Cristina Puzzarini

List of Publications by Citations

279 papers	6,745 citations	40 h-index	68 g-index
303 ext. papers	7,509 ext. citations	3.8 avg, IF	6.43 L-index

#	Paper	IF	Citations
279	Systematically convergent basis sets for transition metals. II. Pseudopotential-based correlation consistent basis sets for the group 11 (Cu, Ag, Au) and 12 (Zn, Cd, Hg) elements. *Theoretical Chemistry Accounts*, **2005**, 114, 283-296	1.9	939
278	Quantum-chemical calculation of spectroscopic parameters for rotational spectroscopy. *International Reviews in Physical Chemistry*, **2010**, 29, 273-367	7	237
277	Theoretical models on the Cu2O2 torture track: mechanistic implications for oxytyrosinase and small-molecule analogues. *Journal of Physical Chemistry A*, **2006**, 110, 1991-2004	2.8	157
276	The accuracy of rotational constants predicted by high-level quantum-chemical calculations. I. molecules containing first-row atoms. *Journal of Chemical Physics*, **2008**, 128, 194108	3.9	121
275	Accurate Harmonic/Anharmonic Vibrational Frequencies for Open-Shell Systems: Performances of the B3LYP/N07D Model for Semirigid Free Radicals Benchmarked by CCSD(T) Computations. *Journal of Chemical Theory and Computation*, **2010**, 6, 828-38	6.4	109
274	Accuracy and Interpretability: The Devil and the Holy Grail. New Routes across Old Boundaries in Computational Spectroscopy. *Chemical Reviews*, **2019**, 119, 8131-8191	68.1	103
273	Accurate structure, thermodynamic and spectroscopic parameters from CC and CC/DFT schemes: the challenge of the conformational equilibrium in glycine. *Physical Chemistry Chemical Physics*, **2013**, 15, 10094-111	3.6	102
272	Semi-experimental equilibrium structure determinations by employing B3LYP/SNSD anharmonic force fields: validation and application to semirigid organic molecules. *Journal of Physical Chemistry A*, **2015**, 119, 2058-82	2.8	101
271	Extending the molecular size in accurate quantum-chemical calculations: the equilibrium structure and spectroscopic properties of uracil. *Physical Chemistry Chemical Physics*, **2011**, 13, 7189-97	3.6	97
270	Accurate Anharmonic Vibrational Frequencies for Uracil: The Performance of Composite Schemes and Hybrid CC/DFT Model. *Journal of Chemical Theory and Computation*, **2011**, 7, 3702-10	6.4	96
269	Glycine conformers: a never-ending story?. *Physical Chemistry Chemical Physics*, **2013**, 15, 1358-63	3.6	75
268	Extrapolation to the complete basis set limit of structural parameters: comparison of different approaches. *Journal of Physical Chemistry A*, **2009**, 113, 14530-5	2.8	73
267	The Genealogical Tree of Ethanol: Gas-phase Formation of Glycolaldehyde, Acetic Acid, and Formic Acid. *Astrophysical Journal*, **2018**, 854, 135	4.7	71
266	Accurate Characterization of the Peptide Linkage in the Gas Phase: A Joint Quantum-Chemical and Rotational Spectroscopy Study of the Glycine Dipeptide Analogue. *Journal of Physical Chemistry Letters*, **2014**, 5, 534-40	6.4	70
265	Seeds of Life in Space (SOLIS). *Astronomy and Astrophysics*, **2017**, 605, L3	5.1	67
264	Characterization of the Elusive Conformers of Glycine from State-of-the-Art Structural, Thermodynamic, and Spectroscopic Computations: Theory Complements Experiment. *Journal of Chemical Theory and Computation*, **2013**, 9, 1533-47	6.4	66
263	A variational method for the calculation of spin-rovibronic energy levels of triatomic molecules with three interacting electronic states. *Molecular Physics*, **2000**, 98, 1697-1712	1.7	66

262	CC/DFT Route toward Accurate Structures and Spectroscopic Features for Observed and Elusive Conformers of Flexible Molecules: Pyruvic Acid as a Case Study. *Journal of Chemical Theory and Computation*, **2015**, 11, 4342-63	6.4	65
261	Anharmonic theoretical simulations of infrared spectra of halogenated organic compounds. *Journal of Chemical Physics*, **2013**, 139, 074310	3.9	64
260	Integrated computational approaches for spectroscopic studies of molecular systems in the gas phase and in solution: pyrimidine as a test case. *Theoretical Chemistry Accounts*, **2012**, 131, 1	1.9	63
259	A new experimental absolute nuclear magnetic shielding scale for oxygen based on the rotational hyperfine structure of H(2)(17)O. *Journal of Chemical Physics*, **2009**, 131, 234304	3.9	63
258	The He + H2+ reaction: a dynamical test on potential energy surfaces for a system exhibiting a pronounced resonance pattern. *Chemical Physics Letters*, **2000**, 318, 619-628	2.5	63
257	Ab initio dynamics of the He + H+ 2 -eHeH+ +H reaction: a new potential energy surface and quantum mechanical cross-sections. *Molecular Physics*, **2000**, 98, 1835-1849	1.7	63
256	Quantum Chemistry Meets Spectroscopy for Astrochemistry: Increasing Complexity toward Prebiotic Molecules. *Accounts of Chemical Research*, **2015**, 48, 1413-22	24.3	61
255	The Lamb-dip spectrum of methylcyanide: Precise rotational transition frequencies and improved ground-state rotational parameters. *Journal of Molecular Spectroscopy*, **2006**, 240, 153-163	1.3	61
254	Accurate molecular structure and spectroscopic properties of nucleobases: a combined computational-microwave investigation of 2-thiouracil as a case study. *Physical Chemistry Chemical Physics*, **2013**, 15, 16965-75	3.6	60
253	Rotational spectroscopy meets theory. *Physical Chemistry Chemical Physics*, **2013**, 15, 6595-607	3.6	55
252	Accurate molecular structures and infrared spectra of trans-2,3-dideuterooxirane, methyloxirane, and trans-2,3-dimethyloxirane. *Journal of Chemical Physics*, **2014**, 141, 034107	3.9	51
251	Diving for Accurate Structures in the Ocean of Molecular Systems with the Help of Spectroscopy and Quantum Chemistry. *Accounts of Chemical Research*, **2018**, 51, 548-556	24.3	50
250	Theory Meets Experiment for Noncovalent Complexes: The Puzzling Case of Pnicogen Interactions. *Angewandte Chemie - International Edition*, **2018**, 57, 13853-13857	16.4	48
249	The HCSHSC and HCS+HSC+ systems: molecular properties, isomerization, and energetics. *Journal of Chemical Physics*, **2005**, 123, 24313	3.9	48
248	Comparison of the experimental, semi-experimental and ab initio equilibrium structures of acetylene: influence of relativisitic effects and of the diagonal Born-Oppenheimer corrections. *Journal of Chemical Physics*, **2011**, 134, 064119	3.9	47
247	The rotational spectra of HD17O and D2(17)O: experiment and quantum-chemical calculations. *Journal of Chemical Physics*, **2012**, 137, 154311	3.9	46
246	Millimeter- and submillimeter-wave spectrum of C17O. Rotational hyperfine structure analyzed using the Lamb-dip technique. *Physical Chemistry Chemical Physics*, **2002**, 4, 3575-3577	3.6	46
245	Precise Laboratory Frequencies for theJ= 1-0 andJ= 2-1 Rotational Transitions of C18O. *Astrophysical Journal*, **2003**, 592, L95-L98	4.7	45

244	Galatry versus speed-dependent Voigt profiles for millimeter lines of O3 in collision with N2 and O2. *Journal of Molecular Spectroscopy*, **2008**, 251, 282-292	1.3	44
243	Toward spectroscopic accuracy for organic free radicals: Molecular structure, vibrational spectrum, and magnetic properties of F(2)NO. *Journal of Chemical Physics*, **2008**, 129, 084306	3.9	43
242	Multiple bonds to gold: a theoretical investigation of XAuC (X = F, Cl, Br, I) molecules. *Chemical Physics*, **2005**, 311, 177-186	2.3	43
241	Rotational spectra of 1-chloro-2-fluoroethylene. II. Equilibrium structures of the cis and trans isomer. *Journal of Chemical Physics*, **2006**, 125, 054307	3.9	42
240	Accurate ab initio prediction of the equilibrium geometry of HCO+ and of rovibration energy levels of DCO+. *Molecular Physics*, **1996**, 87, 879-898	1.7	42
239	State-of-the-Art Thermochemical and Kinetic Computations for Astrochemical Complex Organic Molecules: Formamide Formation in Cold Interstellar Clouds as a Case Study. *Journal of Chemical Theory and Computation*, **2016**, 12, 5385-5397	6.4	40
238	ACCURATE SPECTROSCOPIC CHARACTERIZATION OF OXIRANE: A VALUABLE ROUTE TO ITS IDENTIFICATION IN TITAN'S ATMOSPHERE AND THE ASSIGNMENT OF UNIDENTIFIED INFRARED BANDS. *Astrophysical Journal*, **2014**, 785,	4.7	39
237	Precise Laboratory Frequencies for the documentclass{aastex} usepackage{amsbsy} usepackage{amsfonts} usepackage{amssymb} usepackage{bm} usepackage{mathrsfs} usepackage{pifont} usepackage{stmaryrd} usepackage{textcomp} usepackage{portland,xspace}	4.7	38
236	The hyperfine structure in the rotational spectrum of water: Lamb-dip technique and quantum-chemical calculations. *Chemical Physics Letters*, **2009**, 473, 21-25	2.5	37
235	Unveiling the Sulfur-Sulfur Bridge: Accurate Structural and Energetic Characterization of a Homochalcogen Intermolecular Bond. *Angewandte Chemie - International Edition*, **2018**, 57, 15822-15826	16.4	36
234	Accurate molecular structures of small- and medium-sized molecules. *International Journal of Quantum Chemistry*, **2016**, 116, 1513-1519	2.1	34
233	Noncovalent Interactions and Internal Dynamics in Pyridine-Ammonia: A Combined Quantum-Chemical and Microwave Spectroscopy Study. *Chemistry - A European Journal*, **2017**, 23, 4876-4883	4.8	33
232	Toward spectroscopic accuracy for open-shell systems: molecular structure and hyperfine coupling constants of H2CN, H2CP, NH2, and PH2 as test cases. *Journal of Chemical Physics*, **2010**, 133, 184301	3.9	33
231	Assessment of a computational strategy approaching spectroscopic accuracy for structure, magnetic properties and vibrational frequencies of organic free radicals: the F(2)CN and F(2)BO case. *Physical Chemistry Chemical Physics*, **2008**, 10, 6991-7	3.6	33
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229	An integrated experimental and quantum-chemical investigation on the vibrational spectra of chlorofluoromethane. *Journal of Chemical Physics*, **2013**, 139, 164302	3.9	32
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221	Sub-Doppler resolution in the THz frequency domain: 1 kHz accuracy at 1 THz by exploiting the Lamb-dip technique. *Journal of Physical Chemistry A*, **2013**, 117, 13759-66	2.8	29
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219	The hyperfine structure in the rotational spectra of bromofluoromethane: Lamb-dip technique and quantum-chemical calculations. *Molecular Physics*, **2008**, 106, 1181-1192	1.7	29
218	A Comparison of Lineshape Models in the Analysis of Modulated and Natural Rotational Line Profiles: Application to the Pressure Broadening of OCS and CO. *Journal of Molecular Spectroscopy*, **2002**, 216, 428-436	1.3	29
217	Molecular structure and spectroscopic signatures of acrolein: theory meets experiment. *Journal of Physical Chemistry A*, **2014**, 118, 6648-56	2.8	28
216	Rotational spectrum of 13C17O and 13C18O: completely resolved nuclear hyperfine structures due to 13C and 17O. *Journal of Molecular Spectroscopy*, **2003**, 217, 19-25	1.3	28
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211	Equilibrium structure of methylcyanide. *Journal of Molecular Spectroscopy*, **2006**, 240, 260-264	1.3	26
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207	Rotational and Infrared Spectroscopy of Ethanimine: A Route toward Its Astrophysical and Planetary Detection. *Astrophysical Journal*, **2018**, 855, 123	4.7	24
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200	Experimental and theoretical investigation on pressure-broadening and pressure-shifting of the 22.2GHz line of water. *Journal of Quantitative Spectroscopy and Radiative Transfer*, **2007**, 105, 438-449	2.1	23
199	Rotational spectra of rare isotopic species of bromofluoromethane: determination of the equilibrium structure from ab initio calculations and microwave spectroscopy. *Journal of Chemical Physics*, **2007**, 127, 164302	3.9	23
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186	The energetics and structural properties of diazomethyl (HCNN) and cyanomidyl (HNCN) radicals and their related cations and anions from ab initio calculations. *Journal of Chemical Physics*, **2005**, 122, 064316	3.9	21
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171	The nuclear-spin-rotation constants of HCY, HSiY, and SiY(2) (Y=F, Cl): an ab initio study. *Journal of Chemical Physics*, **2006**, 124, 64302	3.9	18
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164	The hyperfine structure of the inversion-rotation transition JK = ${1}_{0}$ $leftarrow$ ${0}_{0}$ of NH3 investigated by Lamb-dip spectroscopy. *Astronomy and Astrophysics*, **2009**, 507, 1707-1710	5.1	17
163	Lamb-dip millimeter-wave spectroscopy of HCP: Experimental and theoretical determination of 31P nuclear spin□otation coupling constant and magnetic shielding. *Chemical Physics Letters*, **2005**, 408, 13-18	2.5	17
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140	ACCURATE SPECTROSCOPIC CHARACTERIZATION OF PROTONATED OXIRANE: A POTENTIAL PREBIOTIC SPECIES IN TITAN'S ATMOSPHERE. *Astrophysical Journal*, **2014**, 792,	4.7	12
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