Peter Pulay

List of Publications by Year in Descending Order

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	Breaking established paradigms: a tribute to Wilfried Meyer's contributions to ab initio quantum chemistry. *Molecular Physics*, **2020**, 118, e1730993	1.7	
181	Comparison of Methods for Active Orbital Selection in Multiconfigurational Calculations. *Journal of Chemical Theory and Computation*, **2020**, 16, 7328-7341	6.4	9
180	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
179	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
178	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
177	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
176	Efficient calculation of the density response function from generalized polarizabilities. *Theoretical Chemistry Accounts*, **2016**, 135, 1	1.9	5
175	The vibrational spectrum of 1,4-dioxane in aqueous solution: theory and experiment. *New Journal of Chemistry*, **2016**, 40, 7663-7670	3.6	11
174	Finding symmetry breaking Hartree-Fock solutions: The case of triplet instability. *Journal of Chemical Physics*, **2016**, 145, 164102	3.9	16
173	What Is the Price of Open-Source Software?. *Journal of Physical Chemistry Letters*, **2015**, 6, 2751-4	6.4	8
172	Selection of active spaces for multiconfigurational wavefunctions. *Journal of Chemical Physics*, **2015** , 142, 244104	3.9	73
171	Zundel-type H-bonding in biomolecular ions. *Journal of the American Society for Mass Spectrometry*, **2014**, 25, 1511-4	3.5	5
170	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
169	The accuracy of quantum chemical methods for large noncovalent complexes. *Journal of Chemical Theory and Computation*, **2013**, 9, 3364-3374	6.4	223
168	Ultrafast Quantum Mechanics/Molecular Mechanics Monte Carlo simulations using generalized multipole polarizabilities. *Chemical Physics Letters*, **2012**, 530, 1-9	2.5	13
167	A benchmark comparison of π and π dispersion: the dimers of naphthalene and decalin, and coronene and perhydrocoronene. *Journal of the American Chemical Society*, **2012**, 134, 17520-5	16.4	70
166	Recent developments in the PQS program. *Wiley Interdisciplinary Reviews: Computational Molecular Science*, **2012**, 2, 63-72	7.9	15

165	Convex–concave stacking of curved conjugated networks: Benchmark calculations on the corannulene dimer. *Chemical Physics Letters*, **2011**, 512, 155-160	2.5	63
164	A benchmark quantum chemical study of the stacking interaction between larger polycondensed aromatic hydrocarbons. *Theoretical Chemistry Accounts*, **2011**, 130, 419-427	1.9	12
163	A Festschrift in honor of Shigeru Nagase. *Theoretical Chemistry Accounts*, **2011**, 130, 129-152	1.9	1
162	A perspective on the CASPT2 method. *International Journal of Quantum Chemistry*, **2011**, 111, 3273-3279	2.1	122
161	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
160	Accurate correlated calculation of the intermolecular potential surface in the coronene dimer. *Molecular Physics*, **2010**, 108, 249-257	1.7	66
159	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
158	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
157	Quantum chemistry in parallel with PQS. *Journal of Computational Chemistry*, **2009**, 30, 317-35	3.5	101
156	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
155	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
154	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
153	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
152	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
151	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
150	Analytical Derivative Methods in Quantum Chemistry. *Advances in Chemical Physics*, **2007**, 241-286		119
149	Array files for computational chemistry: MP2 energies. *Journal of Computational Chemistry*, **2007**, 28, 1215-20	3.5	21
148	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

147	New parallel algorithm for MP2 energy gradient calculations. *Journal of Computational Chemistry*, **2007**, 28, 2034-42	3.5	35
146	Parallel DFT gradients using the Fourier Transform Coulomb method. *Journal of Computational Chemistry*, **2007**, 28, 2581-8	3.5	8
145	High accuracy benchmark calculations on the benzene dimer potential energy surface. *Chemical Physics Letters*, **2007**, 447, 27-32	2.5	248
144	A new parallel algorithm of MP2 energy calculations. *Journal of Computational Chemistry*, **2006**, 27, 407-13	3.5	58
143	Das 7-Norbornadienyl-Kation: die NMR/IGLO-Bestätigung seiner mit ab-initio-Methoden berechneten Struktur. *Angewandte Chemie*, **2006**, 101, 1063-1065	3.6	15
142	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
141	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
140	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
139	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
138	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
137	An efficient atomic orbital based second-order Møller-Plesset gradient program. *Journal of Chemical Physics*, **2004**, 120, 11423-31	3.9	24
136	Fock matrix dynamics. *Chemical Physics Letters*, **2004**, 386, 272-278	2.5	80
135	Parallel implementation of Hartree–Fock and density functional theory analytical second derivatives. *Molecular Physics*, **2004**, 102, 2475-2484	1.7	9
134	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
133	Parallel Density Functional Theory Energies using the Fourier Transform Coulomb Method. *Journal of Physical Chemistry A*, **2004**, 108, 3040-3047	2.8	13
132	Parallel stored-integral and semidirect Hartree-Fock and DFT methods with data compression. *Journal of Computational Chemistry*, **2003**, 24, 154-60	3.5	10
131	Assessment of the OLYP and O3LYP density functionals for first-row transition metals. *Journal of Computational Chemistry*, **2003**, 24, 1184-91	3.5	64
130	An improved 6-31G* basis set for first-row transition metals. *Journal of Chemical Physics*, **2003**, 118, 7775-7782	3.9	137

129	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
128	CHO 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
127	Assessment of density functional methods for nuclear magnetic resonance shielding calculations. *Journal of Chemical Physics*, **2003**, 119, 1350-1357	3.9	72
126	Second-order MllerPlesset calculations with dual basis sets. *Journal of Chemical Physics*, **2003**, 118, 9497-9503	3.9	92
125	Accurate prediction of proton chemical shifts. II. Peptide analogues. *Journal of Computational Chemistry*, **2002**, 23, 492-7	3.5	33
124	An efficient parallel algorithm for the calculation of canonical MP2 energies. *Journal of Computational Chemistry*, **2002**, 23, 1150-6	3.5	36
123	Newtonian molecular dynamics in general curvilinear internal coordinates. *Chemical Physics Letters*, **2002**, 353, 400-406	2.5	12
122	Reply to the comments on 'Efficient calculation of canonical MP2 energies' by A. Kn and C. Httig. *Chemical Physics Letters*, **2002**, 358, 354-356	2.5	2
121	Assessment of the HandyCohen optimized exchange density functional for organic reactions. *Journal of Chemical Physics*, **2002**, 117, 1441-1449	3.9	116
120	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
119	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
118	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
117	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
116	Accurate prediction of proton chemical shifts. I. Substituted aromatic hydrocarbons. *Journal of Computational Chemistry*, **2001**, 22, 1887-1895	3.5	45
115	Efficient calculation of canonical MP2 energies. *Chemical Physics Letters*, **2001**, 344, 543-552	2.5	41
114	A low-scaling method for second order MllerPlesset calculations. *Journal of Chemical Physics*, **2001**, 115, 3975-3983	3.9	84
113	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
112	Efficient geometry optimization of molecular clusters. *Journal of Computational Chemistry*, **2000**, 21, 69-76	3.5	15

111	Geometry optimization of large biomolecules in redundant internal coordinates. *Journal of Chemical Physics*, **2000**, 113, 6566-6572	3.9	44
110	Density functional implementation of a Gaussian-weighted operator for spin densities. *Physical Chemistry Chemical Physics*, **2000**, 2, 2131-2135	3.6	7
109	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
108	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
107	DFT-SQM Force Field for Nickel Porphine: Intrinsic Ruffling. *Journal of Physical Chemistry A*, **1999**, 103, 1357-1366	2.8	95
106	Stability of Novel Oxo- and Chloro-Substituted Trioxanes. *Journal of the American Chemical Society*, **1999**, 121, 8544-8548	16.4	7
105	Multipole approximation of distant pair energies in local MP2 calculations. *Chemical Physics Letters*, **1998**, 290, 143-149	2.5	167
104	Raman spectrum of coronene: a scaled quantum mechanical force field study. *Journal of Raman Spectroscopy*, **1998**, 29, 473-481	2.3	22
103	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
102	Integral transformation with low-order scaling for large local second-order M□ller□lesset calculations **1998**, 19, 1241-1254		70
101	The unrestricted natural orbital-restricted active space method: methodology and implementation. *Theoretical Chemistry Accounts*, **1998**, 100, 12-20	1.9	18
100	Analytical energy gradients for local second-order Mo/ller□lesset perturbation theory. *Journal of Chemical Physics*, **1998**, 108, 5185-5193	3.9	190
99	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
98	An efficient direct method for geometry optimization of large molecules in internal coordinates. *Journal of Chemical Physics*, **1998**, 109, 6571-6576	3.9	40
97	The size consistency of multi-reference M□ller□lesset perturbation theory. *Molecular Physics*, **1998** , 93, 431-439	1.7	31
96	The inner-hydrogen migration in free base porphyrin. *Theoretical Chemistry Accounts*, **1997**, 97, 59-66	1.9	62
95	Density functional based vibrational study of conformational isomers: Molecular rearrangement of benzofuroxan. *Journal of Computational Chemistry*, **1997**, 18, 489-500	3.5	34
94	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

93	Ab initio geometry optimization for large molecules **1997**, 18, 1473-1483		127
92	Ab initio geometry optimization for large molecules **1997**, 18, 1473		2
91	Ab initio geometry optimization for large molecules **1997**, 18, 1473		1
90	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
89	Considerations regarding the local treatment of Laplace transform MPPT. *Chemical Physics Letters*, **1996**, 248, 223-227	2.5	13
88	Geometry optimization of atomic microclusters using inverse-power distance coordinates. *Journal of Chemical Physics*, **1996**, 105, 11100-11107	3.9	23
87	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
86	An accurate in-plane force field for porphine. A scaled quantum mechanical study. *Chemical Physics Letters*, **1995**, 247, 379-385	2.5	65
85	Possibilities and limitations of ab initio calculation of vibrational spectra. *Journal of Molecular Structure*, **1995**, 347, 293-308	3.4	49
84	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
83	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
82	Modeling localized electron pair correlation energies. *Journal of Chemical Physics*, **1995**, 103, 5662-5673	3.9	14
81	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
80	ANALYTICAL DERIVATIVE TECHNIQUES AND THE CALCULATION OF VIBRATIONAL SPECTRA. *Advanced Series in Physical Chemistry*, **1995**, 1191-1240		61
79	Chemical shift anisotropies in silicon containing three-membered rings. An ab initio study. *Chemical Physics Letters*, **1995**, 241, 393-398	2.5	9
78	Basis set and correlation effects in the calculation of selenium NMR shieldings. *Chemical Physics Letters*, **1994**, 225, 280-284	2.5	32
77	Can (semi)local density functional theory account for the London dispersion forces?. *Chemical Physics Letters*, **1994**, 229, 175-180	2.5	888
76	Structure and fundamental vibrations of phenoxyl radical. *Journal of Chemical Physics*, **1994**, 100, 5023-5035	3.9	79

75	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
74	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
73	Comparison of the boys and Pipek–Mezey localizations in the local correlation approach and automatic virtual basis selection. *Journal of Computational Chemistry*, **1993**, 14, 736-740	3.5	243
72	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
71	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
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 tautomers of uracil: A local correlation treatment. *International Journal of Quantum Chemistry*, **1993**, 47, 49-58	2.1	33
68	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
67	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
66	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
65	The geometries of chlorobenzenes as obtained from ab initio calculations empirically corrected by offset forces. *Computational and Theoretical Chemistry*, **1992**, 277, 147-160		2
64	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
63	A space-saving modification of Davidson's eigenvector algorithm. *Journal of Computational Chemistry*, **1990**, 11, 1164-1168	3.5	78
62	Ab initio prediction of vibrational spectra: A database approach. *Vibrational Spectroscopy*, **1990**, 1, 159-165	2.1	68
61	Methods for finding unrestricted Hartree-Fock solutions and multiple solutions. *The Journal of Physical Chemistry*, **1990**, 94, 5548-5551		24
60	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
59	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
58	The 7-Norbornadienyl Cation: An NMR/IGLO Validation of its ab initio Structure. *Angewandte Chemie International Edition in English*, **1989**, 28, 1042-1044		28

57	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
56	Generalized Mo/llerPlesset 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
55	The unrestricted natural orbitalomplete active space (UNOCAS) method: An inexpensive alternative to the complete active spaceelf-consistent-field (CASCF) method. *Journal of Chemical Physics*, **1989**, 90, 3637-3646	3.9	180
54	UHF natural orbitals for defining and starting MC-SCF calculations. *Journal of Chemical Physics*, **1988**, 88, 4926-4933	3.9	210
53	The local correlation treatment. II. Implementation and tests. *Journal of Chemical Physics*, **1988**, 88, 1884-1890	3.9	241
52	Vibrational energy levels of methyl fluoride. *Journal of Chemical Physics*, **1987**, 86, 5088-5093	3.9	46
51	Fourth-order Mo/llerPlessett perturbation theory in the local correlation treatment. I. Method. *Journal of Chemical Physics*, **1987**, 86, 914-922	3.9	411
50	Scaled quantum mechanical (SQM) force field and vibrational assignment for hexatriene. *Computational and Theoretical Chemistry*, **1987**, 151, 341-354		32
49	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
48	The ring puckering potential of oxetane: local correlation results. *Chemical Physics Letters*, **1986**, 132, 29-31	2.5	8
47	A test of the approximate coupled cluster doubles approximation. *Chemical Physics Letters*, **1986**, 131, 384-388	2.5	14
46	Orbital-invariant formulation and second-order gradient evaluation in Mller-Plesset perturbation theory. *Theoretica Chimica Acta*, **1986**, 69, 357-368		466
45	Vibrational energy levels of hydrogen cyanide. *Journal of Chemical Physics*, **1986**, 85, 5838-5846	3.9	64
44	The force constants of benzene: Local many-body perturbation theory vs new experiment. *Journal of Chemical Physics*, **1986**, 85, 1703-1704	3.9	47
43	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
42	Local configuration interaction: An efficient approach for larger molecules. *Chemical Physics Letters* , **1985**, 113, 13-18	2.5	398
41	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
40	An efficient reformulation of the closed-shell self-consistent electron pair theory. *Journal of Chemical Physics*, **1984**, 81, 1901-1905	3.9	163

39	The adiabatic correction to molecular potential surfaces in the SCF approximation. *Chemical Physics Letters*, **1984**, 103, 463-465	2.5	97
38	The computed force constants and vibrational spectra of cubane. *Journal of Molecular Spectroscopy* , **1984**, 103, 268-280	1.3	22
37	Geometry optimization by direct inversion in the iterative subspace. *Journal of Molecular Structure*, **1984**, 114, 31-34	3.4	461
36	On the calculation of elastic electron scattering cross sections from molecular wavefunctions: CF4 and CH4. *Computational and Theoretical Chemistry*, **1984**, 108, 149-159		10
35	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
34	Localizability of dynamic electron correlation. *Chemical Physics Letters*, **1983**, 100, 151-154	2.5	684
33	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
32	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
31	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
30	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
29	Comment on □orce in SCF theories□*Journal of Chemical Physics*, **1983**, 79, 2491-2492	3.9	5
28	Theoretical equilibrium geometry, vibrational frequencies and the first electronic transition energy of HCC. *Molecular Physics*, **1983**, 50, 139-151	1.7	33
27	The molecular structure, vibrational force field, spectral frequencies, and infrared intensities of CH3POF2. *Computational and Theoretical Chemistry*, **1982**, 87, 113-124		31
26	The structure of some nitrogen heteroaromatics. *Computational and Theoretical Chemistry*, **1982**, 88, 79-89		39
25	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
24	Structures of some fluorinated benzenes determined by ab initio computation. *Journal of Computational Chemistry*, **1982**, 3, 344-353	3.5	52
23	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
22	Convergence acceleration of iterative sequences. the case of scf iteration. *Chemical Physics Letters*, **1980**, 73, 393-398	2.5	1825

21	The molecular structure of toluene. *Journal of Molecular Structure*, **1980**, 66, 281-287	3.4	68
20	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
19	The geometry of some amides obtained from ab initio calculations. *Journal of Molecular Structure*, **1979**, 57, 259-270	3.4	73
18	An efficient ab initio gradient program. *Theoretica Chimica Acta*, **1979**, 50, 299-312		448
17	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
16	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
15	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
14	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
13	Ab initio Hartree-Fock calculation of the force constants and geometry of HNF2 and H2NF. *Molecular Physics*, **1977**, 33, 1565-1570	1.7	36
12	The tilt and asymmetry of methyl groups in asymmetric environments. *Journal of the American Chemical Society*, **1977**, 99, 5570-5574	16.4	61
11	Direct Use of the Gradient for Investigating Molecular Energy Surfaces **1977**, 153-185		141
10	The in-plane force field of nitryl fluoride. *Molecular Physics*, **1976**, 32, 169-176	1.7	6
9	Force constants, vibrational assignment and geometry of methyl amine from hartree-fock calculations. *Journal of Molecular Structure*, **1975**, 29, 239-246	3.4	34
8	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
7	Ab initio study of the force constants of inorganic molecules ONF and NF3. *Journal of Molecular Spectroscopy*, **1974**, 51, 135-141	1.3	26
6	Vibrational assignment of SF4. *Journal of Molecular Structure*, **1974**, 21, 158-164	3.4	11
5	Comparison of the ab initio force constants of ethane, ethylene and acetylene. *Molecular Physics*, **1974**, 27, 473-490	1.7	113
4	Hartree-Fock calculation of the harmonic force constants and equilibrium geometry of formaldehyde. *Theoretica Chimica Acta*, **1974**, 32, 253-264		87

3	Calculation of fully optimized geometries of five- and six-membered heterocycles by the CNDO force method. *Theoretica Chimica Acta*, **1973**, 32, 145-150		12
2	Force Constants and Dipole Moment Derivatives of Ammonia from Hartree-Fock Calculations. *Journal of Chemical Physics*, **1972**, 57, 3337-3340	3.9	73
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