Sebastian Ehlert

List of Publications by Year
in descending order

300 papers	111,326 citations	7069 78 h-index	261 299 g-index
312 all docs	312 docs citations	312 times ranked	65687 citing authors

#	Article	IF	Citations
1	Computerâ€aided simulation of infrared spectra of ethanol conformations in gas, liquid and in <scp>CCl₄</scp> solution. Journal of Computational Chemistry, 2022, 43, 279-288.	1.5	12
2	HFIPâ€Assisted Single Cå^'F Bond Activation of Trifluoromethyl Ketones using Visibleâ€Light Photoredox Catalysis. Angewandte Chemie - International Edition, 2022, 61, .	7.2	54
3	Increased Antiaromaticity through Pentalene Connection in [n]Cyclo-1,5-dibenzopentalenes. Organic Letters, 2022, 24, 983-988.	2.4	13
4	Frustrated Lewis pair catalyzed hydrodehalogenation of benzyl-halides. Chemical Communications, 2022, 58, 1175-1178.	2.2	11
5	Hydrocarbon Macrocycle Conformer Ensembles and ¹³Câ€NMR Spectra. Angewandte Chemie - International Edition, 2022, 61, .	7.2	10
6	Stereochemical Behavior of Pairs of Pâ€stereogenic Phosphanyl Groups at the Dimethylxanthene Backbone. Chemistry - A European Journal, 2022, , .	1.7	2
7	The long-awaited synthesis and self-assembly of a small rigid C₃-symmetric trilactam. Chemical Communications, 2022, 58, 3751-3754.	2.2	1
8	The State of Fortran. Computing in Science and Engineering, 2022, 24, 63-72.	1.2	9
9	Benchmark Study on the Calculation of ¹¹⁹Sn NMR Chemical Shifts. Inorganic Chemistry, 2022, 61, 3903-3917.	1.9	11
10	The Varied Frustrated Lewis Pair Reactivity of the Germylene Phosphaketene (CH{(CMe)(2,6â€ⁱPr₂C₆H₃N)}₂)GePCO. Chemistry - A European Journal, 2022, 28, .	1.7	5
11	Intermolecular Carbosilylation of Î±â€Olefins with C(sp3)â€“C(sp) Bond Formation Involving Siliumâ€Ion Regeneration. Angewandte Chemie - International Edition, 2022, , .	7.2	12
12	Dispersion corrected r2SCAN based global hybrid functionals: r2SCANh, r2SCAN0, and r2SCAN50. Journal of Chemical Physics, 2022, 156, 134105.	1.2	32
13	Quantum Chemistryâ€based Molecular Dynamics Simulations as a Tool for the Assignment of ESIâ€MS/MS Spectra of Drug Molecules. Chemistry - A European Journal, 2022, 28, .	1.7	8
14	The Nonâ€Ancillary Nature of Trimethylsilylamide Substituents in Boranes and Borinium Cations. Chemistry - A European Journal, 2022, 28, .	1.7	4
15	Quantum Chemical Calculation and Evaluation of Partition Coefficients for Classical and Emerging Environmentally Relevant Organic Compounds. Environmental Science & Technology, 2022, 56, 379-391.	4.6	18
16	Itâ€™s Complicated: On Relativistic Effects and Periodic Trends in the Melting and Boiling Points of the Group 11 Coinage Metals. Journal of the American Chemical Society, 2022, 144, 485-494.	6.6	6
17	Computational study of groundâ€state properties of Î¼ ₂ â€bridged group 14 porphyrinic sandwich complexes. Journal of Computational Chemistry, 2022, , .	1.5	1
18	Towards understanding solvation effects on the conformational entropy of non-rigid molecules. Physical Chemistry Chemical Physics, 2022, 24, 12249-12259.	1.3	15

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19	Automated Molecular Cluster Growing for Explicit Solvation by Efficient Force Field and Tight Binding Methods. Journal of Chemical Theory and Computation, 2022, 18, 3174-3189.	2.3	45
20	Conformational Energy Benchmark for Longer n-Alkane Chains. Journal of Physical Chemistry A, 2022, 126, 3521-3535.	1.1	16
21	The Role of Packing, Dispersion, Electrostatics, and Solvation in Highâ€Affinity Complexes of Cucurbit[n]urils with Uncharged Polar Guests. Chemistry - A European Journal, 2022, 28, .	1.7	15
22	Optimization of the r²SCAN-3c Composite Electronic-Structure Method for Use with Slater-Type Orbital Basis Sets. Journal of Physical Chemistry A, 2022, 126, 3826-3838.	1.1	8
23	Extended <scp>tightâ€binding</scp> quantum chemistry methods. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2021, 11, e1493.	6.2	596
24	Mechanistic Insights for Dimethyl Sulfoxide Catalyzed Aromatic Chlorination Reactions. ChemCatChem, 2021, 13, 207-211.	1.8	9
25	Quantification of Noncovalent Interactions in Azideâ€“Pnictogen, â€“Chalcogen, and â€“Halogen Contacts. Chemistry - A European Journal, 2021, 27, 4627-4639.	1.7	25
26	Sensory Perception of Nonâ€Deuterated and Deuterated Organic Compounds. Chemistry - A European Journal, 2021, 27, 1046-1056.	1.7	1
27	Theoretical study on conformational energies of transition metal complexes. Physical Chemistry Chemical Physics, 2021, 23, 287-299.	1.3	52
28	Oxidation Under Reductive Conditions: From Benzylic Ethers to Acetals with Perfect Atomâ€Economy by Titanocene(III) Catalysis. Angewandte Chemie - International Edition, 2021, 60, 5482-5488.	7.2	20
29	Oxidation Under Reductive Conditions: From Benzylic Ethers to Acetals with Perfect Atomâ€Economy by Titanocene(III) Catalysis. Angewandte Chemie, 2021, 133, 5542-5548.	1.6	10
30	Comprehensive Benchmark Study on the Calculation of ²⁹Si NMR Chemical Shifts. Inorganic Chemistry, 2021, 60, 272-285.	1.9	14
31	Calculation of absolute molecular entropies and heat capacities made simple. Chemical Science, 2021, 12, 6551-6568.	3.7	83
32	Benchmarking London dispersion corrected density functional theory for noncovalent ionâ€“ï€ interactions. Physical Chemistry Chemical Physics, 2021, 23, 11635-11648.	1.3	31
33	Lithium Dicyclohexylamide in Transition-Metal-Free Fischerâ€“Tropsch Chemistry. Journal of the American Chemical Society, 2021, 143, 634-638.	6.6	47
34	The power of trichlorosilylation: isolable trisilylated allyl anions, allyl radicals, and allenyl anions. Chemical Science, 2021, 12, 12419-12428.	3.7	4
35	Mechanistic Insights for Nitromethane Activation into Reactive Nitrogenating Reagents. ChemCatChem, 2021, 13, 2132-2137.	1.8	11
36	Oxâ€SLIM: Synthesis of and Siteâ€Specific Labelling with a Highly Hydrophilic Trityl Spin Label. Chemistry - A European Journal, 2021, 27, 5292-5297.	1.7	36

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37	Single-Point Hessian Calculations for Improved Vibrational Frequencies and Rigid-Rotor-Harmonic-Oscillator Thermodynamics. Journal of Chemical Theory and Computation, 2021, 17, 1701-1714.	2.3	49
38	r2SCAN-3c: A â€œSwiss army knifeâ€•composite electronic-structure method. Journal of Chemical Physics, 2021, 154, 064103.	1.2	290
39	r2SCAN-D4: Dispersion corrected meta-generalized gradient approximation for general chemical applications. Journal of Chemical Physics, 2021, 154, 061101.	1.2	70
40	Mechanistic Insights for Acidâ€catalyzed Rearrangement of Quinoxalinâ€2â€one with Diamine and Enamine. ChemCatChem, 2021, 13, 1503-1508.	1.8	5
41	Chiral Dibenzopentaleneâ€Based Conjugated Nanohoops through Stereoselective Synthesis. Angewandte Chemie, 2021, 133, 10775-10784.	1.6	9
42	Chiral Dibenzopentaleneâ€Based Conjugated Nanohoops through Stereoselective Synthesis. Angewandte Chemie - International Edition, 2021, 60, 10680-10689.	7.2	29
43	Efficient Quantum Chemical Calculation of Structure Ensembles and Free Energies for Nonrigid Molecules. Journal of Physical Chemistry A, 2021, 125, 4039-4054.	1.1	105
44	Perspective on Simplified Quantum Chemistry Methods for Excited States and Response Properties. Journal of Physical Chemistry A, 2021, 125, 3841-3851.	1.1	15
45	Comment on â€œThe Nature of Chalcogenâ€Bondingâ€Type Telluriumâ€“Nitrogen Interactionsâ€• Fixing the Description of Finiteâ€Temperature Effects Restores the Agreement Between Experiment and Theory. Angewandte Chemie, 2021, 133, 13252-13257.	1.6	4
46	Titanoceneâ€Catalyzed [2+2] Cycloaddition of Bisenones and Comparison with Photoredox Catalysis and Established Methods. Angewandte Chemie - International Edition, 2021, 60, 14339-14344.	7.2	14
47	Predicting the Mass Spectra of Environmental Pollutants Using Computational Chemistry: A Case Study and Critical Evaluation. Journal of the American Society for Mass Spectrometry, 2021, 32, 1508-1518.	1.2	7
48	Titanoceneâ€Catalyzed [2+2] Cycloaddition of Bisenones and Comparison with Photoredox Catalysis and Established Methods. Angewandte Chemie, 2021, 133, 14460-14465.	1.6	4
49	Comment on â€œThe Nature of Chalcogenâ€Bondingâ€Type Telluriumâ€“Nitrogen Interactionsâ€• Fixing the Description of Finiteâ€Temperature Effects Restores the Agreement Between Experiment and Theory. Angewandte Chemie - International Edition, 2021, 60, 13144-13149.	7.2	8
50	Efficient Quantum-Chemical Calculations of Acid Dissociation Constants from Free-Energy Relationships. Journal of Physical Chemistry A, 2021, 125, 5681-5692.	1.1	18
51	LiAlH 4 â€catalyzed Imine Hydrogenation with Dihydrogen: New DFT Mechanistic Insights. ChemCatChem, 2021, 13, 3401-3404.	1.8	9
52	Robust and Efficient Implicit Solvation Model for Fast Semiempirical Methods. Journal of Chemical Theory and Computation, 2021, 17, 4250-4261.	2.3	186
53	From QCEIMS to QCxMS: A Tool to Routinely Calculate CID Mass Spectra Using Molecular Dynamics. Journal of the American Society for Mass Spectrometry, 2021, 32, 1735-1751.	1.2	30
54	Facile Synthesis of Cyanide and Isocyanides from CO. Angewandte Chemie - International Edition, 2021, 60, 16965-16969.	7.2	15

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55	Frustrated Lewisâ€Pair Neighbors at the Xanthene Framework: Epimerization at Phosphorus and Cooperative Formation of Macrocyclic Adduct Structures. Chemistry - A European Journal, 2021, 27, 12104-12114.	1.7	2
56	Revisiting conformations of methyl lactate in water and methanol. Journal of Chemical Physics, 2021, 155, 024507.	1.2	16
57	[Cl@Si₂₀H₂₀]^{â^'}: Parent Siladodecahedrane with Endohedral Chloride Ion. Journal of the American Chemical Society, 2021, 143, 10865-10871.	6.6	20
58	A Primary Acyl Phosphine Stabilized by a Phosphonium Ylide. Angewandte Chemie, 2021, 133, 18695-18699.	1.6	1
59	A Primary Acyl Phosphine Stabilized by a Phosphonium Ylide. Angewandte Chemie - International Edition, 2021, 60, 18547-18551.	7.2	6
60	High-Throughput Non-targeted Chemical Structure Identification Using Gas-Phase Infrared Spectra. Analytical Chemistry, 2021, 93, 10688-10696.	3.2	4
61	Software for the frontiers of quantum chemistry: An overview of developments in the Q-Chem 5 package. Journal of Chemical Physics, 2021, 155, 084801.	1.2	518
62	PCM-ROKS for the Description of Charge-Transfer States in Solution: Singletâ€“Triplet Gaps with Chemical Accuracy from Open-Shell Kohnâ€“Sham Reaction-Field Calculations. Journal of Physical Chemistry Letters, 2021, 12, 8470-8480.	2.1	23
63	Reactions of a Dilithiomethane with CO and N₂O: An Avenue to an Anionic Ketene and a Hexafunctionalized Benzene. Angewandte Chemie, 2021, 133, 25485-25489.	1.6	5
64	Calculation of improved enthalpy and entropy of vaporization by a modified partition function in quantum cluster equilibrium theory. Journal of Chemical Physics, 2021, 155, 104101.	1.2	12
65	Reactions of a Dilithiomethane with CO and N₂O: An Avenue to an Anionic Ketene and a Hexafunctionalized Benzene. Angewandte Chemie - International Edition, 2021, 60, 25281-25285.	7.2	18
66	Assessing Density Functional Theory for Chemically Relevant Open-Shell Transition Metal Reactions. Journal of Chemical Theory and Computation, 2021, 17, 6134-6151.	2.3	75
67	Steric Influence on Reactions of Benzyl Potassium Species with CO. Chemistry - an Asian Journal, 2021, 16, 3640-3644.	1.7	7
68	All-Atom Quantum Mechanical Calculation of the Second-Harmonic Generation of Fluorescent Proteins. Journal of Physical Chemistry Letters, 2021, 12, 9684-9690.	2.1	5
69	Hydrogenation of Secondary Amides using Phosphane Oxide and Frustrated Lewis Pair Catalysis. Chemistry - A European Journal, 2021, 27, 14179-14183.	1.7	9
70	Hydrogen atom transfer rates from Tp-containing metal-hydrides to trityl radicals. Canadian Journal of Chemistry, 2021, 99, 216-220.	0.6	5
71	Selective Catalytic Frustrated Lewis Pair Hydrogenation of CO₂ in the Presence of Silylhalides. Angewandte Chemie - International Edition, 2021, 60, 25771-25775.	7.2	26
72	Supramolecular Nanopatterns of Molecular Spoked Wheels with Orthogonal Pillars: The Observation of a Fullerene Haze. Angewandte Chemie - International Edition, 2021, 60, 27264-27270.	7.2	4

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73	Automated Quantum Chemistry-Based Calculation of Optical Rotation for Large Flexible Molecules. Journal of Organic Chemistry, 2021, 86, 15522-15531.	1.7	18
74	Boron-Catalyzed Hydroarylation of 1,3-Dienes with Arylamines. Organic Letters, 2021, 23, 8952-8957.	2.4	13
75	Ligand Protonation at Carbon, not Nitrogen, during H₂ Production with Amine-Rich Iron Electrocatalysts. Inorganic Chemistry, 2021, 60, 17407-17413.	1.9	6
76	Nanoscale Ï€-conjugated ladders. Nature Communications, 2021, 12, 6614.	5.8	8
77	Quantum Chemistry Common Driver and Databases (QCDB) and Quantum Chemistry Engine (QCE<scp>ngine</scp>): Automation and interoperability among computational chemistry programs. Journal of Chemical Physics, 2021, 155, 204801.	1.2	15
78	Quickstart guide to model structures and interactions of artificial molecular muscles with efficient computational methods. Chemical Communications, 2021, 58, 258-261.	2.2	3
79	Designing a Solution-Stable Distannene: The Decisive Role of London Dispersion Effects in the Structure and Properties of {Sn(C₆H₂-2,4,6-Cy₃)₂}₂ (Cy = Cyclohexyl). Journal of the American Chemical Society, 2021, 143, 21478-21483.	6.6	17
80	Influencing the Selfâ€Sorting Behavior of [2.2]Paracyclophaneâ€Based Ligands by Introducing Isostructural Binding Motifs. Chemistry - A European Journal, 2020, 26, 3335-3347.	1.7	12
81	Heterobifunctional Rotaxanes for Asymmetric Catalysis. Angewandte Chemie, 2020, 132, 5140-5145.	1.6	18
82	Heterobifunctional Rotaxanes for Asymmetric Catalysis. Angewandte Chemie - International Edition, 2020, 59, 5102-5107.	7.2	56
83	Comprehensive Assessment of GFN Tight-Binding and Composite Density Functional Theory Methods for Calculating Gas-Phase Infrared Spectra. Journal of Chemical Theory and Computation, 2020, 16, 7044-7060.	2.3	32
84	Mechanistic Insights for Anilineâ€Catalyzed Halogenation Reactions. ChemCatChem, 2020, 12, 5369-5373.	1.8	5
85	Efficient Calculation of Small Molecule Binding in Metalâ€“Organic Frameworks and Porous Organic Cages. Journal of Physical Chemistry C, 2020, 124, 27529-27541.	1.5	32
86	A Unified Strategy for the Chemically Intuitive Interpretation of Molecular Optical Response Properties. Journal of Chemical Theory and Computation, 2020, 16, 7709-7720.	2.3	11
87	Benchmark Study of Electrochemical Redox Potentials Calculated with Semiempirical and DFT Methods. Journal of Physical Chemistry A, 2020, 124, 7166-7176.	1.1	45
88	Efficient Computation of Free Energy Contributions for Association Reactions of Large Molecules. Journal of Physical Chemistry Letters, 2020, 11, 6606-6611.	2.1	49
89	Modeling of spinâ€“spin distance distributions for nitroxide labeled biomacromolecules. Physical Chemistry Chemical Physics, 2020, 22, 24282-24290.	1.3	32
90	Mechanistic Insights for Iodane Mediated Aromatic Halogenation Reactions. ChemCatChem, 2020, 12, 6186-6190.	1.8	5

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91	Simplified time-dependent density functional theory (sTD-DFT) for molecular optical rotation. Journal of Chemical Physics, 2020, 153, 084116.	1.2	25
92	Robust Atomistic Modeling of Materials, Organometallic, and Biochemical Systems. Angewandte Chemie, 2020, 132, 15795-15803.	1.6	40
93	The first microsolvation step for furans: New experiments and benchmarking strategies. Journal of Chemical Physics, 2020, 152, 164303.	1.2	28
94	Building up Strain in One Step: Synthesis of an Edgeâ€Fused Double Silacyclobutene from an Extensively Trichlorosilylated Butadiene Dianion. Angewandte Chemie - International Edition, 2020, 59, 16181-16187.	7.2	6
95	BNB-Doped Phenalenyls: Modular Synthesis, Optoelectronic Properties, and One-Electron Reduction. Journal of the American Chemical Society, 2020, 142, 11072-11083.	6.6	63
96	Building up Strain in One Step: Synthesis of an Edgeâ€Fused Double Silacyclobutene from an Extensively Trichlorosilylated Butadiene Dianion. Angewandte Chemie, 2020, 132, 16315-16321.	1.6	2
97	Dynamic Structural Effects on the Second-Harmonic Generation of Tryptophane-Rich Peptides and Gramicidin A. Journal of Physical Chemistry B, 2020, 124, 2568-2578.	1.2	13
98	Extension and evaluation of the D4 London-dispersion model for periodic systems. Physical Chemistry Chemical Physics, 2020, 22, 8499-8512.	1.3	138
99	DFTB+, a software package for efficient approximate density functional theory based atomistic simulations. Journal of Chemical Physics, 2020, 152, 124101.	1.2	589
100	Fast and Accurate Quantum Chemical Modeling of Infrared Spectra of Condensed-Phase Systems. Journal of Physical Chemistry B, 2020, 124, 6664-6670.	1.2	18
101	RÃ¼cktitelbild: Heterobifunctional Rotaxanes for Asymmetric Catalysis (Angew. Chem. 13/2020). Angewandte Chemie, 2020, 132, 5446-5446.	1.6	0
102	Semiautomated Transition State Localization for Organometallic Complexes with Semiempirical Quantum Chemical Methods. Journal of Chemical Theory and Computation, 2020, 16, 2002-2012.	2.3	60
103	Quantum Chemical Calculation of Molecular and Periodic Peptide and Protein Structures. Journal of Physical Chemistry B, 2020, 124, 3636-3646.	1.2	33
104	Exploration of the Solid-State Sorption Properties of Shape-Persistent Macrocyclic Nanocarbons as Bulk Materials and Small Aggregates. Journal of the American Chemical Society, 2020, 142, 8763-8775.	6.6	86
105	Robust Atomistic Modeling of Materials, Organometallic, and Biochemical Systems. Angewandte Chemie - International Edition, 2020, 59, 15665-15673.	7.2	224
106	Frustrated Lewis Pair Catalyzed Reduction of Carbon Dioxide Using Hydroboranes: New DFT Mechanistic Insights. ChemCatChem, 2020, 12, 3656-3660.	1.8	14
107	Automated exploration of the low-energy chemical space with fast quantum chemical methods. Physical Chemistry Chemical Physics, 2020, 22, 7169-7192.	1.3	966
108	Extension of the element parameter set for ultra-fast excitation spectra calculation (sTDA-xTB). Molecular Physics, 2019, 117, 1104-1116.	0.8	4

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109	Isolation and Computational Studies of a Series of Terphenyl Substituted Diplumbynes with Ligand Dependent Leadâ€“Lead Multiple-Bonding Character. Journal of the American Chemical Society, 2019, 141, 14370-14383.	6.6	21
110	Pulsed EPR Dipolar Spectroscopy on Spin Pairs with one Highly Anisotropic Spin Center: The Lowâ€Spin Fe^{III} Case. Chemistry - A European Journal, 2019, 25, 14388-14398.	1.7	22
111	Are Fully Conjugated Expanded Indenofluorenes Analogues and Diindeno[n]thiophene Derivatives Diradicals? A Simplified (Spin-Flip) Time-Dependent Density Functional Theory [(SF-)sTD-DFT] Study. Journal of Physical Chemistry A, 2019, 123, 9828-9839.	1.1	5
112	Boron Lewis Acid-Catalyzed Regioselective Hydrothiolation of Conjugated Dienes with Thiols. ACS Catalysis, 2019, 9, 11627-11633.	5.5	25
113	Catalytic Difunctionalization of Unactivated Alkenes with Unreactive Hexamethyldisilane through Regeneration of Silylium Ions. Angewandte Chemie - International Edition, 2019, 58, 17307-17311.	7.2	26
114	Calculation of Electron Ionization Mass Spectra with Semiempirical GFNn-xTB Methods. ACS Omega, 2019, 4, 15120-15133.	1.6	33
115	Folding of unstructured peptoids and formation of hetero-bimetallic peptoid complexes upon side-chain-to-metal coordination. Chemical Science, 2019, 10, 620-632.	3.7	25
116	Synthesis of Î¼₂â€Oxoâ€Bridged Iron(III) Tetraphenylporphyrinâ€“Spacerâ€“Nitroxide Dimers and their Structural and Dynamics Characterization by using EPR and MD Simulations. Chemistry - A European Journal, 2019, 25, 2586-2596.	1.7	10
117	TEMPO-Mediated Catalysis of the Sterically Hindered Hydrogen Atom Transfer Reaction between (C₅Ph₅)Cr(CO)₃H and a Trityl Radical. Journal of the American Chemical Society, 2019, 141, 1882-1886.	6.6	25
118	A Simplified Spin-Flip Time-Dependent Density Functional Theory Approach for the Electronic Excitation Spectra of Very Large Diradicals. Journal of Physical Chemistry A, 2019, 123, 5815-5825.	1.1	17
119	Structure Optimisation of Large Transitionâ€Metal Complexes with Extended Tightâ€Binding Methods. Angewandte Chemie - International Edition, 2019, 58, 11078-11087.	7.2	72
120	Structure Optimisation of Large Transitionâ€Metal Complexes with Extended Tightâ€Binding Methods. Angewandte Chemie, 2019, 131, 11195-11204.	1.6	21
121	Structural and Conformational Studies on Carboxamides of 5,6-Diaminouracilsâ€”Precursors of Biologically Active Xanthine Derivatives. Molecules, 2019, 24, 2168.	1.7	2
122	Boraneâ€Catalyzed Hydrogenation of Tertiary Amides Activated by Oxalyl Chloride: DFT Mechanistic Insights. European Journal of Organic Chemistry, 2019, 2019, 4609-4612.	1.2	10
123	Exploring the chemical nature of super-heavy main-group elements by means of efficient plane-wave density-functional theory. Physical Chemistry Chemical Physics, 2019, 21, 18048-18058.	1.3	31
124	Pulsed EPR Dipolar Spectroscopy under the Breakdown of the Highâ€Field Approximation: The Highâ€Spin Iron(III) Case. Chemistry - A European Journal, 2019, 25, 8820-8828.	1.7	16
125	A generally applicable atomic-charge dependent London dispersion correction. Journal of Chemical Physics, 2019, 150, 154122.	1.2	697
126	Cooperative Organocatalysis: A Systematic Investigation of Covalently Linked Organophosphoric Acids for the Stereoselective Transfer Hydrogenation of Quinolines. European Journal of Organic Chemistry, 2019, 2019, 5190-5195.	1.2	8

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127	Nonlinear-response properties in a simplified time-dependent density functional theory (sTD-DFT) framework: Evaluation of excited-state absorption spectra. Journal of Chemical Physics, 2019, 150, 094112.	1.2	25
128	Fast Quantum Chemical Simulations of Infrared Spectra of Organic Compounds with the B97-3c Composite Method. Journal of Physical Chemistry A, 2019, 123, 3802-3808.	1.1	26
129	Exploration of Chemical Compound, Conformer, and Reaction Space with Meta-Dynamics Simulations Based on Tight-Binding Quantum Chemical Calculations. Journal of Chemical Theory and Computation, 2019, 15, 2847-2862.	2.3	551
130	The Chiral Trimer and a Metastable Chiral Dimer of Achiral Hexafluoroisopropanol: A Multiâ€Messenger Study. Angewandte Chemie, 2019, 131, 5134-5138.	1.6	20
131	GFN2-xTBâ€"An Accurate and Broadly Parametrized Self-Consistent Tight-Binding Quantum Chemical Method with Multipole Electrostatics and Density-Dependent Dispersion Contributions. Journal of Chemical Theory and Computation, 2019, 15, 1652-1671.	2.3	1,704
132	Reduction of Phosphine Oxide by Using Chlorination Reagents and Dihydrogen: DFT Mechanistic Insights. Chemistry - A European Journal, 2019, 25, 4670-4672.	1.7	16
133	The Chiral Trimer and a Metastable Chiral Dimer of Achiral Hexafluoroisopropanol: A Multiâ€Messenger Study. Angewandte Chemie - International Edition, 2019, 58, 5080-5084.	7.2	46
134	Understanding and Quantifying London Dispersion Effects in Organometallic Complexes. Accounts of Chemical Research, 2019, 52, 258-266.	7.6	117
135	Aggregation Behavior of a Sixâ€Membered Cyclic Frustrated Phosphane/Borane Lewis Pair: Formation of a Supramolecular Cyclooctameric Macrocyclic Ring System. Angewandte Chemie - International Edition, 2019, 58, 882-886.	7.2	29
136	Frustrated Lewis Pair Catalyzed Hydrogenation of Amides: Halides as Active Lewis Base in the Metal-Free Hydrogen Activation. Journal of the American Chemical Society, 2019, 141, 159-162.	6.6	70
137	Efficient structural and energetic screening of fullerene encapsulation in a large supramolecular double decker macrocycle. Journal of the Serbian Chemical Society, 2019, 84, 837-844.	0.4	12
138	Finding the best density functional approximation to describe interaction energies and structures of ionic liquids in molecular dynamics studies. Journal of Chemical Physics, 2018, 148, 193835.	1.2	38
139	Donorâ€"acceptor interactions between cyclic trinuclear pyridinate gold(<scp>i</scp>)-complexes and electron-poor guests: nature and energetics of guest-binding and templating on graphite. Chemical Science, 2018, 9, 3477-3483.	3.7	19
140	Solid state frustrated Lewis pair chemistry. Chemical Science, 2018, 9, 4859-4865.	3.7	35
141	B97-3c: A revised low-cost variant of the B97-D density functional method. Journal of Chemical Physics, 2018, 148, 064104.	1.2	400
142	The furan microsolvation blind challenge for quantum chemical methods: First steps. Journal of Chemical Physics, 2018, 148, 014301.	1.2	44
143	Comprehensive Thermochemical Benchmark Set of Realistic Closed-Shell Metal Organic Reactions. Journal of Chemical Theory and Computation, 2018, 14, 2596-2608.	2.3	202
144	Formation of macrocyclic ring systems by carbonylation of trifunctional P/B/B frustrated Lewis pairs. Chemical Science, 2018, 9, 1544-1550.	3.7	32

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145	Computational Chemistry: The Fate of Current Methods and Future Challenges. Angewandte Chemie - International Edition, 2018, 57, 4170-4176.	7.2	138
146	Raising the Bar in Aromatic Donorâ€“Acceptor Interactions with Cyclic Trinuclear Gold(I) Complexes as Strong Ï€-Donors. Journal of the American Chemical Society, 2018, 140, 17932-17944.	6.6	43
147	Electrophilic Phosphonium Cationâ€Mediated Phosphane Oxide Reduction Using Oxalyl Chloride and Hydrogen. Angewandte Chemie - International Edition, 2018, 57, 15253-15256.	7.2	37
148	Boraneâ€Catalyzed Synthesis of Quinolines Bearing Tetrasubstituted Stereocenters by Hydride Abstractionâ€Induced Electrocyclization. Chemistry - A European Journal, 2018, 24, 16287-16291.	1.7	50
149	Counterintuitive Interligand Angles in the Diaryls E{C₆H₃-2,6-(C₆H₂-2,4,6-ⁱPr₃)₂}<sub> (E = Ge, Sn, or Pb) and Related Species: The Role of London Dispersion Forces. Organometallics, 2018, 37, 2075-2085.	1.1	29
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