

CURRICULUM VITAE – Cristina Puzzarini

□ PERSONAL INFORMATION

Puzzarini, Cristina
Professor of Physical Chemistry
Dept. Chemistry “Giacomo Ciamician”, Università di Bologna
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<https://site.unibo.it/rotational-computational-spectroscopy/en>
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Date of Birth: 2 Dec 1969
Nationality: Italian
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□ EDUCATION

Ph.D. (Chemistry), Università di Bologna, 1997 (Supervisor: Prof. P. Palmieri).
M.Sc. (Chemistry), Università di Bologna, 1993 (cum laude).

□ CURRENT POSITIONS

2018 – to date *Full Professor of Physical Chemistry, University of Bologna.*

□ PREVIOUS POSITIONS

2018 – 2021 Director, STAR – Interuniversity Center for Astrochemistry.
2017 – 2021 Visiting Research Professor, Department of Physics, University of Maryland.
2012 – 2017 Associate Professor of Physical Chemistry, University of Bologna.
2006 – 2012 Assistant Professor of Physical Chemistry, University of Bologna.
2000 – 2006 Research Associate (molecular spectroscopy), University of Bologna.
1998 – 2000 Postdoctoral Scholar (theoretical chemistry), University of Bologna.
1997 Postdoctoral Scholar (theoretical chemistry), University of Marne-la-Vallée.
1994 – 1996 Ph.D. fellowship (theoretical chemistry), University of Bologna.

□ FELLOWSHIPS AND AWARDS

2021 Leadership Award - Frontiers in Astronomy and Space Sciences
2017 Invited Professor, University of Valladolid
2016 LabEx fellowship, Invited Professor, Université Paris-Est
2004 Galilei fellowship, Research Associate, Université de Lille I, France
2004 Marco Polo fellowship, Visiting Research Associate, Washington State University
2001 Visiting Research Associate, Universität Göttingen

□ RESEARCH INTERESTS

Research activity is characterized by the synergic interplay of experiment and theory:

- Astrochemistry: spectroscopic support to astronomical observations, chemistry of the interstellar medium, fundamental questions about the origin of life.
- Molecular physical chemistry: studied via the fields of rotational spectroscopy and state-of-the-art computational methods.
- Effective communication of science through presentations and writing (e.g. an educational book on Astrochemistry has been published by “Il Corriere della Sera” and outreach talks).

The leading expertise in both experimental and computational fields at a national and international level applied to astrochemistry has led to the coordination as principal investigator (national coordinator) of three national projects:

2011-2013 PRIN 2009 Project "*Molecular Spectroscopy for Atmospheric and Astrochemical Research: Experiment, Theory and Applications*";
2014-2017 PRIN 2012 Project "*STAR: Spectroscopic and computational Techniques for Astrophysical and atmospheric Research*";
2022-2025 PRIN 2020 Project "*ARES: A Road from Earth to the Stars*";
2024-2026 PRIN 2022 PNRR Project "*GASCHEM4air – GAS-phase CHEMistry for AIR quality modeling*";

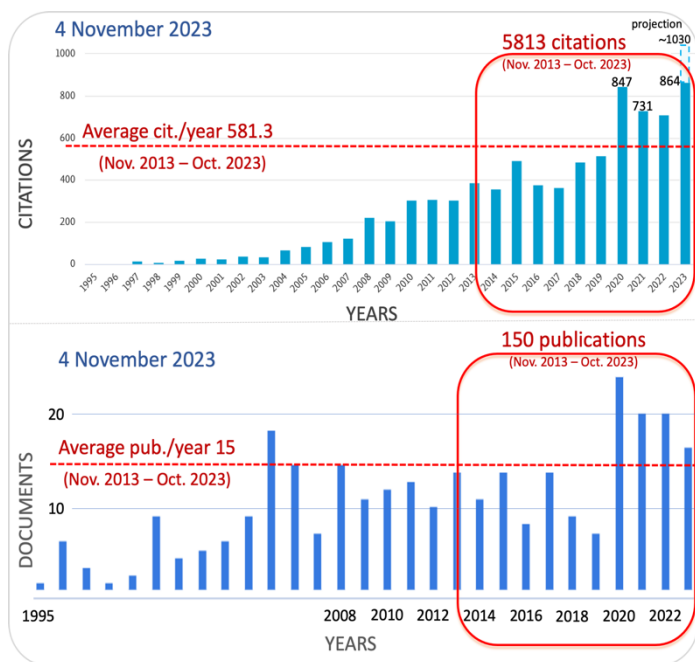
and to the coordination of a local research unit (co-PI) of national projects:

2017-2020 PRIN 2015 Project "STARS in the CAOS (Simulation Tools for Astrochemical Reactivity and Spectroscopy in the Cyberinfrastructure for Astrochemical Organic Species)"

2021-2025 Co-ordination of the project: *Astrochemistry - Materials Under Extreme Conditions: Clues From The Gas Phase*. An INSTM-UniBO-SNS joint PROJECT in the framework of SKIES-VILLAGE (https://www.instm.it/ricerca/cr_instm/schede_cr/village.aspx)

□ PUBLICATIONS, TALKS AND SEMINARS

According to PLOS Biology (*J.P.A. Ioannidis, J. Baas, R. Klavans, K. W. Boyack, "A standardized citation metrics author database annotated for scientific field", doi:10.1371/journal.pbio.3000384*), I am one of the top-100000 world scientists (World's Top 2% Scientists: 62224 in the world, 1289 in Italy), and one of top-200 Italian chemists. According to "August 2021 data-update for "Updated science-wide author databases of standardized citation indicators"" (DOI: 10.17632/btchxktzyw.3): World rank 22438 (**top 1%**). According research.com (<https://research.com/u/cristina-puzzarini>): World rank 12751 (D-index: 45).



Since 1995, I have published about 300 papers [SCOPUS (8/11/2023): 8059 citations, 6146 since 2013; H-index = 44 (49 Google Scholar)], almost all in the areas of high-resolution rotational and computational spectroscopy, quantum chemistry and astrochemistry. In the last five years, I have published more than 90 papers, including several review and perspective articles. The full list of papers is provided below.

I have given more than 130 presentations at scientific meetings (about 90% at international meetings), 78 in the last 10 years and most of them upon invitation. I am frequently chosen to present lectures on the interface between spectroscopy and theory. More and more frequently, I participate or am invited at astrophysical conferences. The full list of talks and seminars is provided below.

□ TEACHING ACTIVITIES

I am fiercely committed to the process and communication of science, and my teaching activities reflect my broad background in both experimental and theoretical chemical physics.

2006 – to date *University of Bologna*: molecular spectroscopy, computational chemistry/spectroscopy, statistical thermodynamics, physical chemistry (kinetics), astrobiology.

2011 – 2013 *Scuola Normale Superiore* (PhD): molecular spectroscopy

2018 – 2021 *Scuola Normale Superiore* (PhD): astrochemistry and molecular astrophysics

2020 – 2022 *IUSS di Pavia* (Corso Ordinario): astrochemistry

Seminar activity for PhD students at *Scuola Normale Superiore* (2017 to date) and *Scuola Superiore Meridionale* (2022 to date).

□ SUPERVISION OF STUDENTS AND POSTDOCTORAL FELLOWS

2006 – to date I have supervised several undergraduate and graduate students as well as postdocs at both my home institution and, since 2015, at *Scuola Normale Superiore di Pisa*.

For the current members of my group see:

<https://site.unibo.it/rotational-computational-spectroscopy/en/people>

□ MAJOR COLLABORATORS

CfA – Harvard-Smithsonian (USA): M.C. McCarthy
CSIC-IFF (Spain): J. Cernicharo
CSIC-INTA (Spain): I. Jiménez-Serra, V.M. Rivilla
MIT (USA): B. McGuire
MPE (Garching, Germany): P. Caselli
MPI (Bonn, Germany): A. Belloche
PoliMI (Italy): C. Cavallotti
Scuola Normale Superiore (Italy): V. Barone
U. Ca'Foscari (Venice, Italy): A. Pietropolli-Charmet, P. Stoppa.
U. Chongqing (China): Q. Gou, G. Feng
U. Florida (USA): J.F. Stanton
U. Hannover (Germany): J.-U. Grabow
U. Kassel (Germany): T. Giesen
U. Mainz (Germany): J. Gauss
U. Maryland (USA): A. Ali, H.D. Drew, T.E. Murphy
U. Paris-Est (France): M. Hochlaf, R. Linguerrri
U. Rennes (France): F. Lique, J.-C. Guillemin
U. Shanghai (China): M. Biczysko
U. Valladolid (Spain): J.L. Alonso

□ ORGANISATION OF INTERNATIONAL SCIENTIFIC MEETINGS

2024 (July 13-21) COSPAR - F3.1, co-Chair, Busan, South Korea
2023 – to date [Member of the International Advisory Committee, *International Symposium on Molecular Spectroscopy*, Urbana-Champaign, IL \(USA\)](#)
2022 (Nov 10-11) Winter Modeling (special edition: 70th birthday V. Barone) 2022bis, co-chair, Naples, Italy.
2022 (July 16-24) COSPAR - F3.1, co-Chair, Athens, Greece
2022 (Jun 27-Jul 1) EAS2022/S9, SOC Member, Valencia, Spain
2022 (Feb 14-15) Winter Modeling (on Valentine day, 2nd edition) 2022, Co-chair, Naples, Italy.
2019 (March 4-8) APS Focus Topic Symposium “Bridging the gap between theory and experiment in gas-phase spectroscopy”, Chair, Boston, USA
2019 (Feb 27-Mar 1) 4th MOLIM Cost General Meeting, Chair, Bologna, Italy
2019 (Feb 14) Winter Modeling (on Valentine day, 1st edition) 2019, Co-chair, Naples, Italy.
2018 (Sept 10-12) Faraday Discussion, Scientific Advisory Board, Edinburgh, UK
2018 (July 14-22) COSPAR - F3.5: The Evolving Universe and the Origin of Life, SOC, Caltech, Pasadena, USA
2018 (June, 25-28) National meeting of the Physical Chemistry Division of the Italian Chemistry Society (SCI), LOC, Bologna, Italy
2018 (June, 13-16) 2nd Italian Workshop on Astrochemistry, Co-chair, Follonica (GR), Italy
2018 (February 15-16) ASTRO-Winter Modeling, Chair, Bologna, Italy
2014 (Nov 23-30) QUITEL 2014, Scientific Advisory Board, Galapagos, Ecuador
2013 (July 2-5) IMAMPC 2013, Scientific Advisory Board, Lille, France
2012 (Sept 12-14) IMAMPC 2012, Chair, Scuola Normale Superiore di Pisa, Italy

□ INSTITUTIONAL / INTERNATIONAL RESPONSIBILITIES

2022 – to date [Vice Chair, COST Action CA21101 “COSY”](#)
2021 – 2023 [Head of the Panel Chemistry, Research Evaluation Committee, U. Bologna, Italy](#)
2021 – to date Member of the Doctoral School Board, MOSES, Scuola Superiore Meridionale, Naples, Italy
2018 – to date Member of the Research Evaluation Committee of the Dept. Chemistry “Giacomo Ciamician”, Univ. Bologna, Italy

- 2018 – 2021 Member of the Doctoral School Board, Astrochemistry, Scuola Normale di Pisa, Italy
- 2016 – 2021 Member of the Admission and Didactics Committee, Master Degree in Chemistry, Dept. Chemistry “Giacomo Ciamician”, Univ. Bologna, Italy
- 2016 – to date Member/President of selection committee for academic positions: national (for assistant-/associate-/full-professor position) and international (U. Leuven 2018, 2019; U. Torun 2021)
- 2014 – 2021 Member of the Research Evaluation Committee, Panel Chemistry, Univ. Bologna, Italy
- 2017 – 2019 Board member, Theoretical and Computational Chemistry Division, Italian Chemistry Society
- 2015 – 2019 Management Committee Member, COST Action CM1405 “MOLIM”
- 2016 – 2018 Member of the Doctoral School Board, Methods and Models for Molecular Sciences, Scuola Normale di Pisa, Italy
- 2012 – 2016 Member of the Admission and Didactics Committee, Master Degree in Photochemistry, Univ. Bologna, Dept. Chemistry “Giacomo Ciamician”, Italy
- 2007 – 2011 Board member, Physical Chemistry Division, Italian Chemistry Society

□ **REVIEWING / EDITORIAL ACTIVITIES**

- 2023 – to date Editorial Advisory Board, *Journal of Physical Chemistry A/B/C*
 - 2022 – to date Editorial Board, *Scientific Reports*
 - 2021 – to date Editorial Board, *Journal of Molecular Spectroscopy*
 - 2020 – to date Chief Editor, *Frontiers Astrochemistry* (section of “Frontiers in Astronomy and Space Sciences”)
 - 2016 – to date Editorial Board, *Journal of Molecular Structure*
 - 2023 NWO: DAN-JWST Assessment Committee
 - 2017 – to date Reviewer of international projects (ERC StG 2021,2023; ACS PRF, NSF & DOE, USA; I-SITE ULNE excellence in research, Univ. Lille-Nord & ANR, France; DFG, Germany; NWO, The Netherlands; SNSF, Swiss; FONDECYT-CHILE, Chile; CYCLONE, Cyprus; NRD, Hungary; OSF, Poland)
 - 2010 – to date Reviewer of the Assessment of Quality in Scientific Research (VQR)
 - 2010 – to date Reviewer of national MUR projects (PRIN, FIRB, SIRI)
 - 2010 – 2013 Editorial Board, *Journal of Molecular Spectroscopy*
- I regularly serve as a reviewer for ACS (JPCA, JPCL, JCTC, ACS Earth Space Chem., JACS); RSC (PCCP, Chem. Comm.); Elsevier (JQSRT, JMS, JMStruct, New Astronomy); Wiley-VCH (Angew. Chem., IJQC, Chem. Eur. J.); AIP (JCP); AAS (Astrophys. J., Astrophys. J. Lett., Astrophys. J. Suppl. Ser.); Astron. Astrophys.; MNRAS.

Guest editor:

- PCCP themed issue (2019 - Challenges in spectroscopy: accuracy versus interpretation from isolated molecules to condensed phases)
- PCCP themed collection (2022 - Stability and properties of new-generation metal and metal-oxide clusters down to the subnanometer scale: synthesis, experimental characterization, and theory)
- JPCA (2022 - Vincenzo Barone Festschrift: honoring his 70th birthday)
- Molecules (2023 - Spectroscopic and Theoretical Methods to Investigate Interstellar Medium)

□ **MEMBERSHIPS OF SCIENTIFIC SOCIETIES**

- 2019 Co-founder of the Italian Institute of Astrobiology (<https://astrobiologia.weebly.com/istituto-astrobiologico-italiano.html>)
- 2016 – to date Associated Member, INAF, Italy
- 2014 – to date Associated Member, INFN, Italy
- 2009 – to date Associated Member, INSTM Consortium, Italy
- 2012 – to date Member of American Chemical Society (ACS)

2007 – to date Member of Italian Chemical Society (SCI)

2015 – 2019 Member, COST Action CM1401 “Our Astro-Chemical History”

□ **CARRIER BREAK**

2006 (Jul 8 – Dec 8) Maternity leave (5 months)

FULL LIST OF PUBLICATIONS

Book Chapters:

- 8bc}** C. Puzzarini, V. Barone, "Interstellar Complex Organic Molecules: A Step Toward Biomolecule Building Blocks in the Skies" in *Prebiotic Photochemistry: From Urey–Miller-like Experiments to Recent Findings*, F. Saija, G. Cassone (Eds.), RCS (2021), chapter 10, pp 195-218 (<https://doi.org/10.1039/9781839164354>).
- 7bc}** V. Barone, C. Puzzarini, "Interpretability meets Accuracy in Computational Spectroscopy: The Virtual Multifrequency Spectrometer" in *Molecular Spectroscopy: A Quantum Chemistry Approach*, M. Wojcik, Y. Ozaki, J. Popp (Eds.), Wiley (2019), pp 1-42.
- 6bc}** C. Puzzarini, "Structure Prediction", Reference Module in Chemistry, Molecular Sciences and Chemical Engineering (2015) <http://dx.doi.org/10.1016/B978-0-12-409547-2.10884-4>
- 5bc}** C. Puzzarini, M. Biczysko, "Computational spectroscopy tools for molecular structure analysis" in *Tools in Structure Determination of Organic Molecules and Complexes*, Magdalena Cid (Ed.), Wiley (2015) pp 27-64.
- 4bc}** C. Puzzarini, "Computational Astrochemistry and Molecular Astrophysics", Reference Module in Chemistry, Molecular Sciences and Chemical Engineering (2014) <http://dx.doi.org/10.1016/B978-0-12-409547-2.10836-4>
- 3bc}** C. Puzzarini, "Computational Approach to Rotational Spectroscopy" in *Computational Strategies for Spectroscopy: from Small Molecules to Nano Systems*, Vincenzo Barone (Ed.), Wiley (2011) pp 263-307.
- 2bc}** G. Cazzoli, C. Puzzarini, G. Buffa, O. Tarrini, "Pressure-broadening of the 22.2 GHz line of Water: basic results for Remote Sensing of the Atmosphere", in *Remote Sensing of the Atmosphere for Environmental Security*, NATO ARW Series, Series C: Environmental Security, A. Perrin, N. Ben Sari-Zizi and J. Demaison (Eds.), Springer (2006), pp 237-255.
- 1bc}** C. Puzzarini, "How accurately can structural, spectroscopic and thermochemical properties be predicted by ab initio computations?", Lecture Series on Computer and Computational Science, **6** (2006), 416. (Edited by G. Maroulis and T. Simons, Brill Academic Publisher)

Research articles:

- 299}** M. Melosso, S. Alessandrini, L. Spada, A. Melli, X. Wang, Y. Zheng, C. Duan, J. Li, W. Du, Q. Gou, L. Bizzocchi, L. Dore, V. Barone, C. Puzzarini
"Rotational spectra and semi-experimental structures of furonitrile and its water cluster"
Phys. Chem. Chem. Phys, in press (2023) DOI: [10.1039/d3cp03984f](https://doi.org/10.1039/d3cp03984f)
- 298}** F. Tonolo, L. Bizzocchi, V. M. Rivilla, F. Lique, M. Melosso, C. Puzzarini
"Collisional excitation of PO⁺ by para-H₂: Potential Energy Surface, Scattering Calculations and Astrophysical Applications"
MNRAS, in press (2023) DOI: [10.1093/mnras/stad3140](https://doi.org/10.1093/mnras/stad3140)
- 297}** C. Puzzarini*, R. Linguetti*, M. Hochlaf*
"Insights into the molecular structure and spectroscopic properties of HONCO: An accurate ab initio study"
J. Phys. Chem. A, in press (2023) DOI: [10.1021/acs.jpca.3c05741](https://doi.org/10.1021/acs.jpca.3c05741)
- 296}** N. Balucani, M. Brann, S. Brünken, C. Ceccarelli, M. Cordiner, E.M. Crump, K.M. Douglas, A.J. Fleisher, A. Flint, J. Fulker, R.T. Garrod, M.S. Gudipati, D. Gupta, J. Halpern, D.E. Heard, E. Herbst, E.K. Hockey, K.-Y. Huang, U. Jacovella, I. Kamp, A.K. Lemmens, N. Madhusudhan, M.R.S. McCoustra, B. McGuire, A. Meijer, C. Puzzarini, D.B. Rap, I.R. Sims, M.H. Stockett, A. Sturm, A.G. Suits, E. F. van Dishoeck, S. Viti, N. Walker, S. Widicus Weaver, L. Wiesenfeld, O.H. Wilkins
"Laboratory astrochemistry of the gas phase: general discussion"
Farad. Discuss. **245** (2023) 391
- 295}** C. Puzzarini*, S. Alessandrini, L. Bizzocchi*, M. Melosso*
"Hunting for interstellar molecules: Rotational spectra of reactive species"
Farad. Discuss. **245** (2023) 309
- 294}** H. Ye, S. Alessandrini*, C. Puzzarini*
"Gas-phase formation route for *trans*-HC(O)SH and its isomers under interstellar conditions: A state-of-the-art quantum-chemical study"
MNRAS **525** (2023) 1158
- 293}** C. Puzzarini*, S. Alessandrini, L. Bizzocchi, M. Melosso, V.M. Rivilla
"From the laboratory to the interstellar medium: A strategy to search for exotic molecules in space"
Front. Astron. Space Sci. **10** (2023) 1211784

- 292}** P. Stoppa, A. Pietropolli Charmet, F. Tamassia, E. Cané, M. Melosso, A. Achilli, L. Dore, [C. Puzzarini](#), “High resolution FTIR spectrum of CH₂D³⁷Cl: ν_4 and ν_8 fundamental bands”
J. Quantit. Spectrosc. Radiat. Transfer **309** (2023) 108703
- 291}** N. Marcelino, [C. Puzzarini](#), M. Agúndez, R. Fuentetaja, B. Tercero, P. de Vicente, J. Cernicharo
“First detection in space of the HSO radical”
Astron. Astrophys. (Letter) **674** (2023) L13
- 290}** A. Pietropolli Charmet, P. Stoppa, A. De Lorenzi, M. Melosso, A. Achilli, L. Dore, [C. Puzzarini](#), E. Cané, F. Tamassia
“Computational, rotational and ro-vibrational experimental investigation of monodeuterated Chloromethane”
J. Quantit. Spectrosc. Radiat. Transfer **305** (2023) 108624
- 289}** M. Melosso,* N. Jiang, J. Gauss, [C. Puzzarini](#),*
“Hyperfine-resolved spectra of HDS together with a global ro-vibrational analysis”
J. Chem. Phys. **158** (2023) 174310
- 288}** V. Barone,* M. Fusè, R. Aguado, S. Potenti, I. León, E. R. Alonso, S. Mata, F. Lazzari, G. Mancini, L. Spada, A. Gualandi, P. G. Cozzi, [C. Puzzarini](#),* J. L. Alonso*
“Bringing Machine-Learning Enhanced Quantum Chemistry and Microwave Spectroscopy to Conformational Landscape Exploration: The Paradigmatic Case of 4-Fluoro-Threonine”
Chem. Eur. J. **29** (2023) e202203990
- 287}** V. Barone*, [C. Puzzarini](#)*
“Gas-phase Computational Spectroscopy: The Challenge of Molecular Bricks of Life”
Ann. Rev. Phys. Chem. **74** (2023) 29
- 286}** M.P. de Lara-Castells,* [C. Puzzarini](#),* V. Bonačić-Koutecky,* M.A. López-Quintela,* S. Vajda
“Stability and properties of new-generation metal and metal-oxide clusters down to subnanometer scale”
Phys. Chem. Chem. Phys. **25** (2023) 15081
- 285}** S. Alessandrini*, M. Melosso, V.M. Rivilla, L. Bizzocchi, [C. Puzzarini](#),*
“Computational Protocol for the Identification of Candidates for Radioastronomical Detection and its Application to the C₃H₃NO Family of Isomers”
Molecules **28** (2023) 3226
- 284}** J.-T. Spaniol, K. L. K. Lee, O. Pirali, [C. Puzzarini](#)*, M.-A. Martin-Drumel*
“A rotational investigation of the three isomeric forms of cyanoethynylbenzene (HCC-C₆H₄-CN): Benchmarking experiments and calculations using the "Lego brick" approach”
Phys. Chem. Chem. Phys. **25** (2023) 6397
- 283}** N. Jiang, M. Melosso*, S. Alessandrini, L. Bizzocchi, M.-A. Martin-Drumel, O. Pirali, [C. Puzzarini](#)*
“Insights into the molecular structure and infrared spectrum of the prebiotic species aminoacetonitrile”
Phys. Chem. Chem. Phys. **25** (2023) 4754
- 282}** S. Alessandrini, L. Bizzocchi, M. Melosso, [C. Puzzarini](#)
“Protonation of apolar species: from Cl₂H⁺ to (E)-NCCCHCHCNH⁺ through computational investigations”
Front. Astron. Space Sci. **10** (2023) 1128896
- 281}** [C. Puzzarini](#)*, J.F. Stanton
“Connections between the accuracy of rotational constants and equilibrium molecular structures”
Phys. Chem. Chem. Phys. **25** (2023) 1421
- [[invited review article: “Benchmark Experiments for Numerical Quantum Chemistry”](#)]
- 280}** V. Barone, S. Di Grande, [C. Puzzarini](#)*
“Toward accurate yet effective computations of rotational spectroscopy parameters for biomolecule building blocks”
Molecules, **28** (2023) 913
- 279}** D. Alberton, L. Bizzocchi, N. Jiang, M. Melosso, V. M. Rivilla, A. Pietropolli Charmet, B.M. Giuliano, P. Caselli, [C. Puzzarini](#), S. Alessandrini, L. Dore, I. Jiménez-Serra, J. Martín-Pintado
“Laboratory spectroscopy of allylimine and tentative detection towards the G+0.693-0.027 molecular cloud”
Astron. Astrophys. **669** (2023) A93
- 278}** [C. Puzzarini](#)*, M. Biczysko*, L. Gagliardi*
“A tribute to Vincenzo Barone”
J. Phys. Chem. A **126** (2022) 9141
[[introduction to the Vincenzo Barone special issue](#)]
- 277}** M.L. Diouf, R. Tobiás, F.M. J. Cozijn, E.J. Salumbides, C. Fábri, [C. Puzzarini](#), A.G. Császár, W. Ubachs
“Parity-pair-mixing effects in nonlinear spectroscopy of HDO”

Opt. Express **30** (2022) 46040

276} P. Recio, S. Alessandrini, G. Vanuzzo, G. Pannacci, A. Baggioli, D. Marchione, A. Caracciolo, V.J. Murray, P. Casavecchia, N. Balucani, * C. Cavallotti, * C. Puzzarini, * V. Barone*

“Intersystem-Crossing in the Entrance Channel without Heavy Atoms: the reaction of O(³P) with pyridine”

Nature Chem. **14** (2022) 1405

275} S.B. Howell, V. Izmodenov, S.M. Kopeikin, P. Marziani, C. Puzzarini, M. Rengel, S.W. McIntosh, D. Fraix-Burnet, I. Kanik

“Editorial: Frontiers in astronomy and space sciences: Rising stars”

Front. Astron. Space Sci. **9** (2022) 991696

274} H. Ye, S. Alessandrini, M. Melosso, C. Puzzarini*

“Exploiting the “Lego brick” approach to predict accurate molecular structures of PAHs and PANHs”

Phys. Chem. Chem. Phys. **24** (2022) 23254

[*selected as 2022 PCCP HOT Article*]

273} F. Tonolo, F. Lique, M. Melosso, C. Puzzarini, L. Bizzocchi*

“Hyperfine resolved rate coefficients of HC¹⁷O⁺ with H₂ (*j* = 0)”

MNRAS **516** (2022) 2653

272} A. Melli, M. Melosso*, L. Bizzocchi, S. Alessandrini, N. Jiang, F. Tonolo, S. Boi, G. Castellan, C. Sapienza, J.-C. Guillemin, L. Dore, C. Puzzarini*

“Rotational Spectra of Unsaturated Carbon-Chains Produced by Pyrolysis: The Case of Propadienone, Cyanovinylacetylene, and Allenylacetylene”

J. Phys. Chem. A **126** (2022) 6210

271} I. León, M. Fusè, E.R. Alonso, S. Mata, G. Mancini, C. Puzzarini, J.L. Alonso, V. Barone

“Unbiased disentanglement of conformational baths with the help of microwave spectroscopy, quantum chemistry and artificial intelligence: the puzzling case of homocysteine”

J. Chem. Phys. **157** (2022) 074107

270} I. Jimenez-Serra, L.F. Rodriguez-Almeida, J. Martin-Pintado, V.M. Rivilla, M. Melosso, S. Zeng, L. Colzi, Y. Kawashima, E. Hirota, C. Puzzarini, B. Tercero, P. de Vicente, F. Rico-Villas, M.A. Requena-Torres, S. Martin

“Precursors of fatty alcohols in the ISM: Discovery of n-propanol”

Astron. Astrophys. **662** (2022) A181

269} S.W. McIntosh, P. Marziani, C. Puzzarini, S.B. Howell

“Editorial: Horizons in Astronomy and Astrophysics”

Front. Astron. Space Sci. **9** (2022) 951370

268} L. Bizzocchi, S. Alessandrini, M. Melosso, C. Puzzarini*

“Dipolar spin-spin coupling as auxiliary tool for structure determination of small isolated molecules”

Phys. Chem. Chem. Phys. **24** (2022) 15173

[*invited review article*]

267} A. Melli, M. Melosso*, K.G. Lengsfeld, L. Bizzocchi, V.M. Rivilla, L. Dore, V. Barone, J.-U. Grabow, C. Puzzarini*

“Spectroscopic Characterization of 3-Aminoisoxazole, a Prebiotic Precursor of Ribonucleotides”

Molecules **27** (2022) 3278

266} V.M. Rivilla, L. Colzi, I. Jimenez-Serra, J. Martín-Pintado, A. Megías, M. Melosso, L. Bizzocchi, A. Lopez-Gallifa, A. Martinez-Henares, S. Massalkhi, B. Tercero, P. de Vicente, J.-C. Guillemin, J.G. de la Concepcion, F. Rico-Villas, S. Zeng, S. Martín, M. A. Requena-Torres, F. Tonolo, S. Alessandrini, L. Dore, V. Barone, C. Puzzarini.

“Precursors of the RNA-world in space: Detection of (Z)-1,2-ethenediol in the interstellar medium, a key intermediate in sugar formation”

Astrophys. J. Lett. **929** (2022) L11

265} N. Jiang, M. Melosso*, L. Bizzocchi, S. Alessandrini, J.-C. Guillemin, L. Dore, C. Puzzarini*

“Spectroscopic and Computational Characterization of 2-Aza-1,3-butadiene, a Molecule of Astrochemical Significance”

J. Phys. Chem. A **126** (2022) 1881

264} M. Melosso*, L. Bizzocchi, H. Gazzeh, F. Tonolo, J.-C. Guillemin, S. Alessandrini, V. M. Rivilla, L. Dore, V. Barone, C. Puzzarini*

“Gas-phase identification of (Z)-1,2-ethenediol, a key prebiotic intermediate in the formose reaction”

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- 262}** V. Barone, [C. Puzzarini](#)
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“Synchrotron-based far-infrared spectroscopy of HC₃N: extended ro-vibrational analysis and new line list up to 3360 cm⁻¹”
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- 260}** L. Bizzocchi, S. Alessandrini, M. Melosso, V. M. Rivilla, [C. Puzzarini*](#)
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- 259}** X. Li, L. Spada, S. Alessandrini, Y. Zheng, K.G. Lengsfeld, J.-U. Grabow, G. Feng, [C. Puzzarini](#), V. Barone
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- 258}** F. Tonolo, L. Bizzocchi*, M. Melosso, F. Lique*, L. Dore, V. Barone, [C. Puzzarini*](#)
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- 257}** J. García de la Concepción*, [C. Puzzarini*](#), V. Barone*, I. Jiménez-Serra, O. Roncero
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Astrophys. J. **922** (2021) 169
- 256}** A. Melli, F. Tonolo, V. Barone*, [C. Puzzarini*](#)
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Phys. Life Rev. **37** (2021) 65
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- 240}** S. Alessandrini, F. Tonolo, C. Puzzarini
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“A computational journey in the CH₂O₂S land: an accurate rotational and ro-vibrational analysis of the sulfene molecule and the O,S- and O,O-monothiocarbonic acids”

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[*Invited Article: Special Issue in honor of prof. J. Gauss*]

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“The Italian national project of astrobiology-life in space-origin, presence, persistence of life in space, from molecules to extremophiles”

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“The role of state-of-the-art quantum-chemical calculations in astrochemistry: formation route and spectroscopy of ethanimine as a paradigmatic case”

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[*Special Issue "From Molecules to Origin of Life: The Astrobiology Network"*]

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“Grand Challenges in Astrochemistry”

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[*Speciality Grand Challenge*]

224} C. Puzzarini*, V. Barone

“Collisional broadening and hyperfine structure of rotational transitions. Reply to the comments on “A never-ending story in the sky: The secrets of chemical evolution””

Phys. Life Rev. **32** (2020) 124

223} C. Puzzarini*, V. Barone*

“A never-ending story in the sky: The secrets of chemical evolution”

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222} Z. Salta, N. Tassinato, J. Lupi, R. Boussessi, A. Balbi, C. Puzzarini, V. Barone
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- 9}** C. Degli Esposti, L. Bizzocchi, F. Tamassia, C. Puzzarini, R. Tarroni, Z. Zelinger
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- 1}** E. Canè, C. Puzzarini, R. Tarroni, A. Trombetti

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Technical reports

1} J. Demaison, S. Buehler, N. Koulev, T. Kuhn, C. Verdes, G. Cazzoli, L. Dore, C. Puzzarini, J.-M. Flaud, A. Perrin, B. Bakri, J.-M. Colmont, F. Rohart, G. Wlodarczak,
"Characterization of millimetre-wave spectroscopic signatures",
Final Report, ESA Contract N. 16377/02/NL/FF, ESTEC (2004).

2} C. Puzzarini,

"Triatomic molecules, radicals and ions: how accurate can ab initio calculations be?",

In "*Science & Supercomputing @ CINECA, Report 200*", p. 183.

(Eds.: M. Voli and P. Coluccia; Monograf s.r.l.; Bologna; 2006).

3} A. Gambi, C. Puzzarini,

"Theoretical Investigations of H₂CN₂ molecule, HCN₂ radicals and their Ions",

In "*Science & Supercomputing @ CINECA, Report 2005*", p. 261.

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LIST OF TALKS

Invitations received for 2024:

Invited talk, *QAMTS - XXFst International Workshop on Quantum Atomic and Molecular Tunneling Systems*, 16-21 June 2024, Donostia-San Sebastián (Basque Country), Spain.

Invited talk, *NanoSpace COST Action – 1st WG2 meeting*, 20-23 February 2024, Edinburgh, UK.

Invited talk, *Gordon Research Conference “Molecular and Ionic Clusters”*, 4-9 February 2024, Ventura (CA), USA.

Invited talk, *The Path of Quantum Chemistry into the 21st Century – Symposium Celebrating Prof. Roland Lindh's 65th Birthday*, 16-18 January 2024, ETH Zurich, Switzerland.

Invitations received for 2023:

Invited talk, *Life And Space Conference (LAS 2023)*, 1-3 December 2023, online (Polish Astrobiology Society).

132} *Workshop on Interstellar Matter*, 8-10 November 2023, Sapporo, Japan.

Invited talk: “From the lab to space: An integrated rotational spectroscopy–quantum chemistry strategy”

131} *The van der Waals and London Discussions*, 26-27 October 2023, University of Strasbourg, France.

Plenary lecture: “Accurate structural, energetic and spectroscopic characterization of non-covalent interactions”

130} *Summer Modeling 2023*, 23-30 September 2023, Riva del Sole, Castiglione della Pescaia, Italy

Plenary lecture: “The Role of Quantum Chemistry in Rotational Spectroscopy”

129} *DCTC 2023 - VIII Congresso Nazionale della Divisione di Chimica Teorica e Computazionale della SCI*, 20 - 22 September 2023, Scuola Normale Superiore, Pisa, Italy

Invited talk: “Unveiling exotic chemistry and molecules in the interstellar medium: The role of quantum-chemical calculations”

128} *The 28th Colloquium on High-Resolution Molecular Spectroscopy*, 28 August – 1 September 2023, Dijon, France

Plenary lecture: “Astrochemical challenges: The role of rotational spectroscopy”

127} *ACS Fall 2023 ACS National Meeting - Symposium "The Astrochemistry Subdivision: A Decade of Progress and Prospects for the Next Decade"*, 13-17 August 2023, San Francisco, USA.

Invited talk: “From the lab to space: An integrated rotational spectroscopy–quantum chemistry strategy”

125-126} *76th International Symposium on Molecular Spectroscopy*, 19-23 June 2023, Urbana-Champaign, Illinois (USA)

Oral communication: “Rotational spectroscopy of reactive species in support of the detection of interstellar molecules”

Oral communication: “Insights into the infrared spectrum of a prebiotic species: the case of aminoacetonitrile”

Co-author of one other oral contribution

124} *VII Convegno Nazionale della Società di Astrobiologia*, 12-15 June 2023, Sala Marconi – CNR, Roma.

Oral communication: “Hunting for Prebiotic Molecules in the Interstellar Medium”

123} *Astrochemistry at high resolution Faraday Discussion*, 31 May – 2 June, Space Telescope Science Institute, Baltimore, Maryland (USA).

Oral communication: “Rotational spectra of reactive molecules produced by pyrolysis”

122} *1st General Meeting COSY COST Action*, 1-3 March 2023, Cádiz (Spain)

Invited talk: “Astrochemical challenges: the interplay of quantum chemistry and rotational spectroscopy”

121} *Winter Modeling 2023 – New Frontiers in Astrochemistry and Astrobiology*, 23-24 February 2023, Napoli, Italy

Invited talk: “From the lab to space: In search of building blocks of life”

120} *28th Austin Symposium on Molecular Structure and Dynamics at Dallas (ASMD@D) “Spectroscopy meets Theory”*, 18-20 February 2023, Dallas, USA

Plenary lecture: “Detection of molecules in the interstellar medium: Unstable species produced by pyrolysis”

119} *62nd Sanibel Symposium: The Theory Meeting for Theoreticians*, 12-17 February 2023, St. Augustine Beach, FL, USA

Invited talk: “Astrochemical challenges: the role of quantum chemistry”

118} *International Winter School on Origins of Life – WISOL 23*, 16-19 January 2023, Pavia, Italy

Invited talk: “From the lab to space: the building blocks of prebiotic molecules”

117} *COSY WG1-WG5 meeting*, 15 December 2022 (Virtual)

Invited talk: “Rotational spectroscopy and chemical reactivity in Astrochemistry: experiment and theory”

116} *DIG (Dust, Ice and Gas) Astrochemistry*, 17-18 November 2022 (Virtual)

Invited talk: “Rotational spectroscopy and chemical reactivity in Astrochemistry: experiment and theory”

115} *Ischia Summer Modeling Challenges of molecular sciences towards 2030*, 5-7 September 2022, Ischia (NA), Italy

Invited speaker: “Astrochemical challenges: the role of quantum chemistry”

114} *Opera-2020 (Operators, Perturbations, Electrons, Relativity, and Multi-Scale Applications) – A symposium in honor of professor J. Gauss*, 31 August - 2 September 2022, Ingelheim am Rhein, Germany

Invited speaker: “Hyperfine structure of rotational spectra: the pioneering work of Jürgen Gauss”

113} *ACS National Fall Meeting 2022 – Symposium “Inorganic and Organometallic Astrochemistry”*, 21-25 March 2022, Chicago, Illinois (USA)

Invited speaker: “Detection of molecules in the interstellar medium: the role of rotational spectroscopy and quantum chemistry”

112} *Conference on Chemistry and Physics at Low Temperatures*, 3-8 July 2022, Visegrád, Hungary

Invited speaker: “Rotational spectroscopy and chemical reactivity in Astrochemistry: experiment and theory”

110-111} “75th International Symposium on Molecular Spectroscopy”, 20-24 June 2022, Urbana-Champaign, Illinois (USA)

Oral communication: “Prebiotic molecules in interstellar space: the role of rotational spectroscopy and quantum-chemical calculations”

Oral communication: “The “LEGO brick” approach at work: a cost-effective strategy for predicting accurate rotational constants”

Co-author of other 8 oral contributions

109} *COSYES Summer and Live Meeting 2022*, 2-3 June 2022, CSIC, Madrid, Spain

Invited speaker: “Accurate quantum-chemical composite schemes for interaction energies”

108} *ACS National Meeting 2022 – “The Synergy of Theory and Experiment: A symposium in honor of Prof. John F. Stanton”*, 20-24 March 2022, San Diego, CA (online)

Invited speaker: “The Synergy of Theory and Experiment in Astrochemistry”

107} *PacifiChem 2021 “Misconceptions in Astrochemistry: A Chemist’s Guide”*, 16-21 December 2021 (Honolulu, Hawaii - VIRTUAL)

Invited speaker: “Challenges in astrochemistry: an integrated rotational spectroscopy–quantum chemistry strategy”

106} *Workshop on Interstellar Matter 2021 (Tokyo/VIRTUAL)*, 17-18 November 2021

Oral communication: “Theory and Experiment for Elucidating Chemical Evolution in Space”

105} *International Symposium on Molecular Spectroscopy - VIRTUAL*, 21-25 June 2021.

Oral communication: “Improved centrifugal and hyperfine analysis of ND₂H and NH₂D and its application to the spectral line survey of L1544”

Co-author of other 8 oral contributions

104} *1st Italian Space Agency workshop on Astrobiology*, 27-29 October 2020, ONLINE.

Oral communication: “Theory Meets Experiment for Elucidating Chemical Evolution in Space”

103} *Gordon Research Conference ‘Molecular and Ionic Clusters’*, 26-31 January 2020, Ventura Beach Marriott, Ventura (CA), USA.

Invited speaker: “Accurate Structural and Spectroscopic Characterization of Molecular Complexes by Rotational Spectroscopy”

102} *Workshop “DYMCOM - DYNAmical Methods for COld Molecular collisions, from laboratory to beyond the Earth*, 4-29 November 2019, l’Université Paris-Saclay, Paris, France.

Invited speaker: “The challenge of ions, radicals and unstable species in space: A joint molecular spectroscopy – quantum chemistry approach”

101} *WE-Heraeus Seminar: The chemical evolution of cosmic matter*, 23-25 October 2019, Bad Honnef, Germany.

Invited speaker: “Rotational Spectroscopy, Quantum Chemistry and the Astrochemical Challenges”

100} *10th Congress of the International Society of Theoretical Chemical Physics (ISTCP) - scientific track: ‘Computational Spectroscopy: From X-rays to microwaves’*, 11-17 July 2019, Tromsø, Norway.

Invited speaker: “Rotational Spectroscopy Meets Quantum Chemistry for Elucidating Astrochemical Challenges”

99} “CECAM workshop - Atomistic simulations in prebiotic chemistry – a dialog between experiment and theory”, 1-3 July 2019, Paris, France.

Invited speaker: “Rotational Spectroscopy Meets Quantum Chemistry for Elucidating Astrochemical Challenges”

98} *28th International Symposium on Molecular Beams*, 23-28 June 2019, Edinburgh, UK.

Invited speaker: “Accurate spectroscopic characterization of molecular complexes as a first step toward the understanding of intermolecular interactions”

97} “*74th International Symposium on Molecular Spectroscopy*”, 17-21 June 2019, Urbana-Champaign, Illinois (USA).

Plenary speaker: “The renaissance of rotational spectroscopy: theory meets experiment for new challenges”

96} “*LAU Symposium 350. Laboratory Astrophysics: from Observations to Interpretation*”, 14-19 April 2019, Jesus College, Cambridge, UK.

Invited speaker: “Prebiotic molecules in interstellar space: rotational spectroscopy and quantum chemistry”

95} Focus symposium “*Gas phase clusters - experiment and theory in concert*”, APS meeting, 4-8 March 2019, Boston, USA

Invited speaker: “Accurate Spectroscopic Characterization of Molecular Complexes as a First Step Toward the Understanding of Intermolecular Interactions in Condensed Phase”

94} “Molim COST action working group 3 workshop - Ab-Initio Modelling of Molecular Processes Under Confinement”, 3-5 December 2018, CSIC, Madrid (Spain)

Invited speaker: “Accurate Spectroscopic Characterization of Molecular Complexes as a First Step Toward the Understanding of Intermolecular Interactions in Condensed Phase”

93} “*6th International Conference on Vibrational Optical Activity*”, 9-13 September 2018, Brescia (Italy)

Invited speaker: “From chiral ACOMs to the origin of life: a quantum chemical and spectroscopic journey”

91-92} “*73rd International Symposium on Molecular Spectroscopy*”, 18-22 June 2018, Urbana-Champaign, Illinois (USA)

Oral communication: “Prebiotic molecules in interstellar space: rotational spectroscopy of cyanomethanimine and ethanimine”

Oral communication: “VMS-ROT: a new module of the virtual multifrequency spectrometer for simulation, interpretation, and fitting of rotational spectra”

89-90} “*255th ACS National Meeting – Symposium: Quantum Chemistry, Dynamics and Reaction Modeling for Molecules and Materials in Astrophysical Environments*”, 18-22 March 2018, New Orleans (USA)

Oral communication: “Spectroscopic characterization of key aromatic and heterocyclic molecules: A route toward the origin of life”

Oral communication: “State-of-the-art thermochemical and kinetic computations for complex organic molecules: Gas-phase formation routes in cold interstellar clouds”

88} “*27th Austin Symposium on Molecular Structure and Dynamics*”, 3-5 March 2018, Dallas (USA)

Invited speaker: “Prebiotic molecules in interstellar space: rotational spectroscopy and quantum Chemistry”

87} “ERC AdG – Barone – DREAMS: final meeting Advances in computational modelling: from isolated molecules to soft matter”, 29 November -2 December 2017, Pisa (Italy)

Invited speaker: “Modeling of isolated molecules: a joint computational-spectroscopic approach”

86} “*XVII International Conference on Science, Arts and Culture - SAILING THROUGH THE WONDERS OF ASTROBIOLOGY*”, 25-29 September 2017, Veli Lošinj (Croatia)

Invited speaker: “Prebiotic molecules in interstellar space: rotational spectroscopy and quantum chemistry”

85} “*XXVI Congresso Nazionale della Società Chimica Italiana*”, 10-14 September 2017, Paestum (SA, Italy)

Oral communication: “Astrochemistry: A computational spectroscopy’s view”

83-84} “*254th ACS National Meeting – Symposium: Molecules in Space: Linking the Interstellar Medium to (Exo)-Planets*”, 20-24 August 2017, Washington DC (USA)

Oral communication: “New virtual tools for astrochemistry”

Oral communication: “Rotational spectroscopy as a tool to investigate molecules in space: Laboratory measurements and quantum-chemical calculations.”

81-82} “*72nd International Symposium on Molecular Spectroscopy*”, 19-23 June 2017, Urbana-Champaign, Illinois (USA)

Oral communication: “Zeeman effect in sulfur monoxide: a probe to observe magnetic fields in star forming regions?”

Oral communication: “Non-covalent interactions and internal dynamics in pyridine-ammonia: a combined quantum-chemical and microwave spectroscopy study”

80} “*The quantum world of molecules: from orbitals to spin networks*”, 27-28 April 2017, Accademia dei Lincei, Roma (Italy)

Invited speaker: “Spectroscopic accuracy: the role of electron correlation and basis sets”
79} “*DREAMS@ANACAPRI Development of a Research Environment for Advanced Modelling of Soft Matter*”, 20-22 April 2017, Anacapri (Italy)

Invited speaker: “Accurate Quantum-Chemical Calculations of Building-Blocks of Biomolecules”
78} “*Molecular Properties and Computational Spectroscopy - From Esoteric Effects to Novel Probing Tools - MPCSI7*”, 10-12 April 2017, CNR Pisa (Italy)

Invited speaker: “Molecular Properties: A Joint Quantum-Chemistry and Rotational Spectroscopy Approach”
77} “*European Conference on Laboratory Astrophysics - ECLA2016 'Gas on the Rocks'*”, 21-25 November 2016, CSIC, Madrid (Spain)

Oral communication: “Sulfur-bearing molecular species: Rotational spectroscopy and quantum-chemical computations at the LMSB”
76} “*2nd MOLIM General Meeting*”, 10-12 October 2016, Dubrovnik (Croatia)

Invited speaker: “Astronomical complex organic molecules in space: the crucial frequency information from rotational spectroscopy”
75} “*Workshop - Laboratory Astrophysics*”, 28-30 September 2016, Tagungstätte Schloss Ringberg, Kreuth (Germany)

Oral communication: “Sulfur-bearing molecular species: Rotational spectroscopy and quantum-chemical computations at the LMSB”
74} “*10th Congress on Electronic Structure: Principles and Applications (ESPA2016)*”, 28 June - 1 July 2016, Castellón (Spain)

Keynote speaker: “Extending the molecular size in accurate quantum-chemical calculations: The equilibrium structure and spectroscopic properties of building-blocks of biomolecules”
71-73} “*71st International Symposium on Molecular Spectroscopy*”, 20-24 June 2016, Urbana-Champaign, Illinois (USA)

Oral communication: “Hyperfine structure in rotational spectra of deuterated molecules: The HDS and ND₃ case studies”

Oral communication: “Measurements @ mm-/sub-mm-wave spectroscopy laboratory of Bologna: Rotational spectroscopy applied to atmospheric studies”

Oral communication: “Quantum chemistry meets rotational spectroscopy for astrochemistry: Increasing the molecular complexity”
70} “*1st Italian Workshop on Astrochemistry: Astronomical Complex Organic Molecules in different environments*”, 10 - 11 March 2016, Firenze (Italy)

Invited speaker: “Astronomical complex organic molecules in space: the crucial frequency information from rotational spectroscopy”
69} “*26th Austin Symposium on Molecular Structure and Dynamics at Dallas*”, 5 - 7 March 2016, Dallas (TX, USA)

Invited speaker: “Measurements @ mm-/sub-mm-wave Spectroscopy Laboratory of Bologna: rotational spectroscopy applied to astrochemistry”
68} “*Winter Modeling 2015 – Complex Molecular Systems: Accuracy and Interpretation*”, 18 December 2015, Pisa (Italy)

Oral communication: “Quantum Chemistry Meets Spectroscopy for Astrochemistry: Increasing Complexity toward Prebiotic Molecules”
67} “*Congresso Nazionale della Divisione di Chimica Teorica e Computazionale*”, 14-16 December 2015, Roma (Italy)

Keynote speaker: “Quantum Chemistry Meets Rotational Spectroscopy for Astrochemistry: Increasing Complexity toward Prebiotic Molecules”
66} “*Colloquium: Theory of Gas Phase Scattering and Reactivity for Astrophysics*”, 26-27 November 2015, Max-Planck-Institut für extraterrestrische Physik, Garching (Germany)

Invited speaker: “Rotational spectroscopy as a tool to investigate molecules in space”
65} “*5th Workshop of the Italian Astrobiology Society: Life in a Cosmic Context*”, 15-17 September 2015, Trieste (Italy)

Oral communication: “Quantum Chemistry Meets Spectroscopy for Astrochemistry: Increasing Complexity toward Prebiotic Molecules”
64} “*New Developments in Coupled-Cluster Theory*”, 3-7 August 2015, Telluride, Colorado (USA)

Invited speaker: “Coupled-cluster theory in rotational spectroscopy: Where we are and wish list”

63} "First General Meeting: COST Action Our Astrochemical History CM1401", 25-29 May 2015, Prague (Czech Republic)
Invited speaker: "Astrophysics and Astrochemistry: The role of Rotational Spectroscopy"

62} "AMOC 2015. Anharmonicity in medium-sized molecules and clusters", 26-30 April 2015, CSIC, Madrid (Spain)
Invited speaker: "Rotational spectroscopy in support of astronomical observations: Laboratory measurements and quantum-chemical calculations"

61} "Winter Modeling 2014 – In the framework of DREAMS", 1-2 December 2014, Pisa (Italy)
Invited speaker: "Interplay of experiment and theory in rotational spectroscopy: determination of accurate molecular structure"

60} "The 23rd International Conference on High Resolution Molecular Spectroscopy", 2-6 September 2014, Bologna (Italy)
Oral communication: "Sub-Doppler Resolution in the THz Frequency Domain"

59} "248th ACS National Meeting - Symposium: 'Quantum Chemical Calculation of Molecular Properties: Symposium in Honor of Professor Nicholas C. Handy'", 10-14 August 2014, San Francisco, CA (USA)
Invited speaker: "Quantum chemical calculation of molecular properties of relevance to rotational spectroscopy"

56-58} "69th International Symposium on Molecular Spectroscopy", 16-20 June 2014, Urbana-Champaign, Illinois (USA)
Oral communication: "The rotational spectrum of HDO: Accurate spectroscopic and hyperfine parameters"

Oral communication: "Laboratory measurements in support of astronomical observations: Rotational spectroscopy up to the THz region" – ALMA mini-symposium

Oral communication: "Accurate Characterization of the Peptide Linkage in the Gas Phase: A Joint Quantum-Chemical and Rotational Spectroscopy Study of the Glycine Dipeptide Analogue"

55} "25th Austin Symposium on Molecular Structure and Dynamics at Dallas", 1-4 March 2014, Dallas (USA)
Invited speaker: "Rotational spectroscopy meets theory"

54} "Seminarie sur la DFT and ses Applications", 26-27 October 2013, Sousse (Tunisia)
Invited speaker: "A coupled cluster and DFT joint-venture: Molecular structure and spectroscopic properties".

53} "XLI Congresso Nazionale di Chimica Fisica", 23-27 June 2013, Alessandria (Italy)
Oral communication: "Rotational spectroscopy meets theory: the challenge of biomolecules"

51-52} "68th International Symposium on Molecular Spectroscopy", 17-21 June 2013, Columbus, OHIO (USA)
Invited speaker: "Rotational spectroscopy meets theory"

Oral communication: "Rotational spectrum of H₂S: the H₂³³S isotopologue and the sub-Doppler resolution in the THz regime"

50} "7th Molecular Quantum Mechanics" (Conference in honor of Prof. R.J. Bartlett), Lugano (Switzerland) 2-7 June 2013.
Invited speaker: "Spectroscopy accuracy: why do we need highly accurate quantum-chemical calculations?"

49} "German Bunsen Society annual meeting 2013", Karlsruhe (Germany) 9-11 May 2013.
Invited speaker: "Rotational spectroscopy meets theory"

48} "CODECS COST meeting", El Escorial, Madrid (Spain) 18-22 April 2013.
Invited speaker: "Extending the molecular size in accurate quantum-chemical calculations: the equilibrium structure and spectroscopic properties of biomolecules"

47} "From Astrophysics to Astrochemistry towards Astrobiology – IV Workshop della Società Italiana di Astrobiologia", 19-21 September 2012, Perugia
Oral communication: "Astrophysical investigations: the role of rotational spectroscopy"

46} "22th International Conference on High-Resolution Molecular Spectroscopy", 4-8 September 2012, Prague (Czech Rep.)
Oral communication: "The rotational spectrum of D₂¹⁷O and HD¹⁷O: Accurate spectroscopic and hyperfine parameters"

45} "Theoretical and Computational Astrochemistry", Scuola Normale Superiore, Pisa (Italy), August 30 - September 1, 2012
Invited speaker: "Rotational spectroscopy and astrophysical investigations: the role of quantum-chemical calculations"

44} "The XVII Symposium on High Resolution Molecular Spectroscopy", 2-7 July 2012, Zelenogorsk, St. Petersburg (Russia).
Invited speaker: "Atmospheric and astrophysical investigations: the role of rotational spectroscopy"

43} "Coupled-Cluster Theory and Related Techniques" 1-3 July, Boulder, CO (USA):

Invited speaker: "Quantum-chemical calculations in rotational spectroscopy: when experiment cannot do without theory"

41-42} "67th International Symposium on Molecular Spectroscopy", 18-22 June 2012, Columbus, OHIO (USA)

Oral communication: "Precise THz measurements of HCO^+ , N_2H^+ and CF^+ "

Oral communication: "The rotational spectrum of D_2^{17}O : Accurate spectroscopic and hyperfine parameters"

40} "XXIV Congresso Nazionale della Società Chimica Italiana", 11-16 September 2011, Lecce (Italy)

Oral communication: "Rotational spectroscopy and astrophysical investigations: the role of quantum-chemical calculations"

39} "9th Congress of the World Association of Theoretical and Computational Chemists (WATOC 2011)", 17-22 July 2011, Santiago de Compostela (Spain)

Invited speaker: "Puzzling aspects in rotational spectroscopy: when experiment cannot do without theory"

36-38} "66th International Symposium on Molecular Spectroscopy", 20-24 June 2011, Columbus, OHIO (USA)

Oral communication: "Quantum-chemical calculations of spectroscopic parameters for rotational spectroscopy: the need of the interplay between experiment and theory"

Oral communication: "Rotational spectrum of CH_2FI from 5 GHz up to 1 THz: accurate spectroscopic and hyperfine parameters"

Oral communication: "Rotational spectroscopy for astrophysical applications: the THz frequency region"

35} "European Seminar on Computational Methods in Quantum Chemistry", 16-19 June 2011, Oscarsborg Fortress, Oslo (Norway)

Oral communication: "Benchmarking Quantum Chemistry with Rotational Spectroscopy or Benchmarking Rotational Spectroscopy with Quantum Chemistry?"

34} "Winter Modeling 2011", 13-14 January 2011, SCUOLA NORMALE SUPERIORE, Pisa (Italy)

Invited speaker: "Astrophysical investigations: the computational and spectroscopic approach"

33} "Astrochimica: Molecole nello spazio e nel tempo", 4-5 November 2010, ACCADEMIA NAZIONALE dei LINCEI, Roma (Italy)

Invited contribution: "Rotational spectroscopy for astrophysical investigations"

32} "XXXIX Congresso Nazionale di Chimica Fisica", 20-24 September 2010, Stresa (VB, Italy)

Oral communication: "Benchmarking Quantum Chemistry with Rotational Spectroscopy or Benchmarking Rotational Spectroscopy with Quantum Chemistry?"

31} "The 21st International Conference on High Resolution Molecular Spectroscopy", 7-11 September 2010, Poznan (Poland)

Oral communication: "Investigation of rotational spectra of isotopic species of trans-formic acid: a test case for the interplay between experiment and theory"

30} "EUCMOS2010 - 30th European Congress of Molecular Spectroscopy", 29 August - 30 September 2010, Firenze (Italy)

Oral communication: "Hyperfine structure of rotational spectra: Interplay of experiment and theory"

29} "International Meeting on Atomic and Molecular Physics and Chemistry, IMAMPC 2010", 30 June - 2 July 2010, Madrid (Spain)

Invited speaker: "Molecular structure determination: a testing ground for high-level quantum-chemical computations"

28} "23rd Austin Symposium on Molecular Structure and Dynamics", 6-9 March 2010, Austin (USA)

Oral communication: "Molecular structure determination from quantum-chemical calculations: extrapolation to the complete basis set limit and additivity approximation"

27} "XXXV Congress of Theoretical Chemists of Latin Expression", 18-22 September 2009, San Andres Island (Colombia)

Plenary speaker: "Molecular structure determination: a testing ground for high-level quantum-chemical computations"

26} "21st Colloquium on High Resolution Molecular Spectroscopy", 31 August - 4 September 2009, Castellammare di Stabia (NA)

Plenary speaker: "Hyperfine structure of rotational spectra: state-of-the-art experimental and theoretical determinations"

25} "XXIII Congresso Nazionale della Società Chimica Italiana", 5-10 July 2009, Sorrento (NA)

Oral communication: "Absolute ^{17}O NMR scale: a joint rotational spectroscopy and quantum chemistry study"

Vincitore del Premio Gaussian 2009: "Per il contenuto innovativo e l'originalità dell'attività di ricerca basata su metodologie in silico applicate alle scienze molecolari"

23-24} "OSU International Symposium on Molecular Spectroscopy", 22-26 June 2009, Columbus, OH (USA)

Oral communication: "Silyl fluoride: Lamb-dip spectra and equilibrium structure"

Oral communication: "Absolute ^{17}O NMR scale: a joint rotational spectroscopy and quantum chemistry study "

22} "Advanced workshop on Theoretical and Computational Methods for Molecular Spectroscopy and Collisions: Application to Astrophysical and Atmospheric relevant Systems", 7-10 May 2009, Granada (Spain)

Invited speaker: "Quantum-chemical calculation of spectroscopic parameters for rotational spectroscopy: Application to astrophysics and atmospheric systems".

21} "Winter Modeling '08", 19 December 2008, Pisa (CNR)

Oral communication: "State-of-the-art coupled cluster calculations: molecular and spectroscopic properties"

20} "7th European Conference on Computational Chemistry", 11-15 September 2008, S.Servolo - Venice

Oral communication (Invited): "Toward spectroscopic accuracy for open-shell systems: X_2AB radicals as test cases "

19} "20th International Conference on High Resolution Molecular Spectroscopy", 2-6 September 2008, Prague (Czech Republic)

Oral communication: "Pressure-broadening of Water Lines in the THz Frequency Region: Improvements and Confirmations for Spectroscopic Databases"

18} "XXXIV Congress of Theoretical Chemists of Latin Expression", 3-8 July 2008, Cetraro (CS)

Oral communication: "Benchmark calculations for molecules in the gas phase: state-of-the-art coupled cluster computations"

17} "10th International HITRAN Conference", 22-24 June 2008, Cambridge, Massachusetts (USA) - Harvard-Smithsonian Center for Astrophysics

Oral communication: "Pressure-broadening of Water Lines in the THz Frequency Region: Improvements and Confirmations for Spectroscopic Databases"

16} "22nd Austin Symposium on Molecular Structure", 1-4 March 2008, Austin (USA)

Invited speaker: "High resolution rotational spectroscopy as a source of information on the structure and magneto-electric properties of molecules"

15} "37° Congresso Nazionale della Società di Chimica Italiana – Divisione di Chimica Fisica", 24-29 February 2008, Camogli (Ge)

Oral communication: "Benchmark calculations on Nucleobases: Uracil as a Test Case"

14} "Workshop TheTIS (Theoretical Tools for in-silico Spectroscopy)", 14-16 February 2008, Paris - École nationale supérieure de chimie de Paris (France)

Oral communication: "Interplay of theory and experiment in rotational spectroscopy"

13} "WM07 - Winter Modeling 2007", 23 November 2007, Roma (CNR)

Oral communication: "Benchmark calculations: highly accurate ab initio computations for molecules in the gas phase"

12} "36° Congresso Nazionale della Società di Chimica Italiana – Divisione di Chimica Fisica", 17-22 June 2007, Gallipoli (LE)

Oral communication: "Vibrational Corrections to Dipolar Coupling Constants: an Alternative for Determining Equilibrium Distances from Rotational Spectroscopy"

11} VI Convegno Nazionale Gruppo Interdivisionale di Chimica Computazionale, 18-21 December 2006, Venezia.

Oral communication: "How accurately can structural, spectroscopic and thermochemical properties be predicted by ab initio computations?".

10} Workshop: "Molecular databases for Herschel, ALMA and SOFIA", 6-8 December 2006, Leiden (NL)

Oral communication: "High precision spectroscopic measurements in the millimeter- and submillimeter-wave region".

9} "ICCMSE 2006 – Highlighted Symposium (in honour of B. Roos) : Electron correlation for the whole periodic table", 27/10-1/11 2006, Chania (Crete)

Invited keynote speaker: "How accurately can structural, spectroscopic and thermochemical properties be predicted by ab initio computations?".

8} "The 19th International Conference on High Resolution Molecular Spectroscopy", 29/8-2/9 2006, Prague (Czech Republic)

Plenary speaker: "Rotational Spectroscopy: A Powerful Tool for Atmospheric and Interstellar-Space Chemistry".

7} Mini-symposium: "Accurate calculations and fine-structure operators on transition metal-containing systems", 3 April 2006, Département de Chimie Physique, Université de Geneve, Geneve (Switzerland)

Oral communication: "Structural, spectroscopic and thermochemical properties of transition-metal containing systems: benchmark calculations".

6} "34° Congresso Nazionale della Società di Chimica Italiana – Divisione di Chimica Fisica", 20-24 June 2005, Siena.

Oral communication: "Fine- and hyperfine-structure of rotational spectra: microwave spectroscopy and ab initio computations".

5} VI Conference on "Complex Systems: structure, properties, reactivity and dynamics", 10-13 June 2003, Bologna.

Oral communication: "An ab initio study of trans-1-chloro-2-fluoroethylene: equilibrium structure, molecular properties and anharmonic force field".

4} ESA: ESTEC Contract N. 16377/02/NL/FF "Characterization of Millimetre-Wave Spectroscopic Signatures".

- Oral communication: II progress meeting (21/03/2003 Lille, F):

"N₂- and O₂-broadening of O₃ the 301.8 and 317.2 GHz lines. Preliminary results".

- Oral communication: mid-term (III) meeting (16/05/2003 Estec, Noordwijk, NL):

"N₂- and O₂-broadening of O₃: the 301.8 and 319.9 GHz lines. Final results".

- Oral communication: IV progress meeting (18/07/2003 Bologna, I):

"Air-broadening of HNO₃: the 319.2 and 344.2 GHz lines".

- Oral communication: V progress meeting (24/10/2003 Orsay-Paris, F):

"Air-broadening of HNO₃: the 319.2, 319.9, 320.0, 322.3 and 344.2 GHz lines. Final results".

- Oral communication: final meeting (16/01/2004 Estec, Noordwijk, NL):

"N₂- and O₂-broadening of O₃ and air-broadening of HNO₃: final results obtained at the LMSB Bologna".

3} 'Meeting of the NETWORK THEONET', 26-28 August 1999, Copenhagen (Denmark).

Oral communication: "Potential energy surface for the He + H₂⁺ ground state reaction and a new diabaticization technique for the excited state potentials".

2} IV Conference on "Sistemi Complessi: Struttura, Proprietà, Reattività e Dinamica", 16-18 June 1999, Varenna (LC).

Oral communication: "Potential energy surface for the He + H₂⁺ ground state reaction and a new diabaticization technique for the excited state potentials".

1} 'Workshop: Meeting of the NETWORK SCAMP (CHRXCT 93-0157)', 18-21 February 1996, Luminy-Marsiglia (France).

Oral communication: "Rovibrational energy levels and equilibrium geometry of HCP".

SEMINARS

54-55} COST Training School 2023 – Multiscale modeling of the properties of compounds: From isolated molecules to 3D materials relevant for industrial and astrophysical applications, 19-22 September 2023, Belgrade, Serbia

Seminar 1, "Quantum-chemical composite schemes in gas phase: Accurate molecular structures, spectroscopic properties and energetics"

Seminar 2, "Quantum-chemical composite scheme in gas phase: Application to astrochemistry"

53} "Introduction to Astrochemistry – Part II: In Search of the Origin of Life"

Seminar, May 25 2023, Seminari Frontiere della Chimica, Scuola Normale Superiore, Pisa.

52} "Exotic molecules in the interstellar medium: From the laboratory to space"

Seminar, May 10 2023, virtual International Microwave Seminar series

51} "From the lab to space: in search of building blocks of life. But, where is chirality?"

Seminar, January 30 2023 – CRC seminar, University of Kassel (Germany)

50} "Once upon the time there was ... an astrochemistry story"

Seminar, January 9 2023, Ben-Gurion University, Beersheva (Israel)

49} "Introduction to Astrochemistry"

Seminar, December 22 2022, Scuola Superiore Meridionale, MOSES Doctoral School

48} "Il mistero della chimica dell'universo"

Seminar, December 14 2022, Scuola di Studi Superiori "Carlo Urbani", 14 December 2022

47} "Once upon the time there was ... an astrochemistry story"

Seminar, September 13 2022, University of Florida, Gainesville, FL (USA)

46} "Once upon the time there was ... an astrochemistry story"

Seminar, June 13 2022, University of Maryland, College Park, MA (USA)

45} "Il mistero della chimica dell'universo"

Seminar, May 5 2022, Spazio, Ultima Frontiera II Edizione, Università La Sapienza, Roma

44} "Composite schemes for accurate calculations of energetics, structures and spectroscopic properties"

Seminar, April 14 2022, Scuola Superiore Meridionale, MOSES Doctoral School

43} "Molecules in space and the origin of life"

Seminar, March 17 2022, Seminari Frontiere della Chimica, Scuola Normale Superiore, Pisa.

42} "Introduction to Astrochemistry"

Seminar, February 16 2022, Scuola Superiore Meridionale, MOSES Doctoral School

41} "Theory and Experiment for Elucidating Chemical Evolution in Space"

Seminar, September 8 2021, The Astrochemistry Subdivision of the ACS, Online Seminar Series

40} "Il mistero della chimica dell'universo"

Seminar, September 8 2021, PLS Scuola Estiva Virtuale per Studenti, Università di Napoli, Federico II

37-38} Simulation of Molecular Systems for Chemistry, Materials and Biology, 5-9 July 2021, Polo di Lecco, Politecnico di Milano

Seminar 1, "Composite scheme in quantum chemistry. Part 1: Accurate determination of spectroscopic parameters and energetics"

Seminar 2, Cristina Puzzarini, Composite scheme in quantum chemistry. Part 2: Applications to astrochemistry

39} "Molecules in space and the origin of life"

Seminar, June 7 2021, Seminari Frontiere della Chimica, Scuola Normale Superiore, Pisa.

36} "In search of the origin of Life: the astrochemical point of view"

Seminar, July 23 2020, Seminari Frontiere della Chimica, Scuola Normale Superiore, Pisa.

34} "Rotational Spectroscopy Meets Quantum Chemistry for Elucidating Astrochemical Challenges"

GDCh Seminar, November 14 2019, Göttingen, Germany

33} "In search of the origin of Life: the astrochemical point of view"

Seminar, May 30 2019, Seminari Frontiere della Chimica, Scuola Normale Superiore, Pisa.

32} "Prebiotic molecules in interstellar space: rotational spectroscopy and quantum chemistry"

Seminar, March 18 2019, New York University Abu Dhabi, Abu Dhabi, Emirates

31} "Spectroscopic characterization of sulfur-containing molecular systems. Rotational spectroscopy of radicals and molecular complexes"

Seminar, December 14 2018, Mainz, Germany

30} " In search of the origin of Life: the astrochemical point of view "

Seminar, November 20 2018, International Astro-Spectroscopy Symposium, International Centre for Quantum and Molecular Structures, Shanghai University, Shanghai, China.

29} "In search of the origin of Life: the astrochemical point of view"

Seminar, October 9 2018, Seminari Frontiere della Chimica, Scuola Normale Superiore, Pisa.

28} "Un viaggio negli spazi intersiderali alla ricerca delle basi chimiche della vita"

Seminar, July 5 2018, San Miniato (PI); Scuola di Orientamento Universitario – Scuola Normale Superiore, Scuola Superiore Sant'Anna, IUSS di Pavia

27} "Prebiotic molecules in interstellar space: rotational spectroscopy and quantum chemistry"

Seminar, February 2 2018, Department of Chemistry, Torino

26} "Rotational spectroscopy as a tool to investigate molecules in space: Laboratory measurements and quantum-chemical calculations"

Seminar, December 19 2017, TC Mini Symposium, Mainz, Germany

25} "Once upon a time there was ... a computational astrochemistry and rotational spectroscopy story"

Seminar, March 28 2017, Seminari Frontiere della Chimica, Scuola Normale Superiore, Pisa.

24} "Once upon a time there was ... a computational astrochemistry and rotational spectroscopy story"

Seminar, March 21 2017, Innsbruck University, Physics Colloquium.

23} "Once upon a time there was ... a computational astrochemistry and rotational spectroscopy story"

Seminar, September 2 2016, Scuola Normale Superiore, Pisa.

22} "High-level quantum-chemical calculations applied to atmospheric studies: the HO₂ and HOCH₂OO radicals"

Seminar, July 11 2016, Laboratoire Modelisation et Simulation Multi Echelle (MSME), Université de Marne la Vallée (France). Scientific afternoon in honor of Prof. J. Francisco

21} "Rotational Spectroscopy @LMSB (Laboratory of mm-/submm-wave Spectroscopy in Bologna): Interplay of experiment and quantum-chemical calculations"

Seminar, January 14 2016, Theoretical Chemistry Group, University of Mainz, Mainz (Germany).

20} "Laboratory of mm-/submm-wave Spectroscopy of Bologna, LMSB: sub-Doppler resolution, THz measurements and quantum-chemical calculations"

Seminar, December 3 2015, GEM, University of Valladolid, Valladolid (Spain).

19} "Astrophysical and astrochemical investigations: The contribution of rotational spectroscopy"

Seminar, November 18 2015, INAF, Arcetri, FI (Italy).

18} "Extending the molecular size in accurate quantum-chemical calculations: the equilibrium structure and spectroscopic properties of building-blocks of biomolecules"

Seminar, July 1 2015, Laboratoire Modelisation et Simulation Multi Echelle (MSME), Université de Marne la Vallée (France).

17} "Laboratory of Mm-/submm-wave Spectroscopy of Bologna, LMSB: sub-Doppler resolution, THz measurements and quantum-chemical calculations"

Seminar, February 24 2015, Physikalisches Institut Universität zu Köln, Cologne (Germany)

16} "Hyperfine structure of rotational spectra: sub-Doppler resolution and quantum-chemical calculations"

Seminar, October 23 2014, LENS, Sesto Fiorentino, FI (Italy).

15} "Spectroscopic accuracy: why do we need highly accurate quantum-chemical calculations?"

Seminar, July 4 2013, Laboratoire Modelisation et Simulation Multi Echelle (MSME), Université de Marne la Vallée (France).

14} "Atmospheric and astrophysical investigations: the role of Rotational spectroscopy"

Seminar, Kick-Off Meeting of the International Research Group « HiresMIR », September 27-28, 2012, Université de Lille I, Villeneuve d'Ascq (France).

13} "Rotational spectroscopy and astrophysical investigations: the role of quantum-chemical calculations"

Seminar, 29 Marzo 2012, Scuola Normale Superiore, Pisa.

12} "Toward the spectroscopic accuracy for free radicals: Quantum-chemical calculations of molecular structure and properties"

Seminar, 2 Marzo 2011, Scuola Normale Superiore, Pisa.

11} "A quick introduction to rotational spectroscopy"

Seminar, 25 Gennaio 2011, Institut für Physikalische Chemie, Universität Mainz.

10} Winter School in Theoretical Chemistry "Accurate Molecular Structure by Experiment and Theory", 13-16 Dicembre 2010, Helsinki (Finland).

- "Introductory lecture on rotational spectroscopy"

- "Rotational spectroscopy at work"

9} Doctorate's master "Láseres y Aplicaciones en Química", 5 Febbraio 2010, Universidad Pablo de Olavide (Spain).

"*High-resolution rotational spectroscopy in the millimeter- and submillimeter-wave region*"

8} "*Benchmarking quantum chemistry with high-resolution rotational spectroscopy*"

Seminar, 14 Gennaio 2010, Institut für Physikalische Chemie, Universität Mainz.

7} "*Hyperfine structure in the rotational spectra of $H_2^{17}O$* "

Seminar, 10 Gennaio 2009, Söllerhaus, (Skiing seminars: Universität Mainz-Stuttgart-Karlsruhe).

6} "*Interplay of theory and experiment: measurement at the LMSB*"

Seminar, 31 Gennaio 2008, Institut für Physikalische Chemie, Universität Mainz.

5} "*Accurate electronic structure calculations for accurately predicting rotational spectra*"

Seminar, 17 Aprile 2007, Dipartimento di Chimica Fisica, Università Federico II, Napoli.

4} "*Fine- and hyperfine-structure of rotational spectra: microwave spectroscopy and ab initio computations*"

Seminar, 8 Marzo 2006, Istituto per i Processi Chimico Fisici, CNR, Pisa.

3} "*Struttura e proprietà molecolari: l'approccio dal punto di vista sperimentale e teorico*"

Seminar, 14 Aprile 2005, Dipartimento di Chimica Fisica, Università di Palermo.

2} "*Molecular properties and rotational spectrum: the ab initio and high resolution spectroscopy approaches joint together*"

Seminar, 3 Novembre 2004, Institut für Physikalische Chemie, Universität Mainz.

1} "*Calcoli ab initio applicati alla spettroscopia a microonde: trans-1-cloro-2-fluoroetilene*"

Seminar, 14 Febbraio 2003, Dipartimento di Chimica Fisica dell'Università Ca' Foscari di Venezia.