CURRICULUM VITAE – Cristina Puzzarini

- **PERSONAL INFORMATION**

Puzzarini, Cristina
Professor of Physical Chemistry
Dept. Chemistry "Giacomo Ciamician", Universitá di Bologna
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https://site.unibo.it/rotational-computational-spectroscopy/en
https://www.unibo.it/sitoweb/cristina.puzzarini

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**

2024 Invited professor Univ. Gustave Eiffel
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 four national projects:

2011-2013 PRIN 2009 Project "*Molecular Spectroscopy for Atmospherical 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:

2025-2026 PRIN 2022 "scorrimento" Project "*SMART_H2 – Simulations, Modeling and Applications of Plasma Assisted-conversion of methane to hydrogen and carbon*"

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-coordination 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 *J.P.A. Ioannidis, J. Baas, R. Klavans, K. W. Boyack, "A standardized citation metrics author database annotated for scientific field",* PLOS Biology *doi:10.1371/journal.pbio.3000384*), in 2019, I was one of the top world scientists (Top 2% Scientists: 62224 in the world), and one of top-200 Italian chemists. According to the "August 2024 data-update for "Updated science-wide author databases of standardized citation indicators"" (DOI: 10.17632/btchxktzyw.7; released on September 16, 2024), the world rank improved to 42135. The corresponding (world) rank in the "Chemical Physics" sub-field is 968.

Since 1995 (first publication), I have published more 320 papers (H-index = 49 SCOPUS, 54 Google Scholar; January 2, 2026), ~150 out of them in the last ten years, and 9 book chapters. PI's papers received more than 9800 citations SCOPUS), almost all in the areas of high-resolution rotational and computational spectroscopy, quantum chemistry and astrochemistry. The full list of papers is provided below.

I have given 152 presentations at scientific meetings (about 90% at international meetings), 84 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 (prebiotic chemistry in the early Universe).

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
FELIX Laboratory, Radboud Univ. (NL): S. Brünken

MIT (USA): B. McGuire
MPE (Garching, Germany): P. Caselli
MPI (Bonn, Germany): A. Belloche
PoliMI (Italy): C. Cavallotti
Scuola Normale Superiore (Italy): N. Tasinato
U. Bologna, Dept. Astronomy (Italy): L. Testi
U. Ca'Foscari (Venice, Italy): A. Pietropolli-Charmet, P. Stoppa.
U. Chongqing (China): Q. Gou, G. Feng
U. Cologne (Germany): S. Schlemmer, O. Asvany, S. Thorwirth
U. Gustave Eiffel (France): M. Hochlaf, R. Linguerri
U. Hannover (Germany): J.-U. Grabow
U. Kassel (Germany): T. Giesen
U. Mainz (Germany): J. Gauss
U. Rennes (France): F. Lique, J.-C. Guillemin
U. Valladolid (Spain): C. Pérez
U. Wroclaw (Poland): M. Biczysko

- **ORGANISATION OF INTERNATIONAL SCIENTIFIC MEETINGS**

2026 (August 1-9)	COSPAR (46th Scientific Assembly) - F3.1 & F3.4, SOC member
2026 (June 22-26)	ISMS – Symposium "*Experimentally Inspired Computational Spectroscopy*", co-Chair, Urbana-Champaign, IL (USA)
2026 (June 22-26)	ISMS – Symposium "*Probing Chemical Reactions with High-Resolution Spectroscopy*", co-Chair, Urbana-Champaign, IL (USA)
2025 (July 9-11):	3rd COSY Cost General Meeting, *Chair*, Bologna, Italy
2024 (Sept. 2-6)	17th High-Resolution Molecular Spectroscopy, LOC member, Bologna, Italy
2024 (July 1-2)	EAS2024 – Symposium S6 "European Laboratory Astrophysics in the JWST era", co-Chair, Padova, Italy
2024 (July 13-21)	COSPAR - F3.1, co-Chair, Busan, South Korea
2024 (June 17-21)	ISMS – Symposium "Synergy Between Experiment and Theory", co-Chair, Urbana-Champaign, IL (USA)
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 – Symposium 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**

2025 – to date Coordinator of the Doctoral School in Chemistry, University of Bologna
2024 – to date Member of the Department Board (Giunta), Dept. Chemistry "Giacomo Ciamician"
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* (Nature journal)
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*
2026 NWO Open Competition ENW-XL: Assessment Committee, Member
2025 FWF-Special Research Program (SFB): Assessment Committee, Chair
2023 NWO: DAN-JWST Assessment Committee, Member
2017 – to date Reviewer of international projects (ERC StG 2021,2023; ERC AdG 2024; COST Action 2024; 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; NRDI, Hungary; OSF, Poland; ISF, Israel; FNRS, Belgium; FWF, Austria; DG, Denmark)
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., Chem. Sci.); 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; Nature, Nat. Astron.

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)
- JPCA (2025 - John F. Stanton Memorial Issue)

- **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)
2022 – to date Member, COST Action CA21126 “Nanospace”
2015 – 2019 Member, COST Action CM1401 “Our Astro-Chemical History”

- **CARRIER BREAK**

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

RESEARCH ACHIEVEMENTS

In **2017**, I founded the **ROT&Comp lab** (https://site.unibo.it/rotational-computational-spectroscopy/en): the main research line is the interplay of rotational spectroscopy and computational chemistry/spectroscopy applied to astrochemistry. The PI has made original contributions in the fields of computational chemistry, rotational spectroscopy and astrochemistry.

ASTROCHEMISTRY at the ROT&Comp lab

https://site.unibo.it/rotational-computational-spectroscopy/en/research/astrochemistry

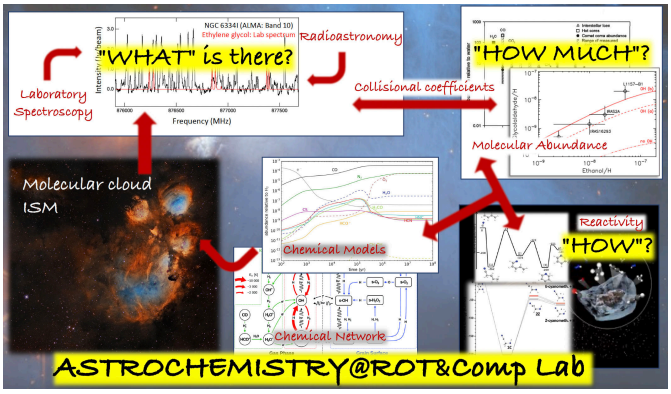
As shown in this figure [adapted from *Figure 1* of C. Puzzarini. *Front. Astron. Space Sci.* 7 (2020) 19], the complete chemical characterization of interstellar clouds is a grand challenge of astrochemistry and involves 4 steps:

1) Unveiling the molecular census – "What" is there?
2) Evaluating molecular abundances – "How much"?
3) Formation and destruction of molecules – "How"?
4) Reaction network & astrochemical model

The research activity of the ROT&Comp lab covers the steps 1 to 3. While the *interplay* of experiment and theory characterizes steps 1 and 2, this proposal is meant to extend this synergy to step 3. The figure above serves as a sort of *manifesto* of the PI's research vision, emphasizing the willingness to cover (in the future) also step 4 and make ROT&Comp lab the reference center for astrochemistry in Italy. Let us summarize the achievements accomplished so far (steps 1-3).

1) "What" is there? Hunting molecules in space.

Because of the extreme conditions of the ISM, the chemical reactivity is unusual and leads to the onset of both transient and stable molecular species. The former are broadly defined as exotic molecules (radicals, ions, unsaturated species, …). Their spectroscopic characterization is a challenge and, at the same time, the required step for astronomical searches. *Faraday Discuss.* 245, 309 (2023) and *Front. Astron. Space Sci.* 10, 1211784 (2023) present the strategy exploited at the ROT&Comp lab, which relies on a strong interplay of experiment and theory. Representative results are the spectroscopic study of (Z)-1,2-ethenediol, a key prebiotic intermediate in the formose reaction (*Chem. Commun.* 58, 2570 (2022)), and its detection (*Astrophys. J. Lett.* 929, L11 (2022)), and the laboratory characterization and tentative identification of allylimine (*Astron. Astrophys.* 669, A93 (2023)). Both molecules were produced by flash vacuum pyrolysis (FVP) and investigated on-the-fly. FVP is also employed for the generation of unsaturated carbon chains (*J. Phys. Chem. A* 126, 6210 (2022), *Faraday Discuss.* 245, 309 (2023)) and radical species (*Faraday Discuss.* 245, 309 (2023)). However, at ROT&Comp lab, the latter are instead usually obtained by applying DC discharge. In this respect, a significant example is provided by the spectroscopy study of HSO (*Astron. Astrophys.* 591, A126 (2016)) and its detection in the ISM (*Astron. Astrophys.* 674, L13 (2023)). The DC discharge system is employed for the production of ions, with *Astrophys. J.* 970, 26 (2024) only providing the latest example. For details on instrumentation: https://site.unibo.it/rotational-computational-spectroscopy/en/research/facilities.



A fundamental aspect of the spectroscopic studies of "new" species is their computational characterization. The leadership of the PI is here testified by invited reviews that have become a reference for the community (*Chem. Rev.* 119, 8131 (2019); *Nat. Rev. Methods Primers* 1, 38 (2021); *PCCP* 25, 1421 (2023)).

Astronomical detections have so far been accomplished owing to strong collaborations with astronomers, but the expertise available at the ROT&Comp lab and our recent involvement with the

Sardinia Radio Telescopes (since 2024: 2 campaigns/year) will allow us to provide first-hand contributions (manuscript is in preparation).

2) "How much"? Collisional studies for non-LTE abundances.

Since at the very low density of the ISM the molecular energy level populations are rarely at the local thermodynamics equilibrium (LTE), collisions compete with radiative processes. Thus, the interpretation of observed interstellar spectra in terms of molecular abundances requires the knowledge of collisional rate coefficients of the molecule under consideration (with the most abundant perturbing species, H_2). While a few experimental studies allow the determination of such parameters (e.g., *Nat. Chem.* 14, 811 (2022)), quantum inelastic scattering calculations offer an accurate and more accessible alternative. Examples of PI's contributions are provided by *J. Chem. Phys.* 155, 234306 (2021), *MNRAS* 516, 2653 (2022), and *MNRAS* 527, 2279 (2024). The accuracy of scattering calculations can be validated through pressure broadening measurements (e.g. *Astrophys. J.* 970, 26 (2024); *JQSRT* 345, 109521 (2025)), pressure-shift and broadening coefficients being related to the imaginary and real part of the scattering matrix. Line-profile analysis is a consolidated expertise at the ROT&Comp lab (e.g. *JQSRT* 109, 1563 (2008); *ibid* 113, 1051 (2012)).

3) "How"? Formation of interstellar molecules.

As mentioned in Section a, molecules in space can be synthesized on grain surfaces or in the gas-phase phase or by both types of chemistries. To be completely characterized, interstellar chemistry requires an investigation of all possible reactions leading to the molecules detected as well as those involving them. The harsh conditions of the ISM (in particular, the low temperatures) put severe constraints on the reactivity: exothermicity, barrierless approach of reactants and submerged barriers. The characterization of reactions cannot be confined to thermochemistry, but kinetic studies are required to establish the definitive feasibility and relevance of the reaction processes under consideration. The major challenges are the exhaustive exploration of reaction mechanisms (all possible reactive channels) and the accurate kinetic description of the barrierless approach of reactants. The PI has provided important contributions to the definition of accurate methodologies for addressing these challenges (e.g. *J. Chem. Theory Comp.* 16, 5090 (2020); *MNRAS* 496, 4298 (2020); *J. Chem. Phys.* 154, 054306 (2021); *Nature Chem.* 14, 1405 (2022)). From a more applicative point of view, representative results of gas-phase studies able to explain detected molecules are *Astrophys. J. Lett.* 903, L35 (2020) (Propargylimine), *Astrophys. J.* 922, 169 (2021) (PO), *MNRAS* 525, 1158 (2023) (trans-HC(O)SH), and *ACS Earth Space Chem.* 9, 1217 (2025) (HC(S)CN). An important contribution to the field is also the definition of general mechanisms, which are crucial steps in the rationalization of interstellar chemistry (*Front. Astron. Space Sci.* 8, 811342 (2022); *Astrophys. J.* 962, 32 (2024)). Finally, the recent collaboration established with A. Rimola (Universitat Autonoma de Barcelona) has allowed the PI to extend the research of the ROT&Comp lab to the chemistry occurring on interstellar grains (*Astron. Astrophys.* 698, A51 (2025)).

ROTATIONAL SPECTROSCOPY at the ROT&Comp Lab

https://site.unibo.it/rotational-computational-spectroscopy/en/research/rotational-spectroscopy

The research activities are mainly related to the point #1 of the previous section (Astrochemsity).

I made important advances in the field of mm-/submm-wave spectroscopy focusing on exploiting sub-Doppler resolution achieved by means of the Lamb-dip technique. In particular, she reported the first exploitation ever of the Lamb-dip effect in the THz region: a result that allows an accuracy of 1 part to 10^9 or better in the retrieved transition frequencies (*J. Phys. Chem. A* 117, 13759 (2013)). Worth of mention is also the work on the characterization of intermolecular complexes (*Angew. Chem. Int. Ed.* 57, 13857 (2018); *ibid* 57, 15822 (2018); *ibid* 58, 13935 (2019); *ibid* 61, 264 (2022)).

2) COMPUTATIONAL CHEMISTRY/SPECTROSCOPY at the ROT&Comp Lab

https://site.unibo.it/rotational-computational-spectroscopy/en/research/computational-spectroscopy

Concerning quantum chemistry, I am a world-leading scientist in the accurate determination of structural, molecular and spectroscopic properties as well as energetics, as mentioned above (points #1 and 3 of achievements in astrochemistry). As far as energetics is concerned, an original contribution is

the development of low-cost yet accurate composite schemes for energetics: junChS and junChS-F12 approaches (*J. Chem. Theory Comput.* 19, 988 (2020); *ibid.* 17, 6974 (2021)), which are extensions of the "cheap" scheme (ChS) originally introduced by the PI for structural and molecular properties, then extended to energetics (e.g. *PCCP* 13, 7158 (2011); *J. Phys. Chem. Lett.* 5, 534 (2014)).

FULL LIST OF PUBLICATIONS

Book Chapters:

9*bc*} C. Puzzarini, S. Alessandrini, "Quantum Chemical Approach to Rotational Spectroscopy", Handbook of Electronic Structure Theory, Elsevier, V. Barone & M. Hochlaf Eds.
8*bc*} 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).
7*bc*} 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.
6*bc*} 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
5*bc*} 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.
4*bc*} 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
3*bc*} 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.
2*bc*} 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.
1*bc*} 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:

331} – 336} in preparation
330} M. Hochlaf,* R. Linguerri, N. Chahinez Kandi, S. Alessandrini, C. Puzzarini*
"Ab Initio Characterization of the $[H2,C,N,O]^+$ Isomeric System: Structures, Spectroscopy, and Electronic States"
Submitted for publication (2026)
329} L. Bizzocchi, M. Melosso, F. Tamassia, M. Taddia, F. Tonolo, S. Alessandrini, G. Panizzi, M. Nonne, M.-A. Martin-Drumel, O. Pirali, L. Dore, I.E. Gordon, C. Puzzarini
"An improved study of the $2\nu_5$ band of HC_3N and ν_4 band of HC_4H with a detailed analysis of the associated resonances"
JQSRT, submitted for publication (2026)
328} C. Puzzarini*, S. Alessandrini
"Chemistry in Extreme Environments: The Mystery of Molecular Complexity in Space"
ACS Central Sci. *in press* (2026) DOI: 10.1021/acscentsci.5c02122
[Invited Outlook]
327} S. Alessandrini*, H. Ye, M. Melosso, C. Puzzarini*
"Computational Study of the Reaction between Ethylene Glycol and the CH Radical: Competition between Carbon Addition and Dehydrogenation"
J. Phys. Chem. A *in press* (2026) DOI: 10.1021/acs.jpca.5c06889
326} M. Nonne, M. Melosso, F. Tonolo, L. Bizzocchi, S. Alessandrini, J.-C. Guillemin, A. Kpoezoun, G. Baba, V.M. Rivilla, I. Jiménez-Serra, C. Puzzarini
"Investigating Enols Chemistry in the Interstellar Medium: Rotational Spectroscopy and Interstellar Search of (*E*)-1-Propenol"
Astrophys. J. *in press* (2026) DOI: 10.3847/1538-4357/ae3729
325} L. Bonah∗, M.-A. Martin-Drumel, O. Pirali, F. Tonolo, M. Nonne, M. Melosso, L. Bizzocchi, C. Puzzarini, J.-C. Guillemin, C.P. Endres, S. Schlemmer, S. Thorwirth

"High-resolution infrared spectroscopy and ASAP analysis of cyclopentadiene. The vibrational modes below 860 cm^{-1} and the ν_{21} mode at 961 cm^{-1}"
ACS Earth Space Chem. *in press* (2026) DOI: 10.1021/acsearthspacechem.5c00349
324} M. Bensberg, S. Alessandrini*, M. Melosso, C. Puzzarini*, M. Reiher*
"Automated Exploration of Radical-Molecule Chemistry: The Case of Oxirane + CH in the ISM"
Astrophys. J. *in press* (2026) DOI: 10.3847/1538-4357/ae2d0a
323} M. Michielan, K. Steenbakkers, D. Ascenzi, J. Diprose, M. Polášek, S. Brünken, C. Romanzin, B.R. Heazlewood, C. Puzzarini, V. Richardson*
"IR-Action Spectroscopy of the Astrochemically Relevant $HCCS^+$ Cation"
ACS Earth Space Chem. **10** (2026) 148
322} A. Savarese, S. Alessandrini*, M. Melosso, G. Panizzi, M. Nonne, L. Bizzocchi, C. Puzzarini*
"Energetic and Spectroscopic Insights into the $C_3H_6O_2$ Isomer Family for Astrochemical Purposes"
ACS Earth Space Chem. **10** (2026) 198
321} N.C. Benmoussa, S. Alessandrini, L. de Boer, S. Azizi, H. Friha, R. Bachir, M. Hochlaf, C. Puzzarini, R. Linguerri
"Computational Characterization of the Energetics, Structure, and Spectroscopy of Biofuel Precursors: The Case of Furfural-Acetone-Furfural"
J. Comp. Chem. **47** (2026) e70297
320} M. Melosso, S. Alessandrini, H. Ye, A.L. Steber, C. Pérez, L. Spada, L. Bizzocchi, C. Puzzarini
"The challenge of the equilibrium structure of cinnamonitrile: Rotational spectroscopy and semi-experimental approach"
J. Mol. Struct. **1353** (2026) 144698
319} D. Comte, M. Melosso, S. Alessandrini, L. Bizzocchi, V.M. Rivilla, I. Jiménez-Serra, C. Puzzarini
"Protonated phosphorus mononitride: Spectroscopic parameters and formation routes relevant for astrochemistry"
J. Chem. Phys. **163** (2025) 214306
318} T. Field-Theodore*, M. Ravasio, S. Alessandrini, C. Cavalloti, C. Puzzarini*
"A theoretical investigation of OH• + H_2CCNH reactivity: interstellar insights into glycolonitrile formation"
Astrophys. J. **993** (2025) 179
317} F. Tonolo, H.J. Jóźwiak, L. Bizzocchi, M. Melosso, P. Wcisło, F. Lique, C. Puzzarini
"Experimental and theoretical investigation on N_2 pressure-induced coefficients of the lowest rotational transitions of HCN"
J. Quantit. Spectrosc. Radiat. Transfer **345** (2025) 109521
316} J. Navarro*, A. G. Fairén, D. Fraix-Burnet, S. B. Howell, P. Marziani, C. Puzzarini, M. Rengel
"Editorial: Frontiers in astronomy and space sciences: a decade of discovery and advancement-10th anniversary conference"
Front. Astron. Space Sci. **12** (2025) 159996
315} M. Melosso, P. Stoppa, D. Alvarado-Jiménez, F. Tamassia, C. Sapienza, L. Bizzocchi, L. Dore, C. Puzzarini*, A. Pietropolli Charmet*, N. Tasinato*
"Completing the Spectral Mosaic of Chloromethane by Adding the CHD_2Cl Missing Piece Through the Interplay of Rotational/Vibrational Spectroscopy and Quantum Chemical Calculations"
Molecules **30** (2025) 1604
314} J. Perrero, S. Alessandrini, H. Ye, C. Puzzarini, A. Rimola
"Formation of the glycine isomer glycolamide ($NH_2C(O)CH_2OH$) on the surfaces of interstellar ice grains: Insights from atomistic simulations"
Astron. Astrophys. **698** (2025) A51
313} J. A. Claus, M. Melosso*, A. Maillard, L. Bizzocchi, V. Barone, C. Puzzarini
"Deciphering the Complexity in the Rotational Spectrum of Deuterated Ethylene Glycol"
ACS Earth Space Chem. **9** (2025) 1267
312} S. Alessandrini*, H. Ye, C. Puzzarini*
"Gas-Phase Reactions of H_2CS and H_2CO with CN: Similarities and Differences from a Computational Study"
ACS Earth Space Chem. **9** (2025) 1217−1226
311} P. Cambianica, G. Munaretto, G. Cremonese, A. Mura, F. La Forgia, L. Bizzocchi, M. Lazzarin, C. Puzzarini, M. Melosso, V. Lorenzi, W. Boschin
"Pre-perihelion observations of the carbon-depleted comet C/2023 A3 (Tsuchinshan-ATLAS). Insights into CN production and molecular upper limits"

Planet. Space Sci. **261** (2025) 106102
310} T. E. Field-Theodore, S. Alessandrini, M. Melosso, C. Puzzarini*
"Extension of the Lego-brick approach to protonated molecules"
Chem. Phys. Lett. **868** (2025) 141978
309} S. Alessandrini, H. Ye, M. Biczysko*, C. Puzzarini*
"Describing the Disulfide Bond: From the Density Functional Theory and Back through the "Lego Brick" Approach"
J. Phys. Chem. A **128** (2024) 9383
308} S. Alessandrini*, M. Melosso, L. Bizzocchi, V. Barone, C. Puzzarini*
"The Semiexperimental Approach at Work: Equilibrium Structure of Radical Species"
J. Phys. Chem. A **128** (2024) 5833
307} M. Nonne, M. Melosso*, F. Tonolo, L. Bizzocchi, S. Alessandrini, J.-C. Guillemin, L. Dore, C. Puzzarini*
"Tracing Prebiotic Molecules: Rotational Spectroscopy of Deuterated Glycolaldehyde and (Z)-1,2-Ethenediol"
J. Phys. Chem. A **128** (2024) 4850
306} L. Bizzocchi, F. Tonolo, B. M. Giuliano, P. Caselli, M. Melosso, L. Dore, S. Alessandrini, C. Puzzarini, A. Pietropolli Charmet
"Millimeter to THz Spectroscopy of $HC^{18}O^+$ and $HC^{17}O^+$: Accurate Rest Frequencies for Astrophysical Studies"
Astrophys. J. **970** (2024) 26
305} C. Puzzarini*, S. Alessandrini
"Carbamic acid and its dimer: A computational study"
J. Comput. Chem. **45** (2024) 2501
304} S. Perri*, E. Yordanova, C. Puzzarini
"Editorial: Women in science: astronomy and space sciences"
Front. Astron. Space Sci. **11** (2024) 1378816
303} J, García de la Concepción, C. Cavallotti, V. Barone, C. Puzzarini, I. Jiménez-Serra
"Relevance of the $P+O_2$ Reaction for PO Formation in Astrochemical Environments: Electronic Structure Calculations and Kinetic Simulations"
Astrophys. J. **963** (2024) 142
302} H. Ye, S. Alessandrini*, C. Puzzarini*
"On the General Mechanism for the Gas-phase Reaction of Methanimine with a Radical Species in the Interstellar Medium: Some Failures and an Important Success"
Astrophys. J. **962** (2024) 32
301} C. Puzzarini*, S. Alessandrini
"Interstellar Ices: A Factory of the Origin-of-Life Molecules"
ACS Cent. Sci. 10 (2024) 13
300} C. Puzzarini*, H. Ye, S. Alessandrini
"Isomerism of CH_2SO: Accurate structural, energetic, and spectroscopic characterization"
J. Comput. Chem. **45** (2024) 777
299} F. Tonolo, L. Bizzocchi, V. M. Rivilla, F. Lique, M. Melosso, C. Puzzarini
"Collisional excitation of PO^+ by para-H_2: Potential Energy Surface, Scattering Calculations and Astrophysical Applications"
MNRAS, **527** (2024) 2279
298} 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, **25** (2023) 31281
297} C. Puzzarini*, R. Linguerri*, M. Hochlaf*
"Insights into the molecular structure and spectroscopic properties of HONCO: An accurate ab initio study"
J. Phys. Chem. A, **127** (2023) 9502
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
[*invited review article*]
292} P. Stoppa, A. Pietropolli Charmet, F. Tamassia, E. Cané, M. Melosso, A. Achilli, L. Dore, C. Puzzarini,
"High resolution FTIR spectrum of $CH_2D^{37}Cl$: 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 C_3H_3NO 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-C_6H_4-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 Cl_2H^+ to (E)-$NCCHCHCNH^+$ 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(^{3}P) 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 $HC^{17}O^+$ with H_2 (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"
Chem. Comm. **58** (2022) 2750
263} C. Puzzarini*
"Gas-phase chemistry in the interstellar medium: the role of laboratory astrochemistry"
Front. Astron. Space Sci. **8** (2022) 811342 DOI: 10.3389/fspas.2021.811342
262} V. Barone, C. Puzzarini
"Toward accurate formation routes of complex organic molecules in the interstellar medium: the paradigmatic cases of acrylonitrile and cyanomethanimine"
Front. Astron. Space Sci. **8** (2022) 814384 DOI: 10.3389/fspas.2021.814384
261} F. Tamassia, L. Bizzocchi, M. Melosso, M.-A. Martin-Drumel, O. Pirali, A. Pietropolli Charmet, E. Cané, L. Dore, I.E. Gordon, J.-C. Guillemin, B.M. Giuliano, P. Caselli, S. Alessandrini, V. Barone, C. Puzzarini
"Synchrotron-based far-infrared spectroscopy of HC_3N: extended ro-vibrational analysis and new line list up to 3360 cm^{-1}"
J. Quantit. Spectrosc. Radiat. Transfer, **279** (2022) 108044
260} L. Bizzocchi, S. Alessandrini, M. Melosso, V. M. Rivilla, C. Puzzarini*
"Ab Initio Study of Fine and Hyperfine Interactions in Triplet POH"
Molecules **27** (2022) 302
259} X. Li, L. Spada, S. Alessandrini, Y. Zheng, K.G. Lengsfeld, J.-U. Grabow, G. Feng, C. Puzzarini, V. Barone
"Stacked but not Stuck: Unveiling the Role of $\pi \rightarrow \pi^*$ Interactions with the Help of the Benzofuran-Formaldehyde Complex"
Angew. Chem. Int. Ed. **61** (2022) 264
258} F. Tonolo, L. Bizzocchi*, M. Melosso, F. Lique*, L. Dore, V. Barone, C. Puzzarini*
"An improved study of HCO^+ and He system: Interaction potential, collisional relaxation, and pressure broadening"
J. Chem. Phys. **155** (2021) 234306
257} J. García de la Concepción*, C. Puzzarini*, V. Barone*, I. Jiménez-Serra, O. Roncero
"Formation of Phosphorus Monoxide (PO) in the Interstellar Medium: Insights from Quantum-chemical and Kinetic Calculations"
Astrophys. J. **922** (2021) 169
256} A. Melli, F. Tonolo, V. Barone*, C. Puzzarini*
"Extending the Applicability of the Semi-experimental Approach by Means of "Template Molecule" and "Linear Regression" Models on Top of DFT Computations"
J. Phys. Chem. A **125** (2021) 9904
255} M. Sheng, F. Silvestrini, M. Biczysko*, C. Puzzarini*
"Structural and Vibrational Properties of Amino Acids from Composite Schemes and Double-Hybrid DFT: Hydrogen Bonding in Serine as a Test Case"
J. Phys. Chem. A **125** (2021) 9099
254} J. Lupi, S. Alessandrini, C. Puzzarini*, V. Barone*
"junChS and junChS-F12 Models: Parameter-free Efficient yet Accurate Composite Schemes for Energies and Structures of Noncovalent Complexes"
J. Chem. Theory Comput. **17** (2021) 6974
253} M. Melosso*, M.L. Diouf, L. Bizzocchi, M.E. Harding*, F.M.J. Cozijn, C. Puzzarini*, W. Ubachs*
"Hyperfine-Resolved Near-Infrared Spectra of $H_2{}^{17}O$"
J. Phys. Chem. A **125** (2021) 7884
252} S. Alessandrini*, M. Melosso, N. Jiang, L. Bizzocchi, L. Dore, C. Puzzarini
"Conformational stability of cyclopropanecarboxaldehyde ruled by vibrational effects"
Mol. Phys. **119** (2021) e1955988

[*Invited Article: Special Issue in honor of prof. J.F. Stanton*]
251} I. Leon, N. Tasinato, L. Spada, E.R. Alonso, S. Mata, A. Balbi, C. Puzzarini*, J.L. Alonso*, V. Barone*
"Looking for the Elusive Imine Tautomer of Creatinine: Different States of Aggregation Studied by Quantum Chemistry and Molecular Spectroscopy"
ChemPlusChem **86** (2021) 1374
250} V. Barone*, C. Puzzarini, G. Mancini
"Integration of theory, simulation, artificial intelligence and virtual reality: a four-pillar approach for reconciling accuracy and interpretability in computational spectroscopy"
Phys. Chem. Chem. Phys. **23** (2021) 17079
[*invited perspective article – selected as 2020 PCCP HOT Article*]
249} V. Barone, S. Alessandrini, M. Biczysko, J.R. Cheeseman, D.C. Clary, A.B. McCoy, R.J. DiRisio, F. Neese, M. Melosso, C. Puzzarini*
"Computational Molecular Spectroscopy"
Nature Reviews Methods Primers **1** (2021) 38
248} S. Potenti, L. Spada, M. Fusé, G. Mancini, A. Gualandi, C. Leonardi, P. G. Cozzi*, C. Puzzarini*, V. Barone*
"4-Fluoro-Threonine: From Diastereoselective Synthesis to pH-Dependent Conformational Equilibrium in Aqueous Solution"
ACS Omega **6** (2021) 13170
247} P. Stoppa, A. Pietropolli Charmet, A. De Lorenzi, F. Tamassia, M. Melosso, E. Cané, L. Dore, C. Puzzarini
"High resolution FTIR study of the ν_5, ν_6, and ν_9 fundamental bands of $CH_2D^{37}Cl$"
J. Quant. Spectrosc. Radiat. Transfer **270** (2021) 107719
246} A. Melli, V. Barone, C. Puzzarini*
"Unveiling Bifunctional Hydrogen Bonding with the Help of Quantum Chemistry: The Imidazole-Water Adduct as Test Case"
J. Phys. Chem. A **125** (2021) 2989
245} E. R. Alonso, M. Fusé, I. León, C. Puzzarini, J. L. Alonso, V. Barone
"Exploring the Maze of Cycloserine Conformers in the Gas Phase Guided by Microwave Spectroscopy and Quantum Chemistry"
J. Phys. Chem. A. **125** (2021) 2121
244} N. Jiang, M. Melosso, F. Tamassia, L. Bizzocchi, L. Dore, E. Canè, D. Fedele, J.-C. Guillemin, C. Puzzarini
"High-resolution infrared spectroscopy of DC_3N in the stretching region"
Front. Astron. Space Sci. **8** (2021) 656295
243} M. d'Ischia, P. Manini, Z. Martins, L. Remusat, C. M. O'D. Alexander, C. Puzzarini, V. Barone, R. Saladino
"Insoluble Organic Matter in Chondrites: Archetypal Melanin-Like PAH-Based Multifunctionality at the Origin of Life?"
Phys. Life Rev. **37** (2021) 65
242} M. Melosso*, L. Bizzocchi, L. Dore, Z. Kisiel, N. Jiang, S. Spezzano, P. Caselli, J. Gauss, C. Puzzarini*
"Improved centrifugal and hyperfine analysis of ND_2H and NH_2D and its application to the spectral line survey of L1544"
J. Mol. Spectrosc. **377** (2021) 111431
241} A.R. Al-Derzi, J. Tennyson, S.N. Yurchenkoa, M. Melosso, N. Jiang, C. Puzzarini, L. Dore, T. Furtenbacher, R. Tobias, A.G. Császár
"An improved rovibrational linelist of formaldehyde, $H_2{}^{12}C^{16}O$"
J. Quantit. Spectrosc. Radiat. Transfer **266** (2021) 107563
240} S. Alessandrini, F. Tonolo, C. Puzzarini
"In Search of Phosphorous in Astronomical Environments: The Reaction Between the CP radical ($X^2\Sigma^+$) and Methanimine"
J. Chem. Phys. **154** (2021) 054306
239} V. Barone*, C. Puzzarini*
"Looking for the bricks of the life in the interstellar medium: The fascinating world of astrochemistry"
EPJ Web of Conferences **246** (2020) 00021 [https://doi.org/10.1051/epjconf/202024600021]
238} A. Melli, S. Potenti, M. Melosso, S. Herbers, L. Spada*, A. Gualandi, K.G. Lengsfeld, L. Dore, P. Buschmann, P.G. Cozzi*, J.-U. Grabow*, V. Barone*, C. Puzzarini*
"A journey from thermally-tunable synthesis to spectroscopy of phenylmethanimine in gas-phase and solution."
Chem. Eur. J. **26** (2020) 15016

237} C. Puzzarini*, V. Barone
"Challenges in Astrochemistry: the spectroscopic point of view. Comment on "Prebiotic chemistry and origins of life research with atomistic computer simulations" by A. Pérez-Villa, F. Pietrucci, and A. M. Saitta"
Phys. Life Rev. **34-35** (2020) 143
236} J. Lupi, C. Puzzarini*, V. Barone*
"Methanimine as a key precursor of imines in the interstellar medium: the case of propargylimine"
Astrophys. J. Lett. **903** (2020) L35
235} J. Lei, S. Alessandrini, J. Chen, Y. Zheng, L. Spada, Q. Gou, C. Puzzarini, V. Barone
"Rotational Spectroscopy Meets Quantum Chemistry for Analyzing Substituent Effects on Non-Covalent Interactions: The Case of the Trifluoroacetophenone-Water Complex"
Molecules 25 (2020) 4899
234} S. Alessandrini*, V. Dell'Isola, L. Spada, V. Barone, C. Puzzarini*
"A computational journey in the CH_2O_2S land: an accurate rotational and ro-vibrational analysis of the sulfene molecule and the O,S- and O,O-monothiocarbonic acids"
Mol. Phys. **118** (2020) e1766707
[*Invited Article: Special Issue in honor of prof. J. Gauss*]
233} C. Puzzarini*
"Prebiotic molecules in interstellar space: rotational spectroscopy and quantum chemistry"
Proc. Int. Astron. Union, **15**(S350), 65-70 (2019). DOI: 10.1017/S1743921319007592
232} M. Melosso, A. Belloche, M.-A. Martin-Drumel, O. Pirali, F. Tamassia, L. Bizzocchi, R.T. Garrod, H.S.P. Müller, K.M. Menten, L. Dore, C. Puzzarini
"Far-infrared laboratory spectroscopy of aminoacetonitrile and first interstellar detection of its vibrationally excited transitions"
Astron. Astrophys. **641** (2020) A160
231} F. Tonolo, J. Lupi, C. Puzzarini*, V. Barone
"The quest for a plausible formation route of formyl cyanide in the interstellar medium: a state-of-the-art quantum-chemical and kinetic approach"
Astrophys. J. **900** (2020) 85
230} J. Lupi, C. Puzzarini, C. Cavallotti, V. Barone
"State-of-the-art quantum chemistry meets variable reaction coordinate transition state theory to solve the puzzling case of the H_2S + Cl system"
J. Chem. Theory Comp. **16** (2020) 5090
229} C. Puzzarini*, Z. Salta, N. Tasinato, J. Lupi, C. Cavallotti, V. Barone*
"A twist on the reaction of the CN radical with methylamine in the interstellar medium: new hints from a state-of-the-art quantum-chemical study"
MNRAS **496** (2020) 4298
228} S. Onofri, N. Balucani, V. Barone, P. Benedetti, D. Billi, A. Balbi, J.R. Brucato, B. Cobucci-Ponzano, G. Costanzo, N. La Rocca, M. Moracci, R. Saladino, G. Vladilo, OPPS Project Team: N. Albertini, M. Battistuzzi, J. Bloino, L. Botta, P. Casavecchia, A. Cassaro, R. Claudi, L. Cocola, A. Coduti, P. Di Donato, E. Di Mauro, L. Dore, S. Falcinelli, M. Fulle, S. Ivanovski, A. Lombardi, G. Mancini, M. Maris, L. Maurelli, G. Murante, R. Negri, C. Pacelli, I. Pagano, D. Piccinino, L. Poletto, G. Prantera, C. Puzzarini, S. Rampino, C. Ripa, M. Rosi, M. Sanna, L. Selbmann, L. Silva, D. Skouteris, A. Strazzulli, N. Tasinato, A.M. Timperio, A. Tozzi, G.P. Tozzi, L. Trainotti, P. Ugliengo, L. Vaccaro, L. Zucconi, Laura
"The Italian national project of astrobiology-life in space-origin, presence, persistence of life in space, from molecules to extremophiles"
Astrobiology **20** (2020) 5; Erratum: *ibid* **20** (2020) 924
227} C. Baiano, J. Lupi, N. Tasinato, C. Puzzarini*, V. Barone*
"The role of state-of-the-art quantum-chemical calculations in astrochemistry: formation route and spectroscopy of ethanimine as a paradigmatic case"
Molecules **25** (2020) 2873
[*Special Issue "From Molecules to Origin of Life: The Astrobiology Network"*]
226} P. Gorai,* M. Sil,* A. Das,* B. Sivaraman, S. K. Chakrabarti, S. Ioppolo,* C. Puzzarini,* Z. Kanuchova, A. Dawes, M. Mendolicchio, G. Mancini, V. Barone,* N. Nakatani, T. Shimonishi, N. Mason
"Systematic Study on the Absorption Features of Interstellar Ices in the Presence of Impurities"
ACS Earth Space Chem. **4** (2020) 920
225} C. Puzzarini*

"Grand Challenges in Astrochemistry"
Front. Astron. Space Sci. **7** (2020) 19 DOI: 10.3389/fspas.2020.00019
[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"
Phys. Life Rev. **32** (2020) 59
[invited article]
222} Z. Salta, N. Tasinato, J. Lupi, R. Boussessi, A. Balbi, C. Puzzarini, V. Barone
"Exploring the Maze of $C_2N_2H_5$ Radicals and Their Fragments in the Interstellar Medium with the Help of Quantum-Chemical Computations"
ACS Earth Space Chem., **4** (2020) 774
221} C. Puzzarini*, L. Spada, S. Alessandrini, V. Barone
"The challenge of non-covalent interactions: theory meets experiment for reconciling accuracy and interpretation"
J. Phys.: Condes. Matter, **32** (2020) 343002
[Invited Topical Review]
220} M. Melosso**,** L. Dore, J. Gauss, C. Puzzarini
"Deuterium hyperfine splittings in the rotational spectrum of NH_2D as revealed by Lamb-dip spectroscopy"
J. Mol. Spectrosc., **370** (2020) 111291
219} H. Ye, M. Mendolicchio, H. Kruse, C. Puzzarini, M. Biczysko, V. Barone
"Structural properties of molecules with disulfide bond: an accurate study of HSSH"
J. Mol. Struct., **1211** (2020) 127933
[Jon T. Hougen – Special Issue]
218} C. Puzzarini*, V. Barone
"The challenging playground of astrochemistry: an integrated rotational spectroscopy – quantum chemistry strategy"
Phys. Chem. Chem. Phys., **22** (2020) 6507
[invited perspective article – selected as 2020 PCCP HOT Article]
217} J. Chen, Y. Zheng, A. Melli, L. Spada, T. Lu, G. Feng, Q. Gou*, V. Barone*, C. Puzzarini*
"Theory meets experiment for elucidating the structure and stability of non-covalent complexes: water-amine interaction as a proof of concept"
Phys. Chem. Chem. Phys., **22** (2020) 5020
216} M. Melosso*****, A. Melli, L. Spada, Y. Zheng, J. Chen, M. Li, T. Lu, G. Feng, Q. Gou*, L. Dore, V. Barone, C. Puzzarini*
"Rich Collection of n-Propylamine and Isopropylamine Conformers: Rotational Fingerprints and State-of-the-Art Quantum Chemical Investigation"
J. Phys. Chem. A, **124** (2020) 1372
[invited article: Virtual Special Issue – 75th International Symposium on Molecular Spectroscopy]
215} S. Alessandrini*, V. Barone*, C. Puzzarini*
"Extension of the "cheap" composite approach to non-covalent interactions: the jun-ChS scheme"
J. Chem. Theory Comp., **16** (2020) 988.
214} M. Fusè, G. Mazzeo, G. Longhi, S. Abbate, M. Masi, A. Evidente, C. Puzzarini, V. Barone
"Unbiased Determination of Absolute Configurations by vis-à-vis Comparison of Experimental and Simulated Spectra: The Challenging Case of Diplopyrone"
J. Phys. Chem. B **123** (2019) 9230.
213} J. Wang, L. Spada, J. Chen, S. Gao, S. Alessandrini, G. Feng*, C. Puzzarini*, Q. Gou*, J.-U. Grabow, V. Barone*
"The unexplored world of cycloalkene-water complexes: primary and assisting interactions unraveled by experimental and computational spectroscopy"
Angew. Chem. Int. Ed. **58** (2019) 13935.
212} M. d'Ischia, P. Manini, M. Moracci, R. Saladino, V. Ball, H. Thissen, R. A. Evans, C. Puzzarini, V. Barone
"Astrochemistry and Astrobiology: Materials Science in Wonderland?"

Int. J. Mol. Sci., **20** (2019) 4079

211} C. Puzzarini*, J. Bloino, N. Tasinato, V. Barone*
"Accuracy and Interpretability: The Devil and the Holy Grail. New Routes Across Old Boundaries in Computational Spectroscopy"
Chem. Rev., **119** (2019) 8131.

210} C. Puzzarini*, M. P. de Lara-Castells*, M. J. Ramos*
"Challenges in spectroscopy: accuracy *versus* interpretation from isolated molecules to condensed phases"
Phys. Chem. Chem. Phys., **21** (2019) 3395.
[Editorial: Themed Issue – Challenges in spectroscopy]

209} C. Puzzarini*, N. Tasinato, J. Bloino, L. Spada, V. Barone*
"State-of-the-art computation of the rotational and IR spectra of the methyl-cyclopropyl cation: hints on its detection in space"
Phys. Chem. Chem. Phys., **21** (2019) 3431.
[invited article: Themed Issue – Challenges in spectroscopy]

208} D. A. Obenchain, L. Spada, S. Alessandrini, S. Rampino, S. Herbers, N. Tasinato, M. Mendolicchio, P. Kraus, J. Gauss, C. Puzzarini, J.-U. Grabow, V. Barone
"Unveiling the sulfur-sulfur bridge: accurate structural and energetic characterization of a homo chalcogen inter-molecular bond"
Angew. Chem. Int. Ed. **57** (2018) 15822.
[selected as Very Important Paper]

207} W. Li, L. Spada*, N. Tasinato*, S. Rampino, L. Evangelisti, A. Gualandi, P.G. Cozzi, S. Melandri, V. Barone, C. Puzzarini*
"Theory meets experiment for noncovalent complexes: the puzzling case of pnicogen interactions"
Angew. Chem. Int. Ed., **57** (2018) 13857.

206} S. Alessandrini, J. Gauss, C. Puzzarini*
"The Accuracy of Rotational Parameters Predicted by High-level Quantum-Chemical Calculations: The Case Study of Sulfur-Containing Molecules of Astrochemical Interest"
J. Chem. Theory Comp. **14** (2018) 5360.

205} C. Degli Esposti, L. Dore, C. Puzzarini, M. Biczysko, J. Bloino, L. Bizzocchi, V. Lattanzi, J.-U. Grabow
"Accurate rest frequencies for propargylamine in the ground and low-lying vibrational states"
Astron. Astrophys. **15** (2018) A176.

204} M. Biczysko, J. Bloino, C. Puzzarini*
"Computational Challenges in Astrochemistry"
WIREs Comput Mol Sci **8** (2018) e1349.

203} A. Melli, M. Melosso, N. Tasinato*, G. Bosi, L. Spada, J. Bloino, M. Mendolicchio, L. Dore, V. Barone, C. Puzzarini*
"Rotational and Infrared Spectroscopy of Ethanimine: A Route toward Its Astrophysical and Planetary Detection"
Astrophys. J. **855** (2018) 123.

202} D. Skouteris, N. Balucani, C. Ceccarelli, F. Vazart, C. Puzzarini, V. Barone, C. Codella, B. Lefloch
"The genealogical tree of ethanol: gas-phase formation of glycolaldehyde, acetic acid and formic acid"
Astrophys. J., **854** (2018) 135.

201} C. Puzzarini*, V. Barone*
"Diving for Accurate Structures in the Ocean of Molecular Systems with the Help of Spectroscopy and Quantum Chemistry"
Acc. Chem. Res. **51** (2018) 548.

200} M. Melosso, A. Melli, C. Puzzarini*, C. Codella, L. Spada, L. Dore, C. Degli Esposti, B. Lefloch, R. Bachiller, C. Ceccarelli, J. Cernicharo, V. Barone
"Laboratory measurements and astronomical search for cyanomethanimine"
Astron. Astrophys., **609** (2018) A121.

199} C. Codella, C. Ceccarelli, P. Caselli, N. Balucani, V. Barone, F. Fontani, B. Lefloch, L. Podio, S. Viti, S. Feng, R. Bachiller, E. Bianchi, F. Dulieu, I. Jiménez-Serra, J. Holdship, R. Neri, J. Pineda, A. Pon, I. Sims, S. Spezzano, A.I. Vasyunin, F. Alves, L. Bizzocchi, S. Bottinelli, E. Caux, A. Chacón-Tanarro, R. Choudhury, A. Coutens, C. Favre, P. Hily-Blant, C. Kahane, A. Jaber Al-Edhari, J. Laas, A. López-Sepulcre, J. Ospina, Y. Oya, A. Punanova, C. Puzzarini, D. Quenard, A. Rimola, N. Sakai, D. Skouteris, V. Taquet, L. Testi, P. Theulé, P. Ugliengo, C. Vastel, F. Vazart, L. Wiesenfeld, and S. Yamamoto. Seeds of Life in Space (SOLIS) II

"Formamide in protostellar shocks: evidence for gas-phase formation"
Astron. Astrophys., **605** (2017) L3. arXiv:1708.04663 [astro-ph.EP]
198} N. Tasinato, C. Puzzarini, V. Barone
"Correct Modeling of Cisplatin: a Paradigmatic Case"
Angew. Chem. Int. Ed., **56** (2017) 13838.
[Hot paper]
197} D. Licari, N. Tasinato, L. Spada, C. Puzzarini, V. Barone
"VMS-ROT: A New Module of the Virtual Multifrequency Spectrometer for Simulation, Interpretation, and Fitting of Rotational Spectra"
J. Chem. Theory Comput., **13** (2017) 4382.
196} G. Ceselin, N. Tasinato, C. Puzzarini, A. Pietropolli Charmet, P. Stoppa, S. Giorgianni
"CO_2-, He- and H_2-broadening coefficients of SO_2 for ν_1 band and ground state transitions for astrophysical applications"
J. Quantit. Spectrosc. Radiat. Transfer, **203** (2017) 367.
195} G. Cazzoli, V. Lattanzi, S. Coriani, J. Gauss, C. Codella, A. Asensio Ramos, J. Cernicharo, C. Puzzarini*
"Zeeman effect in sulfur monoxide. A tool to probe magnetic fields in star forming regions"
Astron. Astrophys., **605** (2017) A20.
194} C. Puzzarini*, A. Baiardi, J. Bloino, V. Barone, T. E. Murphy, H. D. Drew, A. Ali
"Spectroscopic Characterization of Key Aromatic and Heterocyclic Molecules: A Route toward the Origin of Life"
Astron. J. **154** (2017) 82
193} C. Puzzarini, M. Biczysko, K. A. Peterson, J. S. Francisco, R. Linguerri
"Accurate spectroscopic characterization of the HOC(O)O radical: A route toward its experimental identification"
J. Chem. Phys. **147** (2017) 024302
192} G. Ceselin, N. Tasinato, C. Puzzarini, A. Pietropolli Charmet, P. Stoppa, S. Giorgianni
"Collision induced broadening of ν_1 band and ground state spectral lines of sulfur dioxide perturbed by N_2 and O_2"
J. Quantit. Spectrosc. Radiat. Transfer **198** (2017) 155
191} L. Spada, N. Tasinato, G. Bosi, F. Vazart, V. Barone, C. Puzzarini*
"On the competition between weak O-H…F and C-H…F hydrogen bonds, in cooperation with CH…O contacts, in the difluoromethane – tert-butyl alcohol cluster"
J. Mol. Spectrosc. **337** (2017) 90
190} A. Pietropolli Charmet, P. Stoppa, S. Giorgianni, J. Bloino, N. Tasinato, I. Carnimeo, M. Biczysko, C. Puzzarini
"Accurate Vibrational−Rotational Parameters and Infrared Intensities of 1-Bromo-1-fluoroethene: A Joint Experimental Analysis and Ab Initio Study"
J. Phys. Chem. A **121** (2017) 3305
189} R. Linguerri, C. Puzzarini, M. Mogren Al Mogren, J. S. Francisco, M. Hochlaf
"Benchmark study of the structural and spectroscopic parameters of the hydroxymethyl peroxy (HOCH2OO) radical and its decomposition reaction to HO_2 and H_2CO"
J. Chem. Phys. **146** (2017) 144303
188} L. Spada, N. Tasinato, F. Vazart, V. Barone, W. Caminati, C. Puzzarini*
"Noncovalent Interactions and Internal Dynamics in Pyridine–Ammonia: A Combined Quantum-Chemical and Microwave Spectroscopy Study"
Chem. Eur. J. **23** (2017) 4876
187} D. Skouteris, F. Vazart, C. Ceccarelli, N. Balucani, C. Puzzarini, V. Barone
"New quantum chemical computations of formamide deuteration support a gas-phase formation of this prebiotic molecule"
MNRAS Lett. **468** (2017) L1
186} L. Wiesenfeld, W.-F. Thi, P. Caselli, A. Faure, L. Bizzocchi, J. Brandão, D. Duflot, E. Herbst, S. J. Klippenstein, T. Komatsuzaki, C. Puzzarini, O. Roncero, H. Teramoto, M. Toda, A. van der Avoird, H. Waalkens
"Theory of Gas Phase Scattering and Reactivity for Astrochemistry"
White Paper - arXiv:1610.00438v1 [astro-ph.IM]
185} C. Puzzarini*
Perspective - "Astronomical Complex Organic Molecules: Quantum Chemistry meets Rotational Spectroscopy"

Int. J. Quantum Chem. **117** (2017) 129
[invited article: Special Issue - Theoretical and Computational Astrochemistry]
184} C. Puzzarini*
Perspective - "Accurate molecular structures of small- and medium-sized molecules"
Int. J. Quantum Chem., **116** (2016) 1513.
[invited article: Special Issue - Computational and Theoretical Chemistry in Italy]
183} F. Vazart, D. Calderini, C. Puzzarini, D. Skouteris, V. Barone
"State-of-the-art thermochemical and kinetic computations for astrochemical complex organic molecules: formamide formation in cold interstellar clouds as a case study"
J. Chem. Theory Comp., **12** (2016) 5385.
182} G. Cazzoli, V. Lattanzi, T. Kirsch, J. Gauss, B. Tercero, J. Cernicharo, C. Puzzarini*
"Laboratory measurements and astronomical search for the HSO radical"
Astron. Astrophys., **591** (2016) A126.
181} S. Alessandrini, C. Puzzarini*
"Structural and Energetic Characterization of Prebiotic Molecules: The Case Study of Formamide and Its Dimer"
J. Phys. Chem. A, **120** (2016) 5257.
[invited article: Casavecchia & Laganà special issue]
180} R. Linguerri, C. Puzzarini, J. S. Francisco,
"Structure and spectroscopic properties of low-lying states of the HOC(O)O radical"
J. Chem. Phys. **144** (2016) 084306.
179} P. Cacciani, J. Cosléou, M. Khelkhal, P. Čermák, C. Puzzarini*
"Nuclear spin conversion in CH_4: a multi-channel relaxation mechanism",
J. Phys. Chem. A, **120** (2016) 173
178} G. Cazzoli, T. Kirsch, J. Gauss, C. Puzzarini*
"The rotational spectrum of $^{17}O_2$ up to the THz region",
J. Quantit. Spectrosc. Radiat. Transfer, **168** (2016) 10
177} C. Puzzarini*
"Isomerism of cyanomethanimine: Accurate structural, energetic and spectroscopic characterization",
J. Phys. Chem. A, **119** (2015) 11614
[invited article: "Spectroscopy and Dynamics of Medium-Sized Molecules and Clusters: Theory, Experiment, and Applications" special issue]
176} A. Bellili, R. Linguerri, M. Hochlaf, C. Puzzarini*
"Accurate structural and spectroscopic characterization of prebiotic molecules: the neutral and cationic acetyl cyanide and their related species",
J. Chem. Phys., **141** (2015) 204302
175} V. Lattanzi, G. Cazzoli, C. Puzzarini
"Rare isotopic species of sulphur monoxide: the rotational spectrum in the THz region",
Astrophys. J, **813** (2015) 4
174} V. Barone, M. Biczysko, J. Bloino, P. Cimino, E. Penocchio, C. Puzzarini
"CC/DFT Route toward Accurate Structures and Spectroscopic Features for Observed and Elusive Conformers of Flexible Molecules: Pyruvic Acid as a Case Study",
J. Chem. Theo. Comp., **11** (2015) 4342
173} M. Hochlaf, C. Puzzarini, M. L. Senent
"Towards the computations of accurate spectroscopic parameters and vibrational spectra for organic compounds",
Mol. Phys., **113** (2015) 1661
172} C. Puzzarini*, M. Biczysko,
"Microsolvation of 2−Thiouracil: Molecular Structure and Spectroscopic Parameters of the Thiouracil-Water Complex",
J. Phys. Chem. A, **119** (2015) 5386
171} A. Ali, E. C. Sittler Jr, D. Chornay, B. R. Rowe, C. Puzzarini*
"Organic chemistry in Titan's upper atmosphere and its astrobiological consequences: I. Views towards Cassini plasma spectrometer (CAPS) and ion neutral mass spectrometer (INMS) experiments in space",
Plan. Space Sci., **109–110** (2015) 46
170} V. Barone*, M. Biczysko*, C. Puzzarini*

"Quantum Chemistry Meets Spectroscopy for Astrochemistry: Increasing Complexity toward Prebiotic Molecules",
Acc. Chem. Res., **48** (2015) 1413
169} G. Cazzoli, V. Lattanzi, J. L. Alonso, J. Gauss, C. Puzzarini*
"The hyperfine structure of the rotational structure of the rotational spectrum of HDO and its extension to the THz region: Accurate rest frequencies and spectroscopic parameters for astrophysical observations",
Astrophys. J., **806** (2015) 100
168} M. Piccardo, E. Penocchio, C. Puzzarini, M. Biczysko, V. Barone
"Semi-Experimental Equilibrium Structure Determinations by Employing B3LYP/SNSD Anharmonic Force Fields: Validation and Application to Semirigid Organic Molecules",
J. Phys. Chem. A, **119** (2015) 2058; Erratum: J. Phys. Chem. A, **120** (2016) 3754
167} C. Puzzarini*, G. Cazzoli, M. E. Harding, J. Vázquez, J. Gauss
"The hyperfine structure in the rotational spectra of $D_2{}^{17}O$ and $HD^{17}O$: Confirmation of the absolute nuclear magnetic shielding scale for oxygen",
J. Chem. Phys., **142** (2015) 124308
166} G. Cazzoli, C. Puzzarini*
"The Impact of Sub-Doppler Measurements on Centrifugal-Distortion Terms: The Rotational Spectrum of Methyl Fluoride Revisited",
J. Phys. Chem. A, **119** (2015) 1765
[invited article: 25th Austin Symposium on Molecular Structure and Dynamics]
165} L. Bizzocchi, C. Degli Esposti, L. Dore, J. Gauss, C. Puzzarini
"The Born-Oppenheimer equilibrium bond distance of GeO from millimeter and submillimeter-wave spectra and quantum-chemical calculations",
Mol. Phys., **113** (2015) 801
164} C. Puzzarini*, M. L. Senent, R. Domínguez-Gómez, M. Carvajal, M. Hochlaf, M. Mogren Al-Mogren
"Accurate spectroscopic characterization of ethyl mercaptan and dimethyl sulfide isotopologues: A route toward their astrophysical detection",
Astrophys. J., **796** (2014) 50
163} C. Puzzarini*, E. Penocchio, M. Biczysko, V. Barone
"Molecular Structure and Spectroscopic Signatures of Acrolein: Theory Meets Experiment",
J. Phys. Chem. A, **118** (2014) 6648
[invited article: Franco Gianturco Festschrift]
162} M. L. Senent, C. Puzzarini, M. Hochlaf, R. Domínguez-Gómez, M. Carvajal
"Theoretical spectroscopic characterization at low temperatures of S-methyl thioformate and O-methyl thioformate",
J. Chem. Phys., **141** (2014) 104303
161} C. Puzzarini*, A. Ali, M. Biczysko, V. Barone
"Accurate spectroscopic characterization of protonated oxirane: A potential prebiotic species in Titan's atmosphere",
Astrophys. J., **792** (2014) 118
160} V. Barone, M. Biczysko, J. Bloino, C. Puzzarini*
"Accurate molecular structures and infrared spectra of trans-2,3-dideuterooxirane, methyloxirane, and trans-2,3-dimethyloxirane",
J. Chem. Phys. **141** (2014) 034107
159} G. Cazzoli, C. Puzzarini*, J. Gauss
"Rare isotopic species of hydrogen sulfide: the rotational spectrum of $H_2{}^{36}S$",
Astron. Astrophys., **566** (2014) A52
158} C. Puzzarini*, M. Biczysko, J. Bloino, V. Barone
"Accurte spectroscopic characterization of oxirane: A valuable route to its identification in Titan's atmosphere and the assignment of unidentified infrared",
Astrophys. J., **785** (2014) 107
157} C. Puzzarini*, M. Biczysko, V. Barone, L. Largo, I. Peña, C. Cabezas, J. L. Alonso
"Accurate Characterization of the Peptide Linkage in the Gas Phase: A Joint Quantum-Chemical and Rotational Spectroscopy Study of the Glycine Dipeptide Analogue",
J. Phys. Chem. Lett., **5** (2014) 534
156} M. L. Senent, C. Puzzarini, R. Domínguez-Gómez, M. Carvajal, M. Hochlaf

"Theoretical spectroscopic characterization at low temperatures of detectable sulfur-organic compounds: ethyl mercaptan and dimethyl sulfide.",
J. Chem. Phys., **140** (2014) 124302.
155} N. Tasinato, A. Turchetto, C. Puzzarini, P. Stoppa, A. Pietropolli Charmet, S. Giorgianni
"Self-, N_2-, O_2- broadening coefficients and line parameters of HFC-32 for ν_7 band- and ground state- transitions from infrared and microwave spectroscopy",
Mol. Phys. (HRMS special issue), **112** (2014) 2384.
154} G. Cazzoli, C. Puzzarini*
"The rotational spectrum of H_2S: the $H_2{}^{33}S$ and $H_2{}^{32}S$ isotopologues revisited and the sub-doppler resolution in the THz regime.",
J. Mol. Spectrosc., **298** (2014) 31.
153} T. U. Helgaker, J. Gauss, G. Cazzoli, C. Puzzarini
"^{33}S hyperfine interactions in H_2S and SO_2 and revision of the sulfur nuclear magnetic shielding.",
J. Chem. Phys., **139** (2013) 244308.
152} G. Cazzoli, C. Puzzarini*
"Sub-Doppler resolution in the THz frequency domain: 1 kHz accuracy at 1 THz by exploiting the Lamb-dip technique.",
J. Phys. Chem. A, **117** (2013) 13759.
[*invited article: Terry Miller special issue*]
151} A. Ali, E. C. Sittler Jr., D. Chornay, B. R. Rowe, C. Puzzarini*
"Cyclopropenyl Cation - the Simplest Huckel's Aromatic Molecole and its Cyclic Methyl Derivatives in Titan's Upper Atmosphere.",
Plan. Space Sci., **87** (2013) 96.
150} A. Pietropolli Charmet, P. Stoppa, N. Tasinato, S. Giorgianni, V. Barone, M. Biczysko, J. Bloino, C. Cappelli, I. Carnimeo, C. Puzzarini
"An integrated experimental and quantum-chemical investigation on the vibrational spectra of chlorofluoromethane",
J. Chem. Phys., **139** (2013) 164302.
149} N. Tasinato, A. Pietropolli Charmet, P. Stoppa, G. Buffa, C. Puzzarini*
"A complete listing of sulfur dioxide self broadening coefficients for atmospheric applications by coupling infrared and microwave spectroscopy to semiclassical calculations",
J. Quantitative Spectrosc. Radiat. Transfer (HITRAN S.I.), **130** (2013) 233.
148} C. Puzzarini*, M. Biczysko, V. Barone, M. I. Pena, C. Cabezas, J. L. Alonso
"Accurate molecular structure and spectroscopic properties for nucleobases: A combined computational - microwave investigation of 2-thiouracil as a case study.",
Phys. Chem. Chem. Phys., **15** (2013) 16965.
147} C. Puzzarini, J. Gauss
"Quantum-chemical determination of Born-Oppenheimer breakdown
parameters for rotational constants: the open-shell species CN, CO^+ and BO.",
Mol. Phys., **111** (2013) 2204.
[*invited article: M. Quack special issue*]
146} I. Carnimeo, C. Puzzarini, N. Tasinato, P. Stoppa, A. Pietropolli Charmet, M. Biczysko, C. Cappelli, V. Barone
"Anharmonic theoretical simulations of infrared spectra of halogenated organic compounds",
J. Chem. Phys., **139** (2013) 074310.
145} S. Stopkowicz, L. Cheng, M. E. Harding, C. Puzzarini, J. Gauss
"The bromine nuclear quadrupole moment revisited.",
Mol. Phys., **111** (2013) 1382.
[*invited article: T. Helgaker special issue*]
144} V. Barone, M. Biczysko, J. Bloino, F. Egidi, C. Puzzarini
"Accurate structure, thermodynamics and spectroscopy of medium-sized radicals by hybrid CC/DFT approaches: the case of phenyl radical",
J. Chem. Phys., **138** (2013) 234303.
143} V. Barone, M. Biczysko, J. Bloino, C. Puzzarini*
"Accurate structure, thermodynamic and spectroscopic parameters from CC and CC/DFT schemes: the challenge of the conformational equilibrium in glycine.",

Phys. Chem. Chem. Phys., **15** (2013) 10094.
[*invited article: special theme issue*]
142} C. Puzzarini*
"Rotational spectroscopy meets theory",
Phys. Chem. Chem. Phys., **15** (2013) 6595.
[*invited PESPECTIVE article*]
141} V. Barone, M. Biczysko, J. Bloino, C. Puzzarini
"Characterization of the elusive conformers of Glycine from state-of-the-art structural, thermodynamic and spectroscopic computations: theory complements experiment ",
J. Chem. Theory Comp., **9** (2013) 1533.
140} V. Barone, M. Biczysko, J. Bloino, C. Puzzarini
"Glycine conformers: a never-ending story?",
Phys. Chem. Chem. Phys., **15** (2013) 1358.
139} G. Cazzoli, L. Cludi, G. Buffa, C. Puzzarini*
"Precise THz measurements of HCO^+, N_2H^+ and CF^+ for astrophysical observations",
Astrophys. J., **203** (2012) 11.
138} S. Coriani, C. Puzzarini, A. Rizzo
"First-order properties and Buckingham birefringence of OCS and N_2O - A computational (re)investigation",
Mol. Phys. (P.R. Taylor special issue), **110** (2012) 2543.
137} G. Cazzoli, C. Puzzarini*, J. Gauss
"Rotational spectrum of silyl chloride: hyperfine structure and equilibrium geometry",
Mol. Phys. (P.R. Taylor special issue), **110** (2012) 2359.
136} C. Puzzarini*, G. Cazzoli, J. Gauss
"The rotational spectra of $HD^{17}O$ and $D_2{}^{17}O$: experiment and quantum-chemical calculations",
J. Chem. Phys., **137** (2012) 154311.
135} C. Puzzarini*, G. Cazzoli, J.C. López, J.L. Alonso, A. Baldacci, A. Baldan, S. Stopkowicz, L. Cheng, J. Gauss
"Rotational spectra of rare isotopic species of fluoroiodomethane: determination of the equilibrium structure from rotational spectroscopy and quantum-chemical calculations",
J. Chem. Phys., **137** (2012) 024310.
134} C. Puzzarini*
"Molecular structure of thiourea",
J. Phys. Chem. A, **116** (2012) 4381.
133} G. Cazzoli, C. Puzzarini*
"N_2-, O_2-, H_2-, and He-broadening of SO_2 rotational lines in the mm-/submm-wave and THz frequency regions: the J and K_a dependence",
J. Quantitative Spectrosc. Radiat. Transfer (Flaud, Camy-Peyret, Barbe S.I.), **113** (2012) 1051.
132} M. Biczysko, J. Bloino, G. Brancato, I. Cacelli, C. Cappelli, A. Ferretti, A. Lami, S. Monti, A. Pedone, G. Prampolini, C. Puzzarini, F. Santoro, F. Trani, G. Villani
"Integrated computational approaches for spectroscopic studies of molecular systems in the gas phase and in solution: Pyrimidine as a test case",
Theor. Chem. Acc. (V. Barone special issue), **131** (2012) 1201.
131} C. Puzzarini*, A. Gambi
"A theoretical study on CH_2N_2 isomers: structure, isomerization and energetics",
Theor. Chem. Acc. (V. Barone special issue), **131** (2012) 1135.
130} C. Puzzarini*
"A theoretical study of the CX_2N isomers (X=F,Cl,Br): the effect of X substitution on structure, isomerization and energetics",
J. Chem. Phys., **136** (2012) 044316.
129} C. Puzzarini*
"Accurate thermochemistry and spectroscopy of protonated sulfur dioxide",
Phys. Chem. Chem. Phys., **13** (2011) 21319.
128} C. Puzzarini*, M. Biczysko, V. Barone
"Accurate anharmonic vibrational frequencies for uracil: the performance of composite schemes and hybrid CC/DFT model",
J. Chem. Theory Comp., **7** (2011) 3702.

127} G. Cazzoli, A. Baldacci, A. Baldan, C. Puzzarini*
"Improved vibrational ground-state spectroscopic parameters of CH_2FI and assignment the rotational spectrum of the v_6=1 vibrational state",
Mol. Phys. (special issue HRMS: Di Lonardo), **109** (2011) 2245.
126} G. Cazzoli, C. Puzzarini*, S. Stopkowicz, J. Gauss
"Lamb-dip and THz spectra of monodeuterated trans-formic acid isotopologues (DCOOH, HCOOD): improvements for astrophysical detections",
Astrophys. J. Suppl. Ser., **196** (2011) 10.
125} C. Puzzarini*, G. Cazzoli, Z. Kisiel
"Rotational spectrum of the v_{12}=1, v_{13}=1 and v_7=1 vibrational states of CH_3CCCCH",
J. Mol. Spectrosc. (Bunker & Klemperer special issue), **267** (2011) 118.
124} C. Puzzarini*
"Rotational spectroscopy for astrophysical investigations",
Rendiconti Lincei (Special Issue: Convegno *ASTROCHIMICA: MOLECOLE NELLO SPAZIO E NEL TEMPO*, 4-5 November 2010, Roma, Accademia Nazionale dei Lincei), **22** (2011) 165.
123} C. Puzzarini*, G. Cazzoli, J.C. López, J.L. Alonso, A. Baldacci, A. Baldan, S. Stopkowicz, L. Cheng, J. Gauss
"Spectroscopic investigation of fluoroiodomethane, CH_2FI: Fourier-transform microwave and millimeter-/submillimeter-wave spectroscopy and quantum-chemical calculations",
J. Chem. Phys., **134** (2011) 174312.
122} C. Puzzarini*, V. Barone
"Extending the molecular size in accurate quantum-chemical calculations: the equilibrium structure and spectroscopic properties of uracil",
Phys. Chem. Chem. Phys., **13** (2011) 7158.
121} J. Liévin, J. Demaison, M. Herman, A. Fayt, C. Puzzarini
"Comparison of the experimental, semi-experimental and ab initio equilibrium structures of acetylene: influence of relativistic effects and of diagonal Born-Oppenheimer corrections",
J. Chem. Phys., **134** (2011) 064119.
120} G. Cazzoli, L. Cludi, C. Puzzarini*, P. Stoppa, A. Pietropolli Charmet, N. Tasinato, A. Baldacci, A. Baldan, S. Giorgianni, R. W. Larsen, S. Stopkowicz, J. Gauss
"Microwave, High-Resolution Infrared, and Quantum-Chemical Investigations of $CHBrF_2$: the Ground and v_4 =1 States ",
J. Phys. Chem. A, **115** (2011) 453.
119} G. De Pretis, A. Cartoni, M. Rosi, V. Barone, C. Puzzarini, A. Troiani
"The proton affinity and gas-phase basicity of sulfur dioxide",
ChemPhysChem, **12** (2011) 112.
118} G. Cazzoli, C. Puzzarini*, S. Stopkowicz, J. Gauss
"The rotational spectrum of trans-DCOOD: Lamb-dip measurements, THz spectroscopy and quantum-chemical calculations",
Chem. Phys. Lett., **502** (2011) 42.
117} C. Puzzarini*, V. Barone
"Toward spectroscopic accuracy for open-shell systems: molecular structure and hyperfine coupling constants of H_2CN, H_2CP, NH_2, and PH_2 as test cases",
J. Chem. Phys., **133** (2010) 184301.
116} C. Puzzarini*
"A theoretical study of the CH_2N isomers: molecular structure and energetics",
Int. J. Quantum Chem. (CHITEL09 special issue), **110** (2010) 2483.
115} G. Cazzoli, C. Puzzarini*, S. Stopkowicz, J. Gauss
"Hyperfine structure in the rotational spectrum of trans-formic acid: Lamb-dip measurements and quantum-chemical calculations",
Astron. Astrophys., **520** (2010) A64.
114} G. Cazzoli, L. Dore, C. Puzzarini*, J. Gauss
"The hyperfine structure in the rotational spectra of D_2O: Lamb-dip measurements and quantum-chemical calculations",
Mol. Phys. (Special Issue: 21st Colloquium on High Resolution Spectroscopy - 2009), **108** (2010) 2335.
[*invited article*]

113} C. Puzzarini*, G. Cazzoli, J. Gauss
"Rotational spectra of isotopic species of silyl fluoride. Part II: theoretical and empirical equilibrium structure",
J. Mol. Spectrosc., **262** (2010) 37.
112} C. Puzzarini*, J. F. Stanton, J. Gauss
"Quantum-chemical calculation of spectroscopic parameter for rotational spectroscopy"
Int. Rev. Phys. Chem., **29** (2010) 273.
[*review article*]
111} P. C. Gómez, O. Gálvez, R. G. Mosteo, C. Puzzarini, R. Escribano
"Clusters of atmospheric relevance: $H_2O/HCl/HNO_3$. Prediction of IR and MW spectra ",
Phys. Chem. Chem. Phys., **12** (2010) 4617.
110} J. Gauss, C. Puzzarini
"Quantum-chemical calculation of Born-Oppenheimer breakdown parameters to rotational constants"
Mol. Phys. (H.-J. Werner special issue), **108** (2010) 269.
[*invited article*]
109} C. Puzzarini*, M. Biczysko, V. Barone
"Accurate harmonic/anharmonic vibrational frequencies for open-shell systems: performance of the B3LYP/N07D model for semirigid free radicals benchmarked by CCSD(T) computations",
J. Chem. Theory Comp., **6** (2010) 828.
108} G. Cazzoli, C. Puzzarini*, J. Gauss
"Rotational spectra of isotopic species of silyl fluoride. Part I: Lamb-dip measurements and quantum-chemical calculations",
J. Mol. Spectrosc., **259** (2010) 93.
[*feature article*]
107} G. Cazzoli, L. Cludi, C. Puzzarini*, J. Gauss
"Rotational spectra of CF^+ and $^{13}CF^+$: accurate rest frequencies and spectroscopic parameters",
Astron. Astrophys., **509** (2010) A1.
106} C. Puzzarini*, V. Barone
"Benchmark calculations for molecules in the gas phase: state-of-the-art coupled-cluster computations",
Int. J. Quantum Chem. (CHITEL08 special issue), **110** (2010) 637.
105} C. Puzzarini*
"Extrapolation to the complete basis set limit of structural parameters: comparison of different approaches",
J. Phys. Chem. A (V. Aquilanti special issue), **113** (2009) 14530.
104} C. Puzzarini*, G. Cazzoli, M. E. Harding, J. Vázquez, J. Gauss
"A new experimental absolute nuclear magnetic shielding scale for oxygen based on the rotational hyperfine structure of $H_2{}^{17}O$",
J. Chem. Phys., **131** (2009) 234304.
103} G. Cazzoli, L. Dore, C. Puzzarini*
"The hyperfine structure of the inversion-rotation transition $J_K = 1_0 - 0_0$ of NH_3 investigated by Lamb-dip spectroscopy",
Astron. Astrophys., **507** (2009) 1701.
102} C. Puzzarini*, V. Barone
"On the stability of X_2NO radicals (X=F,Cl,Br,I)",
Phys. Chem. Chem. Phys., **11** (2009) 11463.
101} P. Cacciani, J. Cosléou, M. Khelkhal, M. Tutorie, C. Puzzarini, P. Pracna
"Nuclear spin conversion in NH_3",
Phys. Rev. A, **80** (2009) 042507.
100} C. Puzzarini, V. Barone
"A theoretical study of the X_2NO systems (X=F,Cl,Br,I): effects of halogen substitution on structural and spectroscopic properties",
J. Chem. Theory Comp., **5** (2009) 2378.
99} C. Puzzarini*, G. Cazzoli
"Equilibrium structure of protonated cyanogen, $HNCCN^+$",
J. Mol. Spectrosc. (PRAHA08 special issue), **256** (2009) 53.
98} G. Cazzoli, C. Puzzarini*, M. E. Harding, J. Gauss
"The hyperfine structure in the rotational spectrum of water: Lamb-dip technique and quantum-chemical calculations",

Chem. Phys. Lett., **473** (2009) 21.
97} G. Cazzoli, C. Puzzarini, G. Buffa, O. Tarrini
"Pressure-broadening of water lines in the THz frequency region: improvements and confirmations for spectroscopic databases. Part II.",
J. Quantitative Spectrosc. Radiat. Transfer (HITRAN special issue), **110** (2009) 609.
96} G. Cazzoli, C. Puzzarini*
"Rotational spectrum of the v_{11}=1 and v_{14}=1 vibrational states of CH_3CCCCH",
J. Mol. Spectrosc., **253** (2009) 106.
95} C. Puzzarini*, V. Barone
"The role of accurate quantum mechanical computations in the assignment of vibrational spectra for unstable free radicals: H_2CN and F_2CN as test cases ",
Chem. Phys. Lett., **467** (2009) 276.
94} C. Puzzarini*, V. Barone
"Assessment of a computational strategy approaching spectroscopic accuracy for structure, magnetic properties and vibrational frequencies of organic free radicals: the F_2CN and F_2BO case",
Phys. Chem. Chem. Phys., **10** (2008) 6991.
93} G. Cazzoli, C. Puzzarini, G. Buffa, O. Tarrini
"Pressure-broadening of water lines in the THz frequency region: improvements and confirmations for spectroscopic databases. Part I.",
J. Quantit. Spectrosc. Radiat. Transfer, **109** (2008) 2820.
92} G. Cazzoli, C. Puzzarini, S. Stopkowicz, J. Gauss
"The hyperfine structure in the rotational spectra of bromofluoromethane isotopologues: Lamb-dip technique and quantum-chemical calculations",
Mol. Phys. (Special Issue: 20th Colloquium on High Resolution Spectroscopy - 2007), **106** (2008), 1181.
91} F. Rohart, J.-M. Colmont, G. Wlodarczak, G. Cazzoli, L. Dore, C. Puzzarini*
"Galatry versus Speed Dependent Voigt Profiles for Millimeter Lines of O_3 in Collision with N_2 and O_2",
J. Mol. Spectrosc. (special issue in honor of E.A. Cohen & H.M. Pickett), **251** (2008), 282.
90} G. Cazzoli, L. Cludi, M. Contento, C. Puzzarini
"Rotational spectrum of $CH_3C^{13}CCCH$: determination of the equilibrium structure of methyldiacetylene from microwave spectroscopy and ab initio calculations",
J. Mol. Spectrosc. (special issue in honor of E.A. Cohen & H.M. Pickett), **251** (2008), 229.
89} C. Puzzarini*, V. Barone
"Toward spectroscopic accuracy for organic free radicals: molecular structure, vibrational spectrum and magnetic properties of F_2NO",
J. Chem. Phys., **129** (2008), 084306.
88} C. Puzzarini, V. Barone
"A critical analysis of the structure and vibrational frequencies of F_2NO^+ and Cl_2NO^+ from accurate quantum chemical computations",
Chem. Phys. Lett., **462** (2008), 49.
87} G. Cazzoli, C. Puzzarini
"Lamb-dip spectrum of methylacetylene and methyldiacetylene: precise rotational transition frequencies and parameters of the main isotopic species",
Astron. Astrophys., **487** (2008), 1197.
86} C. Puzzarini*
"Ab initio characterization of XH_3 (X=N,P). II. Electric, magnetic and spectroscopic properties of ammonia and phosphine",
Theor. Chem. Acc., **121** (2008), 1.
85} C. Puzzarini*
"Ab initio characterization of XH_3 (X=N,P). I. Ammonia, phosphine, and their related ions and radicals: structure and thermochemistry",
Theor. Chem. Acc. (special issue in honor of Prof. N. Russo), **120** (2008), 325.
84} C. Puzzarini*, M. Heckert, Jürgen Gauss
"The accuracy of rotational constants predicted by high-level quantum-chemical calculations. I. Molecules containing first-row atoms",
J. Chem. Phys., **128** (2008), 194108.
83} G. Cazzoli, C. Puzzarini, G. Buffa, O. Tarrini

"Pressure-broadening in the THz frequency region: the 1.113 THz line of Water",
J. Quantit. Spectrosc. Radiat. Transfer, **109** (2008), 1563.
82} C. Puzzarini*
"A theoretical investigation on the HCCS radical and its ions",
Chem. Phys. (special issue in honor of P. Botschwina), **346** (2008), 45.
81} G. Cazzoli, C. Puzzarini, F. Tamassia, L. Fusina
"Rotational spectra of deuterated acetylenes: DCCH, $D^{13}CCH$ and $DC^{13}CH$",
J. Mol. Spectrosc., **247** (2008), 115.
80} C. Puzzarini*, G. Cazzoli, A. Baldacci, A. Baldan, C. Michauk, J. Gauss
"Rotational spectra of rare isotopic species of bromofluoromethane: determination of its equilibrium structure from ab initio calculations and microwave spectroscopy",
J. Chem. Phys., **127** (2007), 164302.
79} A. Baldacci, P. Stoppa, A. Pietropolli Charmet, S. Giorgianni, G. Cazzoli, L. Cludi, C. Puzzarini, R. W. Larsen
"Spectroscopic constants of the ground and low vibrational states of $CH_2{}^{81}BrF$: a combined study from high resolution FTIR and microwave spectra",
J. Mol. Spectrosc., **246** (2007), 126.
78} A. Baldacci, P. Stoppa, A. Pietropolli Charmet, S. Giorgianni, G. Cazzoli, C. Puzzarini, R. W. Larsen
"High resolution FTIR, microwave, and ab initio investigations of $CH_2{}^{79}BrF$: the ground, $v_5 = 1$, and $v_6 = 1, 2$ state constants",
J. Phys. Chem. A, **111** (2007), 7090.
77} C. Puzzarini*
"Ab initio anharmonic force field and equilibrium structure of the sulfonium ion",
J. Mol. Spectrosc., **242** (2007), 70.
76} G. Cazzoli, C. Puzzarini, G. Buffa, O. Tarrini
"Experimental and theoretical investigation on pressure-broadening and pressure-shifting of the 22.2 GHz line of Water",
J. Quantit. Spectrosc. Radiat. Transfer, **105** (2007), 438.
75} G. Cazzoli, C. Puzzarini, A. Baldacci, A. Baldan
"Determination of the molecular dipole moment of bromofluoromethane: microwave Stark spectra and ab initio calculations",
J. Mol. Spectrosc., **241** (2007), 115.
74} C. Puzzarini*, G. Cazzoli
"Equilibrium structure of methylcyanide",
J. Mol. Spectrosc., **240** (2006), 260.
73} G. Cazzoli, C. Puzzarini
"The Lamb-dip spectrum of methylcyanide: precise rotational transition frequencies and improved ground state rotational parameters",
J. Mol. Spectrosc., **240** (2006), 153.
72} L. Bizzocchi, C. Degli Esposti, C. Puzzarini
"Millimeter-wave spectroscopy and ab initio calculations for fluorophosphaethine (FCP)",
Mol. Phys. (Special Issue: 19th Colloquium on High Resolution Spectroscopy - 2005), **104** (2006), 2627.
71} G. Cazzoli, C. Puzzarini
"Observation of OD^- using microwave spectroscopy: a new candidate for astrophysical detection?",
Astrophys. J., **648** (2006), L79.
70} C. Puzzarini*, G. Cazzoli, A. Gambi, J. Gauss
"Rotational spectra of 1-chloro-2-fluoroethylene. II. Equilibrium structure of the cis and trans isomers",
J. Chem. Phys., **125** (2006), 05-4307.
69} G. Cazzoli, C. Puzzarini, A. Gambi, J. Gauss
"Rotational spectra of 1-chloro-2-fluoroethylene. I. Main isotopologues and deuterated species of the trans isomer",
J. Chem. Phys., **125** (2006), 05-4313.
68} G. Cazzoli, C. Puzzarini
"The Lamb-dip spectrum of phosphine: the nuclear hyperfine structure due to hydrogen and phosphorus",
J. Mol. Spectrosc., **239** (2006), 64.
67} G. Cazzoli, C. Puzzarini

"Ground state rotational spectrum of nitrogen trifluoride: the K=3 splittings of $^{14}NF_3$ and $^{15}NF_3$",
J. Mol. Spectrosc., **239** (2006), 59.

66} M. Tudorié, P. Cacciani, J. Cosléou, F. Herlemont, M. Khelkhal, C. Puzzarini, S. Maret, C. Kahane
"Nuclear spin conversion of formaldehyde in protostars environments induced by non reactive collisions",
Astron. & Astrophys., **453** (2006), 755.

65} M. Mladenović, P. Botschwina, C. Puzzarini
"Six-dimensional potential energy surface and rovibrational energies of the HCCN radical in the ground electronic state",
J. Phys. Chem. A (special issue: John C. Light Festschrift), **110** (2006), 5520.

64} A. Rizzo, C. Puzzarini, S. Coriani, J. Gauss
"The nuclear spin rotation constants of HCY, HSiY, and SiY_2 (Y=F, Cl). An ab initio study",
J. Chem. Phys., **124** (2006), 06-4302.

63} C. J. Cramer, M. Włoch, P. Piecuch, C. Puzzarini, L. Gagliardi
"Theoretical Models on the Cu_2O_2 Torture Track. Mechanistic Implications for Oxytyrosinase and Small-molecule Analogs",
J. Phys. Chem. A, **110** (2006), 1991; J. Phys. Chem. A, **111** (2007), 4871(E).

62} G. Cazzoli, C. Puzzarini, F. Tamassia, S. Borri, S. Bartalini
"Improved ground state rotational parameters of deuterium fluoride, DF",
J. Mol. Spectrosc., **235** (2006), 263.

61} G. Cazzoli, L. Cludi, C. Puzzarini
"Microwave spectrum of $P^{14}N$ and $P^{15}N$: spectroscopic constants and molecular structure",
J. Mol. Struct. (special issue in honor of Jean Demaison) , **780-781** (2006), 260.

60} C. Puzzarini *
"Theoretical study of XPO (X=H,F,Cl,Br) molecules: structural and molecular properties",
J. Mol. Struct. (special issue in honor of Jean Demaison), **780-781** (2006), 238.

59} K. A. Peterson, C. Puzzarini
"Systematically convergent basis sets for transition metals. II. Pseudopotential-based correlation consistent basis sets for group 11 (Cu, Ag, Au) and 12 (Zn, Cd, Hg) elements",
Theor. Chem. Acc. (special issue in honor of Hermann Stoll's 60th birthday), **114** (2005), 283.

58} G. Cazzoli, C. Puzzarini
"The Lamb-dip spectrum of the $J + 1 \leftarrow J$ (J=0,1,3-8) transitions of $H^{13}CN$: the nuclear hyperfine structure due to H, ^{13}C and ^{14}N",
J. Mol. Spectrosc., **233** (2005), 280.

57} G. Cazzoli, C. Puzzarini
"Observation of OD^- by microwave spectroscopy",
J. Chem. Phys., **123** (2005), 04-1101.

56} C. Puzzarini*
"The HCS/HSC and HCS^+/HSC^+ systems: molecular properties, isomerization, and energetics",
J. Chem. Phys., **123** (2005), 02-4313.

55} G. Cazzoli, C. Puzzarini, J. Gauss
"The rare isotopomers of HCN: $HC^{15}N$ and $DC^{15}N$. Rotational spectrum and resolved nuclear hyperfine structures due to ^{15}N and D",
Astrophys. J. Suppl. Ser., **159** (2005), 181.

54} A. Perrin, C. Puzzarini, J.-M. Colmont, C. Verdes, G. Wlodarczk, G. Cazzoli, S. Buehler, J.-M. Flaud, J. Demaison
"Molecular line parameters for "MASTER" (Millimeter wave Acquisitions for Stratosphere/Troposphere Exchange Research) database",
Journal of Atmospheric Chemistry, **50** (2005), 161.

53} C. Puzzarini*, S. Coriani, A. Rizzo, J. Gauss
"Critical analysis of the spin-rotation constants of CF_2 and CCl_2: a theoretical study",
Chem. Phys. Lett., **409** (2005), 118.

52} L. Bizzocchi, C. Degli Esposti, L. Dore, C. Puzzarini
"Lamb-dip millimetre-wave spectroscopy of HCP: experimental and theoretical determination of ^{31}P nuclear spin-rotation coupling constant and magnetic shielding",
Chem. Phys. Lett., **408** (2005), 13.

51} G. Brizzi, C. Puzzarini, A. Perrin, J. Orphal, H. Willner, and P. Garcia

"High resolution Fourier transform infrared spectrum of $^{79}Br^{14}N^{18}O$: Analysis of the ν_1 band",
J. Mol. Struct. (special issue in honor of Walter Lafferty), **742** (2005), 37.
50} J.-M. Colmont, B. Bakri, F. Rohart, G. Wlodarczak, J. Demaison, G. Cazzoli, L. Dore, C. Puzzarini
"Intercomparison between ozone broadening parameters retrieved from millimetre-wave measurements by using different techniques",
J. Mol. Spectrosc., **231** (2005), 171.
49} C. Puzzarini*, K. A. Peterson
"Multiple bonds to gold: A theoretical investigation of XAuC (X=F,Cl,Br,I) molecules",
Chem. Phys. (special issue on relativistic effects), **311** (2005), 177.
48} C. Puzzarini*, K. A. Peterson
"An ab initio study of the lowest electronic states of yttrium dicarbide, YC_2",
J. Chem. Phys., **122** (2005), 08-4323.
47} G. Cazzoli, C. Puzzarini
"The Lamb-dip spectrum of the $J = 1 \leftarrow 0$ transition of DF: crossing resonances and hyperfine components",
J. Mol. Spectrosc., **231** (2005), 124.
46} C. Puzzarini*, A. Gambi
"The energetics and structural properties of diazomethyl (HCNN) and cyanomidyl (HNCN) radicals and their related cations and anions from ab initio calculations",
J. Chem. Phys., **122** (2005), 06-4316.
45} C. Puzzarini, P. R. Taylor
"An *ab initio* study of the structure, torsional potential energy function and electric properties of disilane, ethane and their deuterated isotopomers",
J. Chem. Phys., **122** (2005), 05-4315.
44} C. Puzzarini, J. Cosléou, P. Cacciani, F. Herlemont, M. Khelkhal
"CH_3F: the magnetic interactions at the origin of the nuclear spin conversion",
Chem. Phys. Lett., **401** (2005), 357.
43} C. L. Verdes, S. Buehler, A. Perrin, J.-M. Flaud, J. Demaison, G. Wlodarczk, J.-M. Colmont, G. Cazzoli, C. Puzzarini
"A sensitive study on spectroscopic parameters accuracies for a mm/sub-mm limb sounder instrument",
J. Mol. Spectrosc., **229** (2005), 266.
42} G. Cazzoli, L. Dore, C. Puzzarini*, B. Bakri, J.-M. Colmont, F. Rohart, G. Wlodarczak
"Experimental determination of air-broadening parameters of pure rotational transitions of HNO_3: intercomparison of measurements by using different techniques",
J. Mol. Spectrosc., **229** (2005), 158.
41} G. Cazzoli, C. Puzzarini
"The hyperfine structure of the $J = 1 \leftarrow 0$ and and $J = 2 \leftarrow 1$ transitions $D^{35}Cl$ and $D^{37}Cl$",
Phys. Chem. Chem. Phys., **6** (2004), 5133.
40} C. Puzzarini*, A. Gambi
"A theoretical study of diazirine (H_2CN_2), diazirinyl radical (HCN_2) and their related cations ($H_2CN_2^+$, HCN_2^+): molecular structure, energetics and ionization potential",
Chem. Phys., **306** (2004), 131.
39} G. Cazzoli, C. Puzzarini, A. V. Lapinov
"Precise laboratory frequencies for the J+1 - J (J=0,1,2,3) rotational transitions of ^{13}CO",
Astrophys. J., **611** (2004), 620.
38} C. Puzzarini*, A. Gambi, G. Cazzoli
"An *ab initio* study of diazirine: equilibrium structure and molecular properties",
J. Mol. Struct., **695-696** (2004), 203. (B.P. and M. Winnewisser special issue)
37} G. Cazzoli, C. Puzzarini
"Hyperfine structure of $J = 1 \leftarrow 0$ transition of $H^{35}Cl$ and $H^{37}Cl$: improved ground state parameters",
J. Mol. Spectrosc., **226** (2004), 161.
36} C. Puzzarini*, A. Gambi
"An accurate determination of the equilibrium and vibrationally averaged structure and molecular properties of difluoromethanimine (F_2CNH) from ab initio calculations",
J. Phys. Chem. A, **108A** (2004), 4138.
35} G. Cazzoli, C. Puzzarini, A. Gambi
"Trans-1-chloro-2-fluoroethylene: microwave spectra and anharmonic force field",

J. Chem. Phys., **120** (2004), 6495.
34} C. Puzzarini*
"An improved determination of the equilibrium structure and molecular properties of XBS and XCP (X = H, F, Cl) molecules from ab initio calculations",
Phys. Chem. Chem. Phys., **6** (2004), 344.
33} G. Cazzoli, C. Puzzarini, L. Dore
"Self-, N_2- and O_2-broadening of pure rotational transitions of HFC-134a",
J. Quantitative Spectrosc. Radiat. Transfer, **83** (2004), 699.
32} G. Cazzoli, C. Puzzarini, A. V. Lapinov
"Precise laboratory frequencies of the $J = 1$-0 and $J = 2$-1 rotational transitions of $C^{18}O$",
Astrophys. J., **592** (2003), L95.
31} L. Dore, S. Beninati, C. Puzzarini, G. Cazzoli
"Study of vibrational interactions in DCO^+ by millimeter-wave spectroscopy and determination of the equilibrium structure of formyl ion",
J. Chem. Phys., **118** (2003), 7857.
30} C. Puzzarini*, L. Dore, L. Cludi, G. Cazzoli
"An improved determination of the molecular dipole moment of HFC-134a: microwave Stark spectra and *ab initio* calculations",
Phys. Chem. Chem. Phys., **5** (2003), 1519.
29} C. Puzzarini*
"Accurate structure and torsional barrier height of disilane",
Phys. Chem. Chem. Phys., **5** (2003), 26.
28} C. Puzzarini*, G. Cazzoli, A. Gambi
"An *ab initio* study of trans-1-chloro-2-fluoroethylene: equilibrium structure and molecular properties",
J. Chem. Phys., **118** (2003), 2647.
27} C. Puzzarini, L. Dore, G. Cazzoli
"Rotational spectrum of $^{13}C^{17}O$ and $^{13}C^{18}O$. Completely resolved nuclear hyperfine structures due to ^{13}C and ^{17}O",
J. Mol. Spectrosc., **217** (2003), 19.
26} A. Gambi, C. Puzzarini, G. Cazzoli, L. Dore, P. Palmieri
"The anharmonic force field of cis-1-chloro-2-fluoroethylene",
Mol. Phys, **100** (2002), 3535.
25} C. Puzzarini*, L. Dore, G. Cazzoli
"A comparison of line shape models in the analysis of modulated and natural rotational line profiles. Application to the pressure broadening of OCS and CO",
J. Mol. Spectrosc., **216** (2002), 428. (special issue)
24} L. Bizzocchi, C. Degli Esposti, C. Puzzarini
"Millimeter-wave spectroscopy of ClBS: an improved evaluation of the equilibrium structure of chlorothioborine",
J. Mol. Spectrosc., **216** (2002), 177. (special issue)
23} G. Cazzoli, L. Dore, C. Puzzarini, S. Beninati
"Millimeter- and Submillimeter-wave Spectrum of $C^{17}O$. Rotational Hyperfine Structure analyzed using the Lamb-dip Technique",
Phys. Chem. Chem. Phys., **4** (2002), 3575.
22} G. Cazzoli, L. Dore, L. Cludi, C. Puzzarini, S. Beninati
"Hyperfine structure of $J = 1 \leftarrow 0$ transition of ^{13}CO",
J. Mol. Spectrosc., **215** (2002), 160.
21} C. Puzzarini*, G. Cazzoli, L. Dore, A. Gambi
"Molecular structure of cis-1-chloro-2-fluoroethylene from *ab initio* calculations and microwave spectroscopy",
Phys. Chem. Chem. Phys., **3** (2001), 4189.
20} P. Botschwina, C. Puzzarini
"CCSD(T) spectroscopic constants and an accurate equilibrium structure for HC_4F",
J. Mol. Spectrosc., **208** (2001), 292.
19} L. Dore, C. Puzzarini, G. Cazzoli
"Millimeter wave spectrum of $HC^{17}O^+$. Experimental and theoretical determination of the quadrupole coupling constant of the ^{17}O nucleus",

Can. J. Phys., **79** (2001), 359. (special issue)
18} L. Dore, C. Puzzarini, G. Cazzoli, A. Gambi
"Nuclear quadrupole tensors for ^{35}Cl and ^{37}Cl in cis-1-chloro-2-fluoroethylene obtained by detection of perturbation allowed ΔJ=2 and ΔJ =3 transitions",
J. Mol. Spectrosc., **204** (2000), 262.
17} P. Palmieri, C. Puzzarini, V. Aquilanti, G. Capecchi, S. Cavalli, D. De Fazio, A. Aguilar, X. Gimenez, J. M. Lucas
"*Ab initio* dynamics of the He + $H_2^+ \rightarrow HeH^+ + H$ reaction: a new potential energy surface and quantum mechanical cross sections",
Mol. Phys., **98** (2000), 1835. (special issue)
16} S. Carter, N. C. Handy, C. Puzzarini, R. Tarroni, P. Palmieri
"A variational method for the calculation of spin-rovibronic energy levels of triatomic molecules with three interacting potential energy surfaces",
Mol. Phys., **98** (2000), 1697. (special issue)
15} A. O. Mitrushenkov, P. Palmieri, C. Puzzarini, R. Tarroni
"Numerical techniques for the evaluation of the non-adiabatic interactions and the generation of quasi-diabatic potential energy surfaces using Configuration Interaction methods",
Mol. Phys. **98** (2000), 1677. (special issue)
14} A. Gambi, G. Cazzoli, L. Dore, A. Mazzavillani, C. Puzzarini, P. Palmieri, A. Baldan
"Theoretical molecular structure and experimental dipole moment of cis-1-chloro-2-fluoroethylene",
Phys. Chem. Chem. Phys., **2** (2000), 1639.
13} V. Aquilanti, G. Capecchi, S. Cavalli, D. De Fazio, C. Puzzarini, P. Palmieri, A. Aguilar, X. Gimenez, J. M. Lucas
"The He + H_2^+ reaction: a dynamical test on potential energy surfaces for a system exhibiting a pronunced resonance pattern",
Chem. Phys. Lett., **318** (2000), 619.
12} C. Leonard, F. Le Quere, P. Rosmus, C. Puzzarini, M. P. de Lara-Castells
"Selective vibrational excitations in the OX (X=F,Cl,Br,I) molecules",
Phys. Chem. Chem. Phys., **2** (2000), 1117.
11} C. Puzzarini*, M. P. de Lara-Castells, R. Tarroni, P. Palmieri, J. Demaison
"Accurate *ab initio* prediction of the rovibrational energy levels and equilibrium geometry of OCSe",
Phys. Chem. Chem. Phys. **1** (1999), 3955.
10} L. Dore, L. Cludi, A. Mazzavillani, G. Cazzoli, C. Puzzarini
"Lamb-dip millimeter-wave spectrum, structure and dipole moment of HCCCCF",
Phys. Chem. Chem. Phys., **1** (1999), 2275.
9} C. Degli Esposti, L. Bizzocchi, F. Tamassia, C. Puzzarini, R. Tarroni, Z. Zelinger
"Millimeter-wave and diode laser spectroscopy of $IC^{15}N$: anharmonic force field of cianogen iodide from spectroscopic data and *ab initio* calculations",
Mol. Phys., **93** (1998), 95; Mol. Phys., **98** (2000), 327 (E).
8} P. Palmieri, C. Puzzarini, R. Tarroni, A. O. Mitrushenkov,
"On the refinement of the force field of BrNO"
Spectrochim. Acta A, **53** (1997), 1139. (special issue: ab initio and ab intio derived force fields: state of the science)
7} C. Puzzarini*, R. Tarroni, P. Palmieri
"The anharmonic force field of chlorofluoromethane",
Spectrochim. Acta A, **53** (1997), 1123. (special issue: ab initio and ab intio derived force fields: state of the science)
6} C. Puzzarini*, R. Tarroni, P. Palmieri, S. Carter
"Isomerism and spin-rovibronic energy levels of SiNO",
J. Chem. Soc. Faraday Trans., **92** (1996),4361.
5} C. Degli Esposti, F. Tamassia, C. Puzzarini, R. Tarroni, Z. Zelinger
"Millimeter-wave and infrared spectroscopy of $Br^{13}CN$: anharmonic force field of cianogen bromide from spectroscopic data and *ab initio* calculations",
Mol. Phys., **88** (1996), 1603; Mol. Phys., **90** (1997), 495 (E).
4} C. Puzzarini, R. Tarroni, P. Palmieri, J. Demaison, M.L. Senent
"Rovibrational energy levels and equilibrium geometry of HCP",

J. Chem. Phys., **105** (1996), 3132.
3} P. Palmieri, C. Puzzarini, R. Tarroni
"The potential energy and dipole moment surfaces of HOBr",
Chem. Phys. Lett., **256** (1996), 409.
2} C. Puzzarini, R. Tarroni, P. Palmieri, S. Carter, L. Dore
"Accurate *ab initio* prediction of the equilibrium geometry of HCO^+ and of rovibration energy levels of DCO^+",
Mol. Phys., **87** (1996), 879.
1} E. Canè, C. Puzzarini, R. Tarroni, A. Trombetti
"The Gas Phase Infrared Spectrum of 1-azaindolizine: The Scaled Quantum Mechanical Force Field and Spectrum Assignment",
J. Chem. Soc. Faraday Trans., **91** (1995), 3741.

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 H_2CN_2 molecule, HCN_2 radicals and their Ions",
In "*Science & Supercomputing @ CINECA, Report 2005*", p. 261.
(Eds.: M. Voli and P. Coluccia; Monograf s.r.l.; Bologna; 2006).

LIST OF TALKS

Invitation received for 2026:

- *46th COSPAR Scientific Assembly. Symposium F3.1*, "Chemical Complexity of Molecular Universe", 1-9 August 2026, Firenze, Italy
- *65th Sanibel Symposium: The Theory Meeting for Theoreticians*, 22-27 February 2026, St. Augustine Beach, FL, USA
- *Beyond the Quantum Year: Theoretical Chemistry Meets the Scuola Superiore Meridionale* (QMChem@SSM), 4-6 February 2026, Scuola Superiore Meridionale, Naples, Italy

152} *Convegno Donegani: 1925: dai numeri quantici al sistema periodico. Una rivoluzione in chimica*, 25-26 November 2025, Accademia Nazionale dei Lincei, Roma
Invited talk: Nessuno è isolato: molecole nell'atmosfera e nello spazio
151} *COSY Academy Day*, 2-3 October 2025, CSIC, Madrid; Spain (virtual participation)
Overview talk: Overview on Astrochemistry
150} *3rd International Conference on Physical Chemistry and Spectroscopy*, 24-26 September 2025, Patras, Greece (virtual participation)
Invited talk: Discovery of molecules in space: the role of rotational spectroscopy
149} *X Scuola Nazionale di Didattica della Chimica "Giuseppe Del Re"*, 15-17 September 2025, Rimini
Invited talk: Il mistero della chimica dell'universo
148} *Summer School 'Modern Wavefunction Based Methods in Electronic Structure Theory' (MWM25)*, 31 August – 5 September 2025, Pisa
Keynote talk: Quantum Chemistry Among the Stars: Unlocking the Secrets of Interstellar Molecules
147} *COSY WG5 Meeting*, 8 July 2025, Bologna
Invited talk: Unveiling exotic chemistry and molecules in the interstellar medium
145-46} *78th International Symposium on Molecular Spectroscopy*, 23-27 June 2025, Urbana-Champaign, Illinois (USA) (virtual participation)
Oral communication: The Lego-brick approach for accurate molecular structures: virtues and vices
Oral communication: Gas-phase reactivity and new potential astrochemical species
144} *Workshop "Physical and Chemical processes of astrophysical interest: astrochemistry in the JWST era"*, 9-12 June 2025, St. Florent, Corsica (F)
Invited talk: Unveiling exotic chemistry and molecules in the interstellar medium
143} *11th Molecular Quantum Mechanics Conference (MQM2025)*, 23-28 May 2025, Kyoto, Japan
Invited talk: Modeling of gas-phase reactions
142} *Winter Modeling 2025 - Napoli Edition: From Ab-Initio to Data Driven,* 13-14 February 2025, Napoli
Invited talk: Unveiling exotic chemistry and molecules in the interstellar medium: The role of quantum-chemical calculations
141} *Simposio Colombiano de Astroquimica*, 23-25 October 2024, Bogotà, Colombia (virtual participation)
Invited talk: From the lab to space: Unveiling exotic chemistry and molecules in the interstellar medium
140} *COSY WG1-WG5 Meeting. Spectroscopic and Collisional Phenomena in Atmospheric Photochemistry, Astrochemistry and Planetary Sciences*, 4-5 July 2025, Torun, Poland
Invited talk: Astrochemistry @ROT&Comp Lab: Unveiling exotic chemistry and molecules in the interstellar medium
139} *2st General Meeting COSY COST Action*, 1-3 July 2024, Wroclaw, Poland
Invited overview talk: Astrochemistry: challenges and perspectives
138} *77th International Symposium on Molecular Spectroscopy*, 17-21 June 2024, Urbana-Champaign, Illinois (USA)
Oral communication: Laboratory data of deuterated-prebiotic species for astronomical searches
137} *QUANTUMGRAIN Workshop: Emerging Horizons in the Chemistry of the Universe*, 9-12 June 2024, Barcelona, Spain.
Invited talk: Astrochemistry @ROT&Comp Lab: Unveiling exotic chemistry and molecules in the interstellar medium
136} *NanoSpace COST Action – 1st WG2 meeting*, 20-23 February 2024, Edinburgh, UK.
Invited talk: Hunting for interstellar molecules
135} *Gordon Research Conference "Molecular and Ionic Clusters*", 4-9 February 2024, Ventura (CA), USA.
Invited talk: Toward the Accurate Description of Non-Covalent Interactions

134} *The Path of Quantum Chemistry into the 21st Century – Symposium Celebrating Prof. Roland Lindh's 65th Birthday,* 16-18 January 2024, ETH Zurich, Switzerland.
Invited talk: Unveiling exotic chemistry and molecules in the interstellar medium: The role of quantum-chemical calculations
133} *Life And Space Conference (LAS 2023)*, 1-3 December 2023, online (Polish Astrobiology Society).
Invited talk: Prebiotic molecules and chemistry in space: A laboratory perspective
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 ND_2H and NH_2D 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} "*IAU 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 - MPCS17*", 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 ND_3 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 astroschemistry"
68} "Winter Modeling 2015 – Complex Molecular Systems: Accuracy and Interpretation", 18 December 2015, Pisa (Italy)
Oral comunication: "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} "Colloqiuum: 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 H_2S: the $H_2{}^{33}S$ 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 Societá 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 $D_2{}^{17}O$ and $HD^{17}O$: 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 Septmber 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 Septmber 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 Septmber 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 Societa' 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 Atmospherical relevant Systems", 7-10 May 2009, Granada (Spain)
Invited speaker: “Quantum-chemical calculation of spectroscopic parameters for rotational spectroscopy: Application to astrophysics and atmospherical systems".

21} "Winter Modeling '08", 19 December 2008, Pisa (CNR)
Oral communication: "State-of-the-art coupled custer 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, Departement de Chimie Physique, Universitè 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):
"N_2- and O_2-broadening of O_3 the 301.8 and 317.2 GHz lines. Preliminary results".
- Oral communication: mid-term (III) meeting (16/05/2003 Estec, Noordwijk, NL):
"N_2- and O_2-broadening of O_3: the 301.8 and 319.9 GHz lines. Final results".
- Oral communication: IV progress meeting (18/07/2003 Bologna, I):
"Air-broadening of HNO_3: the 319.2 and 344.2 GHz lines".
- Oral communication: V progress meeting (24/10/2003 Orsay-Paris, F):
"Air-broadening of HNO_3: 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):
"N_2- and O_2-broadening of O_3 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 comunication: "Potential energy surface for the He + H_2^+ ground state reaction and a new diabatization 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 + H_2^+ ground state reaction and a new diabatization 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

To come:
"***Once upon the time there was … an astrochemistry story***"
Webinar, February 12 2026, COST "COSY" Action

59} "***Chemical Reactivity under Extreme Conditions: A Quantum-Chemical View of Astrochemistry***"
Seminar, January 16 2026, Mainz, Germany
58} "***The Lego-brick approach for accurate molecular structures: virtues and vices***"
Seminar, January 31 2025, Mainz, Germany
57} "***From Lab to Space: Unveiling exotic chemistry and molecules in the interstellar medium***"
Seminar, September 19 2024, Santiago de Compostela, Spain
56} "***From the lab to space: An integrated rotational spectroscopy-quantum chemistry strategy***"
Seminar, January 23 2024, Mainz, Germany
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 HOCOO and $HOCH_2OO$ 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.