Henry F Schaefer

List of Publications by Year in Descending Order

1,004 papers	50,170 citations	103 h-index	188 g-index
1,026 ext. papers	52,901 ext. citations	4.6 avg, IF	7.41 L-index

#	Paper	IF	Citations
1004	Fermi.jl: A Modern Design for Quantum Chemistry.. *Journal of Chemical Theory and Computation*, **2022**,	6.4	3
1003	Hydrogen bonding as a probe of electron density Variations: Substituted pyridines. *Chemical Physics Letters*, **2022**, 791, 139378	2.5	1
1002	A Cationic Magnesium-Based Dithiolene Radical. *Organometallics*, **2022**, 41, 527-531	3.8	
1001	An Undergraduate Chemistry Lab Exploring Computational Cost and Accuracy: Methane Combustion Energy. *Journal of Chemical Education*, **2022**, 99, 1479-1487	2.4	
1000	Mini-Review on Structure-Reactivity Relationship for Aromatic Molecules: Recent Advances.. *ACS Omega*, **2022**, 7, 8199-8208	3.9	0
999	Cumulants as the variables of density cumulant theory: A path to Hermitian triples.. *Journal of Chemical Physics*, **2021**, 155, 244105	3.9	
998	Substituent Effects on Aluminyl Anions and Derived Systems: A High-Level Theory. *Journal of Physical Chemistry A*, **2021**, 125, 10379-10391	2.8	1
997	Quantum Chemistry Common Driver and Databases (QCDB) and Quantum Chemistry Engine (QCEngine): Automation and interoperability among computational chemistry programs. *Journal of Chemical Physics*, **2021**, 155, 204801	3.9	3
996	Potential energy profile for the Cl + (HO) -eHCl + (HO)OH reaction. A CCSD(T) study. *Physical Chemistry Chemical Physics*, **2021**, 23, 26837-26842	3.6	1
995	Kinetic Stability of Pentazole. *Journal of Physical Chemistry A*, **2021**, 125, 9092-9098	2.8	0
994	Contrasting the Mechanism of H Activation by Monomeric and Potassium-Stabilized Dimeric Al Complexes: Do Potassium Atoms Exert any Cooperative Effect?. *Chemistry - A European Journal*, **2021**, 27, 17369-17378	4.8	2
993	Binuclear Cobalt Paddlewheel-Type Complexes: Relating Metal-Metal Bond Lengths to Formal Bond Orders. *Inorganic Chemistry*, **2021**, 60, 584-596	5.1	2
992	Heteroatom (N, P, As, Sb, Bi) Effects on the Resonance-Stabilized 2-, 3-, and 4-Picolyl Radicals. *Inorganic Chemistry*, **2021**, 60, 5860-5867	5.1	1
991	Arbitrary-Order Derivatives of Quantum Chemical Methods via Automatic Differentiation. *Journal of Physical Chemistry Letters*, **2021**, 12, 3232-3239	6.4	8
990	Highly Strained Pn(CH) (Pn = N, P, As, Sb, Bi) Tetrahedranes: Theoretical Characterization. *Journal of Physical Chemistry A*, **2021**, 125, 2612-2621	2.8	1
989	Carbonylic-Carbon-Centered Mechanism for Catalytic Methylation. *Organometallics*, **2021**, 40, 2420-2429	3.8	2
988	Automated theoretical chemical kinetics: Predicting the kinetics for the initial stages of pyrolysis. *Proceedings of the Combustion Institute*, **2021**, 38, 375-384	5.9	7

987	Reaction mechanisms of a cyclic ether intermediate: Ethyloxirane. *International Journal of Chemical Kinetics*, **2021**, 53, 43-59	1.4	6
986	Isomer-dependent reaction mechanisms of cyclic ether intermediates:cis-2,3-dimethyloxirane andtrans-2,3-dimethyloxirane. *International Journal of Chemical Kinetics*, **2021**, 53, 127-145	1.4	6
985	Coupled Cluster Externally Corrected by Adaptive Configuration Interaction. *Journal of Chemical Theory and Computation*, **2021**, 17, 182-190	6.4	7
984	The HOX?SO (X=F, Cl, Br, I) Binary Complexes: Implications for Atmospheric Chemistry. *ChemPhysChem*, **2021**, 22, 112-126	3.2	
983	Fluorine Migration from Carbon to Iron and Fluorine□Iron Dative Bonds in Octafluorocyclohexadiene Iron Carbonyl Chemistry. *Organometallics*, **2021**, 40, 397-407	3.8	1
982	Catalyzed reaction of isocyanates (RNCO) with water. *Physical Chemistry Chemical Physics*, **2021**, 23, 18535-18546	3.6	1
981	Synthesis of Methanesulfonic Acid Directly from Methane: The Cation Mechanism or the Radical Mechanism?. *Journal of Physical Chemistry Letters*, **2021**, 12, 6486-6491	6.4	0
980	Lantern-Type Divanadium Complexes with Bridging Ligands: Short Metal-Metal Bonds with High Multiple Bond Orders. *ChemPhysChem*, **2021**, 22, 2014-2024	3.2	1
979	Group 15 and 16 Nitrene-Like Pnictinidenes. *Chemistry - A European Journal*, **2021**, 27, 14461-14471	4.8	1
978	Carbene-Stabilized Dithiolene (L0) Zwitterions. *Angewandte Chemie*, **2021**, 133, 22888	3.6	
977	Carbene-Stabilized Dithiolene (L) Zwitterions. *Angewandte Chemie - International Edition*, **2021**, 60, 22706-22710	16.1	3
976	Energetics and kinetics of various cyano radical hydrogen abstractions. *Physical Chemistry Chemical Physics*, **2021**, 23, 3389-3400	3.6	1
975	Carbene-mediated synthesis of a germanium tris(dithiolene)dianion. *Chemical Communications*, **2021**, 57, 2543-2546	5.8	2
974	Assessing the orbital-optimized unitary Ansatz for density cumulant theory. *Journal of Chemical Physics*, **2020**, 153, 244102	3.9	2
973	Carbene-Stabilized Disilicon as a Silicon-Transfer Agent: Synthesis of a Dianionic Silicon Tris(dithiolene) Complex. *Angewandte Chemie*, **2020**, 132, 8949-8952	3.6	2
972	C5 Metalation of Imidazole-Based Monothiolates en Route to Selenothiolates. *Organometallics*, **2020**, 39, 4178-4182	3.8	1
971	Psi4 1.4: Open-source software for high-throughput quantum chemistry. *Journal of Chemical Physics* , **2020**, 152, 184108	3.9	158
970	Binding modes of cabazitaxel with the different human □tubulin isotypes: DFT and MD studies. *Journal of Molecular Modeling*, **2020**, 26, 162	2	5

969	Unusual Structures of the Parent Molecules Diarsene, Distibene, and Dibismuthene: Toward Their Observation. *Chemistry - A European Journal*, **2020**, 26, 14159-14166	4.8	1
968	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	3.6	
967	Carbene-Stabilized Disilicon as a Silicon-Transfer Agent: Synthesis of a Dianionic Silicon Tris(dithiolene) Complex. *Angewandte Chemie - International Edition*, **2020**, 59, 8864-8867	16.4	10
966	Reduction of Dinitrogen via 2,3'-Bipyridine-Mediated Tetraboration. *Journal of the American Chemical Society*, **2020**, 142, 6244-6250	16.4	12
965	Perfluoroolefin complexes versus perfluorometallacycles and perfluorocarbene complexes in cyclopentadienylcobalt chemistry. *Physical Chemistry Chemical Physics*, **2020**, 22, 7616-7624	3.6	1
964	Energetics and mechanisms for the acetonyl radical + O reaction: An important system for atmospheric and combustion chemistry. *Journal of Chemical Physics*, **2020**, 152, 114301	3.9	4
963	Increasing the Ligand Field Strength in Butadiene Open Sandwich Compounds from the First to the Second Row Transition Metals. *ChemistrySelect*, **2020**, 5, 6350-6359	1.8	
962	Substituted -Benzynes: Properties of the Triple Bond. *Journal of Organic Chemistry*, **2020**, 85, 9905-9914	4.2	2
961	Conclusive determination of ethynyl radical hydrogen abstraction energetics and kinetics*. *Molecular Physics*, **2020**, 118, e1769214	1.7	5
960	Formation of Formic Acid Derivatives through Activation and Hydroboration of CO by Low-Valent Group 14 (Si, Ge, Sn, Pb) Catalysts. *Journal of Physical Chemistry A*, **2020**, 124, 1121-1133	2.8	10
959	Assessing the Viability of the Methylsulfinyl Radical-Ozone Reaction. *ChemPhysChem*, **2020**, 21, 1289-1294	3.2	1
958	Is silver a mere terminal oxidant in palladium catalyzed C-H bond activation reactions?. *Chemical Science*, **2020**, 11, 208-216	9.4	29
957	Sulfurous and sulfonic acids: Predicting the infrared spectrum and setting the surface straight. *Journal of Chemical Physics*, **2020**, 152, 024302	3.9	4
956	A Stable Naked Dithiolene Radical Anion and Synergic THF Ring-Opening. *Journal of the American Chemical Society*, **2020**, 142, 17301-17305	16.4	6
955	Agostic Hydrogens in 1-Norbornyl Metal Cyclopentadienyl Structures. *European Journal of Inorganic Chemistry*, **2020**, 2020, 4180-4188	2.3	
954	Dibridged, Monobridged, Vinylidene-Like, and Linear Structures for the Alkaline Earth Dihydrides BeH, MgH, CaH, SrH, and BaH. Proposals for Observations. *Inorganic Chemistry*, **2020**, 59, 10404-10408	5.1	2
953	Comparative Study of the Thermal Stabilities of the Experimentally Known High-Valent Fe(IV) Compounds Fe(1-norbornyl) and Fe(cyclohexyl). *Journal of Physical Chemistry A*, **2020**, 124, 6867-6876	2.8	2
952	High level investigation of the catalytic effect of water on formic acid decomposition and isomerization. *Physical Chemistry Chemical Physics*, **2020**, 22, 25638-25651	3.6	2

951	The atmospheric importance of methylamine additions to Criegee intermediates. *Physical Chemistry Chemical Physics*, **2020**, 22, 22555-22566	3.6	1
950	Reduced Density Matrix Cumulants: The Combinatorics of Size-Consistency and Generalized Normal Ordering. *Journal of Chemical Theory and Computation*, **2020**, 16, 6150-6164	6.4	6
949	Vibrational analysis of the ubiquitous interstellar molecule cyclopropenylidene (c-C3H2): the importance of numerical stability. *Molecular Physics*, **2020**, 118, e1589007	1.7	4
948	The water trimer reaction OH + (HO)-(HO)OH + HO. *Physical Chemistry Chemical Physics*, **2020**, 22, 9767-9774	3.6	0
947	Riddles of the structure and vibrational dynamics of HO resolved near the ab initio limit. *Journal of Chemical Physics*, **2019**, 151, 094304	3.9	8
946	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	6.4	26
945	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	2.8	2
944	Substituent effects on the aromaticity of benzene-An approach based on interaction coordinates. *Journal of Chemical Physics*, **2019**, 150, 214108	3.9	5
943	Lewis base-complexed magnesium dithiolenes. *Chemical Communications*, **2019**, 55, 8087-8089	5.8	9
942	tert-Butyl peroxy radical: ground and first excited state energetics and fundamental frequencies. *Physical Chemistry Chemical Physics*, **2019**, 21, 9747-9758	3.6	4
941	Convergent energies and anharmonic vibrational spectra of CaH and CaH constitutional isomers. *Physical Chemistry Chemical Physics*, **2019**, 21, 10914-10922	3.6	3
940	Designing new Togni reagents by computation. *Chemical Communications*, **2019**, 55, 5667-5670	5.8	7
939	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	3.6	1
938	Multi-fidelity Gaussian process modeling for chemical energy surfaces. *Chemical Physics Letters: X*, **2019**, 3, 100022	2	9
937	Ethyl + O in Helium Nanodroplets: Infrared Spectroscopy of the Ethylperoxy Radical. *Journal of Physical Chemistry A*, **2019**, 123, 3558-3568	2.8	12
936	Alternative modes of bonding of C4F8 units in mononuclear and binuclear iron carbonyl complexes. *New Journal of Chemistry*, **2019**, 43, 6932-6942	3.6	1
935	Cyclobutyne: Minimum or Transition State?. *Journal of Organic Chemistry*, **2019**, 84, 5548-5553	4.2	3
934	Redox chemistry of an anionic dithiolene radical. *Dalton Transactions*, **2019**, 48, 3543-3546	4.3	9

933	Decomposition of the electronic activity in competing [5,6] and [6,6] cycloaddition reactions between C and cyclopentadiene. *Physical Chemistry Chemical Physics*, **2019**, 21, 5039-5048	3.6	7
932	A remarkable case of basis set dependence: the false convergence patterns of the methyl anion** A contribution to the Special Issue in Memory of Professor Dieter Cremer.View all notes. *Molecular Physics*, **2019**, 117, 1069-1077	1.7	3
931	The addition of methanol to Criegee intermediates. *Physical Chemistry Chemical Physics*, **2019**, 21, 17760-17771	3.6	18
930	Unsaturation in binuclear iron carbonyl complexes of the split (3 + 2) five-electron donor hydrocarbon ligand bicyclo[3.2.1]octa-2,6-dien-4-yl: Role of agostic hydrogen atoms. *International Journal of Quantum Chemistry*, **2019**, 119, e26010	2.1	
929	Janus: An Extensible Open-Source Software Package for Adaptive QM/MM Methods. *Journal of Chemical Theory and Computation*, **2019**, 15, 4362-4373	6.4	4
928	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	2.8	6
927	Characterization of the 2-methylvinoxy radical + O reaction: A focal point analysis and composite multireference study. *Journal of Chemical Physics*, **2019**, 151, 124302	3.9	8
926	Unusual -Coordinated Alkyne and Alkene Complexes. *Chemistry - A European Journal*, **2019**, 25, 15628-15633	4.8	4
925	Hydrogen Bonding Probes Chemical Reactivity: Bromination of a CC Double Bond and Electrophilic Aromatic Benzylation. *ChemistrySelect*, **2019**, 4, 10934-10942	1.8	0
924	A comparison between hydrogen and halogen bonding: the hypohalous acid-water dimers, HOXHO (X = F, Cl, Br). *Physical Chemistry Chemical Physics*, **2019**, 21, 6160-6170	3.6	22
923	Important features of the potential energy surface of the methylamine plus O(D) reaction. *Physical Chemistry Chemical Physics*, **2019**, 21, 24194-24205	3.6	2
922	Relatives of cyanomethylene: replacement of the divalent carbon by B, N, Al, Si, P, Ga, Ge, and As. *Physical Chemistry Chemical Physics*, **2019**, 21, 26438-26452	3.6	2
921	Labile Imidazolium Cyclopentadienides. *Organometallics*, **2019**, 38, 4578-4584	3.8	4
920	The Nature of Lithium Bonding in C2H2Li2, C6Li6, and Lithium Halide Dimers. *Organometallics*, **2019**, 38, 4708-4716	3.8	0
919	The conformational preferences of polychlorocyclohexanes. *New Journal of Chemistry*, **2019**, 43, 18546-18558	3.3	1
918	Stabilizing Borinium Cations [X-B-X] through Conjugation and Hyperconjugation Effects. *Inorganic Chemistry*, **2019**, 58, 243-249	5.1	1
917	Hydrogen Bonding Probes the Reactivity of Aromatic Compounds: Nitration of Substituted Benzenes. *Journal of Physical Chemistry A*, **2019**, 123, 1069-1076	2.8	5
916	Hydrogen Abstraction Reaction HSe + OH HO + SeH: Comparison with the Analogous Hydrogen Sulfide and Water Reactions. *Inorganic Chemistry*, **2019**, 58, 2069-2079	5.1	1

915	The reaction of alkyl hydropersulfides (RSSH, R = CH and Bu) with HS in the gas phase and in aqueous solution. *Physical Chemistry Chemical Physics*, **2019**, 21, 537-545	3.6	2
914	Re-examining ammonia addition to the Criegee intermediate: converging to chemical accuracy. *Physical Chemistry Chemical Physics*, **2018**, 20, 7479-7491	3.6	28
913	Carbon-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	2.8	1
912	The multichannel n-propyl + O2 reaction surface: Definitive theory on a model hydrocarbon oxidation mechanism. *Journal of Chemical Physics*, **2018**, 148, 094303	3.9	11
911	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	6.4	25
910	Spin-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	6.4	6
909	The Structure and Cl-O Dissociation Energy of the ClOO Radical: Finally, the Right Answers for the Right Reason. *Journal of Physical Chemistry A*, **2018**, 122, 2604-2610	2.8	4
908	CO2 Reduction Pathways on MnBr(N-C)(CO)3 Electrocatalysts. *Organometallics*, **2018**, 37, 337-342	3.8	16
907	Butadiene as a ligand in open sandwich compounds. *Physical Chemistry Chemical Physics*, **2018**, 20, 5683-5691	3.6	3
906	Alkali-Metal Trihalides: MX Ion Pair or MX-X Complex?. *Journal of Physical Chemistry B*, **2018**, 122, 3339-3353	3.4	5
905	Conformers, properties, and docking mechanism of the anticancer drug docetaxel: DFT and molecular dynamics studies. *Journal of Computational Chemistry*, **2018**, 39, 889-900	3.5	8
904	Reinterpreting the infrared spectrum of H + HCN: Methylene amidogen radical and its coproducts. *Journal of Chemical Physics*, **2018**, 148, 014305	3.9	5
903	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	5.1	1
902	Quantification of Aromaticity of Heterocyclic Systems Using Interaction Coordinates. *Journal of Physical Chemistry A*, **2018**, 122, 6953-6960	2.8	16
901	Prototypical Transition-Metal Carbenes, (CO)Cr?CH, (CO)Fe?CH, (CO)Ni?CH, (CO)Mo?CH, (CO)Ru?CH, (CO)Pd?CH, (CO)W?CH, (CO)Os?CH, and (CO)Pt?CH: Challenge to Experiment. *Journal of Physical Chemistry A*, **2018**, 122, 6570-6577	2.8	2
900	Metal-Substrate Cooperation Mechanism for Dehydrogenative Amidation Catalyzed by a PNN-Ru Catalyst. *Inorganic Chemistry*, **2018**, 57, 8778-8787	5.1	15
899	Student-Friendly Guide to Molecular Integrals. *Journal of Chemical Education*, **2018**, 95, 1572-1578	2.4	0
898	Stable Boron Dithiolene Radicals. *Angewandte Chemie - International Edition*, **2018**, 57, 7865-7868	16.4	17

897	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	3.9	20
896	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	4.3	5
895	The bismuth tetramer Bi: the key to experimental observation. *Physical Chemistry Chemical Physics*, **2018**, 20, 21881-21889	3.6	2
894	Hyperconjugative effects in hydrogen bonding: Theory and experiment. *Journal of Computational Chemistry*, **2018**, 39, 527-534	3.5	4
893	The non-covalently bound SOHO system, including an interpretation of the differences between SOHO and OHO. *Physical Chemistry Chemical Physics*, **2018**, 20, 28840-28847	3.6	3
892	Mechanisms of the Ethynyl Radical Reaction with Molecular Oxygen. *Journal of Physical Chemistry A* , **2018**, 122, 9498-9511	2.8	4
891	Metal-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	68.1	69
890	Fundamental Vibrational Analyses of the HCN Monomer, Dimer and Associated Isotopologues. *ChemPhysChem*, **2018**, 19, 3257	3.2	3
889	Reinterpretation of the electronic absorption spectrum of the methylene amidogen radical (HCN). *Journal of Chemical Physics*, **2018**, 149, 094302	3.9	1
888	Noncovalent Interactions between Molecular Hydrogen and the Alkali Fluorides: H-H F-M (M = Li, Na, K, Rb, Cs). High Level Theoretical Predictions and SAPT Analysis. *Journal of Chemical Theory and Computation*, **2018**, 14, 5118-5127	6.4	1
887	Psi4NumPy: An Interactive Quantum Chemistry Programming Environment for Reference Implementations and Rapid Development. *Journal of Chemical Theory and Computation*, **2018**, 14, 3504-3511	6.4	72
886	Stable Boron Dithiolene Radicals. *Angewandte Chemie*, **2018**, 130, 7991-7994	3.6	5
885	High-level theoretical characterization of the vinoxy radical (CHCHO) + O reaction. *Journal of Chemical Physics*, **2018**, 148, 184308	3.9	14
884	Nucleophilic Influences and Origin of the S 2 Allylic Effect. *Chemistry - A European Journal*, **2018**, 24, 11637811648	4.8	11
883	Vibrational frequencies, structures, and energetics of the highly challenging alkali metal trifluorides MF (M = Li, Na, K, Rb, and Cs). *Physical Chemistry Chemical Physics*, **2018**, 20, 18986-18994	3.6	7
882	Prediction and Characterization of Alkaline-Earth (M=Be, Mg, Ca, Sr, and Ba) Metallacyclopentadienes and Relevant Derivatives. *ChemistrySelect*, **2017**, 2, 1442-1453	1.8	7
881	Thioformaldehyde S-Sulfide, Sulfur Analogue of the Criegee Intermediate: Structures, Energetics, and Rovibrational Analysis. *Journal of Physical Chemistry A*, **2017**, 121, 998-1006	2.8	4
880	Structural Distortions Accompanying Noncovalent Interactions: Methane-Water, the Simplest C-H Hydrogen Bond. *Journal of Chemical Theory and Computation*, **2017**, 13, 1478-1485	6.4	9

879	A Stable Anionic Dithiolene Radical. *Journal of the American Chemical Society*, **2017**, 139, 6859-6862	16.4	35
878	Psi4 1.1: An Open-Source Electronic Structure Program Emphasizing Automation, Advanced Libraries, and Interoperability. *Journal of Chemical Theory and Computation*, **2017**, 13, 3185-3197	6.4	733
877	Positional selectivity in the interaction of toluene with nitronium ion. *Molecular Physics*, **2017**, 115, 2782-2788	1.7	2
876	The fate of the tert-butyl radical in low-temperature autoignition reactions. *Journal of Chemical Physics*, **2017**, 146, 194304	3.9	9
875	The water dimer reaction OH + (HO) -e(HO)-OH + HO. *Physical Chemistry Chemical Physics*, **2017**, 19, 18279-18287	3.6	3
874	Ethylperoxy radical: approaching spectroscopic accuracy via coupled-cluster theory. *Physical Chemistry Chemical Physics*, **2017**, 19, 15715-15723	3.6	3
873	Structures of dimetallocenes M2(C5H5)2 (M = Zn, Cu, Ni, Co, Fe) and their perfluorinated derivatives. *New Journal of Chemistry*, **2017**, 41, 5924-5933	3.6	1
872	Metal□metal bonding in biscycloheptatrienyl dimetal compounds of the second-row transition metals. *International Journal of Quantum Chemistry*, **2017**, 117, e25374	2.1	
871	Phosgene at the complete basis set limit of CCSDT(Q): Molecular structure and rovibrational analysis. *Chemical Physics Letters*, **2017**, 683, 12-17	2.5	4
870	Applying a Smolyak collocation method to Cl2CO. *Molecular Physics*, **2017**, 115, 1775-1785	1.7	13
869	Enhanced Relative Stability of Metallabenzenes versus Metallocenes upon Ring Perfluorination: Nickel, Palladium, and Platinum Systems. *European Journal of Inorganic Chemistry*, **2017**, 2017, 4714-4721	2.3	1
868	Facile Conversion of Bis-Silylene to Cyclic Silylene Isomers: Unexpected C-N and C-H Bond Cleavage. *Journal of the American Chemical Society*, **2017**, 139, 16109-16112	16.4	14
867	C-H□O Hydrogen Bonding. The Prototypical Methane-Formaldehyde System: A Critical Assessment. *Journal of Chemical Theory and Computation*, **2017**, 13, 5379-5395	6.4	14
866	Stabilizing a different cyclooctatetraene stereoisomer. *Proceedings of the National Academy of Sciences of the United States of America*, **2017**, 114, 9803-9808	11.5	17
865	Radicals derived from acetaldehyde and vinyl alcohol. *Physical Chemistry Chemical Physics*, **2017**, 19, 27275-27287	3.6	4
864	Fast construction of the exchange operator in an atom-centred basis with concentric atomic density fitting. *Molecular Physics*, **2017**, 115, 2065-2076	1.7	5
863	Quantification of Hydrogen Bond Strength Based on Interaction Coordinates: A New Approach. *Journal of Physical Chemistry A*, **2017**, 121, 6090-6103	2.8	23
862	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	6.4	11

861	Binuclear Cyclopentadienylmetal Methylene Sulfur Dioxide Complexes of Rhodium and Iridium Related to a Photochromic Metal Dithionite Complex. *Inorganic Chemistry*, **2017**, 56, 14486-14493	5.1	2
860	A Twist of the Twist Mechanism, 2-Iodoxybenzoic Acid (IBX)-Mediated Oxidation of Alcohol Revisited: Theory and Experiment. *Organic Letters*, **2017**, 19, 6502-6505	6.2	29
859	The Hydrogen Abstraction Reaction HS + OH -dHO + SH: Convergent Quantum Mechanical Predictions. *Journal of Physical Chemistry A*, **2017**, 121, 9136-9145	2.8	8
858	1,3,2-Diazaborole-derived carbene complexes of boron. *Dalton Transactions*, **2017**, 47, 41-44	4.3	2
857	The Reaction between Bromine and the Water Dimer and the Highly Exothermic Reverse Reaction. *Journal of Computational Chemistry*, **2016**, 37, 177-82	3.5	3
856	CO reduction with Re(i)-NHC compounds: driving selective catalysis with a silicon nanowire photoelectrode. *Chemical Communications*, **2016**, 52, 14258-14261	5.8	27
855	Mn-NHC Electrocatalysts: Increasing Acidity Lowers the Reduction Potential and Increases the Turnover Frequency for CO Reduction. *Inorganic Chemistry*, **2016**, 55, 9509-9512	5.1	45
854	The methylsulfinyl radical CH3SO examined. *Physical Chemistry Chemical Physics*, **2016**, 18, 22293-9	3.6	12
853	Binuclear iron carbonyl complexes of thialene. *RSC Advances*, **2016**, 6, 82661-82668	3.7	4
852	Effect of metal complexation on the equilibrium between methylphosphepine and methylphosphanorcaradiene and their benzo analogues. *New Journal of Chemistry*, **2016**, 40, 7804-7813	3.6	
851	Electrophilic Aromatic Substitution: New Insights into an Old Class of Reactions. *Accounts of Chemical Research*, **2016**, 49, 1191-9	24.3	88
850	Toward unsaturated stannylenes Y2ZSn: and related compounds with triplet electronic ground states. *RSC Advances*, **2016**, 6, 53749-53759	3.7	3
849	Reductive coupling of carbon monoxide to glycolaldehyde and hydroxypyruvaldehyde polyanions in binuclear cyclopentadienyl lanthanum and lutetium derivatives: analogies to cyclooctatetraene thorium chemistry. *Theoretical Chemistry Accounts*, **2016**, 135, 1	1.9	1
848	Chlorine peroxide (Cl2O2) and its isomers: structures, spectroscopy, formation and thermochemistry. *Molecular Physics*, **2016**, 114, 1135-1147	1.7	6
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