Peter M W Gill

List of Publications by Year
in descending order

189 papers	18,818 citations	34105 52 h-index	11939 134 g-index
190 all docs	190 docs citations	190 times ranked	12121 citing authors

#	Article	IF	Citations
1	Software for the frontiers of quantum chemistry: An overview of developments in the Q-Chem 5 package. Journal of Chemical Physics, 2021, 155, 084801.	3.0	518
2	Q-MP2-OS: MÃ¸llerâ€“Plesset Correlation Energy by Quadrature. Journal of Chemical Theory and Computation, 2020, 16, 1568-1577.	5.3	9
3	Assessment of DFT Methods for Transition Metals with the TMC151 Compilation of Data Sets and Comparison with Accuracies for Main-Group Chemistry. Journal of Chemical Theory and Computation, 2019, 15, 3610-3622.	5.3	85
4	Tribute to Leo Radom. Journal of Physical Chemistry A, 2019, 123, 10347-10347.	2.5	0
5	Efficient Method for Calculating Effective Core Potential Integrals. Journal of Physical Chemistry A, 2018, 122, 3066-3075.	2.5	10
6	Simple Models for Difficult Electronic Excitations. Journal of Chemical Theory and Computation, 2018, 14, 1501-1509.	5.3	133
7	Excitation Number: Characterizing Multiply Excited States. Journal of Chemical Theory and Computation, 2018, 14, 9-13.	5.3	39
8	Molecular electronic structure in one-dimensional Coulomb systems. Physical Chemistry Chemical Physics, 2017, 19, 3987-3998.	2.8	8
9	Two-Electron Integrals over Gaussian Geminals. Journal of Chemical Theory and Computation, 2016, 12, 4915-4924.	5.3	15
10	The uniform electron gas. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2016, 6, 410-429.	14.6	98
11	Many-Electron Integrals over Gaussian Basis Functions. I. Recurrence Relations for Three-Electron Integrals. Journal of Chemical Theory and Computation, 2016, 12, 1735-1740.	5.3	13
12	Communication: Three-electron coalescence points in two and three dimensions. Journal of Chemical Physics, 2015, 143, 181101.	3.0	7
13	Uniform electron gases. III. Low-density gases on three-dimensional spheres. Journal of Chemical Physics, 2015, 143, 084114.	3.0	10
14	Chem1D: a software package for electronic structure calculations on one-dimensional systems. Molecular Physics, 2015, 113, 1843-1857.	1.7	6
15	MP2[V] â€“ A Simple Approximation to Second-Order MÃ¸llerâ€“Plesset Perturbation Theory. Journal of Chemical Theory and Computation, 2015, 11, 1639-1644.	5.3	7
16	Chemistry in one dimension. Physical Chemistry Chemical Physics, 2015, 17, 3196-3206.	2.8	15
17	Advances in molecular quantum chemistry contained in the Q-Chem 4 program package. Molecular Physics, 2015, 113, 184-215.	1.7	2,561
18	Basis functions for electronic structure calculations on spheres. Journal of Chemical Physics, 2014, 141, 244102.	3.0	6

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19	Uniform electron gases. II. The generalized local density approximation in one dimension. Journal of Chemical Physics, 2014, 140, 18A524.	3.0	21
20	Exact wave functions for concentric two-electron systems. Physics Letters, Section A: General, Atomic and Solid State Physics, 2014, 378, 329-333.	2.1	4
21	Communication: Hartree-Fock description of excited states of H2. Journal of Chemical Physics, 2014, 141, 111104.	3.0	50
22	Performance of Density Functional Theory Procedures for the Calculation of Proton-Exchange Barriers: Unusual Behavior of M06-Type Functionals. Journal of Chemical Theory and Computation, 2014, 10, 3777-3783.	5.3	44
23	Mixed Rampâ€“Gaussian Basis Sets. Journal of Chemical Theory and Computation, 2014, 10, 4369-4376.	5.3	17
24	Resolutions of the Coulomb Operator: VII.ÂEvaluationÂofÂLong-RangeÂCoulombÂandÂExchangeÂMatrices. Journal of Chemical Theory and Computation, 2013, 9, 863-867.	5.3	6
25	Qâ€Chem: an engine for innovation. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2013, 3, 317-326.	14.6	287
26	Uniform electron gases. I. Electrons on a ring. Journal of Chemical Physics, 2013, 138, 164124.	3.0	31
27	Distribution of r12Â· p12in quantum systems. Molecular Physics, 2013, 111, 2414-2426.	1.7	6
28	Performance of Gradient-Corrected and Hybrid Density Functional Theory: Role of the Underlying Local Density Approximation and the Gradient Correction. Journal of Chemical Theory and Computation, 2012, 8, 4899-4906.	5.3	16
29	Harmonically trapped jellium. Molecular Physics, 2012, 110, 2337-2342.	1.7	7
30	Gaussian Expansions of Orbitals. Journal of Chemical Theory and Computation, 2012, 8, 4891-4898.	5.3	20
31	Distributions of r₁Â·r₂ and p₁Â·p₂ in Atoms. Journal of Chemical Theory and Computation, 2012, 8, 1657-1662.	5.3	8
32	Resolutions of the Coulomb operator. VI. Computation of auxiliary integrals. Journal of Chemical Physics, 2012, 136, 104102.	3.0	11
33	Leadingâ€order behavior of the correlation energy in the uniform electron gas. International Journal of Quantum Chemistry, 2012, 112, 1712-1716.	2.0	8
34	A remarkable identity involving Bessel functions. Proceedings of the Royal Society A: Mathematical, Physical and Engineering Sciences, 2012, 468, 2667-2681.	2.1	9
35	Exact Wave Functions of Two-Electron Quantum Rings. Physical Review Letters, 2012, 108, 083002.	7.8	53
36	Uniform electron gases. Theoretical Chemistry Accounts, 2012, 131, 1.	1.4	31

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37	Uniform electron gases. , 2012, , 121-129.		0
38	Intracule functional models. V. Recurrence relations for two-electron integrals in position and momentum space. Physical Chemistry Chemical Physics, 2011, 13, 2972-2978.	2.8	20
39	Resolutions of the Coulomb Operator: V. The Long-Range Ewald Operator. Journal of Chemical Theory and Computation, 2011, 7, 2353-2357.	5.3	10
40	Intracule functional models. Annual Reports on the Progress of Chemistry Section C, 2011, 107, 229.	4.4	14
41	Resolutions of the Coulomb Operator: IV. The Spherical Bessel Quasi-Resolution. Journal of Chemical Theory and Computation, 2011, 7, 830-833.	5.3	10
42	The nature of electron correlation in a dissociating bond. Journal of Chemical Physics, 2011, 134, 224103.	3.0	24
43	The two faces of static correlation. Journal of Chemical Physics, 2011, 134, 114111.	3.0	103
44	Communication: A new approach to dual-basis second-order MÃ¸llerâ€“Plesset calculations. Journal of Chemical Physics, 2011, 134, 081103.	3.0	15
45	Thinking outside the box: The uniform electron gas on a hypersphere. Journal of Chemical Physics, 2011, 135, 214111.	3.0	28
46	Correlation energy of anisotropic quantum dots. Physical Review A, 2011, 84, .	2.5	8
47	Exact energy of the spin-polarized two-dimensional electron gas at high density. Physical Review B, 2011, 83, .	3.2	14
48	Correlation energy of the spin-polarized uniform electron gas at high density. Physical Review B, 2011, 84, .	3.2	22
49	Intracule Functional Theory. , 2011, , 1-23.		2
50	Communication: Efficient counterpoise corrections by a perturbative approach. Journal of Chemical Physics, 2011, 135, 081105.	3.0	10
51	A tale of two electrons: Correlation at high density. Chemical Physics Letters, 2010, 500, 1-8.	2.6	30
52	Invariance of the Correlation Energy at High Density and Large Dimension in Two-Electron Systems. Physical Review Letters, 2010, 105, 113001.	7.8	31
53	Hartreeâ€“Fock perturbative corrections for total and reaction energies. Journal of Chemical Physics, 2010, 133, 044116.	3.0	11
54	Ground state of two electrons on concentric spheres. Physical Review A, 2010, 81, .	2.5	19

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55	Distribution ofrÂ·pin Atomic Systems. Journal of Physical Chemistry A, 2010, 114, 11984-11991.	2.5	2
56	Posmom: The Unobserved Observable. Journal of Physical Chemistry Letters, 2010, 1, 1254-1258.	4.6	8
57	Correlation energy of two electrons in a ball. Journal of Chemical Physics, 2010, 132, 234111.	3.0	24
58	Excited states of spherium. Molecular Physics, 2010, 108, 2527-2532.	1.7	40
59	Diagnostics of molecular orbital quality. Canadian Journal of Chemistry, 2010, 88, 754-758.	1.1	2
60	Density functional triple jumping. Physical Chemistry Chemical Physics, 2010, 12, 10759.	2.8	14
61	Can correlation bring electrons closer together?. Molecular Physics, 2009, 107, 1089-1093.	1.7	30
62	Intracule functional models. IV. Basis set effects. Journal of Chemical Physics, 2009, 130, 164110.	3.0	22
63	The distribution ofrÂ·pin quantum mechanical systems. New Journal of Physics, 2009, 11, 083015.	2.9	9
64	An efficient algorithm for the generation of two-electron repulsion integrals over gaussian basis functions. International Journal of Quantum Chemistry, 2009, 36, 269-280.	2.0	29
65	Rydberg states of the helium atom. International Journal of Quantum Chemistry, 2009, 109, 1915-1919.	2.0	12
66	Resolutions of the Coulomb operator: II. The Laguerre generator. Chemical Physics, 2009, 356, 86-90.	1.9	30
67	Ground state of two electrons on a sphere. Physical Review A, 2009, 79, .	2.5	54
68	Two Electrons on a Hypersphere: A Quasiexactly Solvable Model. Physical Review Letters, 2009, 103, 123008.	7.8	83
69	Correlation energy of two electrons in the high-density limit. Journal of Chemical Physics, 2009, 131, 241101.	3.0	35
70	Approaching the Hartreeâ€“Fock limit by perturbative methods. Journal of Chemical Physics, 2009, 130, 231101.	3.0	25
71	Self-consistent-field calculations of core excited states. Journal of Chemical Physics, 2009, 130, 124308.	3.0	254
72	Resolutions of the Coulomb operator : Part III. Reduced-rank SchrÃ¶dinger equations. Physical Chemistry Chemical Physics, 2009, 11, 9176.	2.8	15

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73	The role of exchange in systematic DFT errors for some organic reactions. Physical Chemistry Chemical Physics, 2009, 11, 1138.	2.8	60
74	Calculating molecular vibrational spectra beyond the harmonic approximation. Theoretical Chemistry Accounts, 2008, 120, 23-35.	1.4	61
75	Explicit-r12 correlation methods and local correlation methods. Physical Chemistry Chemical Physics, 2008, 10, 3318.	2.8	9
76	Variable Scan Rate Cyclic Voltammetry and Theoretical Studies on Tocopherol (Vitamin E) Model Compounds. Journal of Physical Chemistry B, 2008, 112, 6847-6855.	2.6	22
77	Self-Consistent Field Calculations of Excited States Using the Maximum Overlap Method (MOM). Journal of Physical Chemistry A, 2008, 112, 13164-13171.	2.5	435
78	Resolutions of the Coulomb operator. Journal of Chemical Physics, 2008, 128, 201104.	3.0	31
79	Intracule functional models : Part III. The dot intracule and its Fourier transform. Physical Chemistry Chemical Physics, 2008, 10, 3447.	2.8	22
80	Long-Lived Radical Cations as Model Compounds for the Reactive One-Electron Oxidation Product of Vitamin E. Journal of Physical Chemistry B, 2008, 112, 10367-10374.	2.6	19
81	A generalized Poisson equation and short-range self-interaction energies. Journal of Chemical Physics, 2008, 128, 241101.	3.0	3
82	Computation and interpretation of molecular Omega intracules. Journal of Chemical Physics, 2007, 127, 014101.	3.0	18
83	Intracule functional models. II. Analytically integrable kernels. Journal of Chemical Physics, 2007, 127, 141103.	3.0	27
84	Intracule functional models: I. Angle-corrected correlation kernels. Physical Chemistry Chemical Physics, 2007, 9, 5340.	2.8	21
85	Self-Consistent Hartree-Fock-Wigner Calculations: A Two-Electron-Density Functional Theory. ACS Symposium Series, 2007, , 27-35.	0.5	0
86	BFW:Â A Density Functional for Transition Metal Clusters. Journal of Physical Chemistry A, 2007, 111, 2625-2628.	2.5	8
87	Picosecond time-resolved infrared study of 2-aminopurine ionisation in solution. Photochemical and Photobiological Sciences, 2007, 6, 949.	2.9	4
88	Efficient calculation ofp-values in linear-statistic permutation significance tests. Journal of Statistical Computation and Simulation, 2007, 77, 55-61.	1.2	24
89	Interfacing Q-Chem and CHARMM to perform QM/MM reaction path calculations. Journal of Computational Chemistry, 2007, 28, 1485-1502.	3.3	190
90	A point-charge model for electrostatic potentials based on a local projection of multipole moments. Molecular Simulation, 2006, 32, 1249-1253.	2.0	6

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91	A family of intracules, a conjecture and the electron correlation problem. Physical Chemistry Chemical Physics, 2006, 8, 15-25.	2.8	61
92	Highly Oxidized Ruthenium Organometallic Compounds. The Synthesis and One-Electron Electrochemical Oxidation of [Cp*RuIVCl2(S2CR)] (Cp* = Î·5-C5Me5, R = NMe2, NEt2, OiPr). Organometallics, 2006, 25, 6134-6141.	2.3	16
93	Advances in methods and algorithms in a modern quantum chemistry program package. Physical Chemistry Chemical Physics, 2006, 8, 3172-3191.	2.8	2,597
94	SG-0: A small standard grid for DFT quadrature on large systems. Journal of Computational Chemistry, 2006, 27, 730-739.	3.3	40
95	Finite jellium models. I. Restricted Hartreeâ€“Fock calculations. Journal of Chemical Physics, 2005, 122, 154108.	3.0	9
96	Decay behavior of least-squares coefficients in auxiliary basis expansions. Journal of Chemical Physics, 2005, 123, 061101.	3.0	17
97	Electron correlation in Hookeâ€™s law atom in the high-density limit. Journal of Chemical Physics, 2005, 122, 094110.	3.0	36
98	Benchmark correlation energies for small molecules. Molecular Physics, 2005, 103, 763-766.	1.7	48
99	Auxiliary basis expansions for large-scale electronic structure calculations. Proceedings of the National Academy of Sciences of the United States of America, 2005, 102, 6692-6697.	7.1	184
100	Transformation of Î±-Tocopherol (Vitamin E) and Related Chromanol Model Compounds into Their Phenoxonium Ions by Chemical Oxidation with the Nitrosonium Cation. Journal of Organic Chemistry, 2005, 70, 10466-10473.	3.2	63
101	An optimal point-charge model for molecular electrostatic potentials. Molecular Physics, 2005, 103, 2789-2793.	1.7	15
102	Atomic and molecular intracules for excited states. Journal of Chemical Physics, 2004, 120, 7290-7297.	3.0	19
103	The role of vibrational doorway states in positron annihilation with large molecules. Nuclear Instruments & Methods in Physics Research B, 2004, 221, 30-35.	1.4	25
104	Wigner intracule for the Kellner helium-like ions. International Journal of Quantum Chemistry, 2004, 100, 166-171.	2.0	10
105	Extracting atoms from molecular electron densities via integral equations. Journal of Chemical Physics, 2004, 120, 7887-7893.	3.0	14
106	Remembrance: John A. Pople (1925â€“2004). Journal of Chemical Physics, 2004, 120, 9445-9445.	3.0	2
107	EDF2: A Density Functional for Predicting Molecular Vibrational Frequencies. Australian Journal of Chemistry, 2004, 57, 365.	0.9	139
108	Radial quadrature for multiexponential integrands. Journal of Computational Chemistry, 2003, 24, 732-740.	3.3	39

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109	Stereoselective Association of Binuclear Metallacycles in Coordination Polymers. Journal of the American Chemical Society, 2003, 125, 6753-6761.	13.7	106
110	Wave functions and two-electron probability distributions of the Hookeâ€™s-law atom and helium. Physical Review A, 2003, 68, .	2.5	45
111	Two-electron distribution functions and intracules. Theoretical Chemistry Accounts, 2003, 109, 241-250.	1.4	45
112	Empirical density functional and the adsorption of organic molecules on Si(100). Physical Review B, 2003, 67, .	3.2	18
113	Computation of molecular Hartreeâ€“Fock Wigner intracules. Journal of Chemical Physics, 2003, 118, 2033-2038.	3.0	21
114	Probing the Reactivity of Photoinitiators for Free Radical Polymerization:Â Time-Resolved Infrared Spectroscopic Study of Benzoyl Radicals. Journal of the American Chemical Society, 2002, 124, 14952-14958.	13.7	128
115	Computation and analysis of molecular Hartreeâ€”Fock momentum intracules. Molecular Physics, 2002, 100, 1763-1770.	1.7	20
116	Title is missing!. Australian Journal of Chemistry, 2001, 54, 661.	0.9	39
117	Rapid evaluation of two-center two-electron integrals. Journal of Computational Chemistry, 2000, 21, 1505-1510.	3.3	9
118	Q-Chem 2.0: a high-performanceab initio electronic structure program package. Journal of Computational Chemistry, 2000, 21, 1532-1548.	3.3	617
119	Parallelization of SCF calculations within Q-Chem. Computer Physics Communications, 2000, 128, 170-177.	7.5	23
120	Methods for constructing Stewart atoms. Computational and Theoretical Chemistry, 2000, 500, 363-374.	1.5	6
121	Insights from Coulomb and exchange intracules. Computational and Theoretical Chemistry, 2000, 506, 303-312.	1.5	26
122	Q-Chem 2.0: a high-performance ab initio electronic structure program package. , 2000, 21, 1532.		2
123	Rapid evaluation of twoâ€center twoâ€electron integrals. Journal of Computational Chemistry, 2000, 21, 1505-1510.	3.3	1
124	Decomposition of exchange-correlation energies. Chemical Physics Letters, 1999, 312, 511-521.	2.6	4
125	Computation of Coulomb and exchange radial intracule densities. Chemical Physics Letters, 1999, 313, 271-278.	2.6	28
126	Efficient calculation of short-range Coulomb energies. Journal of Computational Chemistry, 1999, 20, 921-927.	3.3	68

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127	Empirical density functionals. Chemical Physics Letters, 1998, 284, 6-11.	2.6	95
128	Coulomb energies via Stewart densities. Chemical Physics Letters, 1998, 286, 226-232.	2.6	10
129	A tensor approach to two-electron matrix elements. Journal of Chemical Physics, 1997, 107, 124-131.	3.0	31
130	Optimal partition of the Coulomb operator. Physical Review A, 1997, 55, 3233-3235.	2.5	23
131	Effects of Coulomb attenuation on chemical properties. Computational and Theoretical Chemistry, 1997, 398-399, 45-54.	1.5	6
132	A new expansion of the Coulomb interaction. Chemical Physics Letters, 1997, 270, 193-195.	2.6	27
133	An ab initio study of anharmonicity and matrix effects on the hydrogen-bonded BrH:NH3 complex. Molecular Physics, 1997, 92, 429-439.	1.7	36
134	A new gradient-corrected exchange functional. Molecular Physics, 1996, 89, 433-445.	1.7	203
135	Coulomb-attenuated exchange energy density functionals. Molecular Physics, 1996, 88, 1005-1009.	1.7	181
136	Advances in methodologies for linear-scaling density functional calculations. Theoretical and Computational Chemistry, 1996, 4, 441-463.	0.4	17
137	Comment on â€œa generalized fast multipole approach for Hartree-Fock and density functional computationsâ€• Chemical Physics Letters, 1996, 248, 482-483.	2.6	9
138	Linear scaling density functional calculations via the continuous fast multipole method. Chemical Physics Letters, 1996, 253, 268-278.	2.6	327
139	Chemistry without Coulomb tails. Chemical Physics Letters, 1996, 254, 329-336.	2.6	72
140	A family of attenuated Coulomb operators. Chemical Physics Letters, 1996, 261, 105-110.	2.6	69
141	Density Functional Partitions. The Journal of Physical Chemistry, 1996, 100, 6348-6353.	2.9	8
142	KWIK:â€‰ Coulomb Energies in O(N) Work. The Journal of Physical Chemistry, 1996, 100, 6272-6276.	2.9	61
143	Extraction of Stewart Atoms from Electron Densities. The Journal of Physical Chemistry, 1996, 100, 15421-15427.	2.9	33
144	Coulomb-attenuated exchange energy density functionals. Molecular Physics, 1996, 88, 1005-1010.	1.7	30

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145	Spin-unrestricted character of Kohn-Sham orbitals for open-shell systems. International Journal of Quantum Chemistry, 1995, 56, 303-305.	2.0	205
146	Beckeâ€“Wigner : a simple but powerful density functional. Journal of the Chemical Society, Faraday Transactions, 1995, 91, 4337-4341.	1.7	17
147	A simple yet powerful upper bound for Coulomb integrals. Chemical Physics Letters, 1994, 217, 65-68.	2.6	43
148	Reply to Comment on â€œComputing molecular electrostatic potentials with the PRISM algorithmâ€. Chemical Physics Letters, 1994, 218, 595-596.	2.6	0
149	Isomers of C24. Density functional studies including gradient corrections. Chemical Physics Letters, 1994, 220, 385-390.	2.6	85
150	A rotationally invariant procedure for density functional calculations. Chemical Physics Letters, 1994, 220, 377-384.	2.6	36
151	The continuous fast multipole method. Chemical Physics Letters, 1994, 230, 8-16.	2.6	370
152	A density functional study of the simplest hydrogen abstraction reaction. Effect of self-interaction correction. Chemical Physics Letters, 1994, 221, 100-108.	2.6	334
153	Molecular integrals Over Gaussian Basis Functions. Advances in Quantum Chemistry, 1994, 25, 141-205.	0.8	192
154	A standard grid for density functional calculations. Chemical Physics Letters, 1993, 209, 506-512.	2.6	438
155	An improved criterion for evaluating the efficiency of two-electron integral algorithms. Chemical Physics Letters, 1993, 206, 225-228.	2.6	13
156	The efficient transformation of (m0|n0) to (ab|cd) two-electron repulsion integrals. Chemical Physics Letters, 1993, 206, 229-238.	2.6	26
157	Computing molecular electrostatic potentials with the PRISM algorithm. Chemical Physics Letters, 1993, 206, 239-246.	2.6	66
158	Isomers of C20. Dramatic effect of gradient corrections in density functional theory. Chemical Physics Letters, 1993, 214, 357-361.	2.6	144
159	The performance of a family of density functional methods. Journal of Chemical Physics, 1993, 98, 5612-5626.	3.0	1,809
160	Exact exchange functional for the hydrogen atom. Physical Review A, 1993, 47, 2383-2385.	2.5	37
161	Modeling the potential of a charge distribution. Journal of Chemical Physics, 1992, 96, 7178-7179.	3.0	49
162	Preliminary results on the performance of a family of density functional methods. Journal of Chemical Physics, 1992, 97, 7846-7848.	3.0	119

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163	An investigation of the performance of a hybrid of Hartree-Fock and density functional theory. International Journal of Quantum Chemistry, 1992, 44, 319-331.	2.0	200
164	Kohnâ€"Sham density-functional theory within a finite basis set. Chemical Physics Letters, 1992, 199, 557-560.	2.6	437
165	The performance of the Beckeâ€"Leeâ€"Yangâ€"Parr (Bâ€"LYP) density functional theory with various basis sets. Chemical Physics Letters, 1992, 197, 499-505.	2.6	875
166	The structure and stability of the O2+2 dication: a dramatic failure of MÃ¸llerâ€"Plesset perturbation theory. Chemical Physics Letters, 1991, 182, 216-224.	2.6	78
167	Two-electron repulsion integrals over Gaussians functions. International Journal of Quantum Chemistry, 1991, 40, 745-752.	2.0	93
168	The prism algorithm for two-electron integrals. International Journal of Quantum Chemistry, 1991, 40, 753-772.	2.0	129
169	Exact and approximate solutions to the one-center McMurchie-Davidson tree-search problem. International Journal of Quantum Chemistry, 1991, 40, 809-827.	2.0	30
170	Efficient computation of two-electron - repulsion integrals and their nth-order derivatives using contracted Gaussian basis sets. The Journal of Physical Chemistry, 1990, 94, 5564-5572.	2.9	88
171	Structures and stabilities of the dimer dications of first- and second-row hydrides. Journal of the American Chemical Society, 1989, 111, 4613-4622.	13.7	34
172	The hemibonded dimer radical cation of thiirane. Journal of the American Chemical Society, 1989, 111, 2782-2785.	13.7	24
173	The ACDCP model for estimating the kinetic energy release and transition structure bond length in the fragmentation of a diatomic dication. Chemical Physics Letters, 1988, 147, 213-218.	2.6	52
174	An algorithm for the location of branching points on reaction paths. Journal of Computational Chemistry, 1988, 9, 465-475.	3.3	98
175	How well can RMP4 theory treat homolytic fragmentations?. Chemical Physics Letters, 1988, 148, 541-549.	2.6	20
176	Simple models for describing the fragmentation behavior of multiply charged cations. International Journal of Quantum Chemistry, 1988, 34, 567-573.	2.0	9
177	Structures and stabilities of singly charged three-electron hemibonded systems and their hydrogen-bonded isomers. Journal of the American Chemical Society, 1988, 110, 4931-4941.	13.7	194
178	Application of semiempirical molecular orbital theory to cationic intermediates involved in the solvolysis of 1-halobicyclo[n.1.1]alkanes. Journal of Organic Chemistry, 1988, 53, 4354-4357.	3.2	13
179	How does a dication lose a proton?. Journal of the American Chemical Society, 1988, 110, 5311-5314.	13.7	36
180	Why does unrestricted Mo/llerâ€"Plesset perturbation theory converge so slowly for spinâ€contaminated wave functions?. Journal of Chemical Physics, 1988, 89, 7307-7314.	3.0	109

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181	Multiply-charged cations: remarkable structures and stabilities. Pure and Applied Chemistry, 1988, 60, 183-188.	1.9	30
182	6-311G(MC)(d,p): a second-row analogue of the 6-311G(d,p) basis set: calculated heats of formation for second-row hydrides. The Journal of Physical Chemistry, 1988, 92, 4875-4880.	2.9	78
183	Fragmentation Mechanisms for Multiply-Charged Cations. , 1988, , 219-225.		1
184	A rationalization of unusually late transition structures for dication fragmentations. Chemical Physics Letters, 1987, 136, 294-298.	2.6	40
185	Deceptive convergence in mÃ¸ller-plesset perturbation energies. Chemical Physics Letters, 1986, 132, 16-22.	2.6	101
186	An Examination of the Relationship Between Transition State Geometry in Hydron Transfer Reactions and the Temperature Dependence of the Primary Kinetic Isotope Effect. Israel Journal of Chemistry, 1985, 26, 378-386.	2.3	2
187	A theoretical approach to molecular conformational analysis. Journal of Molecular Structure, 1985, 126, 271-290.	3.6	48
188	Model calculations of isotope effects. 10. Temperature-independent isotope effects in hydrogen transfer. Do they signify a bent transition state?. Journal of the American Chemical Society, 1985, 107, 2971-2972.	13.7	14
189	The potential energy surface for the [C2H2O]+Ë™ system: The ketene radical cation [CH2ï£¾Cï£¾O]+Ë™ and its isomers. Organic Mass Spectrometry, 1984, 19, 610-616.	1.3	30