Vicenzo Barone

List of Publications by Year
in descending order

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782 papers	85,136 citations	2427 97 h-index	460 272 g-index
812 all docs	812 docs citations	812 times ranked	43141 citing authors

#	Article	IF	Citations
1	Stacked but not Stuck: Unveiling the Role of Ï€â†'Ï€* Interactions with the Help of the Benzofuranâ€"Formaldehyde Complex. Angewandte Chemie - International Edition, 2022, 61, .	13.8	15
2	Stacked but not Stuck: Unveiling the Role of Ï€ â†' Ï€* Interactions with the Help of the Benzofuranâ€Formaldehyde Complex. Angewandte Chemie, 2022, 134, e202113737.	2.0	2
3	Probing Liquid-Ordered and Disordered Phases in Lipid Model Membranes: A Combined Theoretical and Spectroscopic Study of a Fluorescent Molecular Rotor. Journal of Physical Chemistry B, 2022, , .	2.6	0
4	Toward Accurate Formation Routes of Complex Organic Molecules in the Interstellar Medium: The Paradigmatic Cases of Acrylonitrile and Cyanomethanimine. Frontiers in Astronomy and Space Sciences, 2022, 8, .	2.8	7
5	Gas-phase far-infrared spectroscopy of <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" altimg="si1.svg"><mml:mrow><mml:msub><mml:mrow><mml:mi mathvariant="normal">HC</mml:mi></mml:mrow><mml:mn>3</mml:mn></mml:msub><mml:mi mathvariant="normal">N</mml:mi></mml:mrow></mml:math>: Extended ro-vibrational analysis and new line list up to 3360 cm<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" altimg="si2.svg">	2.3	1
6	Gas-phase identification of (Z)-1,2-ethenediol, a key prebiotic intermediate in the formose reaction. Chemical Communications, 2022, 58, 2750-2753.	4.1	14
7	Welcome to Physchem: Status and Prospects. Physchem, 2022, 2, 16-17.	1.1	0
8	Molecular Dynamics Simulations Enforcing Nonperiodic Boundary Conditions: New Developments and Application to the Solvent Shifts of Nitroxide Magnetic Parameters. Journal of Chemical Theory and Computation, 2022, , .	5.3	5
9	Accurate Quantum Chemical Spectroscopic Characterization of Glycolic Acid: A Route Toward its Astrophysical Detection. Journal of Physical Chemistry A, 2022, 126, 2373-2387.	2.5	16
10	Development, Validation, and Pilot Application of a Generalized Fluctuating Charge Model for Computational Spectroscopy in Solution. ACS Omega, 2022, 7, 13382-13394.	3.5	1
11	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.	8.3	43
12	Gliding on Ice in Search of Accurate and Cost-Effective Computational Methods for Astrochemistry on Grains: The Puzzling Case of the HCN Isomerization. Journal of Chemical Theory and Computation, 2022, 18, 3111-3121.	5.3	4
13	Spectroscopic Characterization of 3-Aminoisoxazole, a Prebiotic Precursor of Ribonucleotides. Molecules, 2022, 27, 3278.	3.8	2
14	PROTEUS: an immersive tool for exploring the world of cultural heritage across space and time scales. Heritage Science, 2022, 10, .	2.3	0
15	Dipolar 1,3â€cycloaddition of thioformaldehyde S â€methylide (<scp> CH ₂ SCH) Tj ETQq1 1 0.784314 rgBT /Over ₃ </scp> , <scp> SO ₂ </scp> , <scp>. Journal of Computational Chemistry, 2022, 43, 1420-1433.	3.3	6
16	Unbiased disentanglement of conformational baths with the help of microwave spectroscopy, quantum chemistry, and artificial intelligence: The puzzling case of homocysteine. Journal of Chemical Physics, 2022, 157, .	3.0	12
17	PhysChem: A New Physical Chemistry Journal. Physchem, 2021, 1, 1-3.	1.1	0
18	Isomerization and Fragmentation Reactions on the [C₂SH₄] Potential Energy Surface: The Metastable Thione S-Methylide Isomer. Journal of Organic Chemistry, 2021, 86, 2941-2956.	3.2	11

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19	Transverseâ€“Spin Quark Distributions from Asymmetry Data and Symmetry Arguments. Symmetry, 2021, 13, 116.	2.2	1
20	1,2-Disubstituted Planar Chiral Ferrocene Derivatives from Sulfonamide-Directed ortho-Lithiation: Synthesis, Absolute Configuration, and Chiroptical Properties. Organometallics, 2021, 40, 578-590.	2.3	14
21	A computational insight into the relationship between side chain IR line shapes and local environment in fibril-like structures. Journal of Chemical Physics, 2021, 154, 084105.	3.0	1
22	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.	2.5	19
23	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.	2.5	13
24	Gas-Phase Formation and Isomerization Reactions of Cyanoacetaldehyde, a Prebiotic Molecule of Astrochemical Interest. ACS Earth and Space Chemistry, 2021, 5, 1071-1082.	2.7	10
25	Accuracy and Reliability in the Simulation of Vibrational Spectra: A Comprehensive Benchmark of Energies and Intensities Issuing From Generalized Vibrational Perturbation Theory to Second Order (GVPT2). Frontiers in Astronomy and Space Sciences, 2021, 8, .	2.8	32
26	Computational molecular spectroscopy. Nature Reviews Methods Primers, 2021, 1, .	21.2	73
27	4-Fluoro-Threonine: From Diastereoselective Synthesis to pH-Dependent Conformational Equilibrium in Aqueous Solution. ACS Omega, 2021, 6, 13170-13181.	3.5	4
28	Interplay of stereo-electronic, vibronic and environmental effects in tuning the chiroptical properties of an Ir(III) cyclometalated N-heterocyclic carbene. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2021, 254, 119631.	3.9	4
29	General Perturb-Then-Diagonalize Model for the Vibrational Frequencies and Intensities of Molecules Belonging to Abelian and Non-Abelian Symmetry Groups. Journal of Chemical Theory and Computation, 2021, 17, 4332-4358.	5.3	15
30	Insoluble organic matter in chondrites: Archetypal melanin-like PAH-based multifunctionality at the origin of life?. Physics of Life Reviews, 2021, 37, 65-93.	2.8	18
31	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	14
32	Development and Validation of a Parameter-Free Model Chemistry for the Computation of Reliable Reaction Rates. Journal of Chemical Theory and Computation, 2021, 17, 4913-4928.	5.3	34
33	High Water Density at Non-Ice-Binding Surfaces Contributes to the Hyperactivity of Antifreeze Proteins. Journal of Physical Chemistry Letters, 2021, 12, 8777-8783.	4.6	11
34	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.	2.8	17
35	Accurate Biomolecular Structures by the Nano-LEGO Approach: Pick the Bricks and Build Your Geometry. Journal of Chemical Theory and Computation, 2021, 17, 7290-7311.	5.3	45
36	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.	5.3	30

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37	Enhancing the Accuracy of Ab Initio Molecular Dynamics by Fine Tuning of Effective Two-Body Interactions: Acetonitrile as a Test Case. Journal of Physical Chemistry A, 2021, 125, 10475-10484.	2.5	4
38	Analysis of L-DOPA and droxidopa binding to human Î²2-adrenergic receptor. Biophysical Journal, 2021, , .	0.5	1
39	Extending the Applicability of the Semi-experimental Approach by Means of â€œTemplate Moleculeâ€•and â€œLinear Regressionâ€•Models on Top of DFT Computations. Journal of Physical Chemistry A, 2021, 125, 9904-9916.	2.5	28
40	Formation of Phosphorus Monoxide (PO) in the Interstellar Medium: Insights from Quantum-chemical and Kinetic Calculations. Astrophysical Journal, 2021, 922, 169.	4.5	21
41	An improved study of HCO+ and He system: Interaction potential, collisional relaxation, and pressure broadening. Journal of Chemical Physics, 2021, 155, 234306.	3.0	5
42	A Computational Journey across Nitroxide Radicals: From Structure to Spectroscopic Properties and Beyond. Molecules, 2021, 26, 7404.	3.8	5
43	A never-ending story in the sky: The secrets of chemical evolution. Physics of Life Reviews, 2020, 32, 59-94.	2.8	28
44	Extension of the â€œCheapâ€•Composite Approach to Noncovalent Interactions: The jun-ChS Scheme. Journal of Chemical Theory and Computation, 2020, 16, 988-1006.	5.3	73
45	Unraveling the role of additional OH-radicals in the Hâ€“Abstraction from Dimethyl sulfide using quantum chemical computations. Chemical Physics Letters, 2020, 739, 136963.	2.6	9
46	Challenges in astrochemistry: The spectroscopic point of view. Physics of Life Reviews, 2020, 34-35, 143-146.	2.8	1
47	Unsupervised search of low-lying conformers with spectroscopic accuracy: A two-step algorithm rooted into the island model evolutionary algorithm. Journal of Chemical Physics, 2020, 153, 124110.	3.0	30
48	Computational Spectroscopy in Solution by Integration of Variational and Perturbative Approaches on Top of Clusterized Molecular Dynamics. Journal of Chemical Theory and Computation, 2020, 16, 5747-5761.	5.3	5
49	Discovering the Elusive Global Minimum in a Ternary Chiral Cluster: Rotational Spectra of Propylene Oxide Trimer. Angewandte Chemie, 2020, 132, 22613-22616.	2.0	11
50	CPL Spectra of Camphor Derivatives in Solution by an Integrated QM/MD Approach. Frontiers in Chemistry, 2020, 8, 584.	3.6	8
51	A Journey from Thermally Tunable Synthesis to Spectroscopy of Phenylmethanimine in Gas Phase and Solution. Chemistry - A European Journal, 2020, 26, 15016-15022.	3.3	7
52	Interplay of Stereoelectronic and Vibrational Modulation Effects in Tuning the UPS Spectra of Unsaturated Hydrocarbon Cage Compounds. Journal of Chemical Theory and Computation, 2020, 16, 5218-5226.	5.3	1
53	Discovering the Elusive Global Minimum in a Ternary Chiral Cluster: Rotational Spectra of Propylene Oxide Trimer. Angewandte Chemie - International Edition, 2020, 59, 22427-22430.	13.8	47
54	Accuracy Meets Interpretability for Computational Spectroscopy by Means of Hybrid and Double-Hybrid Functionals. Frontiers in Chemistry, 2020, 8, 584203.	3.6	50

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55	Rotational Spectroscopy Meets Quantum Chemistry for Analyzing Substituent Effects on Non-Covalent Interactions: The Case of the Trifluoroacetophenone-Water Complex. Molecules, 2020, 25, 4899.	3.8	8
56	Collisional broadening and hyperfine structure of rotational transitions. Reply to the comments on â€œA never-ending story in the sky: The secrets of chemical evolutionâ€• Physics of Life Reviews, 2020, 32, 124-128.	2.8	0
57	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	1
58	A reinvestigation of the deceptively simple reaction of toluene with OH, and the fate of the benzyl radical: a combined thermodynamic and kinetic study on the competition between OH-addition and H-abstraction reactions. Theoretical Chemistry Accounts, 2020, 139, 1.	1.4	5
59	Reinvestigation of the Deceptively Simple Reaction of Toluene with OH and the Fate of the Benzyl Radical: The â€œHiddenâ€•Routes to Cresols and Benzaldehyde. Journal of Physical Chemistry A, 2020, 124, 5917-5930.	2.5	18
60	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.	4.4	24
61	Chemical bonding in cuprous complexes with simple nitriles: octet rule and resonance concepts versus quantitative charge-redistribution analysis. Physical Chemistry Chemical Physics, 2020, 22, 20238-20247.	2.8	3
62	A General User-Friendly Tool for Kinetic Calculations of Multi-Step Reactions within the Virtual Multifrequency Spectrometer Project. Applied Sciences (Switzerland), 2020, 10, 1872.	2.5	8
63	Sextic centrifugal distortion constants: interplay of density functional and basis set for accurate yet feasible computations. Molecular Physics, 2020, 118, e1734678.	1.7	12
64	The challenging playground of astrochemistry: an integrated rotational spectroscopy â€“ quantum chemistry strategy. Physical Chemistry Chemical Physics, 2020, 22, 6507-6523.	2.8	36
65	Length-scale dependence of protein hydration-shell density. Physical Chemistry Chemical Physics, 2020, 22, 7340-7347.	2.8	5
66	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.	2.7	13
67	State-of-the-Art Quantum Chemistry Meets Variable Reaction Coordinate Transition State Theory to Solve the Puzzling Case of the H₂S + Cl System. Journal of Chemical Theory and Computation, 2020, 16, 5090-5104.	5.3	27
68	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, 2873.	3.8	20
69	The challenging equilibrium structure of HSSH: Another success of the rotational spectroscopy / quantum chemistry synergism. Journal of Molecular Structure, 2020, 1211, 127933.	3.6	11
70	Chemical promenades: Exploring potentialâ€energy surfaces with immersive virtual reality. Journal of Computational Chemistry, 2020, 41, 1310-1323.	3.3	21
71	H-Abstraction from Dimethyl Sulfide in the Presence of an Excess of Hydroxyl Radicals. A Quantum Chemical Evaluation of Thermochemical and Kinetic Parameters Unveils an Alternative Pathway to Dimethyl Sulfoxide. ACS Earth and Space Chemistry, 2020, 4, 403-419.	2.7	9
72	Theory meets experiment for elucidating the structure and stability of non-covalent complexes: waterâ€“amine interaction as a proof of concept. Physical Chemistry Chemical Physics, 2020, 22, 5024-5032.	2.8	14

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73	DFT meets the segmented polarization consistent basis sets: Performances in the computation of molecular structures, rotational and vibrational spectroscopic properties. Journal of Molecular Structure, 2020, 1208, 127886.	3.6	23
74	Modeling amino-acid side chain infrared spectra: the case of carboxylic residues. Physical Chemistry Chemical Physics, 2020, 22, 3008-3016.	2.8	10
75	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.	2.5	14
76	Toward Fully Unsupervised Anharmonic Computations Complementing Experiment for Robust and Reliable Assignment and Interpretation of IR and VCD Spectra from Mid-IR to NIR: The Case of 2,3-Butanediol and trans-1,2-Cyclohexanediol. Journal of Physical Chemistry A, 2020, 124, 1011-1024.	2.5	26
77	Molecular Perception for Visualization and Computation: The Proxima Library. Journal of Chemical Information and Modeling, 2020, 60, 2668-2672.	5.4	24
78	The ONIOM/PMM Model for Effective Yet Accurate Simulation of Optical and Chiroptical Spectra in Solution: Camphorquinone in Methanol as a Case Study. Journal of Chemical Theory and Computation, 2020, 16, 3294-3306.	5.3	17
79	Systematic Study on the Absorption Features of Interstellar Ices in the Presence of Impurities. ACS Earth and Space Chemistry, 2020, 4, 920-946.	2.7	6
80	The challenge of non-covalent interactions: theory meets experiment for reconciling accuracy and interpretation. Journal of Physics Condensed Matter, 2020, 32, 343002.	1.8	19
81	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.	4.5	16
82	Methanimine as a Key Precursor of Imines in the Interstellar Medium: The Case of Propargylimine. Astrophysical Journal Letters, 2020, 903, L35.	8.3	24
83	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	3
84	Virtual Reality bridge between Chemistry and Cultural Heritage: the â€œSala degli Stemmiâ€•Case Study.. IOP Conference Series: Materials Science and Engineering, 2020, 949, 012020.	0.6	1
85	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.	2.8	17
86	Two-level stochastic search of low-energy conformers for molecular spectroscopy: implementation and validation of MM and QM models. Physical Chemistry Chemical Physics, 2019, 21, 19921-19934.	2.8	21
87	Hydration Shell of Antifreeze Proteins: Unveiling the Role of Non-Ice-Binding Surfaces. Journal of Physical Chemistry B, 2019, 123, 6474-6480.	2.6	20
88	The Unexplored World of Cycloalkeneâ€“Water Complexes: Primary and Assisting Interactions Unraveled by Experimental and Computational Spectroscopy. Angewandte Chemie, 2019, 131, 14073-14079.	2.0	6
89	The Unexplored World of Cycloalkeneâ€“Water Complexes: Primary and Assisting Interactions Unraveled by Experimental and Computational Spectroscopy. Angewandte Chemie - International Edition, 2019, 58, 13935-13941.	13.8	22
90	Machine Learning of Potential-Energy Surfaces Within a Bond-Order Sampling Scheme. Lecture Notes in Computer Science, 2019, , 388-400.	1.3	2

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91	Virtual reality tools for advanced modeling. AIP Conference Proceedings, 2019, , .	0.4	7
92	Astrochemistry and Astrobiology: Materials Sciencein Wonderland?. International Journal of Molecular Sciences, 2019, 20, 4079.	4.1	29
93	Transversity distributions from difference asymmetries in semi-inclusive DIS. Physical Review D, 2019, 99, .	4.7	6
94	Enthalpies of formation of the benzyloxyl, benzylperoxyl, hydroxyphenyl radicals and related species on the potential energy surface for the reaction of toluene with the hydroxyl radical. Theoretical Chemistry Accounts, 2019, 138, 1.	1.4	3
95	Unbiased Determination of Absolute Configurations by vis-Ã-vis Comparison of Experimental and Simulated Spectra: The Challenging Case of Diplopyrone. Journal of Physical Chemistry B, 2019, 123, 9230-9237.	2.6	29
96	Theory meets experiment for unravelling the C1s X-ray photoelectron spectra of pyridine, 2-fluoropyridine, and 2,6-difluoropyridine. Journal of Chemical Physics, 2019, 151, 124105.	3.0	6
97	Molecular synthons for accurate structural determinations: the equilibrium geometry of 1-chloro-1-fluoroethene. Physical Chemistry Chemical Physics, 2019, 21, 3615-3625.	2.8	15
98	Potential-Energy Surfaces for Ring-Puckering Motions of Flexible Cyclic Molecules through Cremerâ€“Pople Coordinates: Computation, Analysis, and Fitting. Journal of Chemical Theory and Computation, 2019, 15, 4280-4294.	5.3	23
99	Accuracy and Interpretability: The Devil and the Holy Grail. New Routes across Old Boundaries in Computational Spectroscopy. Chemical Reviews, 2019, 119, 8131-8191.	47.7	167
100	Measurement of P-weighted Sivers asymmetries in leptoproduction of hadrons. Nuclear Physics B, 2019, 940, 34-53.	2.5	13
101	Optimization of highly excited matrix product states with an application to vibrational spectroscopy. Journal of Chemical Physics, 2019, 150, 094113.	3.0	29
102	Ferrocenes with simple chiral substituents: an in-depth theoretical and experimental VCD and ECD study. Physical Chemistry Chemical Physics, 2019, 21, 9419-9432.	2.8	19
103	Effective yet reliable computation of hyperfine coupling constants in solution by a QM/MM approach: Interplay between electrostatics and non-electrostatic effects. Journal of Chemical Physics, 2019, 150, 124102.	3.0	42
104	Assessment of Multi-Scale Approaches for Computing UVâ€“Vis Spectra in Condensed Phases: Toward an Effective yet Reliable Integration of Variational and Perturbative QM/MM Approaches. Journal of Chemical Theory and Computation, 2019, 15, 3170-3184.	5.3	17
105	Computational Evidence Suggests That 1-Chloroethanol May Be an Intermediate in the Thermal Decomposition of 2-Chloroethanol into Acetaldehyde and HCl. Journal of Physical Chemistry A, 2019, 123, 1983-1998.	2.5	2
106	Mechanistic insights into metal ions transit through threefold ferritin channel. Biochimica Et Biophysica Acta - General Subjects, 2019, 1863, 472-480.	2.4	7
107	Tailorâ€made computational protocols for precise characterization of small biological building blocks using QM and MM approaches. Biopolymers, 2018, 109, e23109.	2.4	10
108	An ab initio study of Cu-based delafossites as an alternative to nickel oxide in photocathodes: effects of Mg-doping and surface electronic features. Physical Chemistry Chemical Physics, 2018, 20, 14082-14089.	2.8	26

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109	Characterization and Fate of Hydrogen-Bonded Free-Radical Intermediates and Their Coupling Products from the Hydrogen Atom Transfer Agent 1,8-Naphthalenediol. ACS Omega, 2018, 3, 3918-3927.	3.5	28
110	Exploiting coordination geometry to selectively predict the Ïƒ-donor and Ï€-acceptor abilities of ligands: a back-and-forth journey between electronic properties and spectroscopy. Chemical Communications, 2018, 54, 2397-2400.	4.1	24
111	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.	15.6	74
112	On the composition of an arbitrary collection of SU(2) spins: an enumerative combinatoric approach. Journal of Physics A: Mathematical and Theoretical, 2018, 51, 105202.	2.1	3
113	Tuning dispersion correction in DFT-D2 for metal-molecule interactions: A tailored reparameterization strategy for the adsorption of aromatic systems on Ag(1â€¯1â€¯1). Chemical Physics Letters, 2018, 693, 28-33.	2.6	13
114	Computational simulation of vibrationally resolved spectra for spinâ€forbidden transitions. Chirality, 2018, 30, 850-865.	2.6	15
115	Solar collectors based on luminescent 2,5-diarylimidazoles. Dyes and Pigments, 2018, 157, 334-341.	3.7	8
116	Unraveling the role of entropy in tuning unimolecular vs. bimolecular reaction rates: The case of olefin polymerization catalyzed by transition metals. Molecular Catalysis, 2018, 452, 138-144.	2.0	70
117	Rotational and Infrared Spectroscopy of Ethanimine: A Route toward Its Astrophysical and Planetary Detection. Astrophysical Journal, 2018, 855, 123.	4.5	35
118	The Genealogical Tree of Ethanol: Gas-phase Formation of Glycolaldehyde, Acetic Acid, and Formic Acid. Astrophysical Journal, 2018, 854, 135.	4.5	103
119	New atomistic model of pyrrole with improved liquid state properties and structure. International Journal of Quantum Chemistry, 2018, 118, e25554.	2.0	11
120	Force Field Parametrization of Metal Ions from Statistical Learning Techniques. Journal of Chemical Theory and Computation, 2018, 14, 255-273.	5.3	39
121	Effects of music playing on biological molecules. MATEC Web of Conferences, 2018, 210, 05006.	0.2	2
122	Towards the SMART workflow system for computational spectroscopy. Physical Chemistry Chemical Physics, 2018, 20, 26034-26052.	2.8	16
123	Comfort Index CI(bus): A methodology to measure the comfort on board. Procedia Computer Science, 2018, 134, 439-444.	2.0	3
124	Laboratory measurements and astronomical search for cyanomethanimine. Astronomy and Astrophysics, 2018, 609, A121.	5.1	31
125	Time-Dependent Formulation of Resonance Raman Optical Activity Spectroscopy. Journal of Chemical Theory and Computation, 2018, 14, 6370-6390.	5.3	26
126	Diving into chemical bonding: An immersive analysis of the electron charge rearrangement through virtual reality. Journal of Computational Chemistry, 2018, 39, 2607-2617.	3.3	30

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127	Theory Meets Experiment for Noncovalent Complexes: The Puzzling Case of Pnicogen Interactions. Angewandte Chemie, 2018, 130, 14049-14053.	2.0	7
128	Unveiling the Sulfurâ€“Sulfur Bridge: Accurate Structural and Energetic Characterization of a Homochalcogen Intermolecular Bond. Angewandte Chemie - International Edition, 2018, 57, 15822-15826.	13.8	49
129	Unveiling the Sulfurâ€“Sulfur Bridge: Accurate Structural and Energetic Characterization of a Homochalcogen Intermolecular Bond. Angewandte Chemie, 2018, 130, 16048-16052.	2.0	5
130	Extending the perturbed matrix method beyond the dipolar approximation: comparison of different levels of theory. Physical Chemistry Chemical Physics, 2018, 20, 24369-24378.	2.8	49
131	From ascorbic acid to furan derivatives: the gas phase acid catalyzed degradation of vitamin C. Physical Chemistry Chemical Physics, 2018, 20, 17132-17140.	2.8	19
132	Tyrosine absorption spectroscopy: Backbone protonation effects on the side chain electronic properties. Journal of Computational Chemistry, 2018, 39, 1747-1756.	3.3	17
133	Binding of Nucleic Acid Components to the Serpentinite-Hosted Hydrothermal Mineral Brucite. Astrobiology, 2018, 18, 989-1007.	3.0	18
134	Solid State Photochemistry of Hydroxylated Naphthalenes on Minerals: Probing Polycyclic Aromatic Hydrocarbon Transformation Pathways under Astrochemically-Relevant Conditions. ACS Earth and Space Chemistry, 2018, 2, 977-1000.	2.7	16
135	Theory Meets Experiment for Noncovalent Complexes: The Puzzling Case of Pnicogen Interactions. Angewandte Chemie - International Edition, 2018, 57, 13853-13857.	13.8	60
136	The role of the multiconfigurational character of nitronyl-nitroxide in the singletâ€“triplet energy gap of its diradicals. Physical Chemistry Chemical Physics, 2018, 20, 18547-18555.	2.8	3
137	Quantitative prediction and interpretation of spin energy gaps in polyradicals: the virtual magnetic balance. Physical Chemistry Chemical Physics, 2017, 19, 9039-9044.	2.8	4
138	The Borderline between Reactivity and Preâ€reactivity of Binary Mixtures of Gaseous Carboxylic Acids and Alcohols. Angewandte Chemie - International Edition, 2017, 56, 3872-3875.	13.8	14
139	Noncovalent Interactions and Internal Dynamics in Pyridineâ€“Ammonia: A Combined Quantumâ€Chemical and Microwave Spectroscopy Study. Chemistry - A European Journal, 2017, 23, 4876-4883.	3.3	39
140	Fine-tuning of atomic point charges: Classical simulations of pyridine in different environments. Chemical Physics Letters, 2017, 677, 120-126.	2.6	18
141	A Modular Implementation for the Simulation of 1D and 2D Solid-State NMR Spectra of Quadrupolar Nuclei in the Virtual Multifrequency Spectrometerâ€“Draw Graphical Interface. Journal of Chemical Theory and Computation, 2017, 13, 2215-2229.	5.3	18
142	Simulation of Vibronic Spectra of Flexible Systems: Hybrid DVR-Harmonic Approaches. Journal of Chemical Theory and Computation, 2017, 13, 2804-2822.	5.3	40
143	Development and Implementation of Advanced Fitting Methods for the Calculation of Accurate Molecular Structures. Journal of Chemical Theory and Computation, 2017, 13, 3060-3075.	5.3	50
144	Effective Inclusion of Mechanical and Electrical Anharmonicity in Excited Electronic States: VPT2-TDDFT Route. Journal of Chemical Theory and Computation, 2017, 13, 2789-2803.	5.3	23

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145	Electronic absorption spectra of pyridine and nicotine in aqueous solution with a combined molecular dynamics and polarizable QM/MM approach. Journal of Computational Chemistry, 2017, 38, 319-335.	3.3	38
146	Assessment of Electron Propagator Methods for the Simulation of Vibrationally Resolved Valence and Core Photoionization Spectra. Journal of Chemical Theory and Computation, 2017, 13, 3120-3135.	5.3	10
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