

Peter Pulay

List of PR Articles by Year in descending order

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105

PR articles

21,463

PR citations

31116

47

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20722

103

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documents

23066

doc citations

32418

50

h-index

13558

citing authors

#	ARTICLE	IF	PR CITATIONS
1	Compact representation of generalized molecular polarizabilities and efficient calculation of polarization energy in an arbitrary electric field. <i>International Journal of Quantum Chemistry</i> , 2022, , .	2.1	0
2	Comparison of Methods for Active Orbital Selection in Multiconfigurational Calculations. <i>Journal of Chemical Theory and Computation</i> , 2020, 16, 7328-7341.	5.4	34
3	Breaking established paradigms: a tribute to Wilfried Meyer's contributions to ab initio quantum chemistry. <i>Molecular Physics</i> , 2020, 118, e1730993.	2.4	0
4	Analytical Energy Gradients for the Cluster-in-Molecule MP2 Method and Its Application to Geometry Optimizations of Large Systems. <i>Journal of Chemical Theory and Computation</i> , 2019, 15, 3623-3634.	5.4	18
5	Automatic Construction of the Initial Orbitals for Efficient Generalized Valence Bond Calculations of Large Systems. <i>Journal of Chemical Theory and Computation</i> , 2019, 15, 141-153.	5.4	34
6	Benchmark Relative Energies for Large Water Clusters with the Generalized Energy-Based Fragmentation Method. <i>Journal of Chemical Theory and Computation</i> , 2017, 13, 2696-2704.	5.4	41
7	Approximate Force Constants from Uncoupled Self-Consistent Field Perturbation Theory Using Nonhybrid Density Functional Theory. <i>Journal of Physical Chemistry A</i> , 2017, 121, 348-356.	2.7	1
8	The vibrational spectrum of 1,4-dioxane in aqueous solution – theory and experiment. <i>New Journal of Chemistry</i> , 2016, 40, 7663-7670.	2.5	22
9	Finding symmetry breaking Hartree-Fock solutions: The case of triplet instability. <i>Journal of Chemical Physics</i> , 2016, 145, .	2.9	30
10	Selection of active spaces for multiconfigurational wavefunctions. <i>Journal of Chemical Physics</i> , 2015, 142, .	2.9	100
11	Efficient calculation of the density response function from generalized polarizabilities. <i>Theoretical Chemistry Accounts</i> , 2015, 135, .	1.4	8
12	Accuracy of Quantum Chemical Methods for Large Noncovalent Complexes. <i>Journal of Chemical Theory and Computation</i> , 2013, 9, 3364-3374.	5.4	324
13	A Benchmark Comparison of $\tilde{\chi}^{\text{RPA}}/\tilde{\chi}^{\text{RPA}}$ and $\tilde{\chi}^{\text{RPA}}/\tilde{\chi}^{\text{RPA}}$ Dispersion: the Dimers of Naphthalene and Decalin, and Coronene and Perhydrocoronene. <i>Journal of the American Chemical Society</i> , 2012, 134, 17520-17525.	15.1	103
14	Ultrafast Quantum Mechanics/Molecular Mechanics Monte Carlo simulations using generalized multipole polarizabilities. <i>Chemical Physics Letters</i> , 2012, 530, 1-9.	2.8	16
15	The Ethidium – UA/AU Intercalation Site: Effect of Model Fragmentation and Backbone Charge State. <i>Journal of Chemical Theory and Computation</i> , 2011, 7, 2600-2609.	5.4	8
16	Convex – concave stacking of curved conjugated networks: Benchmark calculations on the corannulene dimer. <i>Chemical Physics Letters</i> , 2011, 512, 155-160.	2.8	66
17	A benchmark quantum chemical study of the stacking interaction between larger polycondensed aromatic hydrocarbons. <i>Theoretical Chemistry Accounts</i> , 2011, 130, 419-427.	1.4	16
18	Accurate correlated calculation of the intermolecular potential surface in the coronene dimer. <i>Molecular Physics</i> , 2010, 108, 249-257.	2.4	81

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19	A Reliable and Efficient First Principles-Based Method for Predicting p <i>K</i> _a Values. 1. Methodology. <i>Journal of Physical Chemistry A</i> , 2010, 114, 425-431.	2.7	77
20	A Reliable and Efficient First Principles-Based Method for Predicting p <i>K</i> _a Values. 2. Organic Acids. <i>Journal of Physical Chemistry A</i> , 2010, 114, 432-442.	2.7	93
21	A potential surface for the interaction between water and coronene as a model for a hydrophobic surface. <i>Molecular Physics</i> , 2009, 107, 1197-1207.	2.4	14
22	Efficient Parallel Implementation of the CCSD External Exchange Operator and the Perturbative Triples (T) Energy Calculation. <i>Journal of Chemical Theory and Computation</i> , 2008, 4, 1585-1592.	5.4	72
23	Parallel Calculation of Coupled Cluster Singles and Doubles Wave Functions Using Array Files. <i>Journal of Chemical Theory and Computation</i> , 2007, 3, 1368-1377.	5.4	68
24	High accuracy benchmark calculations on the benzene dimer potential energy surface. <i>Chemical Physics Letters</i> , 2007, 447, 27-32.	2.8	271
25	H ₂ , Ne, and N ₂ Energies of Encapsulation into C ₆₀ Evaluated with the MPWB1K Functional. <i>Journal of Chemical Theory and Computation</i> , 2006, 2, 782-785.	5.4	96
26	The Interpretation of Compliance Constants and Their Suitability for Characterizing Hydrogen Bonds and Other Weak Interactions. <i>Journal of the American Chemical Society</i> , 2006, 128, 11324-11325.	15.1	46
27	Ligand Redox Effects in the Synthesis, Electronic Structure, and Reactivity of an Alkyl ⁺ Alkyl Cross-Coupling Catalyst. <i>Journal of the American Chemical Society</i> , 2006, 128, 13175-13183.	15.1	458
28	Importance of Tensor Asymmetry for the Analysis of ² H NMR Spectra from Deuterated Aromatic Rings. <i>Journal of the American Chemical Society</i> , 2005, 127, 17488-17493.	15.1	19
29	Fock matrix dynamics. <i>Chemical Physics Letters</i> , 2004, 386, 272-278.	2.8	97
30	Parallel implementation of Hartree-Fock and density functional theory analytical second derivatives. <i>Molecular Physics</i> , 2004, 102, 2475-2484.	2.4	12
31	The Performance of the Handy/Cohen Functionals, OLYP and O3LYP, for the Computation of Hydrocarbon Pericyclic Reaction Activation Barriers. <i>Journal of Physical Chemistry A</i> , 2004, 108, 2959-2965.	2.7	57
32	Parallel Density Functional Theory Energies using the Fourier Transform Coulomb Method. <i>Journal of Physical Chemistry A</i> , 2004, 108, 3040-3047.	2.7	14
33	Combined Experimental/Theoretical Refinement of Indole Ring Geometry Using Deuterium Magnetic Resonance and ab Initio Calculations. <i>Journal of the American Chemical Society</i> , 2003, 125, 12268-12276.	15.1	25
34	C ¹⁸ O Hydrogen Bond between N-Methyl Maleimide and Dimethyl Sulfoxide: A Combined NMR and Ab Initio Study. <i>Journal of Physical Chemistry A</i> , 2003, 107, 4683-4687.	2.7	46
35	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. <i>Journal of Biomolecular Structure and Dynamics</i> , 2002, 20, 71-79.	2.8	3
36	Theoretical and Experimental Study of the Vibrational Spectra of the ¹ ±, ¹ ², and ¹ ³ Phases of Octahydro-1,3,5,7-tetranitro-1,3,5,7-tetrazocine (HMX). <i>Journal of Physical Chemistry B</i> , 2002, 106, 10594-10604.	2.8	71

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37	The Fourier transform Coulomb method: Efficient and accurate calculation of the Coulomb operator in a Gaussian basis. <i>Journal of Chemical Physics</i> , 2002, 117, 7827-7835.	2.9	98
38	Newtonian molecular dynamics in general curvilinear internal coordinates. <i>Chemical Physics Letters</i> , 2002, 353, 400-406.	2.8	12
39	Reply to the comments on 'Efficient calculation of canonical MP2 energies' by A. K�hn and C. H�ttig. <i>Chemical Physics Letters</i> , 2002, 358, 354-356.	2.8	3
40	Calculated and Experimental Geometries and Infrared Spectra of Metal Tris-Acetylacetonates:�% Vibrational Spectroscopy as a Probe of Molecular Structure for Ionic Complexes. Part I. <i>Journal of Physical Chemistry A</i> , 2001, 105, 238-244.	2.7	111
41	Efficient calculation of canonical MP2 energies. <i>Chemical Physics Letters</i> , 2001, 344, 543-552.	2.8	43
42	Density functional implementation of a Gaussian-weighted operator for spin densities. <i>Physical Chemistry Chemical Physics</i> , 2000, 2, 2131-2135.	2.8	7
43	GIAO Nuclear Magnetic Shielding Tensors in Free Base Porphyrin and in Magnesium and Zinc Metalloporphyrins. <i>Journal of Physical Chemistry A</i> , 1999, 103, 420-425.	2.7	25
44	DFT-SQM Force Field for Nickel Porphine:�% Intrinsic Ruffling. <i>Journal of Physical Chemistry A</i> , 1999, 103, 1357-1366.	2.7	110
45	Stability of Novel Oxo- and Chloro-Substituted Trioxanes. <i>Journal of the American Chemical Society</i> , 1999, 121, 8544-8548.	15.1	7
46	Multipole approximation of distant pair energies in local MP2 calculations. <i>Chemical Physics Letters</i> , 1998, 290, 143-149.	2.8	196
47	The unrestricted natural orbital-restricted active space method: methodology and implementation. <i>Theoretical Chemistry Accounts</i> , 1998, 100, 12-20.	1.4	19
48	Direct Scaling of Primitive Valence Force Constants:� An Alternative Approach to Scaled Quantum Mechanical Force Fields. <i>Journal of Physical Chemistry A</i> , 1998, 102, 1412-1424.	2.7	501
49	The size consistency of multi-reference M�ller-Plesset perturbation theory. <i>Molecular Physics</i> , 1998, 93, 431-439.	2.4	35
50	The inner-hydrogen migration in free base porphyrin. <i>Theoretical Chemistry Accounts</i> , 1997, 97, 59-66.	1.4	65
51	Comparison of NMR Shieldings Calculated from Hartree-Fock and Density Functional Wave Functions Using Gauge-Including Atomic Orbitals. <i>The Journal of Physical Chemistry</i> , 1996, 100, 6310-6316.	3.1	208
52	Considerations regarding the local treatment of Laplace transform MPPT. <i>Chemical Physics Letters</i> , 1996, 248, 223-227.	2.8	15
53	Vibrational Assignment and Definite Harmonic Force Field for Porphine. 2. Comparison with Nonresonance Raman Data. <i>The Journal of Physical Chemistry</i> , 1996, 100, 13985-13992.	3.1	95
54	Chemical shift anisotropies in silicon containing three-membered rings. An ab initio study. <i>Chemical Physics Letters</i> , 1995, 241, 393-398.	2.8	13

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55	An accurate in-plane force field for porphine. A scaled quantum mechanical study. <i>Chemical Physics Letters</i> , 1995, 247, 379-385.	2.8	66
56	Possibilities and limitations of ab initio calculation of vibrational spectra. <i>Journal of Molecular Structure</i> , 1995, 347, 293-308.	4.2	57
57	A new grid-based method for the direct computation of excited molecular vibrational states: test application to formaldehyde. <i>Computational and Theoretical Chemistry</i> , 1995, 341, 1-11.	1.3	39
58	Identification of Isomers from Calculated Vibrational Spectra. A Density Functional Study of Tetrachlorinated Dibenzodioxins. <i>Journal of the American Chemical Society</i> , 1995, 117, 4167-4172.	15.1	94
59	Basis set and correlation effects in the calculation of selenium NMR shieldings. <i>Chemical Physics Letters</i> , 1994, 225, 280-284.	2.8	37
60	Can (semi)local density functional theory account for the London dispersion forces?. <i>Chemical Physics Letters</i> , 1994, 229, 175-180.	2.8	990
61	Building a database of force constants based on scaled ab initio (SQM) results. I. Chlorobenzenes. <i>Spectrochimica Acta Part A: Molecular Spectroscopy</i> , 1993, 49, 1499-1514.	0.2	16
62	Complete assignment of vibrational spectra of 1,5-cyclooctadiene—a theoretical and experimental infrared and Raman study. <i>Spectrochimica Acta Part A: Molecular Spectroscopy</i> , 1993, 49, 257-270.	0.2	13
63	Theoretical study on the structures, force field, and vibrational spectra of cyclooctatetraene and cyclooctatetraene-d8. <i>Spectrochimica Acta Part A: Molecular Spectroscopy</i> , 1993, 49, 953-964.	0.2	8
64	The calculation of ab initio molecular geometries: efficient optimization by natural internal coordinates and empirical correction by offset forces. <i>Journal of the American Chemical Society</i> , 1992, 114, 8191-8201.	15.1	943
65	The geometries of chlorobenzenes as obtained from ab initio calculations empirically corrected by offset forces. <i>Computational and Theoretical Chemistry</i> , 1992, 277, 147-160.	1.3	4
66	Ab initio prediction of vibrational spectra: A database approach. <i>Vibrational Spectroscopy</i> , 1990, 1, 159-165.	2.6	71
67	Methods for finding unrestricted Hartree-Fock solutions and multiple solutions. <i>The Journal of Physical Chemistry</i> , 1990, 94, 5548-5551.	3.1	30
68	Efficient implementation of the gauge-independent atomic orbital method for NMR chemical shift calculations. <i>Journal of the American Chemical Society</i> , 1990, 112, 8251-8260.	15.1	6,657
69	The 7-Norbornadienyl Cation: An NMR/IGLO Validation of its ab initio Structure. <i>Angewandte Chemie International Edition in English</i> , 1989, 28, 1042-1044.	4.6	38
70	Natural charge densities for the evaluation of MC-SCF energy derivatives without density matrix transformation. <i>Chemical Physics Letters</i> , 1989, 156, 501-504.	2.8	1
71	Das 7-Norbornadienyl-Kation: die NMR/IGLO-Bestätigung seiner mit ab-initio-Methoden berechneten Struktur. <i>Angewandte Chemie</i> , 1989, 101, 1063-1065.	1.4	26
72	Scaled quantum mechanical (SQM) force field and vibrational assignment for hexatriene. <i>Computational and Theoretical Chemistry</i> , 1987, 151, 341-354.	1.3	35

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73	Consistent generalization of the M \ddot{u} ller-Plesset partitioning to open-shell and multiconfigurational SCF reference states in many-body perturbation theory. <i>Chemical Physics Letters</i> , 1987, 140, 225-231.	2.8	167
74	The ring puckering potential of oxetane: local correlation results. <i>Chemical Physics Letters</i> , 1986, 132, 29-31.	2.8	12
75	A test of the approximate coupled cluster doubles approximation. <i>Chemical Physics Letters</i> , 1986, 131, 384-388.	2.8	14
76	Orbital-invariant formulation and second-order gradient evaluation in M \ddot{u} ller-Plesset perturbation theory. <i>Theoretica Chimica Acta</i> , 1986, 69, 357-368.	0.0	533
77	Local configuration interaction: An efficient approach for larger molecules. <i>Chemical Physics Letters</i> , 1985, 113, 13-18.	2.8	444
78	Theoretical prediction of vibrational spectra. 2. Force field, spectroscopically refined geometry, and reassignment of the vibrational spectrum of naphthalene. <i>Journal of the American Chemical Society</i> , 1985, 107, 6487-6494.	15.1	125
79	The adiabatic correction to molecular potential surfaces in the SCF approximation. <i>Chemical Physics Letters</i> , 1984, 103, 463-465.	2.8	111
80	The computed force constants and vibrational spectra of cubane. <i>Journal of Molecular Spectroscopy</i> , 1984, 103, 268-280.	1.3	25
81	Geometry optimization by direct inversion in the iterative subspace. <i>Journal of Molecular Structure</i> , 1984, 114, 31-34.	4.2	525
82	On the calculation of elastic electron scattering cross sections from molecular wavefunctions: CF ₄ and CH ₄ . <i>Computational and Theoretical Chemistry</i> , 1984, 108, 149-159.	1.3	10
83	Theoretical prediction of vibrational spectra. 1. The in-plane force field and vibrational spectra of pyridine. <i>Journal of the American Chemical Society</i> , 1984, 106, 2765-2769.	15.1	134
84	Localizability of dynamic electron correlation. <i>Chemical Physics Letters</i> , 1983, 100, 151-154.	2.8	798
85	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. <i>Journal of the American Chemical Society</i> , 1983, 105, 7037-7047.	15.1	1,517
86	Theoretical equilibrium geometry, vibrational frequencies and the first electronic transition energy of HCC. <i>Molecular Physics</i> , 1983, 50, 139-151.	2.4	36
87	The molecular structure, vibrational force field, spectral frequencies, and infrared intensities of CH ₃ POF ₂ . <i>Computational and Theoretical Chemistry</i> , 1982, 87, 113-124.	1.3	32
88	The structure of some nitrogen heteroaromatics. <i>Computational and Theoretical Chemistry</i> , 1982, 88, 79-89.	1.3	41
89	Force field and vibrational assignment for cyclobutane from a combination of ab initio calculations and experimental data. <i>Computational and Theoretical Chemistry</i> , 1982, 89, 1-13.	1.3	36
90	Convergence acceleration of iterative sequences. the case of scf iteration. <i>Chemical Physics Letters</i> , 1980, 73, 393-398.	2.8	2,369

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91	The molecular structure of toluene. <i>Journal of Molecular Structure</i> , 1980, 66, 281-287.	4.2	73
92	Transition state vibrational analysis for the methyl isocyanide rearrangement, CH ₃ NC → CH ₃ CN. <i>Journal of the American Chemical Society</i> , 1980, 102, 3718-3723.	15.1	32
93	The geometry of some amides obtained from ab initio calculations. <i>Journal of Molecular Structure</i> , 1979, 57, 259-270.	4.2	79
94	An efficient ab initio gradient program. <i>Theoretica Chimica Acta</i> , 1979, 50, 299-312.	0.0	455
95	Systematic ab initio gradient calculation of molecular geometries, force constants, and dipole moment derivatives. <i>Journal of the American Chemical Society</i> , 1979, 101, 2550-2560.	15.1	2,090
96	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. <i>Journal of the American Chemical Society</i> , 1979, 101, 2002-2010.	15.1	71
97	Ab initio Hartree-Fock calculation of the force constants and geometry of HNF ₂ and H ₂ NF. <i>Molecular Physics</i> , 1977, 33, 1565-1570.	2.4	37
98	The tilt and asymmetry of methyl groups in asymmetric environments. <i>Journal of the American Chemical Society</i> , 1977, 99, 5570-5574.	15.1	66
99	The in-plane force field of nitril fluoride. <i>Molecular Physics</i> , 1976, 32, 169-176.	2.4	8
100	Force constants, vibrational assignment and geometry of methyl amine from Hartree-Fock calculations. <i>Journal of Molecular Structure</i> , 1975, 29, 239-246.	4.2	38
101	Ab initio calculation of force constants for the linear molecules HCN, FCN, (CN) ₂ and the ion N ₂ F ⁺ . <i>Molecular Physics</i> , 1975, 30, 1123-1131.	2.4	38
102	Ab initio study of the force constants of inorganic molecules ONF and NF ₃ . <i>Journal of Molecular Spectroscopy</i> , 1974, 51, 135-141.	1.3	30
103	Vibrational assignment of SF ₄ . <i>Journal of Molecular Structure</i> , 1974, 21, 158-164.	4.2	12
104	Comparison of the ab initio force constants of ethane, ethylene and acetylene. <i>Molecular Physics</i> , 1974, 27, 473-490.	2.4	122
105	Calculation of fully optimized geometries of five- and six-membered heterocycles by the CNDO force method. <i>Theoretica Chimica Acta</i> , 1973, 32, 145-150.	0.0	15