Jan M L Martin

List of Publications by Year
in descending order

309 papers	27,879 citations	4388 86 h-index	6836 155 g-index
319 all docs	319 docs citations	319 times ranked	14940 citing authors

#	Article	IF	Citations
1	Development of density functionals for thermochemical kinetics. Journal of Chemical Physics, 2004, 121, 3405-3416.	3.0	1,380
2	Correlation consistent valence basis sets for use with the Stuttgartâ€“Dresdenâ€“Bonn relativistic effective core potentials: The atoms Gaâ€“Kr and Inâ€“Xe. Journal of Chemical Physics, 2001, 114, 3408-3420.	3.0	1,277
3	Towards standard methods for benchmark quality ab initio thermochemistryâ€”W1 and W2 theory. Journal of Chemical Physics, 1999, 111, 1843-1856.	3.0	947
4	Ab initio total atomization energies of small molecules â€” towards the basis set limit. Chemical Physics Letters, 1996, 259, 669-678.	2.6	733
5	Highly Accurate First-Principles Benchmark Data Sets for the Parametrization and Validation of Density Functional and Other Approximate Methods. Derivation of a Robust, Generally Applicable, Double-Hybrid Functional for Thermochemistry and Thermochemical Kinetics. Journal of Physical Chemistry A, 2008, 112, 12868-12886.	2.5	680
6	W4 theory for computational thermochemistry: In pursuit of confident sub-kJ/mol predictions. Journal of Chemical Physics, 2006, 125, 144108.	3.0	646
7	Exploring the Accuracy Limits of Local Pair Natural Orbital Coupled-Cluster Theory. Journal of Chemical Theory and Computation, 2015, 11, 1525-1539.	5.3	544
8	Assessment of W1 and W2 theories for the computation of electron affinities, ionization potentials, heats of formation, and proton affinities. Journal of Chemical Physics, 2001, 114, 6014-6029.	3.0	444
9	Frequency and Zero-Point Vibrational Energy Scale Factors for Double-Hybrid Density Functionals (and Other Selected Methods): Can Anharmonic Force Fields Be Avoided?. Journal of Physical Chemistry A, 2015, 119, 1701-1714.	2.5	441
10	Halogen Bonds: Benchmarks and Theoretical Analysis. Journal of Chemical Theory and Computation, 2013, 9, 1918-1931.	5.3	435
11	W3 theory: Robust computational thermochemistry in the kJ/mol accuracy range. Journal of Chemical Physics, 2004, 120, 4129-4141.	3.0	434
12	â€œTurning Overâ€•Definitions in Catalytic Cycles. ACS Catalysis, 2012, 2, 2787-2794.	11.2	431
13	DSD-PBEP86: in search of the best double-hybrid DFT with spin-component scaled MP2 and dispersion corrections. Physical Chemistry Chemical Physics, 2011, 13, 20104.	2.8	409
14	The anharmonic force field of ethylene, C2H4, by means of accurate ab initio calculations. Journal of Chemical Physics, 1995, 103, 2589-2602.	3.0	381
15	Comment on: â€œEstimating the Hartreeâ€“Fock limit from finite basis set calculationsâ€•[Jensen F (2005) Theor Chem Acc 113:267]. Theoretical Chemistry Accounts, 2006, 115, 330-333.	1.4	367
16	W4-11: A high-confidence benchmark dataset for computational thermochemistry derived from first-principles W4 data. Chemical Physics Letters, 2011, 510, 165-178.	2.6	353
17	DSD-BLYP: A General Purpose Double Hybrid Density Functional Including Spin Component Scaling and Dispersion Correction. Journal of Physical Chemistry C, 2010, 114, 20801-20808.	3.1	329
18	Spinâ€•componentâ€•scaled double hybrids: An extensive search for the best fifthâ€•rung functionals blending DFT and perturbation theory. Journal of Computational Chemistry, 2013, 34, 2327-2344.	3.3	292

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19	IUPAC Critical Evaluation of Thermochemical Properties of Selected Radicals. Part I. Journal of Physical and Chemical Reference Data, 2005, 34, 573-656.	4.2	283
20	Minimally Empirical Double-Hybrid Functionals Trained against the GMTKN55 Database: revDSD-PBEP86-D4, revDOD-PBE-D4, and DOD-SCAN-D4. Journal of Physical Chemistry A, 2019, 123, 5129-5143.	2.5	262
21	Unrestricted Coupled Cluster and Brueckner Doubles Variations of W1 Theory. Journal of Chemical Theory and Computation, 2009, 5, 2687-2693.	5.3	232
22	Explicitly correlated Wn theory: W1-F12 and W2-F12. Journal of Chemical Physics, 2012, 136, 124114.	3.0	229
23	Benchmark Study of DFT Functionals for Late-Transition-Metal Reactionsâ€. Journal of Physical Chemistry A, 2006, 110, 709-716.	2.5	223
24	Double-Hybrid Functionals for Thermochemical Kinetics. Journal of Physical Chemistry A, 2008, 112, 3-8.	2.5	213
25	An accurate ab initio quartic force field and vibrational frequencies for CH4 and isotopomers. Journal of Chemical Physics, 1995, 102, 254-261.	3.0	212
26	Basis set convergence for geometry and harmonic frequencies. Are h functions enough?. Chemical Physics Letters, 1994, 225, 473-479.	2.6	208
27	Benchmark ab Initio Energy Profiles for the Gas-Phase SN2 Reactions Y- + CH3X â†' CH3Y + X- (X,Y = F,Cl,Br). Validation of Hybrid DFT Methods. Journal of Physical Chemistry A, 2001, 105, 895-904.	2.5	199
28	Basis set convergence in second-row compounds. The importance of core polarization functions. Chemical Physics Letters, 1998, 282, 16-24.	2.6	191
29	Structure and vibrational spectra of carbon clusters Cn (n = 2â€“10, 12, 14, 16, 18) using density functional theory including exact exchange contributions. Chemical Physics Letters, 1995, 242, 570-579.	2.6	187
30	Evidence for a terminal Pt(iv)-oxo complex exhibiting diverse reactivity. Nature, 2008, 455, 1093-1096.	27.8	187
31	On the performance of density functional methods for describing atomic populations, dipole moments and infrared intensities. Chemical Physics Letters, 1996, 250, 393-401.	2.6	186
32	The atomization energy and proton affinity of NH3. An ab initio calibration study. Chemical Physics Letters, 1996, 258, 136-143.	2.6	185
33	The S66x8 benchmark for noncovalent interactions revisited: explicitly correlated ab initio methods and density functional theory. Physical Chemistry Chemical Physics, 2016, 18, 20905-20925.	2.8	182
34	The role of the basis set: Assessing density functional theory. Journal of Chemical Physics, 2003, 119, 3005-3014.	3.0	181
35	Basis set convergence study of the atomization energy, geometry, and anharmonic force field of SO2: The importance of inner polarization functions. Journal of Chemical Physics, 1998, 108, 2791-2800.	3.0	173
36	Calculation of molecular electrostatic potentials and Fukui functions using density functional methods. Chemical Physics Letters, 1996, 256, 400-408.	2.6	167

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37	Basis set convergence and performance of density functional theory including exact exchange contributions for geometries and harmonic frequencies. Molecular Physics, 1995, 86, 1437-1450.	1.7	164
38	Formation of Î·2 Câˆ’H Agostic Rhodium Arene Complexes and Their Relevance to Electrophilic Bond Activation. Journal of the American Chemical Society, 1998, 120, 12539-12544.	13.7	164
39	Computational Study of a New Heck Reaction Mechanism Catalyzed by Palladium(II/IV) Species. Chemistry - A European Journal, 2001, 7, 1703-1711.	3.3	160
40	Performance of Ab Initio and Density Functional Methods for Conformational Equilibria of C_nH_{2n+2} Alkane Isomers (n = 4â€“8). Journal of Physical Chemistry A, 2009, 113, 11974-11983.	2.5	156
41	Structure and Vibrational Spectrum of Some Polycyclic Aromatic Compounds Studied by Density Functional Theory. 1. Naphthalene, Azulene, Phenanthrene, and Anthraceneâ€. The Journal of Physical Chemistry, 1996, 100, 15358-15367.	2.9	155
42	Structure and Vibrations of Small Carbon Clusters from Coupled-Cluster Calculations. The Journal of Physical Chemistry, 1996, 100, 6047-6056.	2.9	155
43	Chirality-induced spin polarization places symmetry constraints on biomolecular interactions. Proceedings of the National Academy of Sciences of the United States of America, 2017, 114, 2474-2478.	7.1	155
44	The geometry, vibrational frequencies, and total atomization energy of ethylene. A calibration study. Chemical Physics Letters, 1996, 248, 336-344.	2.6	153
45	From ab initio quantum chemistry to molecular dynamics: The delicate case of hydrogen bonding in ammonia. Journal of Chemical Physics, 2003, 119, 5965-5980.	3.0	153
46	Vibrational Spectra of the Azabenzenes Revisited:Â Anharmonic Force Fieldsâ€. Journal of Physical Chemistry A, 2004, 108, 3085-3096.	2.5	151
47	A Computational Foray into the Formation and Reactivity of Metallabenzenes. Journal of the American Chemical Society, 2004, 126, 11699-11710.	13.7	149
48	The Mechanism of Aluminum-Catalyzed Meerweinâ€“Schmidtâ€“Ponndorfâ€“Verley Reduction of Carbonyls to Alcohols. Journal of the American Chemical Society, 2004, 126, 14796-14803.	13.7	146
49	Photochemical Reduction of Carbon Dioxide Catalyzed by a Rutheniumâ€Substituted Polyoxometalate. Chemistry - A European Journal, 2010, 16, 1356-1364.	3.3	142
50	Basis set convergence of post-CCSD contributions to molecular atomization energies. Journal of Chemical Physics, 2007, 127, 064104.	3.0	139
51	Gd³⁺ Complexes as Potential Spin Labels for High Field Pulsed EPR Distance Measurements. Journal of the American Chemical Society, 2007, 129, 14138-14139.	13.7	138
52	Benchmark quality total atomization energies of small polyatomic molecules. Journal of Chemical Physics, 1997, 106, 8620-8623.	3.0	135
53	On the performance of correlation consistent basis sets for the calculation of total atomization energies, geometries, and harmonic frequencies. Journal of Chemical Physics, 1994, 100, 8186-8193.	3.0	134
54	On the effect of core correlation on the geometry and harmonic frequencies of small polyatomic molecules. Chemical Physics Letters, 1995, 242, 343-350.	2.6	134

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55	What Makes for a Bad Catalytic Cycle? A Theoretical Study on the Suzukiâ^'Miyaura Reaction within the Energetic Span Model. ACS Catalysis, 2011, 1, 246-253.	11.2	134
56	The Rateâ€Determining Step is Dead. Long Live the Rateâ€Determining State!. ChemPhysChem, 2011, 12, 1413-1418.	2.1	129
57	Empirical Doubleâ€Hybrid Density Functional Theory: A â€˜Third Wayâ€™ in Between WFT and DFT. Israel Journal of Chemistry, 2020, 60, 787-804.	2.3	129
58	A purely ab initio spectroscopic quality quartic force field for acetylene. Journal of Chemical Physics, 1998, 108, 676-691.	3.0	128
59	Benchmark Thermochemistry of the C_nH_{2n+2} Alkane Isomers (n = 2â^'8) and Performance of DFT and Composite Ab Initio Methods for Dispersion-Driven Isomeric Equilibria. Journal of Physical Chemistry A, 2009, 113, 8434-8447.	2.5	128
60	An accurate ab initio quartic force field for ammonia. Journal of Chemical Physics, 1992, 97, 8361-8371.	3.0	122
61	Ab initio study of boron, nitrogen, and boronâ€“nitrogen clusters. I. Isomers and thermochemistry of B3, B2N, BN2, and N3. Journal of Chemical Physics, 1989, 90, 6469-6485.	3.0	120
62	W4â€17: A diverse and highâ€confidence dataset of atomization energies for benchmarking highâ€level electronic structure methods. Journal of Computational Chemistry, 2017, 38, 2063-2075.	3.3	120
63	Comparison of Steric and Electronic Requirements for Câ^'C and Câ^'H Bond Activation. Chelating vs Nonchelating Case. Journal of the American Chemical Society, 2001, 123, 9064-9077.	13.7	118
64	On the integration accuracy in molecular density functional theory calculations using Gaussian basis sets. Computer Physics Communications, 2001, 133, 189-201.	7.5	116
65	An Accurate ab Initio Quartic Force Field for Formaldehyde and Its Isotopomers. Journal of Molecular Spectroscopy, 1993, 160, 105-116.	1.2	115
66	The Silabenzenes:Â Structure, Properties, and Aromaticity. Organometallics, 2000, 19, 1477-1487.	2.3	115
67	A simple DFT-based diagnostic for nondynamical correlation. Theoretical Chemistry Accounts, 2013, 132, 1.	1.4	114
68	Metallacarbenes from Diazoalkanes:Â An Experimental and Computational Study of the Reaction Mechanism. Journal of the American Chemical Society, 2003, 125, 6532-6546.	13.7	112
69	Aromatic vs Aliphatic Câ^'H Bond Activation by Rhodium(I) as a Function of Agostic Interactions:Â Catalytic H/D Exchange between Olefins and Methanol or Water. Journal of the American Chemical Society, 2003, 125, 11041-11050.	13.7	111
70	A Thiourea Tether in the Second Coordination Sphere as a Binding Site for CO₂ and a Proton Donor Promotes the Electrochemical Reduction of CO₂ to CO Catalyzed by a Rhenium Bipyridine-Type Complex. Journal of the American Chemical Society, 2018, 140, 12451-12456.	13.7	111
71	Active site electronic structure and dynamics during metalloenzyme catalysis. Nature Structural Biology, 2003, 10, 98-103.	9.7	109
72	Some Observations on Counterpoise Corrections for Explicitly Correlated Calculations on Noncovalent Interactions. Journal of Chemical Theory and Computation, 2014, 10, 3791-3799.	5.3	109

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73	Accurate ab initio quartic force field for trans-HNNH and treatment of resonance polyads. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 1997, 53, 1039-1050.	3.9	105
74	Alkali and alkaline earth metal compounds: coreâ€"valence basis sets and importance of subvalence correlation. Molecular Physics, 2003, 101, 1345-1361.	1.7	103
75	On the performance of large Gaussian basis sets for the computation of total atomization energies. Journal of Chemical Physics, 1992, 97, 5012-5018.	3.0	101
76	orthoCâ^'H Activation of Haloarenes and Anisole by an Electron-Rich Iridium(I) Complex:Â Mechanism and Origin of Regio- andÂChemoselectivity. AnÂExperimental andÂTheoreticalÂStudy. Organometallics, 2006, 25, 3190-3210.	2.3	100
77	Benchmark ab Initio Conformational Energies for the Proteinogenic Amino Acids through Explicitly Correlated Methods. Assessment of Density Functional Methods. Journal of Chemical Theory and Computation, 2016, 12, 444-454.	5.3	99
78	Electron affinities of the first- and second-row atoms: Benchmarkab initioand density-functional calculations. Physical Review A, 1999, 60, 1034-1045.	2.5	95
79	Ab initio study of the infrared spectra of linear Cn clusters (n=6â€"9). Journal of Chemical Physics, 1990, 93, 8850-8861.	3.0	92
80	The harmonic frequencies of benzene. A case for atomic natural orbital basis sets. Chemical Physics Letters, 1997, 275, 414-422.	2.6	92
81	Charge Transport in Conjugated Aromatic Molecular Junctions:â€‰ Molecular Conjugation and Moleculeâ^'Electrode Coupling. Journal of Physical Chemistry C, 2007, 111, 14893-14902.	3.1	91
82	Heats of Formation of Beryllium, Boron, Aluminum, and Silicon Re-examined by Means of W4 Theory. Journal of Physical Chemistry A, 2007, 111, 5936-5944.	2.5	91
83	The Melatonin Conformer Space: Benchmark and Assessment of Wave Function and DFT Methods for a Paradigmatic Biological and Pharmacological Molecule. Journal of Physical Chemistry A, 2013, 117, 2269-2277.	2.5	91
84	Toward a W4-F12 approach: Can explicitly correlated and orbital-based ab initio CCSD(T) limits be reconciled?. Journal of Chemical Physics, 2016, 144, 214101.	3.0	89
85	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.	2.5	87
86	Co-Crystallization of Sym-Triiodo-Trifluorobenzene with Bipyridyl Donors:Â Consistent Formation of Two Instead of Anticipated Three NÂ·Â·Â·I Halogen Bonds. Crystal Growth and Design, 2007, 7, 386-392.	3.0	87
87	Structure and Vibrational Spectra of the Azabenzenes. A Density Functional Study Including Exact Exchange Contributions. The Journal of Physical Chemistry, 1996, 100, 6973-6983.	2.9	86
88	Selective Câ^'C vs Câ^'H Bond Activation by Rhodium(I) PCP Pincer Complexes. A Computational Study. Journal of the American Chemical Society, 2000, 122, 7095-7104.	13.7	85
89	Conventional and Explicitly Correlated ab Initio Benchmark Study on Water Clusters: Revision of the BEGDB and WATER27 Data Sets. Journal of Chemical Theory and Computation, 2017, 13, 3136-3152.	5.3	81
90	Reactions of pulsed laser produced boron and nitrogen atoms in a condensing argon stream. Journal of Chemical Physics, 1993, 98, 922-931.	3.0	79

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91	Structure and relative energetics of C2n+1 (n = 2â^'7) carbon clusters using coupled cluster and hybrid density functional methods. Chemical Physics Letters, 1996, 252, 9-18.	2.6	78
92	Ab initio multireference study of the BN molecule. Journal of Chemical Physics, 1992, 97, 6549-6556.	3.0	77
93	On the structure and vibrational frequencies of C20. Chemical Physics Letters, 1996, 248, 345-352.	2.6	77
94	The ground-state spectroscopic constants of Be2 revisited. Chemical Physics Letters, 1999, 303, 399-407.	2.6	77
95	Post-CCSD(T) ab Initio Thermochemistry of Halogen Oxides and Related Hydrides XOX, XOOX, HOX, XO_n, and HXO_n (X = F, Cl), and Evaluation of DFT Methods for These Systems. Journal of Physical Chemistry A, 2009, 113, 4802-4816.	2.5	77
96	A critical comparison of MINDO/3, MNDO, AM1, and PM3 for a model problem: Carbon clusters C2-C10. An ad hoc reparametrization of MNDO well suited for the accurate prediction of their spectroscopic constants. Journal of Computational Chemistry, 1991, 12, 52-70.	3.3	76
97	Accurate ab initio quartic force fields for the N2O and CO2 molecules. Chemical Physics Letters, 1993, 205, 535-542.	2.6	76
98	Heats of Formation of Alkali Metal and Alkaline Earth Metal Oxides and Hydroxides:â€‰ Surprisingly Demanding Targets for High-Level ab Initio Procedures. Journal of Physical Chemistry A, 2003, 107, 5617-5630.	2.5	76
99	Boraneâ€“Lewis Base Complexes as Homolytic Hydrogen Atom Donors. Chemistry - A European Journal, 2010, 16, 6861-6865.	3.3	75
100	First principles computation of thermochemical properties beyond the harmonic approximation. I. Method and application to the water molecule and its isotopomers. Journal of Chemical Physics, 1992, 96, 7633-7645.	3.0	74
101	Pulsed laser evaporated boron atom reactions with acetylene. Infrared spectra and quantum chemical structure and frequency calculations for several novel organoborane BC2H2 and HBC2 molecules. The Journal of Physical Chemistry, 1993, 97, 5839-5847.	2.9	74
102	Heats of formation of the amino acids re-examined by means of W1-F12 and W2-F12 theories. Theoretical Chemistry Accounts, 2014, 133, 1.	1.4	74
103	Metallabenzene versus Cp Complex Formation:Â A DFT Investigation. Journal of the American Chemical Society, 2003, 125, 13020-13021.	13.7	71
104	Spectroscopic quality ab initio potential curves for CH, NH, OH and HF. A convergence study. Chemical Physics Letters, 1998, 292, 411-420.	2.6	70
105	Ab Initio Geometry Determinations of Proteins. 1. Crambin. Journal of Physical Chemistry A, 1998, 102, 2246-2251.	2.5	67
106	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.	2.0	67
107	Accurate quantum chemical energies for tetrapeptide conformations: why MP2 data with an insufficient basis set should be handled with caution. Physical Chemistry Chemical Physics, 2013, 15, 7028.	2.8	67
108	Abinitiostudy of the structure, infrared spectra, and heat of formation of C4. Journal of Chemical Physics, 1991, 94, 3753-3761.	3.0	66

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109	Selective sp3Câ˜H Activation of Ketones at the Î² Position by Ir(I). Origin of Regioselectivity and Water Effect. Journal of the American Chemical Society, 2006, 128, 12400-12401.	13.7	66
110	Heats of formation of platonic hydrocarbon cages by means of highâ€level thermochemical procedures. Journal of Computational Chemistry, 2016, 37, 49-58.	3.3	66
111	Infrared Spectra of Boron-Ammonia Reaction Products in Solid Argon. The Journal of Physical Chemistry, 1995, 99, 13839-13849.	2.9	65
112	Ab initio study of the spectroscopy and thermochemistry of the C2N and CN2 molecules. Chemical Physics Letters, 1994, 226, 475-483.	2.6	64
113	Anharmonic force field and vibrational frequencies of tetrafluoromethane (CF4) and tetrafluorosilane (SiF4). Journal of Chemical Physics, 2000, 112, 1353-1366.	3.0	64
114	TpPtMe(H)2:Â Why Is There H/D Scrambling of the Methyl Group but Not Methane Loss?. Journal of the American Chemical Society, 2002, 124, 7041-7054.	13.7	63
115	Explicitly correlated benchmark calculations on C₈H₈ isomer energy separations: how accurate are DFT, double-hybrid, and composite ab initio procedures?. Molecular Physics, 2012, 110, 2477-2491.	1.7	63
116	The Unexpected Role of CO in Cï£¿H Oxidative Addition by a Cationic Rhodium(I) Complex. Angewandte Chemie - International Edition, 2007, 46, 1901-1904.	13.8	62
117	Directing Arylâ˜I versus Arylâ˜Br Bond Activation by Nickel via a Ring Walking Process. Inorganic Chemistry, 2008, 47, 5114-5121.	4.0	62
118	Performance of W4 theory for spectroscopic constants and electrical properties of small molecules. Journal of Chemical Physics, 2010, 133, 144102.	3.0	62
119	Assessment of CCSD(T)-F12 Approximations and Basis Sets for Harmonic Vibrational Frequencies. Journal of Chemical Theory and Computation, 2014, 10, 2085-2090.	5.3	61
120	Platinum Stilbazoles:Â Ring-Walking Coupled with Arylâ˜Halide Bond Activation. Journal of the American Chemical Society, 2005, 127, 9322-9323.	13.7	60
121	Benchmark atomization energy of ethane: Importance of accurate zero-point vibrational energies and diagonal Bornâ€“Oppenheimer corrections for a â€˜simpleâ€™ organic molecule. Computational and Theoretical Chemistry, 2007, 811, 345-353.	1.5	60
122	What Can We Learn about Dispersion from the Conformer Surface of n-Pentane?. Journal of Physical Chemistry A, 2013, 117, 3118-3132.	2.5	60
123	Definitive heat of formation of methylenimine, CH2?NH, and of methylenimmonium ion, CH2NH2+, by means of W2 theory. Journal of Computational Chemistry, 2001, 22, 1297-1305.	3.3	59
124	Anharmonic force fields and thermodynamic functions using density functional theory. Molecular Physics, 2005, 103, 863-876.	1.7	59
125	Economical Post-CCSD(T) Computational Thermochemistry Protocol and Applications to Some Aromatic Compounds. Journal of Physical Chemistry A, 2009, 113, 7610-7620.	2.5	59
126	Accurate ab initio quartic force fields for borane and BeH2. Chemical Physics Letters, 1992, 200, 502-510.	2.6	57

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127	Potential energy surface of B4 and total atomization energies of B2, B3, and B4. Chemical Physics Letters, 1992, 189, 529-536.	2.6	57
128	The cc-pV5Z-F12 basis set: reaching the basis set limit in explicitly correlated calculations. Molecular Physics, 2015, 113, 1551-1558.	1.7	57
129	Accurateab initioquartic force fields for the ions HCO+and HOC+. Journal of Chemical Physics, 1993, 99, 286-292.	3.0	56
130	Discovery of the First Metallaquinone. Journal of the American Chemical Society, 2000, 122, 8797-8798.	13.7	55
131	On the structure and vibrational frequencies of C24. Chemical Physics Letters, 1996, 255, 7-14.	2.6	54
132	Heat of atomization of sulfur trioxide, SO3: a benchmark for computational thermochemistry. Chemical Physics Letters, 1999, 310, 271-276.	2.6	53
133	Cycloaddition Reactions of Metalloaromatic Complexes of Iridium and Rhodium:Â A Mechanistic DFT Investigation. Journal of the American Chemical Society, 2003, 125, 11702-11709.	13.7	53
134	Conformational Equilibria in Butane-1,4-diol: A Benchmark of a Prototypical System with Strong Intramolecular H-bonds. Journal of Physical Chemistry A, 2014, 118, 293-303.	2.5	53
135	Note on the vibrational spectrum of C4 and C5. Journal of Chemical Physics, 1989, 90, 3403-3405.	3.0	51
136	What Are the Ground State Structures of C₂₀ and C₂₄? An Explicitly Correlated Ab Initio Approach. Journal of Physical Chemistry A, 2016, 120, 153-160.	2.5	51
137	Accurate ab initio quartic force field and vibrational frequencies of the NH4+ ion and its deuterated forms. Chemical Physics Letters, 1996, 258, 129-135.	2.6	50
138	The aug-cc-pVnZ-F12 basis set family: Correlation consistent basis sets for explicitly correlated benchmark calculations on anions and noncovalent complexes. Journal of Chemical Physics, 2017, 147, 134106.	3.0	50
139	The structure, stability, and infrared spectrum of B2N, B2N+, B2Nâ^', BO, B2O and B2N2.. Chemical Physics Letters, 1992, 193, 243-250.	2.6	49
140	Benchmark ab initio calculations of the total atomization energies of the first-row hydrides AHn (A =) Tj ETQq0 0 0 rgBT /Overlock 10 Tf	2.6	49
141	sp3 Câ€“H and sp2 Câ€“H agostic ruthenium complexes: a combined experimental and theoretical study. Inorganica Chimica Acta, 2004, 357, 1854-1864.	2.4	49
142	Effect of CO on the Oxidative Addition of Arene Cï£¿H Bonds by Cationic Rhodium Complexes. Chemistry - A European Journal, 2010, 16, 328-353.	3.3	49
143	DFT Study of the Structure and Reactivity of the Terminal Pt(IV)-Oxo Complex Bearing No Electron-Withdrawing Ligands. Journal of the American Chemical Society, 2010, 132, 14886-14900.	13.7	49
144	Electron Transfer Oxidation of Benzene and Aerobic Oxidation to Phenol. ACS Catalysis, 2016, 6, 6403-6407.	11.2	48

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145	Do CCSD and approximate CCSD-F12 variants converge to the same basis set limits? The case of atomization energies. Journal of Chemical Physics, 2018, 149, 154109.	3.0	48
146	?-Accepting-Pincer Rhodium Complexes: An Unusual Coordination Mode of PCP-Type Systems. Chemistry - A European Journal, 2005, 11, 2319-2326.	3.3	47
147	Heats of formation of perchloric acid, HClO4, and perchloric anhydride, Cl2O7. Probing the limits of W1 and W2 theory. Computational and Theoretical Chemistry, 2006, 771, 19-26.	1.5	47
148	Chapter 3 Computational Thermochemistry: A Brief Overview of Quantum Mechanical Approaches. Annual Reports in Computational Chemistry, 2005, 1, 31-43.	1.7	46
149	Structure and infrared spectroscopy of the C11 molecule. Chemical Physics Letters, 1991, 187, 367-374.	2.6	45
150	Structure and vibrations of BnNn (n = 3â€“10). Chemical Physics Letters, 1996, 248, 95-101.	2.6	45
151	Energetics of Acetylene Loss from C14H10â€¢+ Cations:â€‰ A Density Functional Calculation. Journal of Physical Chemistry A, 1997, 101, 219-226.	2.5	45
152	Thermochemical analysis of core correlation and scalar relativistic effects on molecular atomization energies. Journal of Chemical Physics, 2000, 113, 1348-1358.	3.0	45
153	What Types of Chemical Problems Benefit from Density-Corrected DFT? A Probe Using an Extensive and Chemically Diverse Test Suite. Journal of Chemical Theory and Computation, 2021, 17, 1368-1379.	5.3	45
154	The total atomization energy and heat of formation of HCN(g). Chemical Physics Letters, 1996, 259, 679-682.	2.6	44
155	NLO Properties of Metallabenzene-Based Chromophores:Â A Time-Dependent Density Functional Study. Journal of Physical Chemistry A, 2005, 109, 5454-5462.	2.5	44
156	Performance of Localized Coupled Cluster Methods in a Moderately Strong Correlation Regime: HÃ¼ckelâ€“MÃ¶bius Interconversions in Expanded Porphyrins. Journal of Chemical Theory and Computation, 2020, 16, 3641-3653.	5.3	44
157	Pulsed laser evaporation of boron/carbon pellets: Infrared spectra and quantum chemical structures and frequencies for BC2. Journal of Chemical Physics, 1993, 99, 12-17.	3.0	43
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