Peter Pulay

List of Publications by Citations

182 papers	25,834 citations	68 h-index	160 g-index
184 ext. papers	26,900 ext. citations	4.6 avg, IF	6.92 L-index

#	Paper	IF	Citations
182	Efficient implementation of the gauge-independent atomic orbital method for NMR chemical shift calculations. *Journal of the American Chemical Society*, **1990**, 112, 8251-8260	16.4	5418
181	Systematic ab initio gradient calculation of molecular geometries, force constants, and dipole moment derivatives. *Journal of the American Chemical Society*, **1979**, 101, 2550-2560	16.4	1942
180	Convergence acceleration of iterative sequences. the case of scf iteration. *Chemical Physics Letters*, **1980**, 73, 393-398	2.5	1825
179	Combination of theoretical ab initio and experimental information to obtain reliable harmonic force constants. Scaled quantum mechanical (QM) force fields for glyoxal, acrolein, butadiene, formaldehyde, and ethylene. *Journal of the American Chemical Society*, **1983**, 105, 7037-7047	16.4	1350
178	Can (semi)local density functional theory account for the London dispersion forces?. *Chemical Physics Letters*, **1994**, 229, 175-180	2.5	888
177	The calculation of ab initio molecular geometries: efficient optimization by natural internal coordinates and empirical correction by offset forces. *Journal of the American Chemical Society*, **1992**, 114, 8191-8201	16.4	852
176	Localizability of dynamic electron correlation. *Chemical Physics Letters*, **1983**, 100, 151-154	2.5	684
175	Direct Scaling of Primitive Valence Force Constants:An Alternative Approach to Scaled Quantum Mechanical Force Fields. *Journal of Physical Chemistry A*, **1998**, 102, 1412-1424	2.8	475
174	Orbital-invariant formulation and second-order gradient evaluation in Mller-Plesset perturbation theory. *Theoretica Chimica Acta*, **1986**, 69, 357-368		466
173	Geometry optimization by direct inversion in the iterative subspace. *Journal of Molecular Structure*, **1984**, 114, 31-34	3.4	461
172	An efficient ab initio gradient program. *Theoretica Chimica Acta*, **1979**, 50, 299-312		448
171	Force field, dipole moment derivatives, and vibronic constants of benzene from a combination of experimental and ab initio quantum chemical information. *Journal of Chemical Physics*, **1981**, 74, 3999-4014	3.9	415
170	Fourth-order Mo/llerPlessett perturbation theory in the local correlation treatment. I. Method. *Journal of Chemical Physics*, **1987**, 86, 914-922	3.9	411
169	Local configuration interaction: An efficient approach for larger molecules. *Chemical Physics Letters* , **1985**, 113, 13-18	2.5	398
168	Ligand redox effects in the synthesis, electronic structure, and reactivity of an alkyl-alkyl cross-coupling catalyst. *Journal of the American Chemical Society*, **2006**, 128, 13175-83	16.4	388
167	High accuracy benchmark calculations on the benzene dimer potential energy surface. *Chemical Physics Letters*, **2007**, 447, 27-32	2.5	248
166	Comparison of the boys and PipekMezey localizations in the local correlation approach and automatic virtual basis selection. *Journal of Computational Chemistry*, **1993**, 14, 736-740	3.5	243

165	The local correlation treatment. II. Implementation and tests. *Journal of Chemical Physics*, **1988**, 88, 1884-1890	3.9	241
164	The accuracy of quantum chemical methods for large noncovalent complexes. *Journal of Chemical Theory and Computation*, **2013**, 9, 3364-3374	6.4	223
163	Second and third derivatives of variational energy expressions: Application to multiconfigurational self-consistent field wave functions. *Journal of Chemical Physics*, **1983**, 78, 5043-5051	3.9	211
162	UHF natural orbitals for defining and starting MC-SCF calculations. *Journal of Chemical Physics*, **1988**, 88, 4926-4933	3.9	210
161	Generalized Mo/ller–Plesset perturbation theory: Second order results for two-configuration, open-shell excited singlet, and doublet wave functions. *Journal of Chemical Physics*, **1989**, 90, 3647-3659	3.9	207
160	Efficient elimination of basis set superposition errors by the local correlation method: Accurate ab initio studies of the water dimer. *Journal of Chemical Physics*, **1993**, 98, 2170-2175	3.9	204
159	Analytical energy gradients for local second-order Mo/ller–Plesset perturbation theory. *Journal of Chemical Physics*, **1998**, 108, 5185-5193	3.9	190
158	Cubic force constants and equilibrium geometry of methane from Hartree–Fock and correlated wavefunctions. *Journal of Chemical Physics*, **1978**, 68, 5077-5085	3.9	185
157	The unrestricted natural orbital–complete active space (UNO–CAS) method: An inexpensive alternative to the complete active space–self-consistent-field (CAS–SCF) method. *Journal of Chemical Physics*, **1989**, 90, 3637-3646	3.9	180
156	Comparison of NMR Shieldings Calculated from Hartree–Fock and Density Functional Wave Functions Using Gauge-Including Atomic Orbitals. *The Journal of Physical Chemistry*, **1996**, 100, 6310-6316		178
155	Multipole approximation of distant pair energies in local MP2 calculations. *Chemical Physics Letters*, **1998**, 290, 143-149	2.5	167
154	An efficient reformulation of the closed-shell self-consistent electron pair theory. *Journal of Chemical Physics*, **1984**, 81, 1901-1905	3.9	163
153	Consistent generalization of the Mller-Plesset partitioning to open-shell and multiconfigurational SCF reference states in many-body perturbation theory. *Chemical Physics Letters*, **1987**, 140, 225-231	2.5	146
152	Direct Use of the Gradient for Investigating Molecular Energy Surfaces **1977**, 153-185		141
151	An improved 6-31G* basis set for first-row transition metals. *Journal of Chemical Physics*, **2003**, 118, 7775-7782	3.9	137
150	Theoretical prediction of vibrational spectra. 1. The in-plane force field and vibrational spectra of pyridine. *Journal of the American Chemical Society*, **1984**, 106, 2765-2769	16.4	131
149	Ab initio geometry optimization for large molecules **1997**, 18, 1473-1483		127
148	A perspective on the CASPT2 method. *International Journal of Quantum Chemistry*, **2011**, 111, 3273-3279	2.1	122

147	Analytical Derivative Methods in Quantum Chemistry. *Advances in Chemical Physics*, **2007**, 241-286		119
146	Theoretical prediction of vibrational spectra. 2. Force field, spectroscopically refined geometry, and reassignment of the vibrational spectrum of naphthalene. *Journal of the American Chemical Society*, **1985**, 107, 6487-6494	16.4	119
145	Assessment of the Handy–Cohen optimized exchange density functional for organic reactions. *Journal of Chemical Physics*, **2002**, 117, 1441-1449	3.9	116
144	Direct inversion in the iterative subspace (DIIS) optimization of open-shell, excited-state, and small multiconfiguration SCF wave functions. *Journal of Chemical Physics*, **1986**, 84, 5728-5734	3.9	115
143	Comparison of the ab initio force constants of ethane, ethylene and acetylene. *Molecular Physics*, **1974**, 27, 473-490	1.7	113
142	Quantum chemistry in parallel with PQS. *Journal of Computational Chemistry*, **2009**, 30, 317-35	3.5	101
141	The adiabatic correction to molecular potential surfaces in the SCF approximation. *Chemical Physics Letters*, **1984**, 103, 463-465	2.5	97
140	A systematic study of the convergence and additivity of correlation and basis set effects on the force constants of small molecules: HF, HCN, and NH3. *Journal of Chemical Physics*, **1983**, 79, 3382-3391	3.9	96
139	DFT-SQM Force Field for Nickel Porphine: Intrinsic Ruffling. *Journal of Physical Chemistry A*, **1999**, 103, 1357-1366	2.8	95
138	Second-order Møller–Plesset calculations with dual basis sets. *Journal of Chemical Physics*, **2003**, 118, 9497-9503	3.9	92
137	Calculated and Experimental Geometries and Infrared Spectra of Metal Tris-Acetylacetonates: Vibrational Spectroscopy as a Probe of Molecular Structure for Ionic Complexes. Part I. *Journal of Physical Chemistry A*, **2001**, 105, 238-244	2.8	91
136	Vibrational Assignment and Definite Harmonic Force Field for Porphine. 2. Comparison with Nonresonance Raman Data. *The Journal of Physical Chemistry*, **1996**, 100, 13985-13992		88
135	H2, Ne, and N2 Energies of Encapsulation into C60 Evaluated with the MPWB1K Functional. *Journal of Chemical Theory and Computation*, **2006**, 2, 782-5	6.4	87
134	Identification of Isomers from Calculated Vibrational Spectra. A Density Functional Study of Tetrachlorinated Dibenzodioxins. *Journal of the American Chemical Society*, **1995**, 117, 4167-4172	16.4	87
133	Hartree-Fock calculation of the harmonic force constants and equilibrium geometry of formaldehyde. *Theoretica Chimica Acta*, **1974**, 32, 253-264		87
132	The Fourier transform Coulomb method: Efficient and accurate calculation of the Coulomb operator in a Gaussian basis. *Journal of Chemical Physics*, **2002**, 117, 7827-7835	3.9	85
131	A low-scaling method for second order Møller–Plesset calculations. *Journal of Chemical Physics*, **2001**, 115, 3975-3983	3.9	84
130	Fock matrix dynamics. *Chemical Physics Letters*, **2004**, 386, 272-278	2.5	80

129	Structure and fundamental vibrations of phenoxyl radical. *Journal of Chemical Physics*, **1994**, 100, 5023-5035	3.9	79
128	A reliable and efficient first principles-based method for predicting pK(a) values. 2. Organic acids. *Journal of Physical Chemistry A*, **2010**, 114, 432-42	2.8	78
127	A space-saving modification of Davidson's eigenvector algorithm. *Journal of Computational Chemistry*, **1990**, 11, 1164-1168	3.5	78
126	Potential symmetry breaking, structure and definite vibrational assignment for azulene: Multiconfigurational and density functional results. *Journal of Chemical Physics*, **1995**, 103, 5650-5661	3.9	77
125	Accuracy of the three-body fragment molecular orbital method applied to Møller-Plesset perturbation theory. *Journal of Computational Chemistry*, **2007**, 28, 1476-1484	3.5	76
124	Selection of active spaces for multiconfigurational wavefunctions. *Journal of Chemical Physics*, **2015** , 142, 244104	3.9	73
123	The geometry of some amides obtained from ab initio calculations. *Journal of Molecular Structure*, **1979**, 57, 259-270	3.4	73
122	Force Constants and Dipole Moment Derivatives of Ammonia from Hartree-Fock Calculations. *Journal of Chemical Physics*, **1972**, 57, 3337-3340	3.9	73
121	Assessment of density functional methods for nuclear magnetic resonance shielding calculations. *Journal of Chemical Physics*, **2003**, 119, 1350-1357	3.9	72
120	Accurate molecular integrals and energies using combined plane wave and Gaussian basis sets in molecular electronic structure theory. *Journal of Chemical Physics*, **2002**, 116, 7795-7805	3.9	71
119	A benchmark comparison of □ and □ dispersion: the dimers of naphthalene and decalin, and coronene and perhydrocoronene. *Journal of the American Chemical Society*, **2012**, 134, 17520-5	16.4	70
118	Integral transformation with low-order scaling for large local second-order Møller-Plesset calculations **1998**, 19, 1241-1254		70
117	Theoretical and Experimental Study of the Vibrational Spectra of the □ and □ Phases of Octahydro-1,3,5,7-tetranitro-1,3,5,7-tetrazocine (HMX). *Journal of Physical Chemistry B*, **2002**, 106, 10594-10604	3.4	68
116	Ab initio prediction of vibrational spectra: A database approach. *Vibrational Spectroscopy*, **1990**, 1, 159-165	2.1	68
115	The molecular structure of toluene. *Journal of Molecular Structure*, **1980**, 66, 281-287	3.4	68
114	Accurate correlated calculation of the intermolecular potential surface in the coronene dimer. *Molecular Physics*, **2010**, 108, 249-257	1.7	66
113	A reliable and efficient first principles-based method for predicting pK(a) values. 1. Methodology. *Journal of Physical Chemistry A*, **2010**, 114, 425-31	2.8	66
112	An accurate in-plane force field for porphine. A scaled quantum mechanical study. *Chemical Physics Letters*, **1995**, 247, 379-385	2.5	65

111	Assessment of the OLYP and O3LYP density functionals for first-row transition metals. *Journal of Computational Chemistry*, **2003**, 24, 1184-91	3.5	64
110	Vibrational energy levels of hydrogen cyanide. *Journal of Chemical Physics*, **1986**, 85, 5838-5846	3.9	64
109	Convex–concave stacking of curved conjugated networks: Benchmark calculations on the corannulene dimer. *Chemical Physics Letters*, **2011**, 512, 155-160	2.5	63
108	The inner-hydrogen migration in free base porphyrin. *Theoretical Chemistry Accounts*, **1997**, 97, 59-66	1.9	62
107	ANALYTICAL DERIVATIVE TECHNIQUES AND THE CALCULATION OF VIBRATIONAL SPECTRA. *Advanced Series in Physical Chemistry*, **1995**, 1191-1240		61
106	Investigation of the basis of the valence shell electron pair repulsion model by ab initio calculation of geometry variations in a series of tetrahedral and related molecules. *Journal of the American Chemical Society*, **1979**, 101, 2002-2010	16.4	61
105	The tilt and asymmetry of methyl groups in asymmetric environments. *Journal of the American Chemical Society*, **1977**, 99, 5570-5574	16.4	61
104	Parallel Calculation of Coupled Cluster Singles and Doubles Wave Functions Using Array Files. *Journal of Chemical Theory and Computation*, **2007**, 3, 1368-77	6.4	60
103	A new parallel algorithm of MP2 energy calculations. *Journal of Computational Chemistry*, **2006**, 27, 407-13	3.5	58
102	Methods for parallel computation of SCF NMR chemical shifts by GIAO method: Efficient integral calculation, multi-Fock algorithm, and pseudodiagonalization. *Journal of Computational Chemistry*, **1997**, 18, 816-825	3.5	52
101	Structures of some fluorinated benzenes determined by ab initio computation. *Journal of Computational Chemistry*, **1982**, 3, 344-353	3.5	52
100	Efficient Parallel Implementation of the CCSD External Exchange Operator and the Perturbative Triples (T) Energy Calculation. *Journal of Chemical Theory and Computation*, **2008**, 4, 1585-92	6.4	50
99	The Performance of the Handy/Cohen Functionals, OLYP and O3LYP, for the Computation of Hydrocarbon Pericyclic Reaction Activation Barriers. *Journal of Physical Chemistry A*, **2004**, 108, 2959-2965	2.8	49
98	Possibilities and limitations of ab initio calculation of vibrational spectra. *Journal of Molecular Structure*, **1995**, 347, 293-308	3.4	49
97	Geometry optimization in delocalized internal coordinates: An efficient quadratically scaling algorithm for large molecules. *Journal of Chemical Physics*, **1999**, 110, 4986-4991	3.9	47
96	The force constants of benzene: Local many-body perturbation theory vs new experiment. *Journal of Chemical Physics*, **1986**, 85, 1703-1704	3.9	47
95	Vibrational energy levels of methyl fluoride. *Journal of Chemical Physics*, **1987**, 86, 5088-5093	3.9	46
94	Ab initio investigation of geometry changes during inversion of NH3, NH2F, NHF2, NF3 and PH3, PH2F, PHF2, PF3. *Journal of Chemical Physics*, **1977**, 66, 5769-5776	3.9	46

93	Accurate prediction of proton chemical shifts. I. Substituted aromatic hydrocarbons. *Journal of Computational Chemistry*, **2001**, 22, 1887-1895	3.5	45
92	Geometry optimization of large biomolecules in redundant internal coordinates. *Journal of Chemical Physics*, **2000**, 113, 6566-6572	3.9	44
91	Analytical derivatives, forces, force constants, molecular geometries, and related response properties in electronic structure theory. *Wiley Interdisciplinary Reviews: Computational Molecular Science*, **2014**, 4, 169-181	7.9	42
90	CHIIIO Hydrogen Bond between N-Methyl Maleimide and Dimethyl Sulfoxide: A Combined NMR and Ab Initio Study. *Journal of Physical Chemistry A*, **2003**, 107, 4683-4687	2.8	41
89	Efficient calculation of canonical MP2 energies. *Chemical Physics Letters*, **2001**, 344, 543-552	2.5	41
88	An efficient direct method for geometry optimization of large molecules in internal coordinates. *Journal of Chemical Physics*, **1998**, 109, 6571-6576	3.9	40
87	A new grid-based method for the direct computation of excited molecular vibrational states: test application to formaldehyde. *Computational and Theoretical Chemistry*, **1995**, 341, 1-11		39
86	The structure of some nitrogen heteroaromatics. *Computational and Theoretical Chemistry*, **1982**, 88, 79-89		39
85	Predicting the vibrational spectra of some simple fluorocarbons by direct scaling of primitive valence force constants. *Journal of Computational Chemistry*, **1998**, 19, 1187-1204	3.5	37
84	The interpretation of compliance constants and their suitability for characterizing hydrogen bonds and other weak interactions. *Journal of the American Chemical Society*, **2006**, 128, 11324-5	16.4	37
83	An efficient parallel algorithm for the calculation of canonical MP2 energies. *Journal of Computational Chemistry*, **2002**, 23, 1150-6	3.5	36
82	Ab initio Hartree-Fock calculation of the force constants and geometry of HNF2 and H2NF. *Molecular Physics*, **1977**, 33, 1565-1570	1.7	36
81	New parallel algorithm for MP2 energy gradient calculations. *Journal of Computational Chemistry*, **2007**, 28, 2034-42	3.5	35
80	Ab initio calculation of force constants for the linear molecules HCN, FCN, (CN)2 and the ion N2F+. *Molecular Physics*, **1975**, 30, 1123-1131	1.7	35
79	Density functional based vibrational study of conformational isomers: Molecular rearrangement of benzofuroxan. *Journal of Computational Chemistry*, **1997**, 18, 489-500	3.5	34
78	Force constants, vibrational assignment and geometry of methyl amine from hartreeFock calculations. *Journal of Molecular Structure*, **1975**, 29, 239-246	3.4	34
77	Accurate prediction of proton chemical shifts. II. Peptide analogues. *Journal of Computational Chemistry*, **2002**, 23, 492-7	3.5	33
76	The tautomers of uracil: A local correlation treatment. *International Journal of Quantum Chemistry*, **1993**, 47, 49-58	2.1	33

75	Theoretical equilibrium geometry, vibrational frequencies and the first electronic transition energy of HCC. *Molecular Physics*, **1983**, 50, 139-151	1.7	33
74	Basis set and correlation effects in the calculation of selenium NMR shieldings. *Chemical Physics Letters*, **1994**, 225, 280-284	2.5	32
73	Scaled quantum mechanical (SQM) force field and vibrational assignment for hexatriene. *Computational and Theoretical Chemistry*, **1987**, 151, 341-354		32
72	Force field and vibrational assignment for cyclobutane from a combination of ab initio calculations and experimental data. *Computational and Theoretical Chemistry*, **1982**, 89, 1-13		32
71	The size consistency of multi-reference MÖller–Plesset perturbation theory. *Molecular Physics*, **1998**, 93, 431-439	1.7	31
70	Half-projected Hartree–Fock natural orbitals for defining CAS–SCF active spaces. *International Journal of Quantum Chemistry*, **1993**, 45, 133-166	2.1	31
69	The molecular structure, vibrational force field, spectral frequencies, and infrared intensities of CH3POF2. *Computational and Theoretical Chemistry*, **1982**, 87, 113-124		31
68	Benchmark Relative Energies for Large Water Clusters with the Generalized Energy-Based Fragmentation Method. *Journal of Chemical Theory and Computation*, **2017**, 13, 2696-2704	6.4	28
67	The 7-Norbornadienyl Cation: An NMR/IGLO Validation of its ab initio Structure. *Angewandte Chemie International Edition in English*, **1989**, 28, 1042-1044		28
66	Transition state vibrational analysis for the methyl isocyanide rearrangement, CH3NC .fwdarw. CH3CN. *Journal of the American Chemical Society*, **1980**, 102, 3718-3723	16.4	27
65	Ab initio study of the force constants of inorganic molecules ONF and NF3. *Journal of Molecular Spectroscopy*, **1974**, 51, 135-141	1.3	26
64	An efficient atomic orbital based second-order MÖller-Plesset gradient program. *Journal of Chemical Physics*, **2004**, 120, 11423-31	3.9	24
63	Combined experimental/theoretical refinement of indole ring geometry using deuterium magnetic resonance and ab initio calculations. *Journal of the American Chemical Society*, **2003**, 125, 12268-76	16.4	24
62	Methods for finding unrestricted Hartree-Fock solutions and multiple solutions. *The Journal of Physical Chemistry*, **1990**, 94, 5548-5551		24
61	GIAO Nuclear Magnetic Shielding Tensors in Free Base Porphyrin and in Magnesium and Zinc Metalloporphyrins. *Journal of Physical Chemistry A*, **1999**, 103, 420-425	2.8	23
60	Geometry optimization of atomic microclusters using inverse-power distance coordinates. *Journal of Chemical Physics*, **1996**, 105, 11100-11107	3.9	23
59	Comments on the molecular geometry of ferrocene: The dangers of using quantum chemistry programs as black boxes. *Journal of Computational Chemistry*, **2009**, 30, 881-3	3.5	22
58	Raman spectrum of coronene: a scaled quantum mechanical force field study. *Journal of Raman Spectroscopy*, **1998**, 29, 473-481	2.3	22

57	The computed force constants and vibrational spectra of cubane. *Journal of Molecular Spectroscopy* , **1984**, 103, 268-280	1.3	22
56	Array files for computational chemistry: MP2 energies. *Journal of Computational Chemistry*, **2007**, 28, 1215-20	3.5	21
55	Hartree□Fock and second-order Mo/ller□Plesset perturbation theory calculations of the 31P nuclear magnetic resonance shielding tensor in PH3. *Journal of Chemical Physics*, **1993**, 99, 7819-7824	3.9	19
54	The unrestricted natural orbital-restricted active space method: methodology and implementation. *Theoretical Chemistry Accounts*, **1998**, 100, 12-20	1.9	18
53	Ab initio Hartree□Fock calculation of the elastic electron scattering cross section of sulphur hexafluoride. *Journal of Chemical Physics*, **1983**, 79, 185-191	3.9	18
52	Importance of tensor asymmetry for the analysis of 2H NMR spectra from deuterated aromatic rings. *Journal of the American Chemical Society*, **2005**, 127, 17488-93	16.4	17
51	Finding symmetry breaking Hartree-Fock solutions: The case of triplet instability. *Journal of Chemical Physics*, **2016**, 145, 164102	3.9	16
50	Recent developments in the PQS program. *Wiley Interdisciplinary Reviews: Computational Molecular Science*, **2012**, 2, 63-72	7.9	15
49	Das 7-Norbornadienyl-Kation: die NMR/IGLO-Best□igung seiner mit ab-initio-Methoden berechneten Struktur. *Angewandte Chemie*, **2006**, 101, 1063-1065	3.6	15
48	Efficient geometry optimization of molecular clusters. *Journal of Computational Chemistry*, **2000**, 21, 69-76	3.5	15
47	A potential surface for the interaction between water and coronene as a model for a hydrophobic surface. *Molecular Physics*, **2009**, 107, 1197-1207	1.7	14
46	Accuracy and efficiency of atomic basis set methods versus plane wave calculations with ultrasoft pseudopotentials for DNA base molecules. *Journal of Computational Chemistry*, **2005**, 26, 599-605	3.5	14
45	Modeling localized electron pair correlation energies. *Journal of Chemical Physics*, **1995**, 103, 5662-5673	3.9	14
44	Building a database of force constants based on scaled ab initio (SQM) results. I. Chlorobenzenes. *Spectrochimica Acta Part A: Molecular Spectroscopy*, **1993**, 49, 1499-1514		14
43	A test of the approximate coupled cluster doubles approximation. *Chemical Physics Letters*, **1986**, 131, 384-388	2.5	14
42	Ultrafast Quantum Mechanics/Molecular Mechanics Monte Carlo simulations using generalized multipole polarizabilities. *Chemical Physics Letters*, **2012**, 530, 1-9	2.5	13
41	Parallel Density Functional Theory Energies using the Fourier Transform Coulomb Method *Journal of Physical Chemistry A*, **2004**, 108, 3040-3047	2.8	13
40	Considerations regarding the local treatment of Laplace transform MPPT. *Chemical Physics Letters*, **1996**, 248, 223-227	2.5	13

39	Ab initio study of the geometry, stretching, vibrations, and assignment of the observed frequencies of the ground state C6H (hexatriynyl) radical. *Journal of Chemical Physics*, **1992**, 97, 1602-1605	3.9	13
38	A benchmark quantum chemical study of the stacking interaction between larger polycondensed aromatic hydrocarbons. *Theoretical Chemistry Accounts*, **2011**, 130, 419-427	1.9	12
37	Efficient calculation of the energy of a molecule in an arbitrary electric field. *International Journal of Quantum Chemistry*, **2009**, 109, 2113-2120	2.1	12
36	Newtonian molecular dynamics in general curvilinear internal coordinates. *Chemical Physics Letters*, **2002**, 353, 400-406	2.5	12
35	Calculation of fully optimized geometries of five- and six-membered heterocycles by the CNDO force method. *Theoretica Chimica Acta*, **1973**, 32, 145-150		12
34	Complete assignment of vibrational spectra of 1,5-cyclooctadiene theoretical and experimental infrared and Raman study. *Spectrochimica Acta Part A: Molecular Spectroscopy*, **1993**, 49, 257-270		11
33	Vibrational assignment of SF4. *Journal of Molecular Structure*, **1974**, 21, 158-164	3.4	11
32	The vibrational spectrum of 1,4-dioxane in aqueous solution theory and experiment. *New Journal of Chemistry*, **2016**, 40, 7663-7670	3.6	11
31	Automatic Construction of the Initial Orbitals for Efficient Generalized Valence Bond Calculations of Large Systems. *Journal of Chemical Theory and Computation*, **2019**, 15, 141-153	6.4	11
30	Parallel stored-integral and semidirect Hartree-Fock and DFT methods with data compression. *Journal of Computational Chemistry*, **2003**, 24, 154-60	3.5	10
29	Ab initio evidence for the stepwise mechanism of the McLafferty rearrangement of the butanal radical cation. *Journal of Computational Chemistry*, **1992**, 13, 183-186	3.5	10
28	On the calculation of elastic electron scattering cross sections from molecular wavefunctions: CF4 and CH4. *Computational and Theoretical Chemistry*, **1984**, 108, 149-159		10
27	Parallel implementation of Hartree Fock and density functional theory analytical second derivatives. *Molecular Physics*, **2004**, 102, 2475-2484	1.7	9
26	Chemical shift anisotropies in silicon containing three-membered rings. An ab initio study. *Chemical Physics Letters*, **1995**, 241, 393-398	2.5	9
25	Characters for symmetric and antisymmetric higher powers of representations: Application to the number of anharmonic force constants in symmetrical molecules. *Journal of Computational Chemistry*, **1989**, 10, 935-938	3.5	9
24	Comparison of Methods for Active Orbital Selection in Multiconfigurational Calculations. *Journal of Chemical Theory and Computation*, **2020**, 16, 7328-7341	6.4	9
23	What Is the Price of Open-Source Software?. *Journal of Physical Chemistry Letters*, **2015**, 6, 2751-4	6.4	8
22	The Ethidium-UA/AU Intercalation Site: Effect of Model Fragmentation and Backbone Charge State. *Journal of Chemical Theory and Computation*, **2011**, 7, 2600-9	6.4	8

21	Parallel DFT gradients using the Fourier Transform Coulomb method. *Journal of Computational Chemistry*, **2007**, 28, 2581-8	3.5	8
20	Theoretical study on the structures, force field, and vibrational spectra of cyclooctatetraene and cyclooctatetraene-d8. *Spectrochimica Acta Part A: Molecular Spectroscopy*, **1993**, 49, 953-964		8
19	The ring puckering potential of oxetane: local correlation results. *Chemical Physics Letters*, **1986**, 132, 29-31	2.5	8
18	Density functional implementation of a Gaussian-weighted operator for spin densities. *Physical Chemistry Chemical Physics*, **2000**, 2, 2131-2135	3.6	7
17	Stability of Novel Oxo- and Chloro-Substituted Trioxanes. *Journal of the American Chemical Society*, **1999**, 121, 8544-8548	16.4	7
16	The in-plane force field of nitryl fluoride. *Molecular Physics*, **1976**, 32, 169-176	1.7	6
15	Analytical Energy Gradients for the Cluster-in-Molecule MP2 Method and Its Application to Geometry Optimizations of Large Systems. *Journal of Chemical Theory and Computation*, **2019**, 15, 3623-3634	6.4	5
14	Efficient calculation of the density response function from generalized polarizabilities. *Theoretical Chemistry Accounts*, **2016**, 135, 1	1.9	5
13	Zundel-type H-bonding in biomolecular ions. *Journal of the American Society for Mass Spectrometry*, **2014**, 25, 1511-4	3.5	5
12	Comment on Force in SCF theories *Journal of Chemical Physics*, **1983**, 79, 2491-2492	3.9	5
11	Backbone structure confirmation and side chain conformation refinement of a bradykinin mimic BKM-824 by comparing calculated (1)H, (13)C and (19)F chemical shifts with experiment. *Journal of Biomolecular Structure and Dynamics*, **2002**, 20, 71-80	3.6	3
10	Reply to the comments on 'Efficient calculation of canonical MP2 energies' by A. Köhn and C. Hättig. *Chemical Physics Letters*, **2002**, 358, 354-356	2.5	2
9	The geometries of chlorobenzenes as obtained from ab initio calculations empirically corrected by offset forces. *Computational and Theoretical Chemistry*, **1992**, 277, 147-160		2
8	Ab initio geometry optimization for large molecules **1997**, 18, 1473		2
7	Approximate Force Constants from Uncoupled Self-Consistent Field Perturbation Theory Using Nonhybrid Density Functional Theory. *Journal of Physical Chemistry A*, **2017**, 121, 348-356	2.8	1
6	A Festschrift in honor of Shigeru Nagase. *Theoretical Chemistry Accounts*, **2011**, 130, 129-152	1.9	1
5	Variational formulation and gradient evaluation for coupled electron pair approximations: A model study. *International Journal of Quantum Chemistry*, **2009**, 24, 257-263	2.1	1
4	Natural charge densities for the evaluation of MC-SCF energy derivatives without density matrix transformation. *Chemical Physics Letters*, **1989**, 156, 501-504	2.5	1

3	Ab initio geometry optimization for large molecules **1997**, 18, 1473	1
2	Breaking established paradigms: a tribute to Wilfried Meyer's contributions to ab initio quantum chemistry. *Molecular Physics*, **2020**, 118, e1730993	1.7
1	Compact representation of generalized molecular polarizabilities and efficient calculation of polarization energy in an arbitrary electric field. *International Journal of Quantum Chemistry*,e26792	2.1