Cristina Puzzarini

List of Publications by Year in Descending Order

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The third column is the impact factor (IF) of the journal, and the fourth column is the number of citations of the article.

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	Synchrotron-based far-infrared spectroscopy of HC3N: Extended ro-vibrational analysis and new line list up to 3360 cm1. *Journal of Quantitative Spectroscopy and Radiative Transfer*, **2022**, 279, 108044	2.1	
278	Gas-phase identification of ()-1,2-ethenediol, a key prebiotic intermediate in the formose reaction.. *Chemical Communications*, **2022**,	5.8	3
277	Gestapelt, nicht geklebt: Enthlung der -Wechselwirkung mithilfe des Benzofuran-Formaldehyd-Komplexes. *Angewandte Chemie*, **2022**, 134, e202113737	3.6	
276	Precursors of the RNA World in Space: Detection of (Z)-1,2-ethenediol in the Interstellar Medium, a Key Intermediate in Sugar Formation. *Astrophysical Journal Letters*, **2022**, 929, L11	7.9	6
275	Spectroscopic Characterization of 3-Aminoisoxazole, a Prebiotic Precursor of Ribonucleotides. *Molecules*, **2022**, 27, 3278	4.8	0
274	junChS and junChS-F12 Models: Parameter-free Efficient yet Accurate Composite Schemes for Energies and Structures of Noncovalent Complexes. *Journal of Chemical Theory and Computation*, **2021**, 17, 6974-6992	6.4	4
273	Extending the Applicability of the Semi-experimental Approach by Means of "Template Molecule" and "Linear Regression" Models on Top of DFT Computations. *Journal of Physical Chemistry A*, **2021**, 125, 9904-9916	2.8	2
272	Formation of Phosphorus Monoxide (PO) in the Interstellar Medium: Insights from Quantum-chemical and Kinetic Calculations. *Astrophysical Journal*, **2021**, 922, 169	4.7	2
271	An improved study of HCO and He system: Interaction potential, collisional relaxation, and pressure broadening.. *Journal of Chemical Physics*, **2021**, 155, 234306	3.9	0
270	Structural and Vibrational Properties of Amino Acids from Composite Schemes and Double-Hybrid DFT: Hydrogen Bonding in Serine as a Test Case. *Journal of Physical Chemistry A*, **2021**, 125, 9099-9114	2.8	2
269	Exploring the Maze of Cycloserine Conformers in the Gas Phase Guided by Microwave Spectroscopy and Quantum Chemistry. *Journal of Physical Chemistry A*, **2021**, 125, 2121-2129	2.8	9
268	Improved centrifugal and hyperfine analysis of ND2H and NH2D and its application to the spectral line survey of L1544. *Journal of Molecular Spectroscopy*, **2021**, 377, 111431	1.3	2
267	Unveiling Bifunctional Hydrogen Bonding with the Help of Quantum Chemistry: The Imidazole-Water Adduct as Test Case. *Journal of Physical Chemistry A*, **2021**, 125, 2989-2998	2.8	3
266	Computational molecular spectroscopy. *Nature Reviews Methods Primers*, **2021**, 1,		18
265	4-Fluoro-Threonine: From Diastereoselective Synthesis to pH-Dependent Conformational Equilibrium in Aqueous Solution. *ACS Omega*, **2021**, 6, 13170-13181	3.9	0
264	An improved rovibrational linelist of formaldehyde, H212C16O. *Journal of Quantitative Spectroscopy and Radiative Transfer*, **2021**, 266, 107563	2.1	7
263	Insoluble organic matter in chondrites: Archetypal melanin-like PAH-based multifunctionality at the origin of life?. *Physics of Life Reviews*, **2021**, 37, 65-93	2.1	8

262	Looking for the Elusive Imine Tautomer of Creatinine: Different States of Aggregation Studied by Quantum Chemistry and Molecular Spectroscopy. *ChemPlusChem*, **2021**, 86, 1374-1386	2.8	4
261	In search of phosphorus in astronomical environments: The reaction between the CP radical (X²Π) and methanimine. *Journal of Chemical Physics*, **2021**, 154, 054306	3.9	3
260	High resolution FTIR study of the ν5, ν6, and ν9 fundamental bands of CH2D37Cl. *Journal of Quantitative Spectroscopy and Radiative Transfer*, **2021**, 270, 107719	2.1	0
259	Hyperfine-Resolved Near-Infrared Spectra of HO. *Journal of Physical Chemistry A*, **2021**, 125, 7884-7890	2.8	2
258	Integration of theory, simulation, artificial intelligence and virtual reality: a four-pillar approach for reconciling accuracy and interpretability in computational spectroscopy. *Physical Chemistry Chemical Physics*, **2021**, 23, 17079-17096	3.6	5
257	Rotational Spectroscopy Meets Quantum Chemistry for Analyzing Substituent Effects on Non-Covalent Interactions: The Case of the Trifluoroacetophenone-Water Complex. *Molecules*, **2020**, 25,	4.8	5
256	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". *Physics of Life Reviews*, **2020**, 32, 124-128	2.1	
255	A computational journey in the CH2O2S land: an accurate rotational and ro-vibrational analysis of the sulfene molecule and the O,S- and O,O-monothiocarbonic acids. *Molecular Physics*, **2020**, 118, e1766707	1.7	
254	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. *Monthly Notices of the Royal Astronomical Society*, **2020**, 496, 4298-4310	4.3	11
253	Grand Challenges in Astrochemistry. *Frontiers in Astronomy and Space Sciences*, **2020**, 7,	3.8	3
252	The challenging playground of astrochemistry: an integrated rotational spectroscopy - quantum chemistry strategy. *Physical Chemistry Chemical Physics*, **2020**, 22, 6507-6523	3.6	24
251	Exploring the Maze of C2N2H5 Radicals and Their Fragments in the Interstellar Medium with the Help of Quantum-Chemical Computations. *ACS Earth and Space Chemistry*, **2020**, 4, 774-782	3.2	9
250	State-of-the-Art Quantum Chemistry Meets Variable Reaction Coordinate Transition State Theory to Solve the Puzzling Case of the HS + Cl System. *Journal of Chemical Theory and Computation*, **2020**, 16, 5090-5104	6.4	11
249	The Role of State-of-the-Art Quantum-Chemical Calculations in Astrochemistry: Formation Route and Spectroscopy of Ethanimine as a Paradigmatic Case. *Molecules*, **2020**, 25,	4.8	7
248	The challenging equilibrium structure of HSSH: Another success of the rotational spectroscopy / quantum chemistry synergism. *Journal of Molecular Structure*, **2020**, 1211, 127933	3.4	5
247	Theory meets experiment for elucidating the structure and stability of non-covalent complexes: water-amine interaction as a proof of concept. *Physical Chemistry Chemical Physics*, **2020**, 22, 5024-5032	3.6	9
246	Rich Collection of n-Propylamine and Isopropylamine Conformers: Rotational Fingerprints and State-of-the-Art Quantum Chemical Investigation. *Journal of Physical Chemistry A*, **2020**, 124, 1372-1381	2.8	8
245	Looking for the bricks of the life in the interstellar medium: The fascinating world of astrochemistry. *EPJ Web of Conferences*, **2020**, 246, 00021	0.3	1

244	The Quest for a Plausible Formation Route of Formyl Cyanide in the Interstellar Medium: a State-of-the-art Quantum-chemical and Kinetic Approach. *Astrophysical Journal*, **2020**, 900, 85	4.7	7
243	Methanimine as a Key Precursor of Imines in the Interstellar Medium: The Case of Propargylimine. *Astrophysical Journal Letters*, **2020**, 903, L35	7.9	7
242	Systematic Study on the Absorption Features of Interstellar Ices in the Presence of Impurities. *ACS Earth and Space Chemistry*, **2020**, 4, 920-946	3.2	4
241	The challenge of non-covalent interactions: theory meets experiment for reconciling accuracy and interpretation. *Journal of Physics Condensed Matter*, **2020**, 32, 343002	1.8	9
240	Extension of the "Cheap" Composite Approach to Noncovalent Interactions: The jun-ChS Scheme. *Journal of Chemical Theory and Computation*, **2020**, 16, 988-1006	6.4	32
239	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. *Physics of Life Reviews*, **2020**, 34-35, 143-146	2.1	1
238	Far-infrared laboratory spectroscopy of aminoacetonitrile and first interstellar detection of its vibrationally excited transitions. *Astronomy and Astrophysics*, **2020**, 641, A160	5.1	7
237	Deuterium hyperfine splittings in the rotational spectrum of NH2D as revealed by Lamb-dip spectroscopy. *Journal of Molecular Spectroscopy*, **2020**, 370, 111291	1.3	7
236	A Journey from Thermally Tunable Synthesis to Spectroscopy of Phenylmethanimine in Gas Phase and Solution. *Chemistry - A European Journal*, **2020**, 26, 15016-15022	4.8	2
235	A never-ending story in the sky: The secrets of chemical evolution. *Physics of Life Reviews*, **2020**, 32, 59-94	4.1	15
234	Astrochemistry and Astrobiology: Materials Sciencein Wonderland?. *International Journal of Molecular Sciences*, **2019**, 20,	6.3	17
233	Unbiased Determination of Absolute Configurations by vis-à-vis Comparison of Experimental and Simulated Spectra: The Challenging Case of Diplopyrone. *Journal of Physical Chemistry B*, **2019**, 123, 9230-9237	3.4	20
232	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
231	Interpretability Meets Accuracy in Computational Spectroscopy: The Virtual Multifrequency Spectrometer **2019**, 1-42		
230	State-of-the-art computation of the rotational and IR spectra of the methyl-cyclopropyl cation: hints on its detection in space. *Physical Chemistry Chemical Physics*, **2019**, 21, 3431-3439	3.6	13
229	The Unexplored World of Cycloalkene–Water Complexes: Primary and Assisting Interactions Unraveled by Experimental and Computational Spectroscopy. *Angewandte Chemie*, **2019**, 131, 14073-14079	3.6	2
228	The Unexplored World of Cycloalkene-Water Complexes: Primary and Assisting Interactions Unraveled by Experimental and Computational Spectroscopy. *Angewandte Chemie - International Edition*, **2019**, 58, 13935-13941	16.4	18
227	Prebiotic molecules in interstellar space: Rotational spectroscopy and quantum chemistry. *Proceedings of the International Astronomical Union*, **2019**, 15, 65-70	0.1	

226	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
225	Rotational and Infrared Spectroscopy of Ethanimine: A Route toward Its Astrophysical and Planetary Detection. *Astrophysical Journal*, **2018**, 855, 123	4.7	24
224	The Genealogical Tree of Ethanol: Gas-phase Formation of Glycolaldehyde, Acetic Acid, and Formic Acid. *Astrophysical Journal*, **2018**, 854, 135	4.7	71
223	Accuracy of Rotational Parameters Predicted by High-Level Quantum-Chemical Calculations: Case Study of Sulfur-Containing Molecules of Astrochemical Interest. *Journal of Chemical Theory and Computation*, **2018**, 14, 5360-5371	6.4	25
222	Theory Meets Experiment for Noncovalent Complexes: The Puzzling Case of Pnicogen Interactions. *Angewandte Chemie - International Edition*, **2018**, 57, 13853-13857	16.4	48
221	Computational challenges in Astrochemistry. *Wiley Interdisciplinary Reviews: Computational Molecular Science*, **2018**, 8, e1349	7.9	19
220	Cover Image, Volume 8, Issue 3. *Wiley Interdisciplinary Reviews: Computational Molecular Science*, **2018**, 8, e1368	7.9	1
219	Laboratory measurements and astronomical search for cyanomethanimine. *Astronomy and Astrophysics*, **2018**, 609,	5.1	24
218	Accurate rest frequencies for propargylamine in the ground and low-lying vibrational states. *Astronomy and Astrophysics*, **2018**, 615, A176	5.1	7
217	Theory Meets Experiment for Noncovalent Complexes: The Puzzling Case of Pnicogen Interactions. *Angewandte Chemie*, **2018**, 130, 14049-14053	3.6	6
216	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
215	Unveiling the Sulfur□Sulfur Bridge: Accurate Structural and Energetic Characterization of a Homochalcogen Intermolecular Bond. *Angewandte Chemie*, **2018**, 130, 16048-16052	3.6	5
214	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
213	Accurate Vibrational-Rotational Parameters and Infrared Intensities of 1-Bromo-1-fluoroethene: A Joint Experimental Analysis and Ab Initio Study. *Journal of Physical Chemistry A*, **2017**, 121, 3305-3317	2.8	15
212	Benchmark study of the structural and spectroscopic parameters of the hydroxymethyl peroxy (HOCHOO) radical and its decomposition reaction to HO and HCO. *Journal of Chemical Physics*, **2017** , 146, 144303	3.9	3
211	Collision induced broadening of □ band and ground state spectral lines of sulfur dioxide perturbed by N2 and O2. *Journal of Quantitative Spectroscopy and Radiative Transfer*, **2017**, 198, 155-163	2.1	2
210	On the competition between weak O-H□□F and C-H□□F hydrogen bonds, in cooperation with C-H□□O contacts, in the difluoromethane - -butyl alcohol cluster. *Journal of Molecular Spectroscopy*, **2017**, 337, 90-95	1.3	20
209	CO2-, He- and H2-broadening coefficients of SO2 for □ band and ground state transitions for astrophysical applications. *Journal of Quantitative Spectroscopy and Radiative Transfer*, **2017**, 203, 367-376	2.1	11

208	Astronomical complex organic molecules: Quantum chemistry meets rotational spectroscopy. *International Journal of Quantum Chemistry*, **2017**, 117, 129-138	2.1	14
207	Zeeman effect in sulfur monoxide: A tool to probe magnetic fields in star forming regions. *Astronomy and Astrophysics*, **2017**, 605,	5.1	3
206	Correct Modeling of Cisplatin: a Paradigmatic Case. *Angewandte Chemie*, **2017**, 129, 14026-14029	3.6	
205	Correct Modeling of Cisplatin: a Paradigmatic Case. *Angewandte Chemie - International Edition*, **2017**, 56, 13838-13841	16.4	18
204	VMS-ROT: A New Module of the Virtual Multifrequency Spectrometer for Simulation, Interpretation, and Fitting of Rotational Spectra. *Journal of Chemical Theory and Computation*, **2017** , 13, 4382-4396	6.4	30
203	Spectroscopic Characterization of Key Aromatic Molecules: A Route toward The Origin of Life. *Astronomical Journal*, **2017**, 154,	4.9	9
202	New quantum chemical computations of formamide deuteration support a gas-phase formation of this prebiotic molecule. *Monthly Notices of the Royal Astronomical Society: Letters*, **2017**, slx012	4.3	25
201	Accurate spectroscopic characterization of the HOC(O)O radical: A route toward its experimental identification. *Journal of Chemical Physics*, **2017**, 147, 024302	3.9	4
200	Seeds of Life in Space (SOLIS). *Astronomy and Astrophysics*, **2017**, 605, L3	5.1	67
199	Accurate molecular structures of small- and medium-sized molecules. *International Journal of Quantum Chemistry*, **2016**, 116, 1513-1519	2.1	34
198	Laboratory measurements and astronomical search for the HSO radical. *Astronomy and Astrophysics* , **2016**, 591,	5.1	18
197	Nuclear Spin Conversion in CH4: A Multichannel Relaxation Mechanism. *Journal of Physical Chemistry A*, **2016**, 120, 173-82	2.8	8
196	The rotational spectrum of 17O2 up to the THz region. *Journal of Quantitative Spectroscopy and Radiative Transfer*, **2016**, 168, 10-16	2.1	
195	Structure and spectroscopic properties of low-lying states of the HOC(O)O radical. *Journal of Chemical Physics*, **2016**, 144, 084306	3.9	1
194	Correction to Semi-Experimental Equilibrium Structure Determinations by Employing B3LYP/SNSD Anharmonic Force Fields: Validation and Application to Semirigid Organic Molecules. *Journal of Physical Chemistry A*, **2016**, 120, 3754	2.8	1
193	Structural and Energetic Characterization of Prebiotic Molecules: The Case Study of Formamide and Its Dimer. *Journal of Physical Chemistry A*, **2016**, 120, 5257-63	2.8	16
192	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
191	THE HYPERFINE STRUCTURE OF THE ROTATIONAL SPECTRUM OF HDO AND ITS EXTENSION TO THE THz REGION: ACCURATE REST FREQUENCIES AND SPECTROSCOPIC PARAMETERS FOR ASTROPHYSICAL OBSERVATIONS. *Astrophysical Journal*, **2015**, 806, 100	4.7	5

190	Quantum Chemistry Meets Spectroscopy for Astrochemistry: Increasing Complexity toward Prebiotic Molecules. *Accounts of Chemical Research*, **2015**, 48, 1413-22	24.3	61
189	The Born□Oppenheimer equilibrium bond distance of GeO from millimetre- and submillimetre-wave spectra and quantum-chemical calculations. *Molecular Physics*, **2015**, 113, 801-807	1.7	3
188	Isomerism of Cyanomethanimine: Accurate Structural, Energetic, and Spectroscopic Characterization. *Journal of Physical Chemistry A*, **2015**, 119, 11614-22	2.8	19
187	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
186	RARE ISOTOPIC SPECIES OF SULFUR MONOXIDE: THE ROTATIONAL SPECTRUM IN THE THz REGION. *Astrophysical Journal*, **2015**, 813, 4	4.7	7
185	Accurate structural and spectroscopic characterization of prebiotic molecules: The neutral and cationic acetyl cyanide and their related species. *Journal of Chemical Physics*, **2015**, 143, 184314	3.9	7
184	The hyperfine structure in the rotational spectra of D2(17)O and HD(17)O: Confirmation of the absolute nuclear magnetic shielding scale for oxygen. *Journal of Chemical Physics*, **2015**, 142, 124308	3.9	14
183	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. *Planetary and Space Science*, **2015**, 109-110, 46-63	2	29
182	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
181	Impact of sub-Doppler measurements on centrifugal-distortion terms: rotational spectrum of methyl fluoride revisited. *Journal of Physical Chemistry A*, **2015**, 119, 1765-73	2.8	3
180	Microsolvation of 2-thiouracil: molecular structure and spectroscopic parameters of the thiouracil-water complex. *Journal of Physical Chemistry A*, **2015**, 119, 5386-95	2.8	22
179	Towards the computations of accurate spectroscopic parameters and vibrational spectra for organic compounds. *Molecular Physics*, **2015**, 113, 1661-1673	1.7	13
178	Structure Prediction **2015**,		
177	Theoretical spectroscopic characterization at low temperatures of detectable sulfur-organic compounds: ethyl mercaptan and dimethyl sulfide. *Journal of Chemical Physics*, **2014**, 140, 124302	3.9	22
176	ACCURATE SPECTROSCOPIC CHARACTERIZATION OF PROTONATED OXIRANE: A POTENTIAL PREBIOTIC SPECIES IN TITAN'S ATMOSPHERE. *Astrophysical Journal*, **2014**, 792,	4.7	12
175	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
174	The rotational spectrum of hydrogen sulfide: The H2. *Journal of Molecular Spectroscopy*, **2014**, 298, 31-37	1.3	12
173	Molecular structure and spectroscopic signatures of acrolein: theory meets experiment. *Journal of Physical Chemistry A*, **2014**, 118, 6648-56	2.8	28

172	Computational Astrochemistry and Molecular Astrophysics **2014**,		
171	Rare isotopic species of hydrogen sulfide: the rotational spectrum of H236S. *Astronomy and Astrophysics*, **2014**, 566, A52	5.1	13
170	Computational Spectroscopy Tools for Molecular Structure Analysis **2014**, 27-64		3
169	Self-, N2-, O2-broadening coefficients and line parameters of HFC-32 for ν band and ground state transitions from infrared and microwave spectroscopy. *Molecular Physics*, **2014**, 112, 2384-2396	1.7	13
168	Theoretical spectroscopic characterization at low temperatures of S-methyl thioformate and O-methyl thioformate. *Journal of Chemical Physics*, **2014**, 141, 104303	3.9	9
167	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
166	ACCURATE SPECTROSCOPIC CHARACTERIZATION OF ETHYL MERCAPTAN AND DIMETHYL SULFIDE ISOTOPOLOGUES: A ROUTE TOWARD THEIR ASTROPHYSICAL DETECTION. *Astrophysical Journal*, **2014**, 796, 50	4.7	15
165	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
164	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
163	Anharmonic theoretical simulations of infrared spectra of halogenated organic compounds. *Journal of Chemical Physics*, **2013**, 139, 074310	3.9	64
162	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
161	Cyclopropenyl cation □the simplest Huckel's aromatic molecule □and its cyclic methyl derivatives in Titan's upper atmosphere. *Planetary and Space Science*, **2013**, 87, 96-105	2	22
160	Glycine conformers: a never-ending story?. *Physical Chemistry Chemical Physics*, **2013**, 15, 1358-63	3.6	75
159	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
158	Rotational spectroscopy meets theory. *Physical Chemistry Chemical Physics*, **2013**, 15, 6595-607	3.6	55
157	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
156	A complete listing of sulfur dioxide self-broadening coefficients for atmospheric applications by coupling infrared and microwave spectroscopy to semiclassical calculations. *Journal of Quantitative Spectroscopy and Radiative Transfer*, **2013**, 130, 233-248	2.1	11
155	An integrated experimental and quantum-chemical investigation on the vibrational spectra of chlorofluoromethane. *Journal of Chemical Physics*, **2013**, 139, 164302	3.9	32

154	Accurate structure, thermodynamics, and spectroscopy of medium-sized radicals by hybrid coupled cluster/density functional theory approaches: the case of phenyl radical. *Journal of Chemical Physics* , **2013**, 138, 234303	3.9	27
153	33S hyperfine interactions in H2S and SO2 and revision of the sulfur nuclear magnetic shielding scale. *Journal of Chemical Physics*, **2013**, 139, 244308	3.9	21
152	The bromine nuclear quadrupole moment revisited. *Molecular Physics*, **2013**, 111, 1382-1389	1.7	7
151	Quantum-chemical determination of Born□Oppenheimer breakdown parameters for rotational constants: the open-shell species CN, CO+ and BO. *Molecular Physics*, **2013**, 111, 2204-2210	1.7	7
150	A theoretical study on CH2N2 isomers: structure and energetics. *Highlights in Theoretical Chemistry*, **2013**, 31-40		
149	Integrated computational approaches for spectroscopic studies of molecular systems in the gas phase and in solution: pyrimidine as a test case. *Highlights in Theoretical Chemistry*, **2013**, 319-337		
148	N2-, O2-, H2-, and He-broadening of SO2 rotational lines in the mm-/submm-wave and THz frequency regions: The J and Ka dependence. *Journal of Quantitative Spectroscopy and Radiative Transfer*, **2012**, 113, 1051-1057	2.1	18
147	Molecular structure of thiourea. *Journal of Physical Chemistry A*, **2012**, 116, 4381-7	2.8	21
146	Rotational spectrum of silyl chloride: hyperfine structure and equilibrium geometry. *Molecular Physics*, **2012**, 110, 2359-2369	1.7	3
145	First-order properties and Buckingham birefringence of N2O and OCS □A computational (re)investigation. *Molecular Physics*, **2012**, 110, 2543-2555	1.7	1
144	A theoretical study on CH2N2 isomers: structure and energetics. *Theoretical Chemistry Accounts*, **2012**, 131, 1	1.9	9
143	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
142	PRECISE THz MEASUREMENTS OF HCO + , N 2 H + , AND CF + FOR ASTROPHYSICAL OBSERVATIONS. *Astrophysical Journal, Supplement Series*, **2012**, 203, 11	8	32
141	A theoretical study of the CX2N radicals (X = F, Cl, Br): the effect of halogen substitution on structure, isomerization, and energetics. *Journal of Chemical Physics*, **2012**, 136, 044316	3.9	1
140	Rotational spectra of rare isotopic species of fluoroiodomethane: determination of the equilibrium structure from rotational spectroscopy and quantum-chemical calculations. *Journal of Chemical Physics*, **2012**, 137, 024310	3.9	23
139	The rotational spectra of HD17O and D2(17)O: experiment and quantum-chemical calculations. *Journal of Chemical Physics*, **2012**, 137, 154311	3.9	46
138	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
137	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

136	Computational Approach to Rotational Spectroscopy **2011**, 261-307		2
135	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
134	The rotational spectrum of trans-DCOOD: Lamb-dip measurements, THz spectroscopy and quantum-chemical calculations. *Chemical Physics Letters*, **2011**, 502, 42-47	2.5	3
133	Rotational spectroscopy for astrophysical investigations. *Rendiconti Lincei*, **2011**, 22, 165-172	1.7	3
132	The proton affinity and gas-phase basicity of sulfur dioxide. *ChemPhysChem*, **2011**, 12, 112-5	3.2	27
131	Accurate thermochemistry and spectroscopy of the oxygen-protonated sulfur dioxide isomers. *Physical Chemistry Chemical Physics*, **2011**, 13, 21319-27	3.6	15
130	Microwave, high-resolution infrared, and quantum chemical investigations of CHBrF2: ground and v4 = 1 states. *Journal of Physical Chemistry A*, **2011**, 115, 453-9	2.8	24
129	Improved ground-state spectroscopic parameters of CH2FI and assignment of the rotational spectrum of the 6 = 1 state. *Molecular Physics*, **2011**, 109, 2245-2249	1.7	2
128	Assignment and analysis of the rotational spectra of the v7=1, v12=1 and v13=1 vibrational states of CH3CCCCH. *Journal of Molecular Spectroscopy*, **2011**, 267, 118-122	1.3	
127	Spectroscopic investigation of fluoroiodomethane, CH2FI: Fourier-transform microwave and millimeter-/submillimeter-wave spectroscopy and quantum-chemical calculations. *Journal of Chemical Physics*, **2011**, 134, 174312	3.9	22
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