Henry F Schaefer

List of Publications by Year
in descending order

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1,011 papers	56,131 citations	1877 105 h-index	2688 199 g-index
1026 all docs	1026 docs citations	1026 times ranked	23892 citing authors

#	Article	IF	Citations
1	Fermi.jl: A Modern Design for Quantum Chemistry. Journal of Chemical Theory and Computation, 2022, 18, 677-686.	2.3	8
2	Substituent, Solvent, and Dispersion Effects on the Zwitterionic Character and Dimerization Thermochemistry of the Group 6 Fulvene Metal Tricarbonyl Complexes. Journal of Physical Chemistry A, 2022, 126, 365-372.	1.1	0
3	Hydrogen bonding as a probe of electron density Variations: Substituted pyridines. Chemical Physics Letters, 2022, 791, 139378.	1.2	3
4	A Cationic Magnesium-Based Dithiolene Radical. Organometallics, 2022, 41, 527-531.	1.1	0
5	An Undergraduate Chemistry Lab Exploring Computational Cost and Accuracy: Methane Combustion Energy. Journal of Chemical Education, 2022, 99, 1479-1487.	1.1	1
6	Acceleration Effect of Bases on Mn Pincer Complex-Catalyzed CO₂ Hydroboration. Inorganic Chemistry, 2022, 61, 3970-3980.	1.9	14
7	Mini-Review on Structureâ€“Reactivity Relationship for Aromatic Molecules: Recent Advances. ACS Omega, 2022, 7, 8199-8208.	1.6	2
8	Adiabatic Electron Detachment Energies, Reaction Barriers, Chemical Balance, and Ligand Effects on the Nucleophilicities of Metal Carbonyl Monoanions. Organometallics, 2022, 41, 1147-1157.	1.1	0
9	Phosphine-Mediated Cleavage of Sulfurâ€“Sulfur Bonds. Organometallics, 2022, 41, 3099-3103.	1.1	1
10	Automated theoretical chemical kinetics: Predicting the kinetics for the initial stages of pyrolysis. Proceedings of the Combustion Institute, 2021, 38, 375-384.	2.4	28
11	Reaction mechanisms of a cyclic ether intermediate: Ethyloxirane. International Journal of Chemical Kinetics, 2021, 53, 43-59.	1.0	20
12	Isomerâ€dependent reaction mechanisms of cyclic ether intermediates: cisâ€2,3â€dimethyloxirane and transâ€2,3â€dimethyloxirane. International Journal of Chemical Kinetics, 2021, 53, 127-145.	1.0	17
13	Coupled Cluster Externally Corrected by Adaptive Configuration Interaction. Journal of Chemical Theory and Computation, 2021, 17, 182-190.	2.3	11
14	The HOXâ‹¯SO₂ (X=F, Cl, Br, I) Binary Complexes: Implications for Atmospheric Chemistry. ChemPhysChem, 2021, 22, 112-126.	1.0	0
15	Fluorine Migration from Carbon to Iron and Fluorineâ€“Iron Dative Bonds in Octafluorocyclohexadiene Iron Carbonyl Chemistry. Organometallics, 2021, 40, 397-407.	1.1	2
16	Catalyzed reaction of isocyanates (RNCO) with water. Physical Chemistry Chemical Physics, 2021, 23, 18535-18546.	1.3	6
17	Heteroatom (N, P, As, Sb, Bi) Effects on the Resonance-Stabilized 2-, 3-, and 4-Picolyl Radicals. Inorganic Chemistry, 2021, 60, 5860-5867.	1.9	4
18	Arbitrary-Order Derivatives of Quantum Chemical Methods via Automatic Differentiation. Journal of Physical Chemistry Letters, 2021, 12, 3232-3239.	2.1	16

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19	A Reflection on Norman Louis Allinger. Journal of Chemical Theory and Computation, 2021, 17, 2013-2013.	2.3	1
20	Highly Strained Pn(CH)3 (Pn = N, P, As, Sb, Bi) Tetrahedranes: Theoretical Characterization. Journal of Physical Chemistry A, 2021, 125, 2612-2621.	1.1	2
21	Tris(Butadiene) Compounds versus Butadiene Oligomerization in Second-Row Transition Metal Chemistry: Effects of Increased Ligand Fields. Molecules, 2021, 26, 2220.	1.7	0
22	Carbonylic-Carbon-Centered Mechanism for Catalytic Î±-Methylation. Organometallics, 2021, 40, 2420-2429.	1.1	6
23	Synthesis of Methanesulfonic Acid Directly from Methane: The Cation Mechanism or the Radical Mechanism?. Journal of Physical Chemistry Letters, 2021, 12, 6486-6491.	2.1	2
24	Lanternâ€Type Divanadium Complexes with Bridging Ligands: Short Metalâ€Metal Bonds with High Multiple Bond Orders. ChemPhysChem, 2021, 22, 2014-2024.	1.0	4
25	Group 15 and 16 Nitreneâ€Like Pnictinidenes. Chemistry - A European Journal, 2021, 27, 14461-14471.	1.7	4
26	Carbeneâ€Stabilized Dithiolene (L 0) Zwitterions. Angewandte Chemie, 2021, 133, 22888.	1.6	0
27	Carbeneâ€Stabilized Dithiolene (L⁰) Zwitterions. Angewandte Chemie - International Edition, 2021, 60, 22706-22710.	7.2	6
28	Four isomers of In ₂ H ₂ : a careful comparison between theory and experiment. Molecular Physics, 2021, 119, .	0.8	5
29	Energetics and kinetics of various cyano radical hydrogen abstractions. Physical Chemistry Chemical Physics, 2021, 23, 3389-3400.	1.3	4
30	Carbene-mediated synthesis of a germanium tris(dithiolene)dianion. Chemical Communications, 2021, 57, 2543-2546.	2.2	3
31	Binuclear Cobalt Paddlewheel-Type Complexes: Relating Metalâ€“Metal Bond Lengths to Formal Bond Orders. Inorganic Chemistry, 2021, 60, 584-596.	1.9	4
32	Kinetic Stability of Pentazole. Journal of Physical Chemistry A, 2021, 125, 9092-9098.	1.1	5
33	Contrasting the Mechanism of H₂Activation by Monomeric and Potassiumâ€Stabilized Dimeric Al^IComplexes: Do Potassium Atoms Exert any Cooperative Effect?. Chemistry - A European Journal, 2021, 27, 17369-17378.	1.7	9
34	Cumulants as the Variables of Density Cumulant Theory: A Path to Hermitian Triples. Journal of Chemical Physics, 2021, 155, 244105.	1.2	0
35	Substituent Effects on Aluminyl Anions and Derived Systems: A High-Level Theory. Journal of Physical Chemistry A, 2021, 125, 10379-10391.	1.1	1
36	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

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37	Potential energy profile for the Cl + (H2O)3 â†' HCl + (H2O)2OH reaction. A CCSD(T) study. Physical Chemistry Chemical Physics, 2021, 23, 26837-26842.	1.3	2
38	Vibrational analysis of the ubiquitous interstellar molecule cyclopropenylidene (c-C₃H₂): the importance of numerical stability. Molecular Physics, 2020, 118, e1589007.	0.8	7
39	Is silver a mere terminal oxidant in palladium catalyzed Câ€“H bond activation reactions?. Chemical Science, 2020, 11, 208-216.	3.7	53
40	Sulfurous and sulfonic acids: Predicting the infrared spectrum and setting the surface straight. Journal of Chemical Physics, 2020, 152, 024302.	1.2	8
41	A Stable Naked Dithiolene Radical Anion and Synergic THF Ring-Opening. Journal of the American Chemical Society, 2020, 142, 17301-17305.	6.6	11
42	Agostic Hydrogens in 1â€Norbornyl Metal Cyclopentadienyl Structures. European Journal of Inorganic Chemistry, 2020, 2020, 4180-4188.	1.0	0
43	Dibridged, Monobridged, Vinylidene-Like, and Linear Structures for the Alkaline Earth Dihydrides Be₂H₂, Mg₂H₂, Ca₂H₂, Sr₂H₂, and Ba₂H₂. Proposals for Observations. Inorganic Chemistry, 2020, 59, 10404-10408.	1.9	3
44	Comparative Study of the Thermal Stabilities of the Experimentally Known High-Valent Fe(IV) Compounds Fe(1-norbornyl)4 and Fe(cyclohexyl)4. Journal of Physical Chemistry A, 2020, 124, 6867-6876.	1.1	2
45	High level ab initio investigation of the catalytic effect of water on formic acid decomposition and isomerization. Physical Chemistry Chemical Physics, 2020, 22, 25638-25651.	1.3	8
46	The atmospheric importance of methylamine additions to Criegee intermediates. Physical Chemistry Chemical Physics, 2020, 22, 22555-22566.	1.3	8
47	Reduced Density Matrix Cumulants: The Combinatorics of Size-Consistency and Generalized Normal Ordering. Journal of Chemical Theory and Computation, 2020, 16, 6150-6164.	2.3	11
48	Assessing the orbital-optimized unitary Ansatz for density cumulant theory. Journal of Chemical Physics, 2020, 153, 244102.	1.2	2
49	Carbeneâ€Stabilized Disilicon as a Siliconâ€Transfer Agent: Synthesis of a Dianionic Silicon Tris(dithiolene) Complex. Angewandte Chemie, 2020, 132, 8949-8952.	1.6	4
50	C5 Metalation of Imidazole-Based Monothiolates en Route to Selenothiolates. Organometallics, 2020, 39, 4178-4182.	1.1	2
51	P<scp>SI4</scp> 1.4: Open-source software for high-throughput quantum chemistry. Journal of Chemical Physics, 2020, 152, 184108.	1.2	440
52	Binding modes of cabazitaxel with the different human Î²-tubulin isotypes: DFT and MD studies. Journal of Molecular Modeling, 2020, 26, 162.	0.8	6
53	Unusual Structures of the Parent Molecules Diarsene, Distibene, and Dibismuthene: Toward Their Observation. Chemistry - A European Journal, 2020, 26, 14159-14166.	1.7	2
54	Unusual effects of the bulky 1-norbornyl group in cobalt carbonyl chemistry: low-energy structures with agostic hydrogen atoms. New Journal of Chemistry, 2020, 44, 8986-8995.	1.4	0

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55	Carbeneâ€Stabilized Disilicon as a Siliconâ€Transfer Agent: Synthesis of a Dianionic Silicon Tris(dithiolene) Complex. Angewandte Chemie - International Edition, 2020, 59, 8864-8867.	7.2	16
56	Reduction of Dinitrogen via 2,3â€²-Bipyridine-Mediated Tetraboration. Journal of the American Chemical Society, 2020, 142, 6244-6250.	6.6	35
57	Perfluoroolefin complexes versus perfluorometallacycles and perfluorocarbene complexes in cyclopentadienylcobalt chemistry. Physical Chemistry Chemical Physics, 2020, 22, 7616-7624.	1.3	2
58	Energetics and mechanisms for the acetonyl radical + O2 reaction: An important system for atmospheric and combustion chemistry. Journal of Chemical Physics, 2020, 152, 114301.	1.2	5
59	Increasing the Ligand Field Strength in Butadiene Open Sandwich Compounds from the First to the Second Row Transition Metals. ChemistrySelect, 2020, 5, 6350-6359.	0.7	0
60	Substituted Ortho-Benzynes: Properties of the Triple Bond. Journal of Organic Chemistry, 2020, 85, 9905-9914.	1.7	6
61	Conclusive determination of ethynyl radical hydrogen abstraction energetics and kinetics*. Molecular Physics, 2020, 118, e1769214.	0.8	7
62	Formation of Formic Acid Derivatives through Activation and Hydroboration of CO₂ by Low-Valent Group 14 (Si, Ge, Sn, Pb) Catalysts. Journal of Physical Chemistry A, 2020, 124, 1121-1133.	1.1	18
63	Assessing the Viability of the Methylsulfinyl Radicalâ€Ozone Reaction. ChemPhysChem, 2020, 21, 1289-1294.	1.0	1
64	The water trimer reaction OH + (H₂O)₃ â†' (H₂O)₂OH + H₂O. Physical Chemistry Chemical Physics, 2020, 22, 9767-9774.	1.3	2
65	A remarkable case of basis set dependence: the false convergence patterns of the methyl anion. Molecular Physics, 2019, 117, 1069-1077.	0.8	3
66	The addition of methanol to Criegee intermediates. Physical Chemistry Chemical Physics, 2019, 21, 17760-17771.	1.3	19
67	Unsaturation in binuclear iron carbonyl complexes of the split (3 + 2) fiveâ€electron donor hydrocarbon ligand bicyclo[3.2.1]octaâ€2,6â€dienâ€4â€yl: Role of agostic hydrogen atoms. International Journal of Quantum Chemistry, 2019, 119, e26010.	1.0	0
68	Janus: An Extensible Open-Source Software Package for Adaptive QM/MM Methods. Journal of Chemical Theory and Computation, 2019, 15, 4362-4373.	2.3	9
69	Dispersion Effects in Stabilizing Organometallic Compounds: Tetra-1-norbornyl Derivatives of the First-Row Transition Metals as Exceptional Examples. Journal of Physical Chemistry A, 2019, 123, 9514-9519.	1.1	11
70	Characterization of the 2-methylvinoxy radical + O2 reaction: A focal point analysis and composite multireference study. Journal of Chemical Physics, 2019, 151, 124302.	1.2	11
71	Unusual Î·¹â€Coordinated Alkyne and Alkene Complexes. Chemistry - A European Journal, 2019, 25, 15628-15633.	1.7	6
72	Ï€â€Hydrogen Bonding Probes Chemical Reactivity: Bromination of a CC Double Bond and Electrophilic Aromatic Benzylation. ChemistrySelect, 2019, 4, 10934-10942.	0.7	2

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73	Riddles of the structure and vibrational dynamics of HO3 resolved near the ab initio limit. Journal of Chemical Physics, 2019, 151, 094304.	1.2	11
74	PES-Learn: An Open-Source Software Package for the Automated Generation of Machine Learning Models of Molecular Potential Energy Surfaces. Journal of Chemical Theory and Computation, 2019, 15, 4386-4398.	2.3	51
75	Tris(butadiene) Metal Complexes of the First-Row Transition Metals versus Coupling of Butadiene to Eight- and Twelve-Carbon Hydrocarbon Chains. Journal of Physical Chemistry A, 2019, 123, 5542-5554.	1.1	4
76	Substituent effects on the aromaticity of benzeneâ€"An approach based on interaction coordinates. Journal of Chemical Physics, 2019, 150, 214108.	1.2	8
77	Lewis base-complexed magnesium dithiolenes. Chemical Communications, 2019, 55, 8087-8089.	2.2	9
78	tert-Butyl peroxy radical: ground and first excited state energetics and fundamental frequencies. Physical Chemistry Chemical Physics, 2019, 21, 9747-9758.	1.3	7
79	Convergent energies and anharmonic vibrational spectra of Ca₂H₂ and Ca₂H₄ constitutional isomers. Physical Chemistry Chemical Physics, 2019, 21, 10914-10922.	1.3	4
80	Designing new Togni reagents by computation. Chemical Communications, 2019, 55, 5667-5670.	2.2	12
81	Higher spin states in some low-energy bis(tetramethyl-1,2-diaza-3,5-diborolyl) sandwich compounds of the first row transition metals: boraza analogues of the metallocenes. New Journal of Chemistry, 2019, 43, 4497-4505.	1.4	1
82	Multi-fidelity Gaussian process modeling for chemical energy surfaces. Chemical Physics Letters: X, 2019, 737, 100022.	2.1	11
83	Ethyl + O₂ in Helium Nanodroplets: Infrared Spectroscopy of the Ethylperoxy Radical. Journal of Physical Chemistry A, 2019, 123, 3558-3568.	1.1	16
84	Alternative modes of bonding of C4F8 units in mononuclear and binuclear iron carbonyl complexes. New Journal of Chemistry, 2019, 43, 6932-6942.	1.4	2
85	Cyclobutyne: Minimum or Transition State?. Journal of Organic Chemistry, 2019, 84, 5548-5553.	1.7	3
86	Redox chemistry of an anionic dithiolene radical. Dalton Transactions, 2019, 48, 3543-3546.	1.6	12
87	Decomposition of the electronic activity in competing [5,6] and [6,6] cycloaddition reactions between C₆₀ and cyclopentadiene. Physical Chemistry Chemical Physics, 2019, 21, 5039-5048.	1.3	11
88	A comparison between hydrogen and halogen bonding: the hypohalous acidâ€"water dimers, HOXâ‹¯H₂O (X = F, Cl, Br). Physical Chemistry Chemical Physics, 2019, 21, 6160-6170.	1.3	28
89	Important features of the potential energy surface of the methylamine plus O(¹D) reaction. Physical Chemistry Chemical Physics, 2019, 21, 24194-24205.	1.3	3
90	Relatives of cyanomethylene: replacement of the divalent carbon by B^{â^'}, N⁺, Al^{â^'}, Si, P⁺, Ga^{â^'}, Ge, and As⁺. Physical Chemistry Chemical Physics, 2019, 21, 26438-26452.	1.3	3

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91	Labile Imidazolium Cyclopentadienides. Organometallics, 2019, 38, 4578-4584.	1.1	4
92	The Nature of Lithium Bonding in C₂H₂Li₂, C₆Li₆, and Lithium Halide Dimers. Organometallics, 2019, 38, 4708-4716.	1.1	1
93	The conformational preferences of polychlorocyclohexanes. New Journal of Chemistry, 2019, 43, 18546-18558.	1.4	2
94	Stabilizing Borinium Cations [Xâ€“Bâ€“X]⁺ through Conjugation and Hyperconjugation Effects. Inorganic Chemistry, 2019, 58, 243-249.	1.9	2
95	Ï€-Hydrogen Bonding Probes the Reactivity of Aromatic Compounds: Nitration of Substituted Benzenes. Journal of Physical Chemistry A, 2019, 123, 1069-1076.	1.1	7
96	Hydrogen Abstraction Reaction H2Se + OH â†' H2O + SeH: Comparison with the Analogous Hydrogen Sulfide and Water Reactions. Inorganic Chemistry, 2019, 58, 2069-2079.	1.9	2
97	The reaction of alkyl hydropersulfides (RSSH, R = CH₃ and ^tBu) with H₂S in the gas phase and in aqueous solution. Physical Chemistry Chemical Physics, 2019, 21, 537-545.	1.3	4
98	Re-examining ammonia addition to the Criegee intermediate: converging to chemical accuracy. Physical Chemistry Chemical Physics, 2018, 20, 7479-7491.	1.3	40
99	Carbonâ€“Hydrogen Activation in Zerovalent Bis(1,5-cyclooctadiene) Complexes of the First Row Transition Metals: A Theoretical Study. Journal of Physical Chemistry A, 2018, 122, 3280-3286.	1.1	1
100	The multichannel n-propyl + O2 reaction surface: Definitive theory on a model hydrocarbon oxidation mechanism. Journal of Chemical Physics, 2018, 148, .	1.2	14
101	Geometric Energy Derivatives at the Complete Basis Set Limit: Application to the Equilibrium Structure and Molecular Force Field of Formaldehyde. Journal of Chemical Theory and Computation, 2018, 14, 1333-1350.	2.3	41
102	Spinâ€“Orbit Coupling via Four-Component Multireference Methods: Benchmarking on p-Block Elements and Tentative Recommendations. Journal of Chemical Theory and Computation, 2018, 14, 1235-1246.	2.3	15
103	The Structure and Clâ€“O Dissociation Energy of the ClOO Radical: Finally, the Right Answers for the Right Reason. Journal of Physical Chemistry A, 2018, 122, 2604-2610.	1.1	5
104	CO₂ Reduction Pathways on MnBr(N-C)(CO)₃ Electrocatalysts. Organometallics, 2018, 37, 337-342.	1.1	20
105	Butadiene as a ligand in open sandwich compounds. Physical Chemistry Chemical Physics, 2018, 20, 5683-5691.	1.3	5
106	Alkali-Metal Trihalides: M+X3â€“Ion Pair or MXâ€“X2Complex?. Journal of Physical Chemistry B, 2018, 122, 3339-3353.	1.2	8
107	Conformers, properties, and docking mechanism of the anticancer drug docetaxel: DFT and molecular dynamics studies. Journal of Computational Chemistry, 2018, 39, 889-900.	1.5	10
108	Reinterpreting the infrared spectrum of H + HCN: Methylene amidogen radical and its coproducts. Journal of Chemical Physics, 2018, 148, 014305.	1.2	5

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109	Hyperconjugative effects in Ï€â€hydrogen bonding: Theory and experiment. Journal of Computational Chemistry, 2018, 39, 527-534.	1.5	6
110	1,3,2-Diazaborole-derived carbene complexes of boron. Dalton Transactions, 2018, 47, 41-44.	1.6	2
111	The non-covalently bound SOâ‹¯H₂O system, including an interpretation of the differences between SOâ‹¯H₂O and O₂â‹¯H₂O. Physical Chemistry Chemical Physics, 2018, 20, 28840-28847.	1.3	5
112	Mechanisms of the Ethynyl Radical Reaction with Molecular Oxygen. Journal of Physical Chemistry A, 2018, 122, 9498-9511.	1.1	4
113	Metalâ€“Metal (MM) Bond Distances and Bond Orders in Binuclear Metal Complexes of the First Row Transition Metals Titanium Through Zinc. Chemical Reviews, 2018, 118, 11626-11706.	23.0	106
114	Fundamental Vibrational Analyses of the HCN Monomer, Dimer and Associated Isotopologues. ChemPhysChem, 2018, 19, 3257-3265.	1.0	6
115	Reinterpretation of the electronic absorption spectrum of the methylene amidogen radical (H2CN). Journal of Chemical Physics, 2018, 149, 094302.	1.2	1
116	Noncovalent Interactions between Molecular Hydrogen and the Alkali Fluorides: Hâ€“HÂ·Â·Â·Fâ€“M (M = Li,) Tj ETQq0 0 0 rgBT /Overloc Computation, 2018, 14, 5118-5127.	2.3	3
117	P<scp>si</scp>4N<scp>um</scp>P<scp>y</scp>: An Interactive Quantum Chemistry Programming Environment for Reference Implementations and Rapid Development. Journal of Chemical Theory and Computation, 2018, 14, 3504-3511.	2.3	106
118	Stable Boron Dithiolene Radicals. Angewandte Chemie, 2018, 130, 7991-7994.	1.6	6
119	High-level theoretical characterization of the vinoxy radical (â€¢CH2CHO) + O2 reaction. Journal of Chemical Physics, 2018, 148, 184308.	1.2	18
120	Nucleophilic Influences and Origin of the S N 2 Allylic Effect. Chemistry - A European Journal, 2018, 24, 11637-11648.	1.7	17
121	Vibrational frequencies, structures, and energetics of the highly challenging alkali metal trifluorides MF3 (M = Li, Na, K, Rb, and Cs). Physical Chemistry Chemical Physics, 2018, 20, 18986-18994.	1.3	9
122	Quantitative Theoretical Predictions and Qualitative Bonding Analysis of the Divinylborinium System and Its Al, Ga, In, and Tl Congeners. Inorganic Chemistry, 2018, 57, 7851-7859.	1.9	3
123	Quantification of Aromaticity of Heterocyclic Systems Using Interaction Coordinates. Journal of Physical Chemistry A, 2018, 122, 6953-6960.	1.1	22
124	Prototypical Transition-Metal Carbenes, (CO)₅Crâ•CH₂, (CO)₄Feâ•CH₂, (CO)₃Niâ•CH₂, (CO)₅Moâ•CH₂, (CO)₄Ruâ•CH₂, (CO)₃Pdâ•CH₂, (CO)₅Wâ•CH₂, (CO)₄Osâ•CH₂, and (CO)₃Ptâ•CH₂: Challenge to Experiment. Journal of Physical Chemistry A, 2018, 122, 6570-6577.	1.1	3
125	Metalâ€“Substrate Cooperation Mechanism for Dehydrogenative Amidation Catalyzed by a PNN-Ru Catalyst. Inorganic Chemistry, 2018, 57, 8778-8787.	1.9	24
126	Student-Friendly Guide to Molecular Integrals. Journal of Chemical Education, 2018, 95, 1572-1578.	1.1	3

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127	Stable Boron Dithiolene Radicals. Angewandte Chemie - International Edition, 2018, 57, 7865-7868.	7.2	23
128	Using an iterative eigensolver and intertwined rank reduction to compute vibrational spectra of molecules with more than a dozen atoms: Uracil and naphthalene. Journal of Chemical Physics, 2018, 149, 064108.	1.2	28
129	Astrophysical sulfur in diffuse and dark clouds: The fundamental vibrational frequencies and spectroscopic constants of hydrogen sulfide cation (H2S+). Monthly Notices of the Royal Astronomical Society, 2018, 480, 3483-3490.	1.6	7
130	The bismuth tetramer Bi4: the Î½3 key to experimental observation. Physical Chemistry Chemical Physics, 2018, 20, 21881-21889.	1.3	3
131	Prediction and Characterization of Alkalineâ€Earth (M=Be, Mg, Ca, Sr, and Ba) Metallacyclopentadienes and Relevant Derivatives. ChemistrySelect, 2017, 2, 1442-1453.	0.7	7
132	Thioformaldehyde S-Sulfide, Sulfur Analogue of the Criegee Intermediate: Structures, Energetics, and Rovibrational Analysis. Journal of Physical Chemistry A, 2017, 121, 998-1006.	1.1	6
133	Structural Distortions Accompanying Noncovalent Interactions: Methaneâ€“Water, the Simplest Câ€“H Hydrogen Bond. Journal of Chemical Theory and Computation, 2017, 13, 1478-1485.	2.3	11
134	A Stable Anionic Dithiolene Radical. Journal of the American Chemical Society, 2017, 139, 6859-6862.	6.6	49
135	<scp>Psi4</scp> 1.1: An Open-Source Electronic Structure Program Emphasizing Automation, Advanced Libraries, and Interoperability. Journal of Chemical Theory and Computation, 2017, 13, 3185-3197.	2.3	961
136	Positional selectivity in the interaction of toluene with nitronium ion. Molecular Physics, 2017, 115, 2782-2788.	0.8	2
137	The fate of the tert-butyl radical in low-temperature autoignition reactions. Journal of Chemical Physics, 2017, 146, 194304.	1.2	17
138	The water dimer reaction OH + (H2O)2 â†' (H2O)â€“OH + H2O. Physical Chemistry Chemical Physics, 2017, 19, 18279-18287.	1.3	3
139	Ethylperoxy radical: approaching spectroscopic accuracy via coupled-cluster theory. Physical Chemistry Chemical Physics, 2017, 19, 15715-15723.	1.3	4
140	Structures of dimetallocenes M₂(C₅H₅)₂ (M = Zn, Cu,) Tj ETQq0 0 0 rgBT /Overloc	1.4	1
141	Metalâ€“metal bonding in biscycloheptatrienyl dimetal compounds of the secondâ€row transition metals. International Journal of Quantum Chemistry, 2017, 117, e25374.	1.0	0
142	Phosgene at the complete basis set limit of CCSDT(Q): Molecular structure and rovibrational analysis. Chemical Physics Letters, 2017, 683, 12-17.	1.2	4
143	Applying a Smolyak collocation method to Cl₂CO. Molecular Physics, 2017, 115, 1775-1785.	0.8	16
144	Enhanced Relative Stability of Metallabenzenes versus Metallocenes upon Ring Perfluorination: Nickel, Palladium, and Platinum Systems. European Journal of Inorganic Chemistry, 2017, 2017, 4714-4721.	1.0	1

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145	Facile Conversion of Bis-Silylene to Cyclic Silylene Isomers: Unexpected Câ€“N and Câ€“H Bond Cleavage. Journal of the American Chemical Society, 2017, 139, 16109-16112.	6.6	17
146	Câ€“HÂ·Â·Â·O Hydrogen Bonding. The Prototypical Methane-Formaldehyde System: A Critical Assessment. Journal of Chemical Theory and Computation, 2017, 13, 5379-5395.	2.3	17
147	Stabilizing a different cyclooctatetraene stereoisomer. Proceedings of the National Academy of Sciences of the United States of America, 2017, 114, 9803-9808.	3.3	26
148	Radicals derived from acetaldehyde and vinyl alcohol. Physical Chemistry Chemical Physics, 2017, 19, 27275-27287.	1.3	6
149	Fast construction of the exchange operator in an atom-centred basis with concentric atomic density fitting. Molecular Physics, 2017, 115, 2065-2076.	0.8	5
150	Quantification of Hydrogen Bond Strength Based on Interaction Coordinates: A New Approach. Journal of Physical Chemistry A, 2017, 121, 6090-6103.	1.1	31
151	Analytic Energy Gradients for Variational Two-Electron Reduced-Density-Matrix-Driven Complete Active Space Self-Consistent Field Theory. Journal of Chemical Theory and Computation, 2017, 13, 4113-4122.	2.3	14
152	Binuclear Cyclopentadienylmetal Methylene Sulfur Dioxide Complexes of Rhodium and Iridium Related to a Photochromic Metal Dithionite Complex. Inorganic Chemistry, 2017, 56, 14486-14493.	1.9	2
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