran profile

Magdalena Konefał; Michał Słowiński; Mikołaj Zaborowski; Daniel Lisak; Piotr Wcisło

P2.9. Far– and mid–infrared spectroscopy of matrix–isolated clusters and matrix–sublimated ice of D_2O

Hirokazu Nasu; Kazuki Niwata; Yuichi Azuma; Toshiya Tanaka; Ichiro Arakawa; Koichiro Yamakawa

P2.10. Laser absorption spectroscopy of $^{13}CH_4$ at 80 K and 296 K near 1.73 μm

Magdalena Konefał; Mélanie Ghysels; Didier Modelain; Samir Kassi; Alain Campargue

P2.11. Nuclear spin conversion in matrix–isolated water monomer and dimer

Koichiro Yamakawa; Kiwa Yamaguchi; Ichiro Arakawa

P2.12. Understanding metal compound chemistry in Late-Type star environments using chirped-pulse FT millimeter Wave Spectroscopy of supersonic Jets

Pascal Stahl; Guido W. Fuchs; Thomas F. Giesen

P2.13. Tropospheric reactions of triazoles with hydroxyl radicals

Najoua Derbel; Olfa Ferchichi; Alexander Alijah

P2.14. Flexibility at the fringes: conformations of the steroid hormone β-estradiol

Sabrina Zinn; Melanie Schnell

P2.15. Franck-Condon simulated electronic spectra of gold carbene complexes

Agnes H H Chang; Bing Jian Sun; Ian J. Lin

P2.16. FTIR measurements of the third overtone band of $^{12}C^{16}O$

Gang Li; Alexandra Domanskaya; Alekandra Kyuberis; Volker Ebert

P2.17. High resolution Ro-Vibrational analysis of C_2HD_3 in the region of 600 – 1150 cm^{-1}

Olga Gromova; Nadezda V. Kashirina; Elena S. Bekhtereva; Sigurd Bauerecker; Christian Sydow; Oleg N. Ulenikov

P2.18. Fourier transform spectrum of $^{34}SO_2$ in the region of the ν_2 bending fundamental band

Anastasiia G. Ziatkova; Olga V. Gromova; Elena S. Bekhtereva; Sigurd Bauerecker; Christian Sydow; Georg Mellau; Martin Quack; Oleg N. Ulenikov

P2.19. Realistic vibrational spectra of Ethylene Based on a 3-band model

Sergey Yurchenko; Barry Mant; Jonathan Tennyson; Andrey Yachmenev

P2.20. Line positions and strengths in the ν_{10}/ν_7 bands of the C_2D_4 molecule

Anna Fomchenko; Elena S. Bekhtereva; Olga V. Gromova; Maria A. Merkulova; Sigurd Bauerecker; Christian Sydow; Oleg N. Ulenikov

P2.21. Direct deperturbation analysis of the L-mixed $B^1\Pi$ and $C^1\Sigma^+$ states of LiRb

Ekaterina Bormotova; Elena Pazyuk; Andrei Stolyarov; Asen Pashov

P2.22. High resolution study of the decades of H_2S

Tolganay Yersin; Fangce Zhang; Elena S. Bekhtereva; Olga V. Gromova; Sigurd Bauerecker; Christian Sydow; Oleg N. Ulenikov

P2.23. Absolute line strengths in bands ν_9 and ν_{11} of the $^{12}C_2H_4$ molecule

Yulia S. Aslapovskaya; Aleksei V. Kuznetsov; Olga V. Gromova; Elena S. Bekhtereva; Sigurd Bauerecker; Christian Sydow; Oleg N. Ulenikov

P2.24. Analysis of resonance interactions in the bands located in the region of 1500—1750 cm^{-1} in the $C_2H_2D_2$—cis molecule

Yuliya V. Konova; Ivan A. Konov; Olga V. Gromova; Elena S. Bekhtereva; Sigurd Bauerecker; Christian Sydow; Oleg N. Ulenikov

P2.25. High resolution study of $^{73}GeH_4$ in the dyad and pentade regions

Natalia I. Raspopova; Olga V. Gromova; Elena S. Bekhtereva; Petr G. Sennikov; Maxim A. Koshelev; Irina A. Velmuzhova; Aleksandr P. Velmuzhov; Oleg N. Ulenikov

P2.26. High resolution study of Hexades of H_2MS

Fangce Zhang; Petr A. Glushkov; Anastasiia S. Belova; Elena S. Bekhtereva; Olga V. Gromova; Sigurd Bauerecker; Christian Sydow; Christof Maul; Oleg N. Ulenikov

P2.27. First high resolution analysis of SiD_4 in the dyad region

Natalia Raspopova; Olga V. Gromova; Elena S. Bekhtereva; Christian Sydow; Sigurd Bauerecker; Oleg N Ulenikov

P2.28. Ab initio calculations of the potential energy curves and intramolecular interactions in LiRb and LiCs including spin-dependent effects

Ekaterina Bormotova; Alexander Medvedev

P2.29. Comprehensive update of structural data in the MOGADOC database

Rainer Rudert; Natalja Vogt; Jürgen Vogt

P2.30. A highly accurate ab initio dipole moment surface for water: transitions extending into the ultraviolet

Aleksandra Kiuberis; Eamon Conway; Oleg Polyansky; Irina Mizus; Jonathan Tennyson; Nikolay Zobov

P2.31. Far IR continuum absorption of $H_2{}^{16}O$ and $H_2{}^{18}O$

Mikhail Tretyakov; Tatyana Odintsova; Aleksandra Zibarova; Olivier Pirali; Pascale Roy; Alain Campargue

P2.32. A complete and coherent spectral line parameter set for the full $2\nu_3$–band of $^{14}N_2{}^{16}O$ including line strengths, air– and self–induced broadening and shift coefficients

Gang Li; Viktor Werwein; Olav Werhahn; Volker Ebert

P2.33. Rovibrational laser jet–cooled spectroscopy of the NH_3—Ar complex in the ν_2 umbrella region of NH_3: comparison between new infrared data and an ab initio calculated spectrum

Yacine Belkhodja; Pierre Asselin; Atef Jabri; Alexey Potapov; Jérôme Loreau; Ad van der Avoird

P2.34. Exploring interstellar chemical processes of polycyclic aromatic hydrocarbons using opposite sides of the electromagnetic spectrum

Pragya Chopra; Donatella Loru; Sébastien Gruet; Amanda Steber; Hansjochen Köckert; Jasper Peschel; Jan Lahl; Sylvain Maclot; Jason Lee; Rebecca Boll; Simon Dörner; Sadia Bari; Benjamin Erk; Lanhai He; Mehdi Mohammad Kazemi; Alexander Lemmens; Felix Allum; Robert Mason; David Heathcote; Michael Burt; Dimitrios Rompotis; Pavel Olshin; Christopher Passow; Daniel Ramm; Farzaneh Ziaee; Xuemei Cheng; Nora Schirmel; Joss Wiese; Melby Johny; Daniel Rolles; Sebastian Trippel; Terrence Mullins; Anouk Rijs; Jochen Küpper; Mark Brouard; Claire Vallance; Per Johnsson; Bastian Manschwetus; Melanie Schnell

P2.35. Laser–based hydrogen chloride measurements for biogas and biomethane applications

Javis Nwaboh; Alexandra Domanskaya; Zhechao Qu; Olav Werhahn; Volker Ebert

P2.36. Bimolecular absorption in dry atmospheric gases at millimeter waves: new experimental data and high accuracy modeling

Mikhail Tretyakov; Evgeny Serov; Aleksandr Balashov; Tatyana Odintsova; Maksim Koshelev; Aleksandra Zibarova

P2.37. Exoplanetary atlas of molecular opacities: ExoMol Gallery

Sergei N Yurchenko; Jonathan Tennyson; Oleg N. Polyansky; ExoMol team

P2.38. Advanced fitting method for mid–infrared spectra

Risto Sarjonen; Teemu Kääriäinen; Albert Manninen

P2.39. Nuclear spin conversion among three isomers in crystal II methane measured by infrared spectroscopy

Takeru Sugimoto; Hirokazu Nasu; Ichiro Arakawa; Koichiro Yamakawa

P2.40. LED–based Fourier transform spectroscopy of $HD^{16}O$ and $H_2{}^{16}O$ in 14800—15500 cm^{-1} spectral region

Irina Vasilenko; Victor Serdyukov; Olga Naumenko; Leonid Sinitsa

P2.41. Collisional broadenings and shifts in the $S_0(0)$, $S_0(1)$ and $S_0(2)$ rotational lines of HD perturbed by He.

Raúl Martínez Torres; Dionisio Bermejo; Franck Thibault; Piotr Wcisło

P2.42. Terahertz spectra of Ambroxol

Jan Koucký; Tereza Uhlíková; Jitka Bartnická; Ivana Wurmová; Patrik Kania; Štěpán Urban

P2.43. Rotational spectra of 1,2,3,4–Tetrahydroquinoline

Karel Vávra; Kateřina Luková; Patrik Kania; Štěpán Urban

P2.44. Evaluation of the current spectroscopic databases, such as GEISA–2015 and HITRAN–2016, in the frame of the preparation of the new release of GEISA

Agnes Perrin; Raymond Armante; Nicole Jacquinet; Noelle Scott; Alain Chedin

P2.45. High–resolution FTIR spectrum of SO_2 molecule between 2400 and 2650 cm^{-1}

Irina Vasilenko; Olga Naumenko; Veli–Matti Horneman

P2.46. Precision spectroscopy and global deperturbation analysis of the $A^1\Pi(v = 0)$ state in $^{13}C^{18}O$

Rafal Hakalla; Talluri Trivikram; Alan Heays; Edcel Salumbides; Nelson de Oliveira; Robert Field; Wim Ubachs

P2.47. Precision FT spectroscopy and deperturbation analysis of the $A^1\Pi(v = 0)$ state in $^{12}C^{17}O$

Rafal Hakalla; Wojciech Szajna; Alan Heays; Nelson de Oliveira; Edcel Salumbides; Malgorzata Ostrowska-Kopec; Izabela Piotrowska; Przemyslaw Kolek; Miroslaw Zachwieja; Ryszard Kepa; Robert Field; Wim Ubachs

P2.48. Cavity ring-down spectroscopy of CH in the UV

Chris Medcraft; Harold Linnartz; Wim Ubachs

P2.49.THz Spectroscopy: a solution to monitor spoilage indicators. The case of Atlantic salmon

Meriem Mouelhi; Lotta Kuuliala; Cédric Bray; Robin Bocquet; Arnaud Cuisset; Gaël Mouret; Frank Devlieghere; Francis Hindle

P2.50. Structure and dynamics of substituted imidazoles in the gas phase

Eva Gougoula; Nicholas R. Walker

P2.51. New spectral characterization of dimethylether isotopologues in the THz region

José M. Fernández; Guzmán Tejeda; Miguel Carvajal; M. Luisa Senent

P2.52. Ab Initio potential energy surface and vibration-rotation energy levels of Germanium Dicarbide, GeC_2

Jacek Koput

P2.53. The influence of water vapor isotopoloques on the reflection coefficient of multilayer mirrors

Leonid Sinitsa; Victor Serdyukov; Alexei Lugovskoi; Michail Arshinov

P2.54. $H_2{}^{16}O$ and $H_2{}^{18}O$ absorption spectra between 16,460 and 17,200 cm^{-1}

Leonid Sinitsa; Semen Mikhailenko; Victor Serdyukov

P2.55. Monosulfur derivatives of methyl formate: millimeter and submillimeter wave spectra of S- and O-methyl thioformates

Vadym Ilyushyn; Atef Jabri; Roman Motiyenko; Laurent Margulès; Jean-Claude Guillemin; Olga Dorovskaya; Eugene Alekseev; Isabelle Kleiner; Belén Tercero; José Cernicharo

P2.56. Analyses of various ^{17}O and ^{18}O enriched isotopic species of ozone from FTS high resolution spectra

Vladimir Tyuterev; Evgeniya Starikova; Alain Barbe; Marie-Renée De Backer

P2.57. New version of S&MPO database on the ozone spectroscopy

Vladimir Tyuterev; Yurii Babikov; Semen Mikhailenko; Alain Barbe; Evgeniya Starikova

P2.58. Quantitative influence of the ozone potential energy surface upon dynamics of the $^{18}O + {}^{32}O_2$ reaction

Vladimir Tyuterev, Grégoire Guillon; Pascal Honvault; Roman Kochanov

P2.59. Analysis and theoretical modelling of the ^{18}O enriched carbon dioxide spectrum by CRDS near 1.74 µm

Ekaterina Karlovets; Peter Čermák; Didier Mondelain; Samir Kassi; Alain Campargue; Sergey Tashkun; Valery Perevalov

P2.60. Electronic structure of the molecular system HPS^+/HSP^+

B.Mehnen, M. Hochlaf, Saida Ben Yaghlane

P2.61. A global approach for deperturbation of NiH lowest-lying electronic states

Ilvie Havalyova; Ivayla Bozhinova; Amanda Ross; Patrick Crozet; Asen Pashov

P2.62. Dispersed fluorescence from NiD excited with a CW laser, taken in a novel way with a BOMEM DA3 interferometer

Amanda J. Ross, Patrick Crozet, Bradley G. Guislain, Ryan A. R. Harvey, Allan G. Adam, Dennis W. Tokaryk

P2.63. Observation of a periodic many-body system

Klaus Muller-Dethlefs, Francois Michels

P2.64. Creating, imaging, and controlling chiral molecules with electric fields

Andrey Yachmenev, Alec Owens, Jochen Küpper

Friday, September 7, 2018

Morning Sessions

	Plenary Session		
	Chair: **Amanda Ross**, *Université Lyon 1 & CNRS*		
9:00–9:45	**Plenary Lecture 9**		
Mitxelena Auditorium	PT9. Nature and strength of unconventional hydrogen bonds		
	Sanjay Wategaonkar, *Tata Institute of Fundamental Research*		
9:45–10:30	**Plenary Lecture 10**		
Mitxelena Auditorium	PT10. High resolution spectra of floppy molecules: neutral and ionic species		
	Koichi M. T. Yamada, *National Institute of Advanced Industrial Science and Technology*		
10:30–11:00	**Coffee Break**		
Main Hall	**Sponsors Stands will be placed at Main Hall**		
	Oral Sessions 9		
11:00–12:40	**Oral Session A9:**	**Oral Session B9:**	**Oral Session C9:**
	Mitxelena Auditorium	**Baroja Auditorium**	**Oteiza Auditorium**
	Chair: **Walther Caminati**, *University of Bologna*	Chair: **Thomas Giesen**, *University of Kassel*	Chair: **Francisco Basterretxea**, *Universidad del País Vasco (UPV/EHU)*
	HALOGEN AND CHALCOGEN INTERACTIONS	ASTROPHYSICAL MOLECULES	BIOMOLECULES
11:00–11:20	A9.1. Effect of fluorine substitution on non-covalent interactions in molecular complexes of aromatic compounds	B9.1. Spectroscopy of new Imine astrophysics target: Methylimino-acetonitrile (CH_3N=CHCN)	C9.1. Rotational spectroscopy signature of smelling allyl alcohols
	Sonia Melandri, *University of Bologna*	**Laurent Margules,** *Laboratoire PhLAM UMR CNRS 8523*	**Assimo Maris,** *University of Bologna*
11:20–11:40	A9.2. Chalcogen bond formation: The non-covalent, intermolecular sulfur–sulfur interaction of dimethyl sulfide and sulfur dioxide	B9.2. Imidazole rotation spectrum investigation for astrophysical search	C9.2. DNA sugars: in the gas phase and in solution
	Daniel Obenchain, *Leibniz Universität Hannover*	**Barbara Michela Giuliano,** *Max-Planck-Institut für extraterrestrische Physik*	**Iciar Uriarte,** *Universidad del País Vasco (UPV/EHU)*
11:40–12:00	A9.3. Halogen bond and internal dynamics in Perfluorocyclobutane–water	B9.3. Laboratory rotational spectroscopy of isotopic species of Methyl Mercaptan, $CH_3{}^{34}SH$ and CH_3SD, and search for them in ISM	C9.3. Multiresponsive chromic soft materials: formation of macrocycles from carbazole-based biradicaloids
	Qian Gou, *Chongqing University*	**Olena Zakharenko,** *I. Physikalisches Institut, Universität zu Köln*	**Maria Carmen *Ruiz*,** *Universidad de Málaga*

12:00–12:20	A9.4. Rotational spectroscopy of the dimers and monohydrates of furfuryl alcohol and thenyl alcohol	B9.4. Accurate millimetre and submillimetre rest frequencies for cis- and trans-dithioformic acid, HCSSH	C9.4. Raman spectroscopy as a versatile tool to study organic biradicals
	Marcos Juanes, *Universidad de Valladolid*	**Domenico Prudenzano,** *Max-Planck-Institut für extraterrestrische Physik*	**Jose Luis Zafra,** *Universidad de Málaga*
12:20–12:40	A9.5. Microwave spectroscopic characterization of the S···O/N chalcogen bond	B9.5. The nanocosmos gas cell: A broadband Fourier transform millimeterwave spectrometer based on radio astronomy receivers.	C9.5. Molecular spectroscopic study on a natural uric acid type of Kidney Stone
	Gang Feng, *Chongqing University*	**Celina Bermúdez,** *Instituto de Física Fundamental CSIC*	**Mustafa Kumru,** *University of Freiburg*
13:00–14:30	**Lunch Break**		
	Iberdola tower (black tickets) or Deusto Library (white tickets)		
14:30–15:30	**Science Salon: Discussion Forum for students**		
Mitxelena Auditorium	Informal meeting with Dudley R. Herschbach, Nobel Laureate in Chemistry, 1986		

Free Afternoon

21:00–24:00	**Conference Dinner**
	Euskalduna Concert Hall
	Including: – Award of the Plíva Prize, Prizes of the University of Valladolid and PCCP Prize to the best oral presentations from students – Award of the International Mez-Starck Prize 2018 of the Dr. Barbara Mez-Starck Foundation for the Advancement of Science and Research. – Announcement of the 20 student travel grant recipients.

Ab initio calculations of the potential energy curves and intramolecular interactions in LiRb and LiCs including spin-dependent effects

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Ultracold molecules have recommended themselves to be convenient and interesting objects for experimental and theoretical investigations due to the ease of manipulation in laboratory environments. The first step towards making ultracold molecules is conducting a detailed study of the electronic structure of the molecule under examination.

In this work, a two-fold approach has been taken to accurately describe the potential energy curves (PECs) of the LiRb and LiCs heterodimers by looking at both (a) and (c) Hund's coupling cases.

For the latter case, the relativistic PECs of LiRb and LiCs, corresponding to the ground and low-lying excited dissociation limits, were obtained in a wide range of internuclear distances. The inner electronic shells of the Rb and Cs atoms were substituted with shape-consistent relativistic effective core pseudopotentials (ECPs) [1]. For the Li atom, an all-electron basis set [2], augmented by diffuse functions, was used. The energies of the electronic states were calculated using the recently formulated version of the intermediate Hamiltonian relativistic Fock-space coupled-cluster method with singles and doubles (IH FS RCCSD [3,4]). The $[Li-M]^{2+}$ (M={Rb, Cs}) ion served as a vacuum state. The error, associated with the size-inconsistency of the applied method, was insignificant thanks to the dynamically shifted denominators.

As a result of the calculations performed for Hund's coupling case (a) non-relativistic PECs and non-adiabatic matrix elements were obtained in a wide range of internuclear distances. Small-core ECPs with 9 electrons (1 valence + 8 subvalence) for Rb and Cs, and a 1-electron ECP for Li were used within the framework of the internally contracted multi-reference configuration interaction (MRCI) method with state-averaged complete active space self-consistent field (SA-CASSCF) optimization, where core polarization effects were taken into account using *l*-independent core polarization potentials (CPPs).

The calculations were performed within the MOLPRO2010 and the appropriately modified DIRAC17 packages.

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[1] Int. Rev. At. Mol. Phys., 2010, **1**, 63
[2] Theor. Chem. Acc., 2011, **128**, 69
[3] J. Chem. Phys., 2001, **115**, 9720
[4] Phys. Rev. A, 2017, **96**, 022516.