Vicenzo Barone

List of Publications by Year in Descending Order

783 papers	73,105 citations	93 h-index	255 g-index
812 ext. papers	78,965 ext. citations	4.8 avg, IF	8.31 L-index

#	Paper	IF	Citations
783	Synchrotron-based far-infrared spectroscopy of HC3N: Extended ro-vibrational analysis and new line list up to 3360 cm−1. *Journal of Quantitative Spectroscopy and Radiative Transfer*, **2022**, 279, 108044	2.1	
782	Gas-phase identification of ()-1,2-ethenediol, a key prebiotic intermediate in the formose reaction.. *Chemical Communications*, **2022**,	5.8	3
781	Gestapelt, nicht geklebt: Enthüllung der π-π-Wechselwirkung mithilfe des Benzofuran-Formaldehyd-Komplexes. *Angewandte Chemie*, **2022**, 134, e202113737	3.6	
780	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**,	6.4	2
779	Development, Validation, and Pilot Application of a Generalized Fluctuating Charge Model for Computational Spectroscopy in Solution.. *ACS Omega*, **2022**, 7, 13382-13394	3.9	0
778	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
777	Spectroscopic Characterization of 3-Aminoisoxazole, a Prebiotic Precursor of Ribonucleotides. *Molecules*, **2022**, 27, 3278	4.8	0
776	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
775	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	2.8	0
774	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
773	Formation of Phosphorus Monoxide (PO) in the Interstellar Medium: Insights from Quantum-chemical and Kinetic Calculations. *Astrophysical Journal*, **2021**, 922, 169	4.7	2
772	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
771	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	6.4	8
770	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
769	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
768	Gas-Phase Formation and Isomerization Reactions of Cyanoacetaldehyde, a Prebiotic Molecule of Astrochemical Interest. *ACS Earth and Space Chemistry*, **2021**, 5, 1071-1082	3.2	1
767	Computational molecular spectroscopy. *Nature Reviews Methods Primers*, **2021**, 1,		18

766	4-Fluoro-Threonine: From Diastereoselective Synthesis to pH-Dependent Conformational Equilibrium in Aqueous Solution. *ACS Omega*, **2021**, 6, 13170-13181	3.9	0
765	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	4.4	1
764	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	6.4	3
763	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
762	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
761	Isomerization and Fragmentation Reactions on the [CSH] Potential Energy Surface: The Metastable Thione -Methylide Isomer. *Journal of Organic Chemistry*, **2021**, 86, 2941-2956	4.2	4
760	Transverse Spin Quark Distributions from Asymmetry Data and Symmetry Arguments. *Symmetry*, **2021**, 13, 116	2.7	0
759	1,2-Disubstituted Planar Chiral Ferrocene Derivatives from Sulfonamide-Directed ortho-Lithiation: Synthesis, Absolute Configuration, and Chiroptical Properties. *Organometallics*, **2021**, 40, 578-590	3.8	7
758	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	3.9	1
757	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	6.4	6
756	High Water Density at Non-Ice-Binding Surfaces Contributes to the Hyperactivity of Antifreeze Proteins. *Journal of Physical Chemistry Letters*, **2021**, 12, 8777-8783	6.4	4
755	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
754	A Computational Journey across Nitroxide Radicals: From Structure to Spectroscopic Properties and Beyond. *Molecules*, **2021**, 26,	4.8	1
753	Accuracy Meets Interpretability for Computational Spectroscopy by Means of Hybrid and Double-Hybrid Functionals. *Frontiers in Chemistry*, **2020**, 8, 584203	5	18
752	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
751	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	
750	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	
749	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	1.9	4

748	Reinvestigation of the Deceptively Simple Reaction of Toluene with OH and the Fate of the Benzyl Radical: The "Hidden" Routes to Cresols and Benzaldehyde. *Journal of Physical Chemistry A*, **2020**, 124, 5917-5930	2.8	7
747	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
746	Chemical bonding in cuprous complexes with simple nitriles: octet rule and resonance concepts quantitative charge-redistribution analysis. *Physical Chemistry Chemical Physics*, **2020**, 22, 20238-20247	3.6	2
745	A General User-Friendly Tool for Kinetic Calculations of Multi-Step Reactions within the Virtual Multifrequency Spectrometer Project. *Applied Sciences (Switzerland)*, **2020**, 10, 1872	2.6	4
744	Sextic centrifugal distortion constants: interplay of density functional and basis set for accurate yet feasible computations. *Molecular Physics*, **2020**, 118, e1734678	1.7	5
743	The challenging playground of astrochemistry: an integrated rotational spectroscopy - quantum chemistry strategy. *Physical Chemistry Chemical Physics*, **2020**, 22, 6507-6523	3.6	24
742	Length-scale dependence of protein hydration-shell density. *Physical Chemistry Chemical Physics*, **2020**, 22, 7340-7347	3.6	3
741	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
740	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
739	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
738	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
737	Chemical promenades: Exploring potential-energy surfaces with immersive virtual reality. *Journal of Computational Chemistry*, **2020**, 41, 1310-1323	3.5	14
736	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	3.2	5
735	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
734	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	3.4	15
733	Modeling amino-acid side chain infrared spectra: the case of carboxylic residues. *Physical Chemistry Chemical Physics*, **2020**, 22, 3008-3016	3.6	8
732	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
731	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 -1,2-Cyclohexanediol. *Journal of Physical Chemistry A*, **2020**, 124, 1011-1024	2.8	16

730	Molecular Perception for Visualization and Computation: The Proxima Library. *Journal of Chemical Information and Modeling*, **2020**, 60, 2668-2672	6.1	8
729	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	6.4	11
728	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
727	Virtual Reality bridge between Chemistry and Cultural Heritage: the Sala degli Stemmi Case Study.. *IOP Conference Series: Materials Science and Engineering*, **2020**, 949, 012020	0.4	0
726	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
725	Methanimine as a Key Precursor of Imines in the Interstellar Medium: The Case of Propargylimine. *Astrophysical Journal Letters*, **2020**, 903, L35	7.9	7
724	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
723	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
722	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
721	Unraveling the role of additional OH-radicals in the H abstraction from Dimethyl sulfide using quantum chemical computations. *Chemical Physics Letters*, **2020**, 739, 136963	2.5	5
720	Challenges in astrochemistry: The spectroscopic point of view: Comment on "Prebiotic chemistry and origins of life research with atomistic computer simulations" by A. Pez-Villa, F. Pietrucci, and A.M. Saitta. *Physics of Life Reviews*, **2020**, 34-35, 143-146	2.1	1
719	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	3.9	11
718	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	6.4	4
717	Discovering the Elusive Global Minimum in a Ternary Chiral Cluster: Rotational Spectra of Propylene Oxide Trimer. *Angewandte Chemie*, **2020**, 132, 22613-22616	3.6	5
716	CPL Spectra of Camphor Derivatives in Solution by an Integrated QM/MD Approach. *Frontiers in Chemistry*, **2020**, 8, 584	5	6
715	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
714	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	6.4	1
713	Discovering the Elusive Global Minimum in a Ternary Chiral Cluster: Rotational Spectra of Propylene Oxide Trimer. *Angewandte Chemie - International Edition*, **2020**, 59, 22427-22430	16.4	20

712	A never-ending story in the sky: The secrets of chemical evolution. *Physics of Life Reviews*, **2020**, 32, 59-94	4.1	15
711	Virtual reality tools for advanced modeling **2019**,		4
710	Astrochemistry and Astrobiology: Materials Sciencein Wonderland?. *International Journal of Molecular Sciences*, **2019**, 20,	6.3	17
709	Transversity distributions from difference asymmetries in semi-inclusive DIS. *Physical Review D*, **2019**, 99,	4.9	3
708	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	1.9	2
707	Unbiased Determination of Absolute Configurations by vis-□vis Comparison of Experimental and Simulated Spectra: The Challenging Case of Diplopyrone. *Journal of Physical Chemistry B*, **2019**, 123, 9230-9237	3.4	20
706	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	3.9	3
705	Molecular synthons for accurate structural determinations: the equilibrium geometry of 1-chloro-1-fluoroethene. *Physical Chemistry Chemical Physics*, **2019**, 21, 3615-3625	3.6	10
704	Potential-Energy Surfaces for Ring-Puckering Motions of Flexible Cyclic Molecules through Cremer-Pople Coordinates: Computation, Analysis, and Fitting. *Journal of Chemical Theory and Computation*, **2019**, 15, 4280-4294	6.4	13
703	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
702	Measurement of PT-weighted Sivers asymmetries in leptoproduction of hadrons. *Nuclear Physics B*, **2019**, 940, 34-53	2.8	4
701	Interpretability Meets Accuracy in Computational Spectroscopy: The Virtual Multifrequency Spectrometer **2019**, 1-42		
700	Optimization of highly excited matrix product states with an application to vibrational spectroscopy. *Journal of Chemical Physics*, **2019**, 150, 094113	3.9	20
699	Ferrocenes with simple chiral substituents: an in-depth theoretical and experimental VCD and ECD study. *Physical Chemistry Chemical Physics*, **2019**, 21, 9419-9432	3.6	13
698	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	3.9	27
697	Assessment of Multi-Scale Approaches for Computing UV-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	6.4	12
696	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	2.8	2
695	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

694	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	3.6	13
693	Hydration Shell of Antifreeze Proteins: Unveiling the Role of Non-Ice-Binding Surfaces. *Journal of Physical Chemistry B*, **2019**, 123, 6474-6480	3.4	13
692	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
691	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
690	A Modern-Fortran Program for Chemical Kinetics on Top of Anharmonic Vibrational Calculations. *Lecture Notes in Computer Science*, **2019**, 401-412	0.9	3
689	Machine Learning of Potential-Energy Surfaces Within a Bond-Order Sampling Scheme. *Lecture Notes in Computer Science*, **2019**, 388-400	0.9	1
688	Mechanistic insights into metal ions transit through threefold ferritin channel. *Biochimica Et Biophysica Acta - General Subjects*, **2019**, 1863, 472-480	4	5
687	Tailor-made computational protocols for precise characterization of small biological building blocks using QM and MM approaches. *Biopolymers*, **2018**, 109, e23109	2.2	7
686	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	3.6	18
685	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	3.9	16
684	Exploiting coordination geometry to selectively predict the □donor and □acceptor abilities of ligands: a back-and-forth journey between electronic properties and spectroscopy. *Chemical Communications*, **2018**, 54, 2397-2400	5.8	20
683	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
682	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	2
681	Tuning dispersion correction in DFT-D2 for metal-molecule interactions: A tailored reparameterization strategy for the adsorption of aromatic systems on Ag(1 1 1). *Chemical Physics Letters*, **2018**, 693, 28-33	2.5	11
680	Computational simulation of vibrationally resolved spectra for spin-forbidden transitions. *Chirality*, **2018**, 30, 850-865	2.1	11
679	Solar collectors based on luminescent 2,5-diarylimidazoles. *Dyes and Pigments*, **2018**, 157, 334-341	4.6	7
678	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	3.3	42
677	Rotational and Infrared Spectroscopy of Ethanimine: A Route toward Its Astrophysical and Planetary Detection. *Astrophysical Journal*, **2018**, 855, 123	4.7	24

676	The Genealogical Tree of Ethanol: Gas-phase Formation of Glycolaldehyde, Acetic Acid, and Formic Acid. *Astrophysical Journal*, **2018**, 854, 135	4.7	71
675	Tyrosine absorption spectroscopy: Backbone protonation effects on the side chain electronic properties. *Journal of Computational Chemistry*, **2018**, 39, 1747-1756	3.5	10
674	Binding of Nucleic Acid Components to the Serpentinite-Hosted Hydrothermal Mineral Brucite. *Astrobiology*, **2018**, 18, 989-1007	3.7	15
673	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	3.2	7
672	Theory Meets Experiment for Noncovalent Complexes: The Puzzling Case of Pnicogen Interactions. *Angewandte Chemie - International Edition*, **2018**, 57, 13853-13857	16.4	48
671	The role of the multiconfigurational character of nitronyl-nitroxide in the singlet-triplet energy gap of its diradicals. *Physical Chemistry Chemical Physics*, **2018**, 20, 18547-18555	3.6	1
670	New atomistic model of pyrrole with improved liquid state properties and structure. *International Journal of Quantum Chemistry*, **2018**, 118, e25554	2.1	8
669	Force Field Parametrization of Metal Ions from Statistical Learning Techniques. *Journal of Chemical Theory and Computation*, **2018**, 14, 255-273	6.4	35
668	Effects of music playing on biological molecules. *MATEC Web of Conferences*, **2018**, 210, 05006	0.3	1
667	Towards the SMART workflow system for computational spectroscopy. *Physical Chemistry Chemical Physics*, **2018**, 20, 26034-26052	3.6	12
666	Comfort Index CI(bus): A methodology to measure the comfort on board. *Procedia Computer Science*, **2018**, 134, 439-444	1.6	3
665	Laboratory measurements and astronomical search for cyanomethanimine. *Astronomy and Astrophysics*, **2018**, 609,	5.1	24
664	Time-Dependent Formulation of Resonance Raman Optical Activity Spectroscopy. *Journal of Chemical Theory and Computation*, **2018**, 14, 6370-6390	6.4	20
663	Theory Meets Experiment for Noncovalent Complexes: The Puzzling Case of Pnicogen Interactions. *Angewandte Chemie*, **2018**, 130, 14049-14053	3.6	6
662	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
661	Unveiling the Sulfur–Sulfur Bridge: Accurate Structural and Energetic Characterization of a Homochalcogen Intermolecular Bond. *Angewandte Chemie*, **2018**, 130, 16048-16052	3.6	5
660	Extending the perturbed matrix method beyond the dipolar approximation: comparison of different levels of theory. *Physical Chemistry Chemical Physics*, **2018**, 20, 24369-24378	3.6	32
659	From ascorbic acid to furan derivatives: the gas phase acid catalyzed degradation of vitamin C. *Physical Chemistry Chemical Physics*, **2018**, 20, 17132-17140	3.6	9

658	Quantitative prediction and interpretation of spin energy gaps in polyradicals: the virtual magnetic balance. *Physical Chemistry Chemical Physics*, **2017**, 19, 9039-9044	3.6	3
657	The Borderline between Reactivity and Pre-reactivity of Binary Mixtures of Gaseous Carboxylic Acids and Alcohols. *Angewandte Chemie - International Edition*, **2017**, 56, 3872-3875	16.4	10
656	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
655	Fine-tuning of atomic point charges: Classical simulations of pyridine in different environments. *Chemical Physics Letters*, **2017**, 677, 120-126	2.5	13
654	A Modular Implementation for the Simulation of 1D and 2D Solid-State NMR Spectra of Quadrupolar Nuclei in the Virtual Multifrequency Spectrometer-Draw Graphical Interface. *Journal of Chemical Theory and Computation*, **2017**, 13, 2215-2229	6.4	17
653	Simulation of Vibronic Spectra of Flexible Systems: Hybrid DVR-Harmonic Approaches. *Journal of Chemical Theory and Computation*, **2017**, 13, 2804-2822	6.4	28
652	Development and Implementation of Advanced Fitting Methods for the Calculation of Accurate Molecular Structures. *Journal of Chemical Theory and Computation*, **2017**, 13, 3060-3075	6.4	32
651	Effective Inclusion of Mechanical and Electrical Anharmonicity in Excited Electronic States: VPT2-TDDFT Route. *Journal of Chemical Theory and Computation*, **2017**, 13, 2789-2803	6.4	18
650	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	3.5	29
649	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	6.4	8
648	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
647	Magnetic gaps in organic tri-radicals: From a simple model to accurate estimates. *Journal of Chemical Physics*, **2017**, 146, 104103	3.9	3
646	On the relation between carbonyl stretching frequencies and the donor power of chelating diphosphines in nickel dicarbonyl complexes. *Physical Chemistry Chemical Physics*, **2017**, 19, 9028-9038	3.6	18
645	Models of Aged Magnesium Silicate Hydrate Cements Based on the Lizardite and Talc Crystals: A Periodic DFT-GIPAW Investigation. *Journal of Physical Chemistry C*, **2017**, 121, 7319-7330	3.8	12
644	Computational study of the DPAP molecular rotor in various environments: from force field development to molecular dynamics simulations and spectroscopic calculations. *Physical Chemistry Chemical Physics*, **2017**, 19, 30590-30602	3.6	11
643	Encapsulating Iodine and Copper into Copper(I) Clusters Stabilized by Dichalcogenolate Ligands: Stability, Structure, and Optical Properties. *Inorganic Chemistry*, **2017**, 56, 14135-14146	5.1	9
642	General Approach to Coupled Reactive Smoluchowski Equations: Integration and Application of Discrete Variable Representation and Generalized Coordinate Methods to Diffusive Problems. *Journal of Chemical Theory and Computation*, **2017**, 13, 5900-5910	6.4	3
641	Correct Modeling of Cisplatin: a Paradigmatic Case. *Angewandte Chemie*, **2017**, 129, 14026-14029	3.6	

640	Correct Modeling of Cisplatin: a Paradigmatic Case. *Angewandte Chemie - International Edition*, **2017**, 56, 13838-13841	16.4	18
639	Flexible and Comprehensive Implementation of MD-PMM Approach in a General and Robust Code. *Journal of Chemical Theory and Computation*, **2017**, 13, 5506-5514	6.4	12
638	The Sivers asymmetry in Drell□an production at the J/□peak at COMPASS. *Physics Letters, Section B: Nuclear, Elementary Particle and High-Energy Physics*, **2017**, 770, 302-306	4.2	3
637	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
636	Spectroscopic Characterization of Key Aromatic Molecules: A Route toward The Origin of Life. *Astronomical Journal*, **2017**, 154,	4.9	9
635	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
634	Vibrational Density Matrix Renormalization Group. *Journal of Chemical Theory and Computation*, **2017**, 13, 3764-3777	6.4	31
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