Willem Klopper

List of Publications by Year
in descending order

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310 papers	23,269 citations	12303 69 h-index	9311 143 g-index
334 all docs	334 docs citations	334 times ranked	12381 citing authors

#	Article	IF	Citations
1	Basis-set convergence of correlated calculations on water. Journal of Chemical Physics, 1997, 106, 9639-9646.	1.2	2,197
2	Basis-set convergence in correlated calculations on Ne, N2, and H2O. Chemical Physics Letters, 1998, 286, 243-252.	1.2	1,989
3	The <scp>D</scp>alton quantum chemistry program system. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2014, 4, 269-284.	6.2	1,166
4	Turbomole. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2014, 4, 91-100.	6.2	867
5	Basis-set convergence of the energy in molecular Hartreeâ€“Fock calculations. Chemical Physics Letters, 1999, 302, 437-446.	1.2	604
6	Optimized accurate auxiliary basis sets for RI-MP2 and RI-CC2 calculations for the atoms Rb to Rn. Theoretical Chemistry Accounts, 2007, 117, 587-597.	0.5	577
7	Wave functions with terms linear in the interelectronic coordinates to take care of the correlation cusp. I. General theory. Journal of Chemical Physics, 1991, 94, 1985-2001.	1.2	544
8	Explicitly Correlated Electrons in Molecules. Chemical Reviews, 2012, 112, 4-74.	23.0	487
9	R12 methods in explicitly correlated molecular electronic structure theory. International Reviews in Physical Chemistry, 2006, 25, 427-468.	0.9	384
10	Basis set convergence of the interaction energy of hydrogen-bonded complexes. Journal of Chemical Physics, 1999, 111, 9157-9167.	1.2	363
11	Explicitly correlated second-order MÃ¸llerâ€“Plesset methods with auxiliary basis sets. Journal of Chemical Physics, 2002, 116, 6397-6410.	1.2	315
12	Synthesis, Structure, and Characterization of Dinuclear Copper(I) Halide Complexes with P^N Ligands Featuring Exciting Photoluminescence Properties. Inorganic Chemistry, 2013, 52, 2292-2305.	1.9	311
13	MÃ¸ller-plesset calculations taking care of the correlation CUSP. Chemical Physics Letters, 1987, 134, 17-22.	1.2	275
14	Computational determination of equilibrium geometry and dissociation energy of the water dimer. Physical Chemistry Chemical Physics, 2000, 2, 2227-2234.	1.3	249
15	Quintuple-Î¶ quality coupled-cluster correlation energies with triple-Î¶ basis sets. Physical Chemistry Chemical Physics, 2007, 9, 1921-1930.	1.3	244
16	CC-R12, a correlation cusp corrected coupled-cluster method with a pilot application to the Be2 potential curve. Chemical Physics Letters, 1992, 199, 497-504.	1.2	234
17	Basis-set extrapolation techniques for the accurate calculation of molecular equilibrium geometries using coupled-cluster theory. Journal of Chemical Physics, 2006, 125, 044108.	1.2	233
18	New correlation factors for explicitly correlated electronic wave functions. Journal of Chemical Physics, 2005, 123, 074101.	1.2	231

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19	Accuracy of atomization energies and reaction enthalpies in standard and extrapolated electronic wave function/basis set calculations. Journal of Chemical Physics, 2000, 112, 9229-9242.	1.2	224
20	Quantitative quantum chemistry. Molecular Physics, 2008, 106, 2107-2143.	0.8	215
21	Highly accurate calculations of molecular electronic structure. Journal of Physics B: Atomic, Molecular and Optical Physics, 1999, 32, R103-R130.	0.6	214
22	Highly accurate coupled-cluster singlet and triplet pair energies from explicitly correlated calculations in comparison with extrapolation techniques. Molecular Physics, 2001, 99, 481-507.	0.8	209
23	A priori calculation of molecular properties to chemical accuracy. Journal of Physical Organic Chemistry, 2004, 17, 913-933.	0.9	204
24	On the Interaction of Dihydrogen with Aromatic Systemsâ€. Journal of Physical Chemistry A, 2004, 108, 3019-3023.	1.1	181
25	Ab initio Study of the Interactions between CO₂ and Nâ€Containing Organic Heterocycles. ChemPhysChem, 2009, 10, 374-383.	1.0	180
26	Coupled-cluster theory with simplified linear-r12 corrections: The CCSD(R12) model. Journal of Chemical Physics, 2005, 122, 084107.	1.2	167
27	Magnetically Induced Current Densities in Aromatic, Antiaromatic, Homoaromatic, and Nonaromatic Hydrocarbons. Journal of Physical Chemistry A, 2009, 113, 8668-8676.	1.1	164
28	HF dimer: Empirically refined analytical potential energy and dipole hypersurfaces from ab initio calculations. Journal of Chemical Physics, 1998, 108, 10096-10115.	1.2	157
29	Wave functions with terms linear in the interelectronic coordinates to take care of the correlation cusp. II. Secondâ€order Mo/llerâ€“Plesset (MP2â€R12) calculations on closedâ€shell atoms. Journal of Chemical Physics, 1991, 94, 2002-2019.	1.2	156
30	Limiting values for Mo/llerâ€“Plesset secondâ€order correlation energies of polyatomic systems: A benchmark study on Ne, HF, H2O, N2, and He...He. Journal of Chemical Physics, 1995, 102, 6168-6179.	1.2	149
31	Self-consistent treatment of spinâ€“orbit interactions with efficient Hartreeâ€“Fock and density functional methods. Physical Chemistry Chemical Physics, 2008, 10, 1748.	1.3	145
32	Orbital-invariant formulation of the MP2-R12 method. Chemical Physics Letters, 1991, 186, 583-585.	1.2	143
33	Wave functions with terms linear in the interelectronic coordinates to take care of the correlation cusp. III. Secondâ€order Mo/llerâ€“Plesset (MP2â€R12) calculations on molecules of first row atoms. Journal of Chemical Physics, 1991, 94, 2020-2030.	1.2	136
34	An ab initio derived torsional potential energy surface for (H2O)3. II. Benchmark studies and interaction energies. Journal of Chemical Physics, 1995, 103, 1085-1098.	1.2	128
35	MP2-R12 calculations on the relative stability of carbocations. The Journal of Physical Chemistry, 1990, 94, 5625-5630.	2.9	126
36	Anatomy of relativistic energy corrections in light molecular systems. Molecular Physics, 2001, 99, 1769-1794.	0.8	123

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37	A diagonal orbital-invariant explicitly-correlated coupled-cluster method. Chemical Physics Letters, 2008, 452, 326-332.	1.2	118
38	Potential energy surface of the H+3 ground state in the neighborhood of the minimum with microhartree accuracy and vibrational frequencies derived from it. Journal of Chemical Physics, 1994, 101, 2231-2243.	1.2	114
39	Basis-set convergence of the molecular electric dipole moment. Journal of Chemical Physics, 1999, 111, 4424-4430.	1.2	114
40	Gaussian basis sets and the nuclear cusp problem. Computational and Theoretical Chemistry, 1986, 135, 339-356.	1.5	108
41	Synthesis and Properties ofpara-Substituted NCN-Pincer Palladium and Platinum Complexes. Chemistry - A European Journal, 2004, 10, 1331-1344.	1.7	108
42	CH5+: The story goes on. An explicitly correlated coupled-cluster study. Journal of Chemical Physics, 1997, 106, 1863-1869.	1.2	107
43	Accurate Benchmark Calculation of the Reaction Barrier Height for Hydrogen Abstraction by the Hydroperoxyl Radical from Methane. Implications for C_nH_{2n+2} where n = 2 â† 4. Journal of Physical Chemistry A, 2008, 112, 7047-7054.	1.1	105
44	Strong Nâ^'HÂ·Â·Â·Ï€ Hydrogen Bonding in Amideâ^'Benzene Interactions. Journal of Physical Chemistry B, 2009, 113, 2937-2943.	1.2	105
45	An explicitly correlated coupled cluster calculation of the heliumâ€“helium interatomic potential. Journal of Chemical Physics, 1995, 103, 6127-6132.	1.2	103
46	Synthesis of a Pentasilapropellane. Exploring the Nature of a Stretched Siliconâ^'Silicon Bond in a Nonclassical Molecule. Journal of the American Chemical Society, 2010, 132, 10264-10265.	6.6	99
47	The MP2â€F12 method in the T<scp>URBOMOLE</scp> program package. Journal of Computational Chemistry, 2011, 32, 2492-2513.	1.5	98
48	Lowâ€lying stationary points and torsional interconversions of cyclic (H2O)4: An ab initio study. Journal of Chemical Physics, 1995, 103, 6114-6126.	1.2	97
49	Basis Set Limit CCSD(T) Harmonic Vibrational Frequencies. Journal of Physical Chemistry A, 2007, 111, 11242-11248.	1.1	92
50	Atomization energies from coupled-cluster calculations augmented with explicitly-correlated perturbation theory. Chemical Physics, 2009, 356, 14-24.	0.9	92
51	The MP2 limit correction applied to coupled cluster calculations of the electronic dissociation energies of the hydrogen fluoride and water dimers. Molecular Physics, 1999, 96, 559-570.	0.8	89
52	Basis Set Limit Coupled Cluster Study of H-Bonded Systems and Assessment of More Approximate Methods. Journal of Physical Chemistry A, 2007, 111, 11122-11133.	1.1	87
53	Ab initio computations close to the oneâ€particle basis set limit on the weakly bound van der Waals complexes benzeneâ€“neon and benzeneâ€“argon. Journal of Chemical Physics, 1994, 101, 9747-9754.	1.2	86
54	A new ab initio based six-dimensional semi-empirical pair interaction potential for HF. Chemical Physics Letters, 1996, 261, 35-44.	1.2	86

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55	Multiple basis sets in calculations of triples corrections in coupled-cluster theory. Theoretical Chemistry Accounts, 1997, 97, 164-176.	0.5	82
56	Electron correlation: The many-body problem at the heart of chemistry. Journal of Computational Chemistry, 2007, 28, 1307-1320.	1.5	82
57	Robust fitting techniques in the chain of spheres approximation to the Fock exchange: The role of the complementary space. Journal of Chemical Physics, 2013, 139, 094111.	1.2	82
58	Snapshots of the Alï£¿Al Ïƒâ€Bond Formation Starting from {AlR₂} Units: Experimental and Computational Observations. Angewandte Chemie - International Edition, 2009, 48, 8141-8145.	7.2	81
59	Towards the oneâ€particle basis set limit of secondâ€order correlation energies: MP2â€R12 calculations on small Ben and Mgn clusters (n=1â€“4). Journal of Chemical Physics, 1993, 99, 5167-5177.	1.2	80
60	Simple recipe for implementing computation of first-order relativistic corrections to electron correlation energies in framework of direct perturbation theory. Journal of Computational Chemistry, 1997, 18, 20-27.	1.5	80
61	Scope and limitations of the SCS-MP2 method for stacking and hydrogen bonding interactions. Physical Chemistry Chemical Physics, 2008, 10, 2758.	1.3	80
62	Accuracy of spectroscopic constants of diatomic molecules from ab initio calculations. Journal of Chemical Physics, 2003, 118, 2539.	1.2	77
63	Switchable Openâ€Cage Fullerene for Water Encapsulation. Angewandte Chemie - International Edition, 2010, 49, 9935-9938.	7.2	77
64	CID and CEPA calculations with linear r12 terms. Chemical Physics Letters, 1991, 178, 455-461.	1.2	76
65	Assessment of basis sets for F12 explicitly-correlated molecular electronic-structure methods. Molecular Physics, 2009, 107, 963-975.	0.8	76
66	Implementation of the Betheâ€'Salpeter equation in the TURBOMOLE program. Journal of Computational Chemistry, 2017, 38, 383-388.	1.5	76
67	Accuracy Assessment of GW Starting Points for Calculating Molecular Excitation Energies Using the Betheâ€“Salpeter Formalism. Journal of Chemical Theory and Computation, 2018, 14, 2127-2136.	2.3	74
68	The barrier to linearity of water. Journal of Chemical Physics, 1999, 110, 11971-11981.	1.2	73
69	Expanding the Coordination Cage: A Ruthenium(II)â€'Polypyridine Complex Exhibiting High Quantum Yields under Ambient Conditions. Inorganic Chemistry, 2009, 48, 5677-5684.	1.9	73
70	A comparison of linear and nonlinear correlation factors for basis set limit MÃ¸ller-Plesset second order binding energies and structures of He2, Be2, and Ne2. Journal of Chemical Physics, 2006, 125, 094302.	1.2	72
71	Experimental and Theoretical Study of Novel Luminescent Di-, Tri-, and Tetranuclear Copper Triazole Complexes. Organometallics, 2011, 30, 3275-3283.	1.1	70
72	Coupled-cluster reference values for the GW27 and GW100 test sets for the assessment of GW methods. Molecular Physics, 2015, 113, 1952-1960.	0.8	70

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73	Towards the accurate computation of properties of transition metal compounds: the binding energy of ferrocene. Chemical Physics Letters, 1996, 262, 546-552.	1.2	69
74	The accuracy of atomization energies from explicitly correlated coupled-cluster calculations. Journal of Chemical Physics, 2001, 115, 2022-2032.	1.2	69
75	Inclusion of the (T) triples correction into the linear-r12 corrected coupled-cluster model CCSD(R12). International Journal of Quantum Chemistry, 2006, 106, 2306-2317.	1.0	69
76	ortho-Perfluoroalkylation and Ethoxycarbonyldifluoromethylation of Aromatic Triazenes. Journal of Organic Chemistry, 2013, 78, 7938-7948.	1.7	68
77	An ab initio derived torsional potential energy surface for (H2O)3. I. Analytical representation and stationary points. Journal of Chemical Physics, 1995, 103, 1077-1084.	1.2	67
78	The performance of the explicitly correlated coupled cluster method. I. The fourâ€electron systems Be, Liâ^, and LiH. Journal of Chemical Physics, 1995, 103, 309-320.	1.2	67
79	Assessment of various density functionals and basis sets for the calculation of molecular anharmonic force fields. International Journal of Quantum Chemistry, 2005, 104, 830-845.	1.0	67
80	Molecular Hydrogen Interaction with IRMOF-1:â€‰ A Multiscale Theoretical Study. Journal of Physical Chemistry C, 2007, 111, 13635-13640.	1.5	67
81	Nucleobaseâ€“Fluorobenzene Interactions: Hydrogen Bonding Wins over Ï€ Stacking. Angewandte Chemie - International Edition, 2007, 46, 7449-7452.	7.2	66
82	Basis-set extensions for two-component spinâ€“orbit treatments of heavy elements. Physical Chemistry Chemical Physics, 2006, 8, 4862-4865.	1.3	65
83	Cleavage of the N2 Triple Bond by the Ti Dimer: A Route to Molecular Materials for Dinitrogen Activation?. Angewandte Chemie - International Edition, 2006, 45, 2799-2802.	7.2	64
84	Accurate computational thermochemistry from explicitly correlated coupled-cluster theory. Theoretical Chemistry Accounts, 2010, 126, 289-304.	0.5	64
85	Coupled-cluster and explicitly correlated perturbation-theory calculations of the uracil anion. Journal of Chemical Physics, 2007, 126, 085101.	1.2	63
86	Experimental and Theoretical Determination of Dissociation Energies of Dispersion-Dominated Aromatic Molecular Complexes. Chemical Reviews, 2016, 116, 5614-5641.	23.0	62
87	para-Functionalized NCN-Pincer Palladium(II) Complexes: Synthesis, Catalysis and DFT Calculations. European Journal of Inorganic Chemistry, 2003, 2003, 830-838.	1.0	60
88	Equilibrium inversion barrier of NH3from extrapolated coupled-cluster pair energies. Journal of Computational Chemistry, 2001, 22, 1306-1314.	1.5	59
89	Anharmonic force fields and thermodynamic functions using density functional theory. Molecular Physics, 2005, 103, 863-876.	0.8	59
90	Exploring the Boundary between Aromatic and Olefinic Character:â€‰ Bad News for Second-Order Perturbation Theory and Density Functional Schemes. Journal of the American Chemical Society, 1996, 118, 3519-3520.	6.6	57

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91	Anharmonic force field, vibrational energies, and barrier to inversion of SiH3â^'. Journal of Chemical Physics, 2000, 112, 4053-4063.	1.2	57
92	A hybrid scheme for the resolution-of-the-identity approximation in second-order MÃ¸llerâ€“Plesset linear-r12 perturbation theory. Journal of Chemical Physics, 2004, 120, 10890-10895.	1.2	57
93	Oriented Circular Dichroism Analysis of Chiral Surfaceâ€Anchored Metalâ€“Organic Frameworks Grown by Liquidâ€Phase Epitaxy and upon Loading with Chiral Guest Compounds. Chemistry - A European Journal, 2014, 20, 9879-9882.	1.7	57
94	Computation of some new two-electron Gaussian integrals. Theoretica Chimica Acta, 1992, 83, 441-453.	0.9	54
95	Configuration interaction calculations with terms linear in the interelectronic coordinate for the ground state of H+3. A benchmark study. Journal of Chemical Physics, 1993, 99, 8830-8839.	1.2	53
96	Two-dimensional model treatment of torsional motions in the water trimer. Chemical Physics Letters, 1995, 237, 536-544.	1.2	53
97	Pentagerma[1.1.1]propellane: A Combined Experimental and Quantum Chemical Study on the Nature of the Interactions between the Bridgehead Atoms. Angewandte Chemie - International Edition, 2009, 48, 1411-1416.	7.2	49
98	The Formal Combination of Three Singlet Biradicaloid Entities to a Singlet Hexaradicaloid Metalloid Ge₁₄[Si(SiMe₃)₃]₅[Li(THF)₂]₃ Cluster. Journal of the American Chemical Society, 2011, 133, 2518-2524.	6.6	49
99	Ab initio calculation of proton barrier and binding energy of the (H2O)OHâ^' complex. Computational and Theoretical Chemistry, 2002, 586, 201-208.	1.5	48
100	Coupled-cluster response theory with linear-r12 corrections: The CC2-R12 model for excitation energies. Journal of Chemical Physics, 2006, 124, 044112.	1.2	48
101	Ab Initio Study of the Adsorption of Small Molecules on Metalâ€“Organic Frameworks with Oxo-centered Trimetallic Building Units: The Role of the Undercoordinated Metal Ion. Inorganic Chemistry, 2015, 54, 8251-8263.	1.9	48
102	Ionized, electron-attached, and excited states of molecular systems with spinâ€“orbit coupling: Two-component GW and Betheâ€“Salpeter implementations. Journal of Chemical Physics, 2019, 150, 204116.	1.2	48
103	A critical note on extrapolated helium pair potentials. Journal of Chemical Physics, 2001, 115, 761-765.	1.2	46
104	New accurate reference energies for the G2/97 test set. Journal of Chemical Physics, 2012, 136, 164102.	1.2	46
105	An accurate, global,ab initiopotential energy surface for the H⁺₃molecule. Molecular Physics, 2000, 98, 261-273.	0.8	44
106	Parity-violating interaction in H2O2 calculated from density-functional theory. Chemical Physics Letters, 2002, 354, 274-282.	1.2	44
107	The furan microsolvation blind challenge for quantum chemical methods: First steps. Journal of Chemical Physics, 2018, 148, 014301.	1.2	44
108	18-Crown-6 Coordinated Metal Halides with Bright Luminescence and Nonlinear Optical Effects. Journal of the American Chemical Society, 2021, 143, 798-804.	6.6	44

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109	Explicitly correlated coupled cluster calculations of the dissociation energies and barriers to concerted hydrogen exchange of (HF)n oligomers (n = 2,3,4,5). Molecular Physics, 1998, 94, 105-119.	0.8	44
110	High-level ab initio computations of structures and relative energies of two isomers of the CO2 trimer. Journal of Chemical Physics, 1999, 111, 3846-3854.	1.2	43
111	Second-order MÃ¸ller-Plesset perturbation theory with terms linear in the interelectronic coordinates and exact evaluation of three-electron integrals. Theoretical Chemistry Accounts, 2002, 107, 173-179.	0.5	42
112	Spin flipping in ring-coupled-cluster-doubles theory. Chemical Physics Letters, 2011, 510, 147-153.	1.2	42
113	Accurate Quantum-Chemical Prediction of Enthalpies of Formation of Small Molecules in the Gas Phase. ChemPhysChem, 2003, 4, 32-48.	1.0	41
114	Ridge-Tile-like Chiral Topology: Synthesis, Resolution, and Complete Chiroptical Characterization of Enantiomers of Edge-Sharing Binuclear Square Planar Complexes of Ni(II) Bearing Achiral Ligands. Journal of the American Chemical Society, 2010, 132, 10477-10483.	6.6	41
115	Chemical accuracy from â€˜Coulomb holeâ€™ extrapolated molecular quantum-mechanical calculations. Journal of Molecular Structure, 2001, 567-568, 375-384.	1.8	40
116	Photoelectron spectrum of valence anions of uracil and first-principles calculations of excess electron binding energies. Journal of Chemical Physics, 2008, 129, 054309.	1.2	40
117	Explicitly Correlated Coupled-Cluster Theory. Challenges and Advances in Computational Chemistry and Physics, 2010, , 535-572.	0.6	40
118	Global Analytical Potential Energy Surface for Large Amplitude Nuclear Motions in Ammoniaâ€. Journal of Physical Chemistry B, 2005, 109, 8439-8451.	1.2	39
119	Open-shell explicitly correlated F12 methods. Molecular Physics, 2010, 108, 315-325.	0.8	39
120	Basis-set convergence of the two-electron Darwin term. Chemical Physics Letters, 2000, 319, 287-295.	1.2	38
121	Computation of two-electron Gaussian integrals for wave functions including the correlation factor r12exp(â^'Î³r122). Computer Physics Communications, 2002, 149, 1-10.	3.0	38
122	Solid C58 films. Physical Chemistry Chemical Physics, 2005, 7, 2816.	1.3	38
123	Slater-type geminals in explicitly-correlated perturbation theory: application to n-alkanols and analysis of errors and basis-set requirements. Physical Chemistry Chemical Physics, 2008, 10, 3390.	1.3	38
124	Quasirelativistic two-component core excitations and polarisabilities from a damped-response formulation of the Betheâ€“Salpeter equation. Molecular Physics, 2020, 118, e1755064.	0.8	38
125	Extensions of r12 corrections to CC2-R12 for excited states. Journal of Chemical Physics, 2006, 125, 064111.	1.2	37
126	Accurate ab initio computation of thermochemical data for C3Hx species. Chemical Physics, 2008, 346, 56-68.	0.9	37

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127	Automated incremental scheme for explicitly correlated methods. Journal of Chemical Physics, 2010, 132, 164114.	1.2	37
128	Intrinsic fluorescence properties of rhodamine cations in gas-phase: triplet lifetimes and dispersed fluorescence spectra. Physical Chemistry Chemical Physics, 2013, 15, 8162.	1.3	37
129	Sub-meV accuracy in first-principles computations of the ionization potentials and electron affinities of the atoms H to Ne. Physical Review A, 2010, 81, .	1.0	35
130	An improved ab initio relativistic zeroth-order regular approximation correct to order 1/c2. Journal of Chemical Physics, 2000, 113, 9957-9965.	1.2	34
131	Tuning the Gap: Electronic Properties and Radical-Type Reactivities of Heteronuclear [1.1.1]Propellanes of Heavier Group 14 Elements. Organometallics, 2011, 30, 1419-1428.	1.1	34
132	Basis set limit value for the static dipole polarizability of beryllium. Chemical Physics Letters, 1997, 269, 435-440.	1.2	33
133	Accurate molecular geometries of the protonated water dimer. Physical Chemistry Chemical Physics, 2000, 2, 2235-2238.	1.3	33
134	Calculation of Magnetically Induced Currents in Hydrocarbon Nanorings. Journal of Physical Chemistry A, 2008, 112, 13584-13592.	1.1	33
135	The barrier to linearity of hydrogen sulphide. Chemical Physics Letters, 2000, 322, 119-128.	1.2	32
136	Direct perturbation theory of magnetic properties and relativistic corrections for the point nuclear and Gaussian nuclear models. Journal of Chemical Physics, 2001, 115, 7356-7363.	1.2	32
137	Low-lying absorption and emission spectra of pyrene, 1,6-dithiapyrene, and tetrathiafulvalene: A comparison between ab initio and time-dependent density functional methods. Journal of Chemical Physics, 2009, 131, 224315.	1.2	32
138	[2.2]Paracyclophanediyldiphosphane Complexes of Gold. European Journal of Inorganic Chemistry, 2012, 2012, 5033-5042.	1.0	32
139	Non-covalent Interactions of CO₂ with Functional Groups of Metalâ€“Organic Frameworks from a CCSD(T) Scheme Applicable to Large Systems. Journal of Chemical Theory and Computation, 2015, 11, 1574-1584.	2.3	32
140	Explicitly correlated coupled cluster calculations of the dissociation energies and barriers to concerted hydrogen exchange of (HF)n oligomers (n=2,3,4,5). Molecular Physics, 1998, 94, 105-119.	0.8	31
141	Ab Initio Modeling of Methanol Interaction with Single-Walled Carbon Nanotubes. Journal of Physical Chemistry C, 2007, 111, 18917-18926.	1.5	31
142	Heating a bowl of single-molecule-soup: structure and desorption energetics of water-encapsulated open-cage [60] fullerenoid anions in the gas-phase. Physical Chemistry Chemical Physics, 2011, 13, 9818.	1.3	31
143	Effects of counterpoise correction and basis set extrapolation on the MP2 geometries of hydrogen bonded dimers of ammonia, water, and hydrogen fluoride. Physical Chemistry Chemical Physics, 2011, 13, 1230-1238.	1.3	31
144	Theoretical reference values for the AE6 and BH6 test sets from explicitly correlated coupled-cluster theory. Theoretical Chemistry Accounts, 2012, 131, 1.	0.5	31

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145	Extrapolation to the limit of a complete basis set for electronic structure calculations on the N 2 molecule. Theoretical Chemistry Accounts, 1998, 99, 265-271.	0.5	30
146	Accurate computational determination of the binding energy of the SO3â˜™H2O complex. Journal of Chemical Physics, 2006, 125, 054312.	1.2	30
147	Efficient evaluation of three-centre two-electron integrals over London orbitals. Molecular Physics, 2020, 118, e1736675.	0.8	30
148	A closed-shell coupled-cluster treatment of the Breitâ€“Pauli first-order relativistic energy correction. Journal of Chemical Physics, 2004, 121, 6591-6598.	1.2	29
149	Second-order electron-correlation and self-consistent spin-orbit treatment of heavy molecules at the basis-set limit. Journal of Chemical Physics, 2010, 132, 094108.	1.2	29
150	Accurate atomization energies from combining coupled-cluster computations with interference-corrected explicitly correlated second-order perturbation theory. Theoretical Chemistry Accounts, 2014, 133, 1.	0.5	29
151	Modeling the Histidineâ€“Phenylalanine Interaction: The NHÂ·Â·Â·Ï€ Hydrogen Bond of ImidazoleÂ·Benzene. Journal of Physical Chemistry B, 2015, 119, 7778-7790.	1.2	29
152	Density Functional Theory Study of the Formation of Naphthalene and Phenanthrene from Reactions of Phenyl with Vinyl- and Phenylacetylene. Journal of Chemical Theory and Computation, 2007, 3, 139-145.	2.3	28
153	Isomeric Al₂R₄, Mg₂R₂ Species and Oligomerisation Products: Investigation of Alâ€“Al and Mgâ€“Mg Ïƒ Bonding. European Journal of Inorganic Chemistry, 2008, 2008, 4879-4890.	1.0	28
154	The first microsolvation step for furans: New experiments and benchmarking strategies. Journal of Chemical Physics, 2020, 152, 164303.	1.2	28
155	Ab Initio Calculations of the Binding Energies of Small (H₂O)_n Clusters (n =) Tj ETQq1 1 0.784314 rgBT /Ov	0.9	27
156	Explicitly correlated second-order perturbation theory calculations on molecules containing heavy main-group elements. Theoretical Chemistry Accounts, 2008, 121, 11-19.	0.5	27
157	Magnetic Properties of Paddlewheels and Trinuclear Clusters with Exposed Metal Sites. ChemPhysChem, 2011, 12, 3307-3319.	1.0	27
158	Atropisomerization of di-para-substituted propyl-bridged biphenyl cyclophanes. Organic and Biomolecular Chemistry, 2013, 11, 110-118.	1.5	27
159	Communication: A hybrid Betheâ€“Salpeter/time-dependent density-functional-theory approach for excitation energies. Journal of Chemical Physics, 2018, 149, 101101.	1.2	27
160	Extremal Electron Pairs â€” Application to Electron Correlation, Especially the R12 Method. Topics in Current Chemistry, 1999, , 21-42.	4.0	26
161	Low-lying electronic states of the Ti2 dimer: Electronic absorption spectroscopy in rare gas matrices in concert with quantum chemical calculations. Journal of Chemical Physics, 2004, 121, 7195-7206.	1.2	26
162	Reactivity of titanium dimer and molecular nitrogen in rare gas matrices. Vibrational and electronic spectra and structure of Ti2N2. Physical Chemistry Chemical Physics, 2006, 8, 2000-2011.	1.3	26

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163	Nucleophilic Additions to Alkylidene Bis(sulfoxides)â€"Stereoelectronic Effects in Vinyl Sulfoxides. Chemistry - A European Journal, 2008, 14, 4631-4639.	1.7	26
164	Hydrogen abstraction from biphenyl, acenaphthylene, naphthalene and phenanthrene by atomic hydrogen and methyl radical: DFT and G3(MP2)-RAD data. Computational and Theoretical Chemistry, 2010, 940, 115-118.	1.5	26
165	Coinage Metal Complexes of Tris(pyrazolyl)methanide-Based Redox-Active Metalloligands. Organometallics, 2014, 33, 941-951.	1.1	26
166	Computation of Electromagnetic Properties of Molecular Ensembles. ChemPhysChem, 2020, 21, 878-887.	1.0	26
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