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	The MOBH35 Metalâ€“Organic Barrier Heights Reconsidered: Performance of Local-Orbital Coupled Cluster Approaches in Different Static Correlation Regimes. Journal of Chemical Theory and Computation, 2022, 18, 883-898.	5.3	27
2	Heavy-Atom Tunneling in the Covalent/Dative Bond Complexation of Cyclo[18]carbonâ€“Piperidine. Journal of Physical Chemistry B, 2022, 126, 1799-1804.	2.6	5
3	Pure and Hybrid SCAN, rSCAN, and r2SCAN: Which One Is Preferred in KS- and HF-DFT Calculations, and How Does D4 Dispersion Correction Affect This Ranking?. Molecules, 2022, 27, 141.	3.8	10
4	Electron Correlation: Nature's Weird and Wonderful Chemical Glue. Israel Journal of Chemistry, 2022, 62, .	2.3	13
5	Do Double-Hybrid Functionals Benefit from Regularization in the PT2 Term? Observations from an Extensive Benchmark. Journal of Physical Chemistry Letters, 2022, 13, 3499-3506.	4.6	14
6	MP2-F12 Basis Set Convergence near the Complete Basis Set Limit: Are h Functions Sufficient?. Journal of Physical Chemistry A, 2022, 126, 3964-3971.	2.5	3
7	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
8	Prototypical Ï€â€“Ï€ dimers re-examined by means of high-level CCSDT(Q) composite ab initio methods. Journal of Chemical Physics, 2021, 154, 124117.	3.0	9
9	Exploring Avenues beyond Revised DSD Functionals: II. Random-Phase Approximation and Scaled MP3 Corrections. Journal of Physical Chemistry A, 2021, 125, 4628-4638.	2.5	12
10	Exploring Avenues beyond Revised DSD Functionals: I. Range Separation, with xDSD as a Special Case. Journal of Physical Chemistry A, 2021, 125, 4614-4627.	2.5	29
11	Surprisingly Good Performance of XYG3 Family Functionals Using a Scaled KS-MP3 Correlation. Journal of Physical Chemistry Letters, 2021, 12, 9368-9376.	4.6	7
12	Coupled Cluster Benchmark of New DFT and Local Correlation Methods: Mechanisms of Hydroarylation and Oxidative Coupling Catalyzed by Ru(II, III) Chloride Carbonyls. Journal of Physical Chemistry A, 2021, 125, 8987-8999.	2.5	22
13	Energetics of (H2O)20 isomers by means of F12 canonical and localized coupled cluster methods. AIP Conference Proceedings, 2021, , .	0.4	3
14	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
15	Canonical and DLPNO-Based Composite Wavefunction Methods Parametrized against Large and Chemically Diverse Training Sets. 2: Correlation-Consistent Basis Sets, Coreâ€“Valence Correlation, and F12 Alternatives. Journal of Chemical Theory and Computation, 2020, 16, 7507-7524.	5.3	19
16	Canonical and DLPNO-Based G4(MP2)XK-Inspired Composite Wave Function Methods Parametrized against Large and Chemically Diverse Training Sets: Are They More Accurate and/or Robust than Double-Hybrid DFT?. Journal of Chemical Theory and Computation, 2020, 16, 4238-4255.	5.3	30
17	Performance of Electronic Structure Methods for the Description of HÃ¼ckelâ€“MÃ¶bius Interconversions in Extended Ï€-Systems. Journal of Physical Chemistry A, 2020, 124, 2380-2397.	2.5	22
18	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

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19	The Atomic Partial Charges Arboretum: Trying to See the Forest for the Trees. ChemPhysChem, 2020, 21, 688-696.	2.1	43
20	Probing the basis set limit for thermochemical contributions of inner-shell correlation: balance of core-core and core-valence contributions. Molecular Physics, 2019, 117, 1078-1087.	1.7	15
21	A simple model for scalar relativistic corrections to molecular total atomisation energies. Molecular Physics, 2019, 117, 2225-2232.	1.7	5
22	Molecular dynamics simulations of the interaction of Mouse and Torpedo acetylcholinesterase with covalent inhibitors explain their differential reactivity: Implications for drug design. Chemico-Biological Interactions, 2019, 310, 108715.	4.0	11
23	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
24	Some observations on the performance of the most recent exchange-correlation functionals for the large and chemically diverse GMTKN55 benchmark. AIP Conference Proceedings, 2019, , .	0.4	15
25	Tribute to Leo Radom. Journal of Physical Chemistry A, 2019, 123, 10347-10347.	2.5	0
26	Coupled cluster benchmark of new density functionals and of domain pair natural orbital methods: Mechanisms of hydroarylation and oxidative coupling catalyzed by Ru(II) chloride carbonyls. AIP Conference Proceedings, 2019, , .	0.4	10
27	The kinetics and mechanism of oxidation of reduced phosphovanadomolybdates by molecular oxygen: theory and experiment in concert. Physical Chemistry Chemical Physics, 2018, 20, 7579-7587.	2.8	7
28	The X40Ã—10 Halogen Bonding Benchmark Revisited: Surprising Importance of (nâ€“1)d Subvalence Correlation. Journal of Physical Chemistry A, 2018, 122, 2184-2197.	2.5	34
29	A simple â€˜range extenderâ€™ for basis set extrapolation methods for MP2 and coupled cluster correlation energies. AIP Conference Proceedings, 2018, , .	0.4	15
30	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
31	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
32	Prediction of electronic couplings for molecular charge transfer using optimally tuned range-separated hybrid functionals. Molecular Physics, 2018, 116, 2497-2505.	1.7	15
33	The S66 Non-Covalent Interactions Benchmark Reconsidered Using Explicitly Correlated Methods Near the Basis Set Limit. Australian Journal of Chemistry, 2018, 71, 238.	0.9	40
34	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
35	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
36	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

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37	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
38	Surprising performance for vibrational frequencies of the distinguishable clusters with singles and doubles (DCSD) and MP2.5 approximations. AIP Conference Proceedings, 2017, , .	0.4	9
39	MP2-F12 basis set convergence for the S66 noncovalent interactions benchmark: Transferability of the complementary auxiliary basis set (CABS). AIP Conference Proceedings, 2017, , .	0.4	4
40	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
41	Electron Transfer Oxidation of Benzene and Aerobic Oxidation to Phenol. ACS Catalysis, 2016, 6, 6403-6407.	11.2	48
42	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
43	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
44	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
45	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
46	Comment on â€œDoubly hybrid density functional xDH-PBE0 from a parameter-free global hybrid model PBE0â€•[J. Chem. Phys. 136, 174103 (2012)]. Journal of Chemical Physics, 2015, 143, 187101.	3.0	13
47	New Ruthenium Nitrosyl Pincer Complexes Bearing an O2 Ligand. Mono-Oxygen Transfer. Inorganic Chemistry, 2015, 54, 2253-2263.	4.0	12
48	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
49	Explicitly correlated coupled cluster benchmarks with realistic-sized ligands for some late-transition metal reactions: basis sets convergence and performance of more approximate methods. Highlights in Theoretical Chemistry, 2015, , 233-246.	0.0	1
50	The cc-pV5Z-F12 basis set: reaching the basis set limit in explicitly correlated calculations. Molecular Physics, 2015, 113, 1551-1558.	1.7	57
51	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
52	Explicitly correlated coupled cluster benchmarks with realistic-sized ligands for some late-transition metal reactions: basis sets convergence and performance of more approximate methods. Theoretical Chemistry Accounts, 2014, 133, 1.	1.4	37
53	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
54	Equilibrium Gas-Phase Structures of Sodium Fluoride, Bromide, and Iodide Monomers and Dimers. Journal of Physical Chemistry A, 2014, 118, 1927-1935.	2.5	6

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55	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
56	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
57	The eight-valence-electron systems re-examined: convergence of the coupled-cluster series and performance of quasiperturbative methods for quadruple excitations. Molecular Physics, 2014, 112, 785-793.	1.7	26
58	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
59	A simple DFT-based diagnostic for nondynamical correlation. Highlights in Theoretical Chemistry, 2014, , 251-259.	0.0	0
60	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
61	CO-Induced Methyl Migration in a Rhodium Thiophosphoryl Pincer Complex and Its Comparison with Phosphine-Based Complexes: The Divergent Effects of S and P Donor Ligands. Organometallics, 2013, 32, 7163-7180.	2.3	18
62	Benzyl Cation Stabilized by Metal Complexation. Relative Stability of Coordinated Methylene Arenium, Ï€-Benzylic, and Ïƒ-Benzylic Structures. Organometallics, 2013, 32, 4813-4819.	2.3	6
63	Halogen Bonds: Benchmarks and Theoretical Analysis. Journal of Chemical Theory and Computation, 2013, 9, 1918-1931.	5.3	435
64	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
65	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
66	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
67	A simple DFT-based diagnostic for nondynamical correlation. Theoretical Chemistry Accounts, 2013, 132, 1.	1.4	114
68	Polyoxometalate-Catalyzed Insertion of Oxygen from O2 into Tinâ€“Alkyl Bonds. Journal of the American Chemical Society, 2013, 135, 19304-19310.	13.7	38
69	Comment on â€œRevised electron affinity of SF6 from kinetic dataâ€•[J. Chem. Phys. 136, 121102 (2012)]. Journal of Chemical Physics, 2012, 136, 197101.	3.0	13
70	â€œTurning Overâ€•Definitions in Catalytic Cycles. ACS Catalysis, 2012, 2, 2787-2794.	11.2	431
71	O(³P) + CO₂ Collisions at Hyperthermal Energies: Dynamics of Nonreactive Scattering, Oxygen Isotope Exchange, and Oxygen-Atom Abstraction. Journal of Physical Chemistry A, 2012, 116, 64-84.	2.5	19
72	Exclusive Câ€“C Oxidative Addition in a Rhodium Thiophosphoryl Pincer Complex and Computational Evidence for an Î·³-Câ€“Câ€“H Agostic Intermediate. Organometallics, 2012, 31, 505-512.	2.3	33

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73	Explicitly correlated Wn theory: W1-F12 and W2-F12. Journal of Chemical Physics, 2012, 136, 124114.	3.0	229
74	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
75	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
76	What makes for a good catalytic cycle? A theoretical study of the SPhos ligand in the Suzukiâ€“Miyaura reaction. Chemical Communications, 2011, 47, 4935.	4.1	42
77	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
78	Basis set convergence of explicitly correlated double-hybrid density functional theory calculations. Journal of Chemical Physics, 2011, 135, 144119.	3.0	29
79	The Rateâ€Determining Step is Dead. Long Live the Rateâ€Determining State!. ChemPhysChem, 2011, 12, 1413-1418.	2.1	129
80	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
81	Can DFT methods correctly and efficiently predict the coordination number of copper(I) complexes? A case study. Journal of Computational Chemistry, 2010, 31, 75-83.	3.3	20
82	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
83	Photochemical Reduction of Carbon Dioxide Catalyzed by a Rutheniumâ€Substituted Polyoxometalate. Chemistry - A European Journal, 2010, 16, 1356-1364.	3.3	142
84	Boraneâ€“Lewis Base Complexes as Homolytic Hydrogen Atom Donors. Chemistry - A European Journal, 2010, 16, 6861-6865.	3.3	75
85	Performance of W4 theory for spectroscopic constants and electrical properties of small molecules. Journal of Chemical Physics, 2010, 133, 144102.	3.0	62
86	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
87	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
88	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
89	A Coordination Controlled Arylâ€“Halide Oxidative Addition to Platinum. Chemistry - A European Journal, 2009, 15, 10025-10028.	3.3	12
90	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

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91	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
92	Unrestricted Coupled Cluster and Brueckner Doubles Variations of W1 Theory. Journal of Chemical Theory and Computation, 2009, 5, 2687-2693.	5.3	232
93	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
94	Atomization energies of the carbon clusters C_n(n= 2â^'10) revisited by means of W4 theory as well as density functional, Gn, and CBS methods. Molecular Physics, 2009, 107, 977-990.	1.7	41
95	A DFT study on the mechanism of a novel, regioselective, intramolecular Nâ€“Î€ rearrangement of cis and trans-Î·1-N-Cp*Rh-hydroxytamoxifen complexes to their Î·6 derivatives; potential breast cancer pharmaceuticals, and fluorescent probes. Dalton Transactions, 2009, , 4334.	3.3	8
96	The Impact of Weak Cï£¿Hâ‹…â‹…â‹…Rh Interactions on the Structure and Reactivity of transâ€[Rh(CO)₂(phosphine)₂]⁺: An Experimental and Theoretical Examination. Chemistry - A European Journal, 2008, 14, 8183-8194.	3.3	11
97	Fundamental vibrational frequencies and dominant resonances in methylamine isotopologues by ab initio and density functional theory methods. Journal of Computational Chemistry, 2008, 29, 1268-1276.	3.3	16
98	Evidence for a terminal Pt(iv)-oxo complex exhibiting diverse reactivity. Nature, 2008, 455, 1093-1096.	27.8	187
99	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
100	Halogen-Bonded Supramolecular Assemblies Based on Phenylethynyl Pyridine Derivatives: Driving Crystal Packing through Systematic Chemical Modifications. Crystal Growth and Design, 2008, 8, 3066-3072.	3.0	25
101	Double-Hybrid Functionals for Thermochemical Kinetics. Journal of Physical Chemistry A, 2008, 112, 3-8.	2.5	213
102	Directing Arylâ^'I versus Arylâ^'Br Bond Activation by Nickel via a Ring Walking Process. Inorganic Chemistry, 2008, 47, 5114-5121.	4.0	62
103	Basis set convergence of post-CCSD contributions to molecular atomization energies. Journal of Chemical Physics, 2007, 127, 064104.	3.0	139
104	The Protonation Site of Aniline Revisited: A 'Torture Test' for Electron Correlation Methods. ACS Symposium Series, 2007, , 183-192.	0.5	3
105	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
106	W4 thermochemistry of P₂and P₄. Is the CODATA heat of formation of the phosphorus atom correct?. Molecular Physics, 2007, 105, 2499-2505.	1.7	15
107	Polarizability of Small Carbon Cluster Anions from First Principles. Journal of Physical Chemistry A, 2007, 111, 2028-2032.	2.5	15
108	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

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109	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
110	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
111	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
112	Proton Walk in the Aqueous Platinum Complex [TpPtMeCO] via a Sticky Ïƒ-Methane Ligand. Chemistry - A European Journal, 2007, 13, 2812-2823.	3.3	13
113	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
114	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
115	Benchmark Study of DFT Functionals for Late-Transition-Metal Reactionsâ€. Journal of Physical Chemistry A, 2006, 110, 709-716.	2.5	223
116	W4 theory for computational thermochemistry: In pursuit of confident sub-kJ/mol predictions. Journal of Chemical Physics, 2006, 125, 144108.	3.0	646
117	Rozen's Epoxidation Reagent, CH3CNÂ·HOF:Â A Theoretical Study of Its Structure, Vibrational Spectroscopy, and Reaction Mechanismâ€. Journal of Physical Chemistry A, 2006, 110, 8275-8281.	2.5	9
118	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
119	Anharmonic force fields of perchloric acid, HClO4, and perchloric anhydride, Cl2O7. An extreme case of inner polarization. Journal of Molecular Structure, 2006, 780-781, 310-316.	3.6	15
120	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
121	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
122	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
123	The lowest singlet-triplet excitation energy of BN: A converged coupled cluster perspective. Journal of Chemical Physics, 2006, 125, 144313.	3.0	40
124	Is there a satisfactory description of the molecular structure of Roeskyâ€™s ketone?. Chemical Physics Letters, 2005, 413, 440-444.	2.6	11
125	?-Accepting-Pincer Rhodium Complexes: An Unusual Coordination Mode of PCP-Type Systems. Chemistry - A European Journal, 2005, 11, 2319-2326.	3.3	47
126	IUPAC Critical Evaluation of Thermochemical Properties of Selected Radicals. Part 1.. ChemInform, 2005, 36, no.	0.0	1

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127	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
128	Chapter 3 Computational Thermochemistry: A Brief Overview of Quantum Mechanical Approaches. Annual Reports in Computational Chemistry, 2005, 1, 31-43.	1.7	46
129	Anharmonic force fields and thermodynamic functions using density functional theory. Molecular Physics, 2005, 103, 863-876.	1.7	59
130	Structures and Thermochemistry of Calcium-Containing Molecules. Journal of Physical Chemistry A, 2005, 109, 9156-9168.	2.5	17
131	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
132	Platinum Stilbazoles:Â Ring-Walking Coupled with Arylâ^'Halide Bond Activation. Journal of the American Chemical Society, 2005, 127, 9322-9323.	13.7	60
133	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
134	W3 theory: Robust computational thermochemistry in the kJ/mol accuracy range. Journal of Chemical Physics, 2004, 120, 4129-4141.	3.0	434
135	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
136	Vibrational Spectra of the Azabenzenes Revisited:Â Anharmonic Force Fieldsâ€. Journal of Physical Chemistry A, 2004, 108, 3085-3096.	2.5	151
137	Mechanism of the Methylene Transfer Reaction. Câ^'C Activation and Reductive Elimination in One System. A DFT Study. Organometallics, 2004, 23, 2336-2342.	2.3	23
138	Thermodynamic Properties of C1and C2Bromo Compounds and Radicals. A Relativistic ab Initio Study. Journal of Physical Chemistry A, 2004, 108, 7752-7761.	2.5	31
139	Arene Hapticity in (C6H6)Cr(CO)n(n= 1â^'5) Complexes:Â A DFT Study of Singlet and Triplet Energy Surfaces. Organometallics, 2004, 23, 2315-2325.	2.3	24
140	A Computational Foray into the Formation and Reactivity of Metallabenzenes. Journal of the American Chemical Society, 2004, 126, 11699-11710.	13.7	149
141	Development of density functionals for thermochemical kinetics. Journal of Chemical Physics, 2004, 121, 3405-3416.	3.0	1,380
142	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
143	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
144	Novel Azine Reactivity: Facile Nï£¿N Bond Cleavage, Cï£¿H Activation, and Nï£¿N Coupling Mediated by RhI. Angewandte Chemie - International Edition, 2003, 42, 1949-1952.	13.8	39

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145	Density Functional Study of the Complexation Reaction of Sn(CH3)3X (X = F, Cl, Br and I) with Halide Anions. European Journal of Inorganic Chemistry, 2003, 2003, 3803-3810.	2.0	14
146	Active site electronic structure and dynamics during metalloenzyme catalysis. Nature Structural Biology, 2003, 10, 98-103.	9.7	109
147	Metallabenzene versus Cp Complex Formation:Â A DFT Investigation. Journal of the American Chemical Society, 2003, 125, 13020-13021.	13.7	71
148	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
149	The role of the basis set: Assessing density functional theory. Journal of Chemical Physics, 2003, 119, 3005-3014.	3.0	181
150	Catalytic Reduction of Acetone by [(bpy)Rh]+:Â A Theoretical Mechanistic Investigation and Insight into Cooperativity Effects in This System. Journal of the American Chemical Society, 2003, 125, 11430-11441.	13.7	19
151	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
152	Aromatic vs Aliphatic Câˆ'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
153	Alkali and alkaline earth metal compounds: coreâ€"valence basis sets and importance of subvalence correlation. Molecular Physics, 2003, 101, 1345-1361.	1.7	103
154	Mechanistic aspects of acetone addition to metalloaromatic complexes of iridium: a DFT investigationElectronic supplementary information (ESI) available: selected geometric data, calculated structures of all complexes and full computational details. See http://www.rsc.org/suppdata/cc/b2/b210622a/.. Chemical Communications, 2003, , 132-133.	4.1	32
155	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
156	The heats of formation of the haloacetylenes XCCY [X, Y = H, F, Cl]: basis set limitab initioresults and thermochemical analysis. Molecular Physics, 2002, 100, 453-464.	1.7	21
157	Anharmonic force field, structure, and thermochemistry of CF2 and CCl2Electronic supplementary information (ESI) available: Force constants and thermochemical properties of CF2 and CCl2. See http://www.rsc.org/suppdata/cp/b2/b202865d/. Physical Chemistry Chemical Physics, 2002, 4, 3282-3288.	2.8	34
158	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
159	An accurate quartic force field, fundamental frequencies, and binding energy for the high energy density material TdN4. Chemical Physics Letters, 2002, 357, 319-325.	2.6	26
160	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
161	Comparison of Steric and Electronic Requirements for Câˆ'C and Câˆ'H Bond Activation. Chelating vs Nonchelating Case. Journal of the American Chemical Society, 2001, 123, 9064-9077.	13.7	118
162	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

#	Article	IF	Citations
163	Tuning of Au/n-GaAs Diodes with Highly Conjugated Molecules. Journal of Physical Chemistry B, 2001, 105, 12011-12018.	2.6	39
164	Exclusive Câ^'C Activation in the Rhodium(I) PCN Pincer Complex. A Computational Study. Organometallics, 2001, 20, 1783-1791.	2.3	34
165	Tautomerization and Dissociation of Dimethyl Phosphonate Ions(CH3O)2P(H)=Oâ€¢+:Theory and Experiment in Concert. Zeitschrift Fur Physikalische Chemie, 2001, 215, .	2.8	21
166	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
167	A fully ab initio potential curve of near-spectroscopic quality for OHâ^' ion: importance of connected quadruple excitations and scalar relativistic effects. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2001, 57, 875-885.	3.9	22
168	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
169	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
170	On the integration accuracy in molecular density functional theory calculations using Gaussian basis sets. Computer Physics Communications, 2001, 133, 189-201.	7.5	116
171	Fully ab initio atomization energy of benzene via Weizmann-2 theory. Journal of Chemical Physics, 2001, 115, 2051-2054.	3.0	39
172	W1 and W2 Theories, and Their Variants: Thermochemistry in the kJ/mol Accuracy Range. , 2001, , 31-65.		25
173	Anharmonic force field and vibrational frequencies of tetrafluoromethane (CF4) and tetrafluorosilane (SiF4). Journal of Chemical Physics, 2000, 112, 1353-1366.	3.0	64
174	The Silabenzenes:Â Structure, Properties, and Aromaticity. Organometallics, 2000, 19, 1477-1487.	2.3	115
175	Thermochemical analysis of core correlation and scalar relativistic effects on molecular atomization energies. Journal of Chemical Physics, 2000, 113, 1348-1358.	3.0	45
176	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
177	Why Does the Tetrakis(trimethylphosphine)iridium(III) Hydridochloride Cation Adopt the Sterically and Electronically UnfavorableCisGeometry?. Organometallics, 2000, 19, 4608-4612.	2.3	9
178	Discovery of the First Metallaquinone. Journal of the American Chemical Society, 2000, 122, 8797-8798.	13.7	55
179	Structures of Furanosides:â€‰ A Study of the Conformational Space of Methyl Î±-d-Lyxofuranoside by Density Functional Methods. Journal of Physical Chemistry A, 2000, 104, 5291-5297.	2.5	13
180	Electron affinities of the first- and second-row atoms: Benchmarkab initioand density-functional calculations. Physical Review A, 1999, 60, 1034-1045.	2.5	95

#	Article	IF	Citations
181	Benchmark ab initio thermochemistry of the isomers of diimide, N2H2, using accurate computed structures and anharmonic force fields. Molecular Physics, 1999, 96, 681-692.	1.7	41
182	A fully ab initio quartic force field of spectroscopic quality for SO3. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 1999, 55, 709-718.	3.9	31
183	The ground-state spectroscopic constants of Be2 revisited. Chemical Physics Letters, 1999, 303, 399-407.	2.6	77
184	Heat of atomization of sulfur trioxide, SO3: a benchmark for computational thermochemistry. Chemical Physics Letters, 1999, 310, 271-276.	2.6	53
185	Towards standard methods for benchmark quality ab initio thermochemistryâ€"W1 and W2 theory. Journal of Chemical Physics, 1999, 111, 1843-1856.	3.0	947
186	Accurateab initioanharmonic force field and heat of formation for silane. Molecular Physics, 1999, 97, 945-953.	1.7	30
187	Energetics of the naphthalene/azulene monocation isomerization: density functional and coupled cluster calculationsâ€Šâ€â€¡. Journal of the Chemical Society Perkin Transactions II, 1999, , 2383-2387.	0.9	14
188	Structures of Furanosides:Â Density Functional Calculations and High-Resolution X-ray and Neutron Diffraction Crystal Structures. Journal of Physical Chemistry A, 1999, 103, 744-753.	2.5	39
189	Boron Heat of Formation Revisited:Â Relativistic Effects on the BF3Atomization Energy. Journal of Physical Chemistry A, 1999, 103, 7715-7718.	2.5	33
190	A Definitive Heat of Vaporization of Silicon through Benchmarkab InitioCalculations on SiF4. Journal of Physical Chemistry A, 1999, 103, 4427-4431.	2.5	30
191	Ab Initio Thermochemistry Beyond Chemical Accuracy for First-and Second-Row Compounds. , 1999, , 373-415.		7
192	Benchmark ab initio thermochemistry of the isomers of diimide, N2H2, using accurate computed structures and anharmonic force fields. Molecular Physics, 1999, 96, 681-692.	1.7	4
193	Basis set convergence in second-row compounds. The importance of core polarization functions. Chemical Physics Letters, 1998, 282, 16-24.	2.6	191
194	Benchmark ab initio potential curves for the light diatomic hydrides. Unusually large nonadiabatic effects in BeH and BH. Chemical Physics Letters, 1998, 283, 283-293.	2.6	28
195	Modeling stabilization of Siî˜...O bonds by Pd/Pt complexes using density functional theory. Chemical Physics Letters, 1998, 288, 356-362.	2.6	11
196	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
197	Can Siî˜...O bonds be stabilized by Rh/Ir complexes?. Chemical Physics Letters, 1998, 290, 535-542.	2.6	6
198	The impact of larger clusters formation C5, C6, C7, C8, C9, and C10 on the rates of carbon sublimation at elevated temperatures. Journal of Nuclear Materials, 1998, 258-263, 782-786.	2.7	14

#	Article	IF	Citations
199	Ab InitioStudy of the Electronic Spectrum of the SiN Radical. Journal of Molecular Spectroscopy, 1998, 188, 27-36.	1.2	18
200	Anharmonic Force Fields and Accurate Thermochemistry of H2SiO,cis-HSiOH, andtrans-HSiOH. Journal of Physical Chemistry A, 1998, 102, 1394-1404.	2.5	37
201	Ab Initio Calibration Study of the Heat of Formation, Geometry, and Anharmonic Force Field of Fluoroacetylene. Journal of Physical Chemistry A, 1998, 102, 2483-2492.	2.5	35
202	Modeling Proton-Bound Methanol, Ammonia, and Amine Complexes of 12-Crown-4-Ether and Dimethoxyethane (â€œGlymeâ€) Using Density Functional Theory. Journal of Physical Chemistry A, 1998, 102, 6357-6365.	2.5	16
203	Calibration Study of Atomization Energies of Small Polyatomics. ACS Symposium Series, 1998, , 212-236.	0.5	18
204	Formation of Î·2 Câ^'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
205	Ab Initio Geometry Determinations of Proteins. 1. Crambin. Journal of Physical Chemistry A, 1998, 102, 2246-2251.	2.5	67
206	A purely ab initio spectroscopic quality quartic force field for acetylene. Journal of Chemical Physics, 1998, 108, 676-691.	3.0	128
207	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
208	Revised Heat of Formation for Gaseous Boron:Â Basis Set Limit ab Initio Binding Energies of BF3and BF. Journal of Physical Chemistry A, 1998, 102, 2995-2998.	2.5	34
209	Benchmark quality total atomization energies of small polyatomic molecules. Journal of Chemical Physics, 1997, 106, 8620-8623.	3.0	135
210	Structure and Vibrations of the C2P and CNP Radicals and Their Cations Using Density Functional and Coupled Cluster Theories. Journal of Physical Chemistry A, 1997, 101, 8319-8326.	2.5	19
211	Energetics of Acetylene Loss from C14H10â€¢+ Cations:â€‰ A Density Functional Calculation. Journal of Physical Chemistry A, 1997, 101, 219-226.	2.5	45
212	Insertion of Amines and Alcohols into Proton-Bound Dimers. A Density Functional Study. Journal of Physical Chemistry A, 1997, 101, 2597-2606.	2.5	19
213	Very accurate ab initio binding energies â€" a comparison between empirical corrections and extrapolation methods. Computational and Theoretical Chemistry, 1997, 398-399, 135-144.	1.5	27
214	Coupling between the convergence behavior of basis set and electron correlation: a quantitative study. Theoretical Chemistry Accounts, 1997, 97, 227-231.	1.4	25
215	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
216	Time-dependent mass spectra and breakdown graphs. 20. Bromoanthracene. Heat of formation of the anthracenyl ion. International Journal of Mass Spectrometry and Ion Processes, 1997, 160, 39-48.	1.8	8

#	Article	IF	Citations
217	Benchmark ab initio calculations of the total atomization energies of the first-row hydrides AHn (A =) Tj ETQq1 1 0.784314 rgBT /Ove	2.6	49
218	The harmonic frequencies of benzene. A case for atomic natural orbital basis sets. Chemical Physics Letters, 1997, 275, 414-422.	2.6	92
219	Designing low-ionization potential analogs of tetrakis-dimethylamino-ethylene using density functional calculations. Chemical Physics Letters, 1997, 279, 389-395.	2.6	8
220	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
221	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
222	Density-Functional Theory Concepts and Techniques for Studying Molecular Charge Distributions and Related Properties. Theoretical and Computational Chemistry, 1996, , 773-809.	0.4	32
223	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
224	The total atomization energy and heat of formation of HCN(g). Chemical Physics Letters, 1996, 259, 679-682.	2.6	44
225	The vibrational spectra of corannulene and coronene. A density functional study. Chemical Physics Letters, 1996, 262, 97-104.	2.6	38
226	Structure and vibrations of BnNn (n = 3â€“10). Chemical Physics Letters, 1996, 248, 95-101.	2.6	45
227	On the structure and vibrational frequencies of C20. Chemical Physics Letters, 1996, 248, 345-352.	2.6	77
228	The geometry, vibrational frequencies, and total atomization energy of ethylene. A calibration study. Chemical Physics Letters, 1996, 248, 336-344.	2.6	153
229	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
230	Ab initio study of the X2Î£+ and A2Î states of the SiN radical. Chemical Physics Letters, 1996, 252, 398-404.	2.6	36
231	On the structure and vibrational frequencies of C24. Chemical Physics Letters, 1996, 255, 7-14.	2.6	54
232	C28: the smallest stable fullerene?. Chemical Physics Letters, 1996, 255, 1-6.	2.6	36
233	Calculation of molecular electrostatic potentials and Fukui functions using density functional methods. Chemical Physics Letters, 1996, 256, 400-408.	2.6	167
234	The atomization energy and proton affinity of NH3. An ab initio calibration study. Chemical Physics Letters, 1996, 258, 136-143.	2.6	185

#	Article	IF	Citations
235	Ab initio total atomization energies of small molecules â€" towards the basis set limit. Chemical Physics Letters, 1996, 259, 669-678.	2.6	733
236	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
237	Structure and Vibrations of Small Carbon Clusters from Coupled-Cluster Calculations. The Journal of Physical Chemistry, 1996, 100, 6047-6056.	2.9	155
238	Is there evidence for detection of cyclic C4 in IR spectra? An accurate ab initio computed quartic force field. Journal of Chemical Physics, 1996, 104, 4657-4663.	3.0	42
239	Accurate ab-Initio Quartic Force Fields for the Sulfur Compounds H2S, CS2, OCS, and CS. Journal of Molecular Spectroscopy, 1995, 169, 445-457.	1.2	36
240	Structures and thermochemistry of B3N3 and B4N4. Chemical Physics Letters, 1995, 232, 289-294.	2.6	39
241	On the vibrational spectrum of C9, C11 and C13. Chemical Physics Letters, 1995, 240, 521-525.	2.6	25
242	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
243	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
244	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
245	Accurate ab initio total atomization energies of the Cn clusters (n=2â€"10). Journal of Chemical Physics, 1995, 102, 8270-8273.	3.0	41
246	The structure and energetics of B3N2, B2N3, and BN4. Molecular Physics, 1995, 85, 527-537.	1.7	24
247	Accurate ab Initio Quartic Force Fields, Vibrational Frequencies, and Heats of Formation for FCN, FNC, ClCN, and ClNC. The Journal of Physical Chemistry, 1995, 99, 15858-15863.	2.9	35
248	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
249	Infrared Spectra of Boron-Ammonia Reaction Products in Solid Argon. The Journal of Physical Chemistry, 1995, 99, 13839-13849.	2.9	65
250	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
251	The structure, energetics, and harmonic vibrations of B3N and BN3. Molecular Physics, 1994, 82, 155-164.	1.7	25
252	Matrix Infrared Spectrum and ab Initio Calculations on the PNP Radical. The Journal of Physical Chemistry, 1994, 98, 10706-10709.	2.9	3

#	Article	IF	Citations
253	Ab Initio Study of the Isoelectronic Molecules BCN, BNC, and C3 Including Anharmonicity. The Journal of Physical Chemistry, 1994, 98, 6105-6109.	2.9	26
254	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
255	The Anharmonic Force Field of Thioformaldehyde, H2CS, by ab Initio Methods. Journal of Molecular Spectroscopy, 1994, 168, 363-373.	1.2	26
256	Ab initio study of the spectroscopy, kinetics, and thermochemistry of the BN2 molecule. Chemical Physics Letters, 1994, 222, 517-523.	2.6	19
257	Ab initio study of the spectroscopy and thermochemistry of the C2N and CN2 molecules. Chemical Physics Letters, 1994, 226, 475-483.	2.6	64
258	Concerning the heats of formation of the [C, H3, N]+ radical cations. Chemical Physics Letters, 1994, 221, 149-155.	2.6	20
259	Basis set convergence for geometry and harmonic frequencies. Are h functions enough?. Chemical Physics Letters, 1994, 225, 473-479.	2.6	208
260	Abinitiostudy of the molecules BC and B2C. Journal of Chemical Physics, 1994, 100, 9002-9006.	3.0	39
261	Accurate ab Initio Quartic Force Fields and Thermochemistry of FNO and ClNO. The Journal of Physical Chemistry, 1994, 98, 11394-11400.	2.9	22
262	An Accurate ab Initio Quartic Force Field for Formaldehyde and Its Isotopomers. Journal of Molecular Spectroscopy, 1993, 160, 105-116.	1.2	115
263	Accurate ab initio quartic force fields for the N2O and CO2 molecules. Chemical Physics Letters, 1993, 205, 535-542.	2.6	76
264	The structure, energetics and harmonic vibrations of B3N. Chemical Physics Letters, 1993, 201, 54-58.	2.6	22
265	The mechanism of the reaction CH+N2â†'HCN+N. Chemical Physics Letters, 1993, 209, 143-150.	2.6	40
266	On the relative stabilities of the linear and triangular forms of B3N. Chemical Physics, 1993, 178, 77-82.	1.9	12
267	The impact of quantum chemical methods on the interpretation of molecular spectra of carbon clusters. Journal of Molecular Structure, 1993, 294, 21-24.	3.6	25
268	Why computed entropies of quasi-linear species are sometimes random?. Computational and Theoretical Chemistry, 1993, 280, 83-87.	1.5	0
269	Accurateab initioquartic force fields for the ions HCO+and HOC+. Journal of Chemical Physics, 1993, 99, 286-292.	3.0	56
270	Boron atom reactions with acetylene. Ab initio calculated and observed isotopic infrared spectra of the borirene radical BC2H2. A fingerprint match. Journal of the American Chemical Society, 1993, 115, 2510-2511.	13.7	35

#	Article	IF	Citations
271	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
272	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
273	The protonation of N2O reexamined: A case study on the reliability of various electron correlation methods for minima and transition states. Journal of Chemical Physics, 1993, 98, 7951-7957.	3.0	27
274	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
275	Boron atom reactions with acetylene. Ab initio calculated and observed isotopic infrared spectra of the borirene radical BC2H2. A fingerprint match. AIP Conference Proceedings, 1993, , .	0.4	2
276	First principles computation of thermochemical properties beyond the harmonic approximation. II. Application to the amino radical NH2. Journal of Chemical Physics, 1992, 97, 3530-3536.	3.0	17
277	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
278	Ab initio multireference study of the BN molecule. Journal of Chemical Physics, 1992, 97, 6549-6556.	3.0	77
279	An accurate ab initio quartic force field for ammonia. Journal of Chemical Physics, 1992, 97, 8361-8371.	3.0	122
280	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
281	Accurate ab initio quartic force fields for borane and BeH2. Chemical Physics Letters, 1992, 200, 502-510.	2.6	57
282	Potential energy surface of B4 and total atomization energies of B2, B3, and B4. Chemical Physics Letters, 1992, 189, 529-536.	2.6	57
283	The structure, stability, and infrared spectrum of B2N, B2N+, B2Nâ^', BO, B2O and B2N2.. Chemical Physics Letters, 1992, 193, 243-250.	2.6	49
284	Ab initio study of the carbon (C3+) cation using multireference methods. The Journal of Physical Chemistry, 1991, 95, 6530-6534.	2.9	22
285	Structure and infrared spectroscopy of the C11 molecule. Chemical Physics Letters, 1991, 187, 367-374.	2.6	45
286	The rotational partition function of the symmetric top and the effect of K doubling thereon. Chemical Physics Letters, 1991, 187, 375-386.	2.6	5
287	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
288	Ab initio spectroscopy and thermochemistry of the BN molecule. Zeitschrift FÃ¼r Physik D-Atoms Molecules and Clusters, 1991, 21, 47-55.	1.0	14

#	Article	IF	Citations
289	Abinitiostudy of the structure, infrared spectra, and heat of formation of C4. Journal of Chemical Physics, 1991, 94, 3753-3761.	3.0	66
290	On the effect of centrifugal stretching on the rotational partition function of an asymmetric top. Journal of Chemical Physics, 1991, 95, 8374-8389.	3.0	20
291	On the heat of formation of C5 and higher carbon clusters. Journal of Chemical Physics, 1991, 95, 9420-9421.	3.0	27
292	Theoretical study of the proton affinities of 2-, 3-, and 4-monosubstituted phenolate ions in the gas phase by means of MINDO/3, MNDO, and AM1. Journal of Computational Chemistry, 1990, 11, 269-290.	3.3	21
293	Unusually large effects of single excitations on the geometry of radical species and limiting spin-projection invariance of some correlated methods. Chemical Physics Letters, 1990, 166, 295-302.	2.6	9
294	On size-consistency corrections for limited configuration-interaction calculations. Chemical Physics Letters, 1990, 172, 346-353.	2.6	19
295	Some cost-effective approximations to CCSD and QCISD. Chemical Physics Letters, 1990, 172, 354-360.	2.6	8
296	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
297	Accurate ab initio spectroscopic and thermodynamic properties for the SiC molecule. Journal of Chemical Physics, 1990, 92, 6655-6667.	3.0	29
298	The dissociation energy of N3. Journal of Chemical Physics, 1990, 93, 4485-4487.	3.0	31
299	On the geometrical structure of the C+3 cationâ€”an ab initio study. Journal of Chemical Physics, 1990, 93, 5037-5045.	3.0	29
300	Note on the vibrational spectrum of C4 and C5. Journal of Chemical Physics, 1989, 90, 3403-3405.	3.0	51
301	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
302	Combined bond polarization function basis sets for accurate ab initio calculation of the dissociation energies of AHnmolecules (A=LI to F). Journal of Computational Chemistry, 1989, 10, 152-162.	3.3	25
303	Ab initiostudy of the proton affinity of a number of ortho-substituted pyridines. Journal of Computational Chemistry, 1989, 10, 346-357.	3.3	21
304	Theoretical study of the proton affinities of 2-, 3-, and 4-monosubstituted pyridines in the gas phase by means of MINDO/3, MNDO, and AM1. Journal of Computational Chemistry, 1989, 10, 449-467.	3.3	38
305	Combined bond-polarization basis sets for accurate determination of dissociation energies. II. Basis set superposition error as a function of the parent basis set. Journal of Computational Chemistry, 1989, 10, 875-886.	3.3	30
306	Accurate ab initio predictions of the dissociation energy and heat of formation of first-row hydrides. Chemical Physics Letters, 1989, 163, 387-391.	2.6	33

#	Article	IF	Citations
307	On the validity of Pople's infinite-order MÃ¸ller-Plesset extrapolation and an alternative formula within MBP/CC theories. Chemical Physics Letters, 1989, 157, 217-223.	2.6	12
308	Combined bond-polarization basis sets for accurate determination of dissociation energies. Theoretica Chimica Acta, 1989, 76, 195-209.	0.8	38
309	Comment on â€˜â€˜A theoretical study of the dissociation energy of BH using quadratic configuration interactionâ€™â€™. Journal of Chemical Physics, 1989, 91, 4425-4426.	3.0	15