



BOLOGNA2024



The 27th International Conference on High-Resolution Molecular Spectroscopy Bologna, Italy, September 2-6, 2024



Book of abstracts and programme

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ALMA MATER STUDIORUM
UNIVERSITÀ DI BOLOGNA

DEPARTMENT
OF CHEMISTRY
"GIACOMO CIAMICIAN"

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This is the short version of the conference booklet.
Full abstracts with all authors, references, and figures
can be found at:

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Contents

About	4
Useful Information	5
Venue	5
Registration desk	5
University Residence	5
Meals	6
Social program	6
Excursion	7
Detailed Timetable	8

About

BOLOGNA 2024

The International Conference on High-Resolution Molecular Spectroscopy 2024, part of the Prague Spectroscopy Conference Series, marks the 27th edition of the Conference, extending a history that started biannually in 1970 to bring together spectroscopists from the East and West of Europe and all around the Globe. The powerful scientific program will combine ten invited plenary lectures, and contributed oral and poster presentations, emphasizing the contributions of young researchers.

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Useful Information

Venue

Talks and **poster sessions** will be held at teaching building — Complesso Belmeloro located in via B. Andreatta 8, Bologna (see Fig. 1). The registration desk, **coffee breaks** and **sponsor exhibitions** will be located on the ground floor while the sessions will be held in rooms B, C and D on the first floor.

Registration desk

The **registration desk** is located in the teaching building and will be open on:

- Sunday, 1 September from 16:30 until 19:30 (food and drinks will be served for an informal **get together**);
- Monday, 2 September from 8:15 to 12:30;
- Throughout the conference during the breaks.

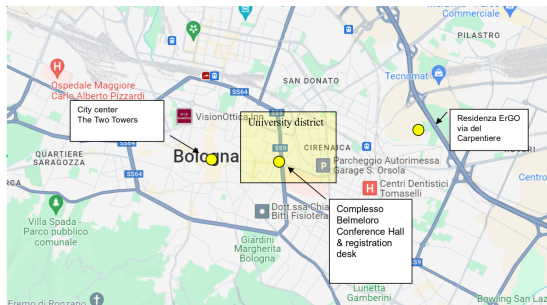


Figure 1: Bologna city center and Residence.

University Residence

The **RESIDENZA ER.GO** is located in via del Carpentiere 58-60, Bologna. From the residence, the conference site can be reached by approximately 20 min bus trip. Walk to the bus stop **Carpentiere** and take bus no. **14** (runs every 15 min). Get off at the bus stop **Porta San Vitale**.

Cross the boulevard and take to your right: in approximately 50 m you will reach via Andreatta. Take via Andreatta: the conference hall is on your right (see Fig. 2).

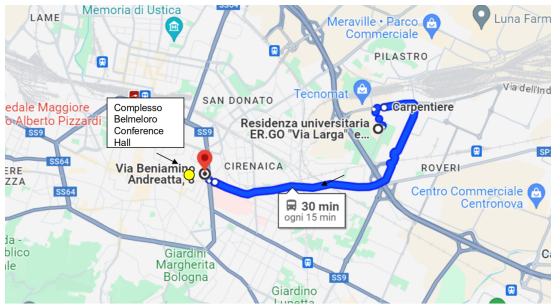


Figure 2: Way from the Residence to the Conference hall.

Meals

A **light breakfast** will be offered at the conference site starting from 8:15. For **lunch** the Mensa Universitaria, Piazza Puntoni 1, is located 400 m from the conference hall. For **supper** the mensa at Ex Scuderie dei Bentivoglio, Piazza Giuseppe Verdi 2, is open (see Fig. 3). The center of Bologna is crowded with small restaurants and bars where small meals are also served.

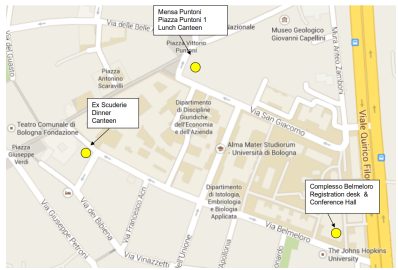


Figure 3: Conference sites.

Social program

The Sunday afternoon/evening **get together**, the **social dinner** and the **chamber concert** on Wednesday are included in the registration fee for both the participants and accompanying persons. The concert will be performed in the **Basilica of San Petronio** in Piazza Maggiore at 18:45.

Since the public will be allowed to enter only from 18:30 (main entrance), we ask you to arrive exactly on time or even a bit earlier to allow everybody to be seated before 18:45. After the concert, the conference dinner¹ at **Circolo Ufficiali** in Palazzo Grassi via Marsala 12 will take place. The dinner starts at 20:00 with an informal “aperitivo” buffet to allow the participants to the concert to walk from the main square to the dinner site (about 8 min, see Fig. 4). *Please, do not forget to bring your tickets to the concert and dinner; they will be required to participate in the events.*

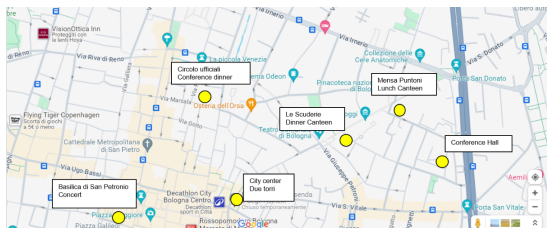


Figure 4: University district, conference & social events sites.

Excursion

On Thursday, an **excursion** (on foot) to the Sanctuary of San Luca (on top of the “Colle della Guardia”, 280 m asl), one of the symbols of Bologna, is organized. At 17:30, from Porta Saragozza, the walk under the world’s longest *portico* (666 arcades) starts. After ~ 1.6 km (in about 25 min), along via Saragozza, the Meloncello Arch is reached. From there, the climbing up to the sanctuary begins (~ 1.9 km, in about 40–45 min). This second part of the walk is quite steep (498 steps) but accessible to everyone (see Fig. 5).

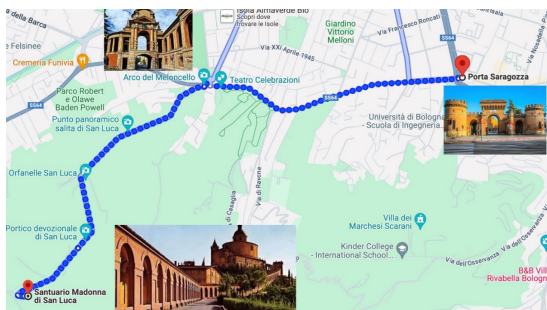


Figure 5: Excursion to San Luca.

¹Vegetarian and vegan choices will be present but catering does not guarantee the absence of cross-contamination for potential allergies such as gluten, shellfish, and nuts.

Detailed Timetable

Session MA — plenary — Monday 2/9, 9:00 – 10:30

Room B, chair: C. Puzzarini

- MA.1** — Missing ions in space and laboratory
O. Asvany, P. C. Schmid, S. Thorwirth, S. Schlemmer
(9:00–9:45)
- MA.2** — Hunting interstellar molecules using rotationally-resolved laboratory spectroscopy
M.-A. Martin-Drumel
(9:45–10:30)

Session MB1 — Monday 2/9, 11:00 – 12:30

Astronomy and atmospheres

Room B, chair: M. Biczysko

- MB1.1** — Millimeter-wave spectroscopy of furoic acids
S. Chawananon, M.-A. Martin-Drumel
(11:00–11:15)
- MB1.2** — Microwave spectroscopy and interstellar search of *n*-propanethiol and *iso*-propanethiol
W. Song, A. Maris, L. Evangelisti, S. Melandri, V. M. Rivilla
(11:15–11:30)
- MB1.3** — Characterization of cyclobutanimine via computational chemistry and microwave spectroscopy
L. Hrubčík, T. Uhlíková, L. Kolesníková, J. Koucký, P. Kania, Š. Urban, J.-C. Guillemin
(11:30–11:45)
- MB1.4** — Quantum chemical and microwave spectroscopic analysis of 1-chloropropene
T. A. Nguyen, I. Kleiner, H. V. L. Nguyen
(11:45–12:00)
- MB1.5** — (Sub)millimeter-wave spectroscopy of naphthalene derivatives
M. R. Bentley, C. Rossi, U. Jacovella, M.-A. Martin-Drumel, O. Pirali
(12:00–12:15)
- MB1.6** — Microwave spectrum of hydantoin in its vibrational excited states
T. Kameyama, H. Ozeki, K. Kobayashi
(12:15–12:30)

Session MC1 — Monday 2/9, 11:00 – 12:30

Structure determination: molecular complexes

Room C, chair: D. A. Obenchain

- MC1.1** — Room temperature detection of the dimer in the absorption spectrum of H₂
H. Fleurbaey, S. Kassi, A. Campargue
(11:00-11:15)
- MC1.2** — High resolution spectrum of D₂O–CO₂ van der Waals complex around the 3OD vibrational excitation
A. S. Bogomolov, R. Glorieux, M. Herman, N. Moazzen-Ahmadi, C. Lauzin
(11:15-11:30)
- MC1.3** — Rotational insights into aggregations of carbon dioxide
Q. Gou, J. Lan, C. Wang, X. Tian, M. Li, X. Wang, J.-U. Grabow
(11:30-11:45)
- MC1.4** — The search for the H₂-benzonitrile complex and the friends we made along the way
B. Hartwig, D. A. Obenchain
(11:45-12:00)
- MC1.5** — Conformational landscape of the complexes isopropanol ··· (carbon dioxide)₂ using broadband chirped-pulse microwave spectroscopy
W. Li, C. Pérez, A. Lesarri
(12:00-12:15)
- MC1.6** — Rotational characterization of the covalently bound dimer of acrolein: 3,4-dihydro-2H-pyran-2-carboxaldehyde (C₈H₈O₂).
S. Herbers, H. V. L. Nguyen
(12:15-12:30)

Session MD1 — Monday 2/9, 11:00 – 12:15

Fundamental physics

Room D, chair: J.-U. Grabow

- MD1.1** — Observation of predissociative Rydberg states in a high-density molecular plasma
F. Michels, K. Müller-Dethlefs
(11:00-11:15)
- MD1.2** — Investigation of the $\nu_2 = 1$, rotation-inversion $2_{1,s} - 1_{1,a}$ transition of ammonia through IR-millimeter-wave double resonance
L. Juppé, O. Pirali, Y. Liu, M. Manceau, B. Darquié, O. Lopez, J. F. Lampin
(11:15-11:30)

- MD1.3** — **Cavity-enhanced spectroscopy of H₂ in a deep cryogenic regime**
 K. Stankiewicz, M. Makowski, M. Stowiński, K. L. Sołtys, B. Bednarski, H. Jóźwiak, N. Stolarczyk, S. Wójtewicz, A. Cygan, G. Kowzan, P. Masłowski, M. Piwiński, D. Lisak, P. Wcisło
 (11:30-11:45)
- MD1.4** — **Probing breakdowns of the impact approximation by cavity ring-down spectroscopy: core line intensity depletion and far-wing absorption**
 Z. D. Reed, J. T. Hodges, H. Tran, J.-M. Hartmann
 (11:45-12:00)
- MD1.5** — **Vibration-rotation linelists and effective Hamiltonians from high-order canonical van Vleck operator perturbation theory**
 S. V. Krasnoshchekov, I. M. Efremov, E. O. Dobrolyubov
 (12:00-12:15)

Session MB2 — Monday 2/9, 14:00 – 16:00

Astronomy and atmospheres

Room B, chair: L. Bizzocchi

- MB2.1** — **Microwave and far-infrared spectroscopy of novel species produced via high-voltage electric discharge**
 J. van Wijngaarden
 (keynote talk: 14:00-14:30)
- MB2.2** — **Rotational action spectroscopy of bare HCN⁺ and HCNH⁺**
 W. G. D. P. Silva, O. Asvany, P. C. Schmid, L. Bonah, D. Gupta, S. Thorwirth, S. Schlemmer
 (14:30-14:45)
- MB2.3** — **Unveil the spectroscopy of the CH₃OCH₂ radical at millimeter wavelengths using Faraday rotation acquisition method**
 R. Chahbazian, O. Pirali
 (14:45-15:00)
- MB2.4** — **High resolution rotational and rovibrational spectroscopy of H₂CCl⁺**
 O. Asvany, W. G. D. P. Silva, M. Fatima, P. C. Schmid, S. Schlemmer, S. Thorwirth, J. L. Doménech
 (15:00-15:15)
- MB2.5** — **¹³C-isotopologues of HC₃N: characterization of the first resonance system for the three monosubstituted isotopomers**
 G. Panizzi, L. Bizzocchi, M. Melosso, S. Alessandrini, C. Puzzarini, M. Nonne
 (15:15-15:30)
- MB2.6** — **Rotational spectroscopy of deuterated species: bis deuterated glycolaldehyde and Z-1,2-ethenediol**
 M. Nonne, M. Melosso, F. Tonolo, L. Bizzocchi, S. Alessandrini, L. Dore, C. Puzzarini, J.-C. Guillemin
 (15:30-15:45)

- MB2.7 — High resolution laboratory spectroscopy of deuterated complex organic molecules (COMs)**
H. A. Bunn, S. Spezzano, C. Endres, V. Lattanzi, L. Coudert, J.-C. Guillemin
(15:45-16:00)

Session MC2 — Monday 2/9, 14:00 – 15:45

Structure determination

Room C, chair: A. Maris

- MC2.1 — Influence of the binding partner on multi-conformational species: clusters analysed by rotational spectroscopy**
M. E. Sanz, V. Tsoi, S. I. Murugachandran
(keynote talk: 14:00-14:30)
- MC2.2 — Investigation of the microsolvation of secondary organic aerosol precursors: microwave spectroscopy of nitromethoxyphenols hydrates**
C. Bracquart, A. Deguine, M. Chrayteh, A. Cuisset, J. A. Claus, M. Goubet
(14:30-14:45)
- MC2.3 — Conformational preferences of gas-phase Gly-Gly-Gly and Ala-Ala-Ala peptides investigated with VUV-IRMPD spectroscopy and quantum chemical calculations**
V. Zhaunerchyk, A. Brandt, Å. Andersson, P. Ferrari
(14:45-15:00)
- MC2.4 — Structural determination of dibenzothiophene and its water complex using broadband rotational spectroscopy**
F. S. Hussain, A. L. Steber, C. Pérez
(15:00-15:15)
- MC2.5 — Conformations of monochloropropionic acids in gas phase and solution**
F. Sun, A. Maris, L. Evangelisti, S. Melandri, C. Calabrese, A. Lesarri
(15:15-15:30)
- MC2.6 — The analysis of coupled torsional and inversion motions in weakly bounded ammonia-water complex**
R. A. Motiyenko, P. Gyawali, L. Margulès, E. A. Alekseev, L. Zou, I. Kleiner
(15:30-15:45)

Session MD2 — Monday 2/9, 14:00 – 16:00

Biology, natural substances

Room D, chair: Q. Gou

- MD2.1** — Simulation of vibrational signatures from the mid infrared (MIR) to the vacuum ultraviolet (VUV) range
M. Biczysko
(keynote talk: 14:00-14:30)
- MD2.2** — Formation and characterization of xanthine complexes via supersonic expansion and laser spectroscopy: a comparative study with crystal sections
I. Usabiaga, P. Pinillos, A. Camiruaga, F. Torres, J. A. Fernández
(14:30-14:45)
- MD2.3** — Exploring DNA derivatives hydration: IR spectroscopy studies on water interactions with theobromine and theophylline
P. Pinillos, A. Camiruaga, J. A. Fernández, I. Usabiaga
(14:45-15:00)
- MD2.4** — The influence of curcumin on tau protein aggregation
M. Urbańska, M. Czaja, E. Lipiec, K. Sofińska
(15:00-15:15)
- MD2.5** — Unveiling 2-aminopyrimidine: insights from rotational spectroscopy from monomer to complexes, from millimeter to centimeter wavelengths
C. Calabrese, M. C. Bermúdez, J. Fernández Sancho, A. Lesarri, E. M. Neeman
(15:15-15:30)
- MD2.6** — The enantioselective interactions of the carvone-1-phenylethanol complex
S. I. Murugachandran, M. E. Sanz
(15:30-15:45)
- MD2.7** — Interactions of a conformationally rich terpenoid with water: the carvone-(H₂O)₁₋₄ complex
S. I. Murugachandran, M. E. Sanz
(15:45-16:00)

Session MB3 — Monday 2/9, 16:30 – 18:15

Astronomy and atmospheres

Room B, chair: A. Campargue

- MB3.1** — High resolution study of the ν_{22} band of pyrrole (C₄H₅N) near 14 μm
C. Silva Tafur, J. Vander Auwera
(16:30-16:45)

- MB3.2** — **Towards mid-IR quantum state-resolved spectroscopy of large molecules for astrochemistry**
D. Charczun, N. Baradaran, T. Nambiar, M. L. Weichman
 (16:45-17:00)
- MB3.3** — **The $^{15}\text{NH}_3$ ammonia spectrum between 4000 and 6350 cm^{-1} .**
P. Cacciani, P. Čermák, J. Vander Auwera, A. Campargue
 (17:00-17:15)
- MB3.4** — **Extended calculations of nitrogen-induced line-broadening coefficients in the ν_7 band of ethylene**
S. Clavier, J. Buldyreva
 (17:15-17:30)
- MB3.5** — **Assignments of methyl chloride CH-stretch overtone spectra using cross-correlation pattern recognition procedure**
O. Votava, J. Rakovský, V. Svoboda
 (17:30-17:45)
- MB3.6** — **CRDS line-shape study of carbon monoxide (7-0) band**
S. Wójtewicz, A. A. Balashov, K. Bielska, J. Domysławska, R. Ciuryło, D. Lisak, G. Li, A. A. Kyuberis, N. F. Zobov, J. Tennyson, O. L. Polyansky
 (17:45-18:00)
- MB3.7** — **The O_2^- and subsequently N_2 -disrupted self-expansion coefficients of the ν_2 , ν_5 and $\nu_3 + \nu_6$ bands of CH_3I**
S. Harbaoui, O. Fathallah, N. Maaroufi, L. Manceron, H. Aroui
 (17:45-18:15)

Session MC3 — Monday 2/9, 16:30 – 18:15

Structure determination: molecules

Room C, chair: I. Kleiner

- MC3.1** — **Low and lower: the torsional barriers of the coupled methyl internal rotations in lutidines studied by microwave spectroscopy**
M. G. Barth, S. Herbers, I. Kleiner, J.-U. Grabow, H. V. L. Nguyen
 (16:30-16:45)
- MC3.2** — **Complex hyperfine-fine structure overlapping observed in the microwave spectrum of 3,4-lutidine**
E. Antonelli, H. V. L. Nguyen
 (16:45-17:00)
- MC3.3** — **Exploring biaryl dithiolthiones using jet-cooled chirped-pulse microwave spectroscopy**
D. Heras, W. Li, M. Juanes, C. Pérez, A. Lesarri
 (17:00-17:15)
- MC3.4** — **The rotational spectra of 3-fluorobenzylamine: conformational analysis and tunnelling effects**
A. Maggio, W. Song, A. Maris, L. Evangelisti, S. Melandri, P. Pinillos
 (17:15-17:30)

- MC3.5** — **Internal rotation and structure of fluoro-substituted methyl benzoates: methyl-2-fluorobenzoate, methyl-3-fluorobenzoate, and methyl-4-fluorobenzoate**
 X. Wang, P. Buschmann
 (17:30-17:45)
- MC3.6** — **Two coupled low-barrier large amplitude motions in 3,5-dimethyl-anisole studied by microwave spectroscopy**
 S. Khemissi, L. Ferres, H. V. L. Nguyen
 (17:45-18:00)
- MC3.7** — **Investigation and characterization of oxyamines: the rotational spectrum of diethylacetyloxyamine**
 F. Baroncelli, S. Melandri, L. Evangelisti, A. Maris, S. Blanco, J. C. López
 (18:00-18:15)

Session MD3 — Monday 2/9, 16:30 – 18:00

Atmospheres

Room D, chair: P. Wcisło

- MD3.1** — **Calculations of collision-induced line-shape parameters for N₂-perturbed lines in HF**
 J. Behrendt, H. Jóźwiak, P. Wcisło
 (16:30-16:45)
- MD3.2** — **Ab initio quantum scattering calculations for rotational lines in HCl perturbed by O₂**
 A. Olejnik, H. Jóźwiak, M. Gancewski, P. Wcisło, R. Dawes, E. Quintas-Sánchez
 (16:45-17:00)
- MD3.3** — **High temperature measurements of polarizability transition moments of CO₂**
 C. Álvarez, G. Tejada, J. M. Fernández
 (17:00-17:15)
- MD3.4** — **Databases of pressure-induced linewidths for infrared absorption by exomolecules**
 J. Buldyreva
 (17:15-17:30)
- MD3.5** — **Heterodyne dispersive cavity ring-down spectroscopy for high-fidelity measurements**
 A. Cygan, S. Wójtewicz, H. Jóźwiak, G. Kowzan, N. Stolarczyk, K. Bielska, P. Wcisło, R. Ciuryło, D. Lisak
 (17:30-17:45)
- MD3.6** — **Physically grounded modeling of the atmospheric gases continuum absorption in subthz range.**
 E. A. Serov, T. A. Galanina, A. O. Koroleva, D. S. Makarov, I. S. Amerkhanov, M. Yu. Tretyakov
 (17:45-18:00)

Session TB1 — Tuesday 3/9, 9:00 – 10:15

Astronomy and atmospheres

Room B, chair: K. Kobayashi

- TB1.1** — **New high resolution microwave and infrared spectra for atmospheric species with large amplitude motions: the case of isoprene**
I. Kleiner, S. Khemissi, S. Herbers, H. V. L. Nguyen, I. Gulaczyk, S. Chawananon, P. Asselin
(keynote talk: 9:00-9:30)
- TB1.2** — **Coupled methyl internal rotations with intermediate and low torsional barriers in 2,5-dimethylanisole investigated by microwave spectroscopy**
H. Sun, I. Kleiner, L. Ferres, H. V. L. Nguyen
(9:30-9:45)
- TB1.3** — **Theoretical structural and spectroscopic characterization of peroxyacetic acid ($\text{CH}_3 - \text{CO} - \text{OOH}$) and dimethyl peroxide ($\text{CH}_3 - \text{OO} - \text{CH}_3$): study of the far infrared region**
M. L. Senent, S. Brahem, D. Missauoia, O. Yazidi, F. Najar
(9:45-10:00)
- TB1.4** — **Extending the rotational spectrum of cyclopentadiene towards higher frequencies and vibrational states**
L. Bonah, B. Helmstaedter, J.-C. Guillemin, S. Thorwirth, S. Schlemmer
(10:00-10:15)

Session TC1 — Tuesday 3/9, 9:00 – 10:30

Combustion, catalysis, kinetics

Room C, chair: T. D. Varberg

- TC1.1** — **Broadband microwave spectra of reactive intermediates**
B. A. Welsh, T. S. Zwiernicki
(keynote talk: 9:00-9:30)
- TC1.2** — **Time resolved measurements of atomic and molecular deuterium densities in a pulsed MW discharge using VUV absorption spectroscopy**
N. De Oliveira, F. J. Iguaz Gutierrez, L. Nahon, S. Bechu, M. Mitrou, P. Svarnas
(9:30-9:45)
- TC1.3** — **Ultraviolet intracavity laser absorption spectroscopy**
U. Zamir, M. Cohen, I. Rozenberg, A. Lerer, Y. Kalisky, A. Kaplan, I. Rahinov, J. H. Baraban
(9:45-10:00)

TC1.4 — Monitoring of the synthesis and temporal evolution of tritiated methane mixtures by Raman spectroscopy

D. Diaz Barrero, T. L. Le, M. Schlösser, H. H. Telle
(10:00-10:15)

TC1.5 — Aqueous-phase photoemission for chemical analysis

L. Tomaník, P. Slaviček, B. Winter
(10:15-10:30)

Session TD1 — Tuesday 3/9, 9:00 – 10:30

Laser spectroscopy

Room D, chair: O. Asvany

TD1.1 — Mass-correlated, high-resolution rotational Raman spectra

T. Schultz, B. R. Özer, I. Heo, J. C. Lee
(keynote talk: 9:00-9:30)

TD1.2 — Development of 14-pole RF ion trap equipped with electrospray ion source high resolution time of flight mass spectrometer

M. Selvaraj, U. Kadhane
(9:30-9:45)

TD1.3 — The double minimum $E^1\Sigma_u^+$ state in CS_2

W. Jastrzebski, J. Szczepkowski, P. Kowalczyk, A. Pashov
(9:45-10:00)

TD1.4 — IR-UV double resonance spectroscopy of formaldehyde. Part I: revealing new vibronic levels of the \bar{A}^1A_2 state

N. Genossar-Dan, M. Cohen, E. Brudner, J. H. Baraban
(10:00-10:15)

TD1.5 — IR-UV double resonance spectroscopy of formaldehyde. Part II: the effect of vibronic coupling on cross anharmonicities

N. Genossar-Dan, M. Cohen, E. Brudner, J. H. Baraban
(10:15-10:30)

Session TB2 — Tuesday 3/9, 11:00 – 12:30

Astronomy and atmospheres

Room B, chair: M. Melosso

TB2.1 — Insights from numerically exact approaches for the calculation of the rovibrational energy structure of tri- and tetratomic molecules

M. Mladenović
(11:00-11:15)

TB2.2 — The semi-experimental equilibrium structures of small radicals and an extension to larger species

S. Alessandrini, M. Melosso, L. Bizzocchi, C. Puzzarini, V. Barone
(11:15-11:30)

- TB2.3** — **An *ab initio* spectroscopic model of the carbon monoxide molecule**
M. Khalil, N. El-Kork, R. P. Brady, S. N. Yurchenko, J. Tennyson, S. J. Evans
(11:30-11:45)
- TB2.4** — **Towards a strict diabatic representation for coupled *N*-state diatomic systems: total rovibronic equivalence**
R. P. Brady, S. N. Yurchenko
(11:45-12:00)
- TB2.5** — **VUV and UV-Vis FT-spectroscopy of CO: analysis of the unimolecular interactions**
R. Hakalla, S. Ryzner, A. Stasik, W. Szajna, R. W. Field, N. De Oliveira, M. I. Malicka, W. Ubachs
(12:00-12:15)
- TB2.6** — **Accessing all vibrationally excited states of the $X^+ 2\Sigma_u^+$ ground electronic state of He_2^+ through multi-step laser excitation**
M. Holdener, H. Schmutz, J. A. Agner, M. Beyer, F. Merkt
(12:15-12:30)

Session TC2 — Tuesday 3/9, 11:00 – 12:30

Instrumental technique demonstration

Room C, chair: C. Pérez

- TC2.1** — **A high-performance tunable THz source for spectroscopy and more**
S. Kassi, L. Lechevallier, L. Djevahirdjian, O. Pirali, M.-A. Martin-Drumel, R. Kassi, G. Ducournau
(11:00-11:15)
- TC2.2** — **Raman thermometry of confined gas micro-flows**
G. Tejeda, S. Bajic, C. Álvarez, J. M. Fernández
(11:15-11:30)
- TC2.3** — **Benchmarking a reduced-footprint broadband microwave spectrometer for simplified structure characterization**
A. Byars, S. Shipman, R. Sonstrom, J. Neill
(11:30-11:45)
- TC2.4** — **Towards electronic spectroscopy of mass and shape selected cationic metal carbides in the context of diffuse interstellar bands**
C. Rossi, B. Gans, U. Jacovella, Y. Žabka, J. Jašík
(11:45-12:00)
- TC2.5** — **Chirped pulse and resonator in one spectrometer (PARIS): a supersonic-jet chirp and tone fourier transform microwave spectrometer for broad acquisition and high resolution.**
H. V. L. Nguyen, S. Herbers, S. Khemissi, M. Schwell, I. Kleiner, X. Landsheere, J.-U. Grabow
(12:00-12:15)

- TC2.6** — Using new DC-discharge sources to investigate the formation of benzonitrile
A. L. Steber, C. Pérez, J. R. Morán, F. Sajeev Hussain, I. Peña, A. Lesarri
(12:15-12:30)

Session TD2 — Tuesday 3/9, 11:00 – 12:30

Linelists and datasets

Room C, chair: F. Tamassia

- TD2.1** — **pyckett and llwp** - new tools to increase the efficiency of spfit/spcat
L. Bonah, S. Schlemmer
(11:00-11:15)
- TD2.2** — Revisiting the 0 – 0 and 1 – 0 bands of the A – X system of CrH with pgopher
A. J. Ross, P. Crozet, A. Genoud, J. Morville
(11:15-11:30)
- TD2.3** — ExoMolHR: a relational database of empirical high-resolution molecular spectra
J. Zhang, J. Tennyson, S. N. Yurchenko, C. Hill
(11:30-11:45)
- TD2.4** — Assignment of measured spectra with the marvelous methane line list
K. Kefala, A. Owens, S. N. Yurchenko, J. Tennyson
(11:45-12:00)
- TD2.5** — Spectroscopic constants from rovibrational configuration interaction calculations
D. F. Dinu, K. R. Liedl, B. Schröder, M. Tschöpe, G. Rauhut
(12:00-12:15)
- TD2.6** — Measurements and modeling of line parameters for the ν_3 , $\nu_3 + \nu_6 - \nu_6$ and $2\nu_3 - \nu_3$ bands of methyl fluoride at 10 μm
M. V. Khan, M. Guinet, D. Jacquemart
(12:15-12:30)

Session TA — plenary — Tuesday 3/9, 14:00 – 15:30

Room B, chair: J. Tennyson

- TA.1** — Ultrafast X-ray scattering: photochemical dynamics and beyond
A. Kirrander
(14:00-14:45)
- TA.2** — Testing the quantum theory with accurate laser spectroscopy
P. Wcisło
(14:45-15:30)

Poster 1 — Tuesday 3/9 16:00 – 17:30

See full list of poster contributions in the abstract book.

Session WA — plenary — Wednesday 4/9, 9:00 – 10:30

Room B, chair: A. Lesarri

WA.1 — Quantitative analysis of isotope mixtures for applications in pharmaceutical chemistry using broadband rotational spectroscopy

B. Pate

(9:00–9:45)

WA.2 — How increased use of remote sensing technique for monitoring the health of our environment translates to additional requirements as to molecular spectroscopy databases

M. De Mazière

(9:45–10:30)

Session WB1 — Wednesday 4/9, 11:00 – 12:45

Atmospheres

Room B, chair: S. Yurchenko

WB1.1 — Oxidation product analysis of an α -pinene discharge by microwave spectroscopy

J. R. Moran, A. L. Steber, I. Peña, C. Cabezas

(11:00–11:15)

WB1.2 — N_2 and O_2 -broadening coefficients of CH_3Br ro-vibrational lines in the ν_2 and ν_5 bands

I. Mejdí, H. Aroui, D. Benabdallah, N. Maaroufi, O. Ben Fathallah, F. Kwabia Tchana

(11:15–11:30)

WB1.3 — Sub-mm line shape analysis of methyl bromide (CH_3Br)

N. Osseiran, W. Tchana Betenga, F. Kwabia Tchana, J. Vander Auwera, F. Hindle, A. Cuisset

(11:30–11:45)

WB1.4 — Isotopologue extrapolation of energy levels for polyatomic molecules: rotation-vibration energies of ammonia $^{15}NH_3$

O. A. Smola, S. N. Yurchenko, J. Tennyson

(11:45–12:00)

WB1.5 — Line positions and intensities of the $\nu_3 + \nu_6$ band of methyl fluoride

H. Ziadi, M. Rey, B. Grouiez, M. Rotger, A. V. Nikitin, H. Aroui

(12:00–12:15)

WB1.6 — High-resolution spectroscopy of protonated diacetylene, $H_2C_4H^+$

D. Gupta, M. Bast, S. J. P. Marlton, S. Thorwirth, O. Asvany, T. Salomon, P. C. Schmid, S. Schlemmer

(12:15–12:30)

- WB1.7** — **Overtone transition $2\nu_1$ of HCO^+ and HOC^+ — origin, radiative lifetime, collisional quenching**
M. Jiménez-Redondo, P. Caselli, P. Jusko, L. Uvarova, M. Kassayová, P. Dohnal
(12:30-12:45)

Session WC1 — Wednesday 4/9, 11:00 – 12:45

Precision spectroscopy

Room C, chair: S. Schlemmer

- WC1.1** — **Precision spectroscopy of tritiated molecules**
V. Hermann
(11:00-11:15)
- WC1.2** — **Precision measurements and tests of fundamental physics with cold molecules**
A. Bonifacio, M. Saffre, Y. Liu, N. Cahuzac, S. Tokunaga, A. Cournol, M. Gonçalves, A. Kaladjian, E. Cantin, O. Lopez, A. Amy-Klein, M. Manceau, B. Darquie
(11:15-11:30)
- WC1.3** — **High (sub-10 mHz) resolution molecular spectroscopy in the mid-IR to THz range using broadband dual frequency comb method**
K. Vodopyanov, D. Konnov, Y.-C. Chan, E. L. Temelkova, A. Muraviev, D. Nesbitt
(11:30-11:45)
- WC1.4** — **Unrivaled accuracy in measuring rotational transitions of greenhouse gases: THz-CRDS of CF_4**
F. Simon, A. Cuisset, C. Elmaleh, F. Hindle, G. Mouret, M. Rey, C. Richard, V. Boudon
(11:45-12:00)
- WC1.5** — **Symmetry aspects and tunneling splittings of the torsional energy levels of the hydroquinone molecule**
G. Pitsevich, A. Malevich
(12:00-12:15)
- WC1.6** — **Si-referenced HCOOH vibrational spectroscopy at the 20 Hz level**
M. Leuliet, A. Mbardi, B. Argence, J.-Ph. Karr, L. Hilico
(12:15-12:30)
- WC1.7** — **A systematic reduction of the effective hamiltonians using normal ordering of cylindrical angular moment operators**
I. M. Efremov, S. V. Krasnoshchekov, D. V. Millionshchikov
(12:30-12:45)

Session WD1 — Wednesday 4/9, 11:00 – 12:30

Laser spectroscopy

Room D, chair: M. Lepère

- WD1.1** — Exploring molecular orbitals and ionization dynamics in 2,3-difluoropyridine: insights from high-resolution VUV-MATI mass spectroscopy
H. Kim, S. M. Park, C. H. Kwon
(11:00-11:15)
- WD1.2** — Study on the conformational preference of morpholine using IR resonant VUV-PI mass spectroscopy
S. M. Park, C. H. Kwon
(11:15-11:30)
- WD1.3** — Elucidating the conformational stability of tetrahydrofuran through conformer-specific vibrational spectroscopy
C. H. Kwon
(11:30-11:45)
- WD1.4** — Dual frequency comb spectroscopy in the UV region with one million spectral data points resolved
K. Vodopyanov, A. Muraviev, D. Konnov, S. Vasilyev
(11:45-12:00)
- WD1.5** — Comparative investigation of the dissociative photoionization of aniline induced by VUV and UV photons
M. Selvaraj, B. Panja, U. Kadhane, R. Richter, P. Bolognesi, L. Avaldi
(12:00-12:15)
- WD1.6** — Analysis of the room temperature absorption spectrum of ethylene in the 6000-8050 cm^{-1} range
O. Ben Fathallah, A. Campargue, S. Beguier, L. Manceron, M. Rey
(12:15-12:30)

Session ThA — plenary — Thursday 5/9, 9:00 – 10:30

Room B, chair: O. Dopfer

- ThA.1** — Precision Rydberg spectroscopy in H, He, H₂ and He₂
F. Merkt
(9:00-9:45)
- ThA.2** — Cold ion trap IR spectroscopy of ion selective molecular systems
I. S. Ishiuchi
(9:45-10:30)

Poster 2 — Thursday 5/9 11:00 – 12:30

See full list of poster contributions in the abstract book.

Session ThB1 — Thursday 5/9, 14:00 – 16:00

Astronomy and atmospheres

Room B, chair: G. Fuchs

- ThB1.1** — Photochemical properties of astrochemically-relevant silicon clusters: bridging the gap between diatomics and silicate grains
O. Dopfer
(keynote talk: 14:00-14:30)
- ThB1.2** — Temperature-dependent photodissociation cross sections and rates for H₂S
A. N. Perri, S. N. Yurchenko, J. Tennyson, A. O. Mitrushchenkov
(14:30-14:45)
- ThB1.3** — Discovery of a new electronic state in iron hydride assigned to (2)⁴Φ
T. Blackmore, D. Tokaryk, A. Adam, P. Crozet, A. J. Ross
(14:45-15:00)
- ThB1.4** — Rotationally resolved PFI-ZEKE photoelectron spectroscopy of the CH₃ radical probing the X⁺ ¹A₁' (ν₂⁺ = 1 and ν₄⁺ = 1) levels of the CH₃⁺ cation
N. Chen, H. Le, B. Gans, S. Boyé-Péronne, P. B. Changala, C. Alcaraz
(15:00-15:15)
- ThB1.5** — Photoelectron spectroscopy of small free radicals at medium- and high-spectral resolution
N. Chen, H. Le, S. Boyé-Péronne, B. Gans
(15:15-15:30)
- ThB1.6** — Stellar wind contribution to origin and transport of water on the surface of oxygen-containing minerals, Part I
S. Civiš, J. Kubišta, J. Plšek, A. Knížek
(15:30-15:45)
- ThB1.7** — Stellar wind contribution to origin and transport of water on the surface of oxygen-containing minerals, Part II
S. Civiš, J. Kubišta, J. Plšek, A. Knížek
(15:45-16:00)

Session ThC1 — Thursday 5/9, 14:00 – 16:00

Non covalent interactions

Room C, chair: H. L. V. Nguyen

- ThC1.1** — Molecular beam microwave spectroscopy: large amplitude motions and non-covalent bonds
E. Arunan
(keynote talk: 14:00-14:30)
- ThC1.2** — Rotational spectroscopic study of the PA-FA-PHS complex
J. Hong, W. Li, M. Zhou
(14:30-14:45)

- ThC1.3** — Interactions of a ketone with a higher number of waters in the gas phase: structures and binding preferences of cyclooctanone ···(H₂O)_{3–8} clusters
 V. Tsoj, E. Burevschi, M. E. Sanz
 (14:45-15:00)
- ThC1.4** — Configurations of *o*-phthalaldehyde-(H₂O)_{1–3} complexes elucidated by rotational spectroscopy
 V. Tsoj, M. E. Sanz
 (15:00-15:15)
- ThC1.5** — Rotational spectroscopy and tautomeric equilibria in complexes formation of benzisothiazolinone
 J. Li, D. Loru, W. Sun, M. Schnell
 (15:15-15:30)
- ThC1.6** — Rotation visualizing solvation: studying oligo hydrates of 4-hydroxy-2-butanone
 M. Li, J.-U. Grabow, W. Li, C. Pérez, A. Lesarri
 (15:30-15:45)
- ThC1.7** — Microwave spectroscopic study of solvation processes in $\pi - \pi$ stacking
 X. Chen, G. Wang, X. Zeng, W. Li, M. Zhou
 (15:45-16:00)

Session ThD1 — Thursday 5/9, 14:00 – 16:00

Laser spectroscopy

Room D, chair: O. Pirali

- ThD1.1** — Jet-cooled mid-infrared laser spectroscopy of centrosymmetric and N-bearing PAHs
 P. Asselin, S. Chawananon, O. Pirali, M. Goubet
 (keynote talk: 14:00-14:30)
- ThD1.2** — Far infrared absorption spectroscopy of the nine stable isotopologues of water vapor
 S. N. Mikhailenko, A. O. Koroleva, E. V. Karlovets, A. Campargue
 (14:30-14:45)
- ThD1.3** — Experimental determination of the Landé *g*-factors for the $N = 1$ rotational energy levels in the ground vibronic state ($X^3\Sigma_g^-, v = 0$) of ¹⁶O₂
 A.-W. Liu, Y.-R. Xu, Z.-T. Zhang, Y.-Q. Cheng, Y. Tan, S.-M. Hu
 (14:45-15:00)
- ThD1.4** — Si-traceable density measurement of H₂ based on polarizability and absorption spectroscopy
 S.-M. Hu, H. Liang, Z.-L. Nie, J. Wang, Y. Tan, C.-L. Hu, C.-F. Cheng, A.-W. Liu, Y. R. Sun
 (15:00-15:15)

- ThD1.5** — **Cavity ring-down spectroscopy of jet-cooled ethylene between 5880 and 6200 cm^{-1}**
S. Perot, J. Lecomte, N. Suas-David, L. Rutkowski, R. Georges, M. Rey, S. Kassi
 (15:15-15:30)
- ThD1.6** — **High resolution dual frequency comb spectroscopy from 1 THz to 1 PHz**
 K. Vodopyanov
 (15:30-15:45)
- ThD1.7** — **Spectroscopic study of a single molecule underneath the STM tip**
A. Farrukh
 (15:45-16:00)

Session FA — plenary — Friday 6/9, 9:00 – 10:30

Room B, chair: M. E. Sanz

- FA.1** — **Magnetic resonance of biomolecules by combining ESR and NMR techniques**
M. Bennati
 (9:00–9:45)
- FA.2** — **Rotational insights into sulfur-mediated non-covalent interactions**
G. Feng, L. Wang, T. Yang, W. Lv, J. Huang, H. Huang, Y. Li, F. Shen, Y. Feng
 (9:45–10:30)

Session FB1 — Friday 6/9, 11:00 – 12:15

Astronomy and atmospheres

Room B, chair: S. Thorwirth

- FB1.1** — **Searching for resonances states by complex scaling**
T. Uhlíková, S. Yurchenko
 (11:00-11:15)
- FB1.2** — **Where experiment meets theory: the way to the new ExoMol line lists–LIV for AIH and AID**
 W. Szajna, R. Hakalla, S. N. Yurchenko, J. Tennyson, M. Semenov, A. Sokolov, R. R. Gamache, Y. Pavlenko, M. R. Schmidt, R. W. Field
 (11:15-11:30)
- FB1.3** — **Towards accurate climate metrics by quantum chemical spectroscopic simulations**
 D. A. Alvarado-Jiménez, N. Tassinato
 (11:30-11:45)

- FB1.4** — **Theoretical vibrational analysis and Raman spectra of acetone isotopologues**
S. Dalbouha, C. Alvarez, G. Tejada, J. M. Fernandez, M. L. Senent
 (11:45-12:00)
- FB1.5** — **Machine learning estimate of the interstellar physical conditions from the observed spectral line profiles**
 E. Mendoza, P. Dall'Olio, M. Carvajal, L. S. Coelho, A. Peregrín, S. López-Domínguez, F. F. S. Van Der Tak
 (12:00-12:15)

Session FC1 — Friday 6/9, 11:00 – 12:30

Linelists and datasets

Room C, chair: A. Ross

- FC1.1** — **Multi-laboratory comparison of $^{12}\text{C}^{16}\text{O}$ (3 – 0) line intensities: towards primary spectroscopic measurements of amount of gas**
 K. Bielska, V. D'Agostino, S. Wójtewicz, A. Cygan, R. Ciuryło, D. Lisak, J. T. Hodges, Z. D. Reed, M. Birk, G. Wagner, C. Röske, R. Guo, G. Li
 (11:00-11:15)
- FC1.2** — **Pressure and temperature dependencies of air-perturbed O_2 B-band line shapes**
 K. Bielska, D. D. Tran, A. A. Balashov, J. Domysławska, S. Wójtewicz, M. Bober, S. Bilicki, R. Ciuryło, D. Lisak
 (11:15-11:30)
- FC1.3** — **Ab initio quantum scattering calculations for N_2 -perturbed R(0) 3–0 line in CO**
 A. Olejnik, H. Jóźwiak, N. Stolarczyk, M. Żółtowski, P. Wcisło, H. Cybulski, B. Fernández, C. Henriksen
 (11:30-11:45)
- FC1.4** — **N_2 -collisional broadening of N_2O lines: high-resolution dual-comb spectroscopy and semi-classical line shape calculations**
 B. Vispoel, R. R. Gamache, M. Lepère
 (11:45-12:00)
- FC1.5** — **Collisional excitation of PO^+ by *para*- H_2**
 F. Tonolo, L. Bizzocchi, M. Melosso, C. Puzzarini, V. M. Rivilla, F. Lique
 (12:00-12:15)
- FC1.6** — **The collision-induced absorption of H_2 near $1.20 \mu\text{m}$: subatmospheric measurements and validation tests of calculations**
 A. O. Koroleva, S. Kassi, H. Fleurbaey, A. Campargue
 (12:15-12:30)

Session FD1 — Friday 6/9, 11:00 – 12:00

Comparing theory and experiment

Room D, chair: S. Alessandrini

- FD1.1** — **A full-symmetry torsion rotation theoretical approach for nitromethane CH_3NO_2**
I. Gulaczyk, M. Kreglewski
(11:00-11:15)
- FD1.2** — **Sweetness and light: computation of the rotational spectra of proto-saccharides**
M. Sang, T. E. Field-Theodore, P. R. Taylor
(11:15-11:30)
- FD1.3** — **Millimeter-wave spectrum of 2-hydroxyacetophenone and 2-aminoacetophenone**
S. Boi, S. Melandri, L. Evangelisti, A. Maris
(11:30-11:45)
- FD1.4** — **Theoretical study of the $\text{CH}_3\text{Br}+\text{N}_2$ van der Waals complex: potential energy surface and applications**
I. Mejdí, D. Benabdallah, H. Aroui, M. Hochlaf
(11:45-12:00)

	Sunday 01/09/24	Monday 02/09/24	Tuesday 03/09/24	Wednesday 04/09/24	Thursday 05/09/24	Friday 06/09/24	
8:45 – 9:00		Opening				Student prizes	
9:00 – 10:30		MA plenary	Sessions TB1/TC1/TD1	WA plenary	ThA plenary	FA plenary	
10:30 – 11:00	Arrival	Break	Break	Break	Break	Break	
11:00 – 12:30		Sessions MB1/MC1/MD1	Sessions TB2/TC2/TD2	Sessions WB1/WC1/WD1	Poster 2	Sessions FB1/FC1/FD1	
12:30 – 14:00		Lunch	Lunch	Lunch [‡]	Lunch	Lunch	
14:00 – 16:00		Sessions MB2/MC2/MD2	TA plenary			Sessions ThB1/ThC1/ThD1	
16:00 – 16:30		Break	Break*	Free afternoon		Break	Departure
16:30 – 18:30	Registration Get together [†]	Sessions MB3/MC3/MD3	Poster 1**		Free time Excursion		
18:30 – 22:30				Concert Social dinner			

[†] Get together until 19:30; * coffee break at 15:30; ** from 16:00 to 17:30; [‡] lunch at 13:00.