Curriculum Vitae

- **PERSONAL INFORMATION**

Puzzarini, Cristina Date of Birt [redacted]
Professor of Physical Chemistry
Dept. Chemistry "Giacomo Ciamician", Universitá di Bologna

- **EDUCATION**

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

- **CURRENT POSITIONS**

– *Full Professor of Physical Chemistry*, University of Bologna, 2018 – to date.
– *Director*, Interuniversity Center for Astrochemistry STAR, 2018 – to date.
– *Research Professor*, Department of Physics – Center for Nanophysics and Advanced Materials, University of Maryland, November 2018 – to date.

- **PREVIOUS POSITIONS**

Associate Professor of Physical Chemistry, University of Bologna, 2012 – 2017.
Assistant Professor of Physical Chemistry, University of Bologna, 2006 – 2012.
Research Associate (molecular spectroscopy), University of Bologna, 2000 – 2006.
Postdoctoral Scholar (theoretical chemistry), University of Bologna, 1998 – 2000.
Postdoctoral Scholar (theoretical chemistry), University of Marne-la-Vallée, 1997.
Ph.D. fellowship (theoretical chemistry), University of Bologna, 1994 – 1996.

- **FELLOWSHIPS AND AWARDS**

Invited Professor, University of Valladolid, 2017.
Invited Professor (LabEx fellowship), Université Paris-Est, 2016.
Research Associate (Galilei fellowship), Université de Lille I, France, 2004.
Visiting Professor, Université de Lille, France, 2004.
Visiting Research Associate (Marco Polo fellowship), Washington State University, 2004.
Visiting Research Associate, Universität Göttingen, 2001.

- **RESEARCH INTERESTS**

Research activity is characterized by the synergic interplay of experiment and theory, often combined with synergistic international collaborations:

- 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 two national projects (PRIN 2009 Project (2011-2013) "*Molecular Spectroscopy for Atmospherical and Astrochemical Research: Experiment, Theory and Applications*" and PRIN 2012 Project (2014-2017) "*STAR: Spectroscopic and computational Techniques for Astrophysical and atmospheric Research*").

- **PUBLICATIONS, TALKS AND SEMINARS**

More than 230 papers [SCOPUS (11/6/2020): 5189 citations, 4247 since 2010; H-index = 35], almost all in the areas of high-resolution rotational and computational spectroscopy, astrochemistry, quantum chemistry. About seventy papers in the last five years, including three review articles. The full list of papers is provided below.

I have given more than 100 presentations at scientific meetings. Of these, only 15 have been in national conferences, while the remaining lectures have been given at international meetings. 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.

According to PLOS Biology (*J. P. A. Ioannidis, J. Baas, R. Klavans, K. W. Boyack, "A standardized citation metrics author database annotated for scientific field", doi:10.1371/journal.pbio.3000384*), I am one of the top-100000 world scientists, and one of top-203 italian chemists.

- **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. Courses that I have taught at my university include those covering molecular spectroscopy (theory and lab), computational chemistry, and physical chemistry. My teaching has been recognized, and I have also been invited to give courses at Scuola Normale Superiore di Pisa (at master and Ph.D. level) and University of Firenze (at the astrophysics graduate school).

- **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, in the last years, 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**

A. Ali (NASA, USA)	J.L. Alonso (U. Valladolid, Spain)	D. Ascenzi (U. Trento, Italy)
N. Balucani (U. Perugia, Italy)	V. Barone (SNS, Italy)	M. Biczysko (U. Shangai, China)
L. Bizzocchi (MPE, Germany)	J. Bloino (SNS, Italy)	P. Caselli (MPE, Germany)
C. Codella (INAF, Italy)	L. Dore (U. Bologna, Italy)	H.D. Drew (U. Maryland, USA)
G.B. Ellison (U. Colorado, USA)	J.S. Francisco (U. Nebraska, USA)	J. Gauss (U. Mainz, Germany)
J.-U. Grabow (U. Hannover, D)	M. Hochlaf (U. Paris-Est, France)	R. Linguerri (U. Paris-Est, France)
G. Mancini (SNS, Italy)	T.E. Murphy (U. Maryland, USA)	K.A. Peterson (WSU, USA)
D. Skouteris (SNS, Italy)	J.F. Stanton (U. Florida, USA)	J. Cernicharo (CSIC, Spain)

- **ORGANISATION OF INTERNATIONAL SCIENTIFIC MEETINGS**

2012 (Sept 12-14)	IMAMPC 2012, Chair, Scuola Normale Superiore di Pisa, Italy
2013 (July 2-5)	IMAMPC 2013, Scientific Advisory Board, Lille, France
2014 (Nov 23-30)	QUITEL 2014, Scientific Advisory Board, Galapagos, Ecuador
2018 (February 15-16)	ASTRO-Winter Modeling, Chair, Bologna, Italy
2018 (June, 13-16)	2nd Italian Workshop on Astrochemistry, Co-chair, Follonica (GR), Italy
2018 (June, 25-28)	National meeting of the Physical Chemistry Division of the Italian Chemistry Society (SCI), LOC, Bologna, Italy
2018 (July 14-22)	COSPAR - F3.5: The Evolving Universe and the Origin of Life, SOC, Caltech, Pasadena, USA
2018 (Sept 10-12)	Faraday Discussion, Scientific Advisory Board, Edinburgh, UK
2019 (Feb 27-Mar 1)	4th MOLIM Cost General Meeting, Chair, Bologna, Italy
2019 (March 4-8)	APS Focus Topic Symposium "Bridging the gap between theory and experiment in gas-phase spectroscopy", Chair, Boston, USA

- **INSTITUTIONAL RESPONSIBILITIES**

2018 – to date Member of the Research Evaluation Committee of the Dept. Chemistry "Giacomo Ciamician", Univ. Bologna, Italy
2018 – to date Member of the Doctoral School Board, Astrochemistry, Scuola Normale di Pisa, Italy
2017 – to date Board member, Theoretical and Computational Chemistry Division, Italian Chemistry Society
2016 – to date Member of the Admission and Didactics Committee, Master Degree in Chemistry, Dept. Chemistry "Giacomo Ciamician", Univ. Bologna, Italy
2014 – to date Member of the Research Evaluation Committee, Panel Chemistry, Univ. Bologna, Italy
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 Fotochemistry, Univ. Bologna, Dept. Chemistry "Giacomo Ciamician", Italy
2007 – 2011 Board member, Physical Chemistry Division, Italian Chemistry Society

- **REVIEWING/EDITORIAL ACTIVITIES**

2020 – to date Chief Editor, Frontiers Astrochemistry (section of "Frontiers in Astronomy and Space Sciences")
2017 – to date Reviewer of international projects (U.S. Department of Energy; ACS Petroleum Research Fund, USA; I-SITE ULNE project excellence in research, Université Lille-Nord, France)
2010 – to date Reviewer of the Assessment of Quality in Scientific Research (VQR)
2010 – to date Reviewer of national MIUR projects (PRIN, FIRB, SIRI)
2016 – to date Editorial Board, Journal of Molecular Structure
2010 – 2013 Editorial Board, Journal of Molecular Spectroscopy

I regularly serve as a reviewer for ACS (JPCA, JPCL, JCTC, Earth and Space Chemistry, JACS), RSC (PCCP), Elsevier (JQSRT, JMS, JMStruct), Wiley-VCH (IJQC,ChemEurJ), OIP (Astrophys. J.) and Astron. Astrophys. I am also the guest editor of the PCCP themed issue (2019 - Challenges in spectroscopy: accuracy versus interpretation from isolated molecules to condensed phases).

- **MEMBERSHIPS OF SCIENTIFIC SOCIETIES**

2016 – to date Associated Member, INAF, Italy
2014 – to date Associated Member, INFN, Italy
2009 – to date Associated Member, INSTM Consortium, Italy
2015 – 2019 Management Committee Member, COST Action CM1405 "MOLIM"
2015 – 2019 Member, COST Action CM1401 "Our Astro-Chemical History"

- **CARRIER BREAK**

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

Full list of Publications

Book Chapters:

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 Papers:

231} 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 Accepted for publication (2020)
[*Special Issue "From Molecules to Origin of Life: The Astrobiology Network"*]
230} 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 In press (2020) DOI: 10.1093/mnras/staa1652
229} 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. In press (2020) DOI: 10.1080/00268976.2020.1766707
228} 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. In press (2020) DOI: 10.1016/j.plrev.2019.11.005
227} C. Puzzarini*
"Prebiotic molecules in interstellar space: rotational spectroscopy and quantum chemistry"
Proc. IAU Symposium No. 350 on Laboratory Astrophysics: from Observations to Interpretation. Accepted for publication (2019)
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) art. 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*
"Challenges in spectroscopy: A route toward the detection in space of the methyl-cyclopropenyl cation"
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-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"
Astronom. 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"
Monthly Not. Royal Astron. Soc. Letter **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*
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68} G. Cazzoli, C. Puzzarini
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48} C. Puzzarini*, K. A. Peterson
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"On the refinement of the force field of BrNO"
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"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)

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"Millimeter-wave and infrared spectroscopy of $BrC^{13}N$: anharmonic force field of cianogen bromide from spectroscopic data and *ab initio* calculations",
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"Rovibrational energy levels and equilibrium geometry of HCP",
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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^+",
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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.
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◊ List of talks

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} "*10^{h} 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 computationsat 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 computationsat 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_2 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 Title: (COMPhandy07) 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 supporto f 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 delle 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*

34} "***Rotational Spectroscopy Meets Quantum Chemistry for Elucidating Astrochemical Challenges***"
GDCh Seminar, November 14, 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$_2$OO 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.