Ernest Davidson

List of Publications by Year
in descending order

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399 papers	35,042 citations	7251 80 h-index	4853 174 g-index
462 all docs	462 docs citations	462 times ranked	12929 citing authors

#	Article	IF	Citations
1	Coherent Xâ€Ray Scattering for the Hydrogen Atom in the Hydrogen Molecule. Journal of Chemical Physics, 1965, 42, 3175-3187.	1.2	5,338
2	Configuration interaction calculations on the nitrogen molecule. International Journal of Quantum Chemistry, 1974, 8, 61-72.	1.0	2,701
3	The iterative calculation of a few of the lowest eigenvalues and corresponding eigenvectors of large real-symmetric matrices. Journal of Computational Physics, 1975, 17, 87-94.	1.9	2,203
4	Ligand spin polarization and antiferromagnetic coupling in transition metal dimers. Chemical Physics, 1986, 109, 131-143.	0.9	904
5	Basis set selection for molecular calculations. Chemical Reviews, 1986, 86, 681-696.	23.0	763
6	Effects of electron repulsion in conjugated hydrocarbon diradicals. Journal of the American Chemical Society, 1977, 99, 4587-4594.	6.6	623
7	Size consistency in the dilute helium gas electronic structure. Chemical Physics Letters, 1977, 52, 403-406.	1.2	573
8	One- and two-electron integrals over cartesian gaussian functions. Journal of Computational Physics, 1978, 26, 218-231.	1.9	562
9	Ground-state correlation energies for atomic ions with 3 to 18 electrons. Physical Review A, 1993, 47, 3649-3670.	1.0	488
10	Comment on â€œComment on Dunning's correlation-consistent basis setsâ€• Chemical Physics Letters, 1996, 260, 514-518.	1.2	375
11	Studies in Configuration Interaction: The First-Row Diatomic Hydrides. Physical Review, 1969, 183, 23-30.	2.7	360
12	Ground-state correlation energies for two- to ten-electron atomic ions. Physical Review A, 1991, 44, 7071-7083.	1.0	360
13	Electronic Population Analysis of Molecular Wavefunctions. Journal of Chemical Physics, 1967, 46, 3320-3324.	1.2	352
14	A Natural Orbital Based Energy Calculation for Helium Hydride and Lithium Hydride. The Journal of Physical Chemistry, 1966, 70, 2675-2685.	2.9	340
15	A test of the Hirshfeld definition of atomic charges and moments. Theoretica Chimica Acta, 1992, 83, 319-330.	0.9	276
16	Porphyrins XXVIII. Extended Hï¿½ckel calculations on metal phthalocyanines and tetrazaporphins. Theoretica Chimica Acta, 1973, 30, 9-30.	0.9	268
17	Asymptotic behavior of atomic and molecular wave functions. Proceedings of the National Academy of Sciences of the United States of America, 1980, 77, 4403-4406.	3.3	268
18	Symmetry breaking in polyatomic molecules: real and artifactual. The Journal of Physical Chemistry, 1983, 87, 4783-4790.	2.9	264

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19	The Importance of Including Dynamic Electron Correlation inab InitioCalculations. Accounts of Chemical Research, 1996, 29, 67-75.	7.6	240
20	Oneâ€electron properties of several small molecules using near Hartreeâ€“Fock limit basis sets. Journal of Chemical Physics, 1987, 86, 3424-3440.	1.2	226
21	The two lowest energy 2Aâ€² states of NO2. Journal of Chemical Physics, 1976, 64, 2908-2917.	1.2	207
22	Properties and Uses of Natural Orbitals. Reviews of Modern Physics, 1972, 44, 451-464.	16.4	204
23	Distribution of effectively unpaired electrons. Chemical Physics Letters, 2000, 330, 161-168.	1.2	197
24	An approximation to frozen natural orbitals through the use of the Hartreeâ€“Fock exchange potential. Journal of Chemical Physics, 1981, 74, 3977-3979.	1.2	188
25	Considerations in constructing a multireference secondâ€order perturbation theory. Journal of Chemical Physics, 1994, 100, 3672-3682.	1.2	181
26	Electron momentum spectroscopy of the valence orbitals of H2O and D2O: Quantitative comparisons using Hartreeâ€”Fock limit and correlated wavefunctions. Chemical Physics, 1987, 113, 19-42.	0.9	177
27	Optimized effective potentials yielding Hartreeâ€“Fock energies and densities. Journal of Chemical Physics, 2006, 124, 141103.	1.2	175
28	Is the Hydrogen Bond in Water Dimer and Ice Covalent?. Journal of the American Chemical Society, 2000, 122, 1210-1214.	6.6	174
29	Ab initio configuration interaction calculations of the hyperfine structure in small radicals. Journal of Chemical Physics, 1984, 80, 1006-1017.	1.2	167
30	Local spin. Journal of Chemical Physics, 2001, 115, 7382-7392.	1.2	165
31	Nature of the Configuration-Interaction Method inAb InitioCalculations. I. Ne Ground State. Physical Review A, 1970, 1, 644-658.	1.0	159
32	An analysis of the hydrogen bond in ice. Journal of Chemical Physics, 1990, 93, 8029-8035.	1.2	154
33	Theoretical studies of diradicals containing four .pi. electrons. Accounts of Chemical Research, 1981, 14, 69-76.	7.6	149
34	Single-Molecule Magnets:Â Two-Electron Reduced Version of a Mn12Complex and Environmental Influences on the Magnetization Relaxation of (PPh4)2[Mn12O12(O2CCHCl2)16(H2O)4]. Journal of the American Chemical Society, 2003, 125, 3576-3588.	6.6	149
35	An ab initio potentialâ€energy surface study of several electronic states of NO2. Journal of Chemical Physics, 1976, 65, 2941-2957.	1.2	148
36	Nature of ground and electronic excited states of higher acenes. Proceedings of the National Academy of Sciences of the United States of America, 2016, 113, E5098-107.	3.3	147

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37	Selection of the Proper Canonical Roothaanâ€Hartreeâ€Fock Orbitals for Particular Applications. I. Theory. Journal of Chemical Physics, 1972, 57, 1999-2005.	1.2	146
38	Spin-restricted open-shell self-consistent-field theory. Chemical Physics Letters, 1973, 21, 565-567.	1.2	140
39	Extended x-ray-absorption fine-structure amplitudesâ€”Wave-function relaxation and chemical effects. Physical Review B, 1978, 17, 560-565.	1.1	140
40	Large Spin Differences in Structurally Related Fe6Molecular Clusters and Their Magnetostructural Explanation. Inorganic Chemistry, 2004, 43, 5505-5521.	1.9	140
41	Global topology of triatomic potential surfaces. Journal of the American Chemical Society, 1977, 99, 397-402.	6.6	138
42	Large Ground-State Entropy Changes for Hydrogen Atom Transfer Reactions of Iron Complexes. Journal of the American Chemical Society, 2007, 129, 5153-5166.	6.6	134
43	Natural Expansion of Exact Wavefunctions. II. The Hydrogenâ€Molecule Ground State. Journal of Chemical Physics, 1962, 37, 2966-2971.	1.2	132
44	Perturbation theory for open shell systems. Chemical Physics Letters, 1991, 187, 451-454.	1.2	132
45	An SCF method for hole states. Journal of Chemical Physics, 1976, 65, 609-613.	1.2	127
46	Improved algorithms for the lowest few eigenvalues and associated eigenvectors of large matrices. Journal of Computational Physics, 1992, 103, 382-389.	1.9	123
47	A possible definition of basis set superposition error. Chemical Physics Letters, 1994, 217, 48-54.	1.2	123
48	Experimental evidence for a C2v (2B1) ground-state structure of the methane cation radical: ESR and ab initio CI investigations of methane cation radicals (CH4+ and CD2H2+) in neon matrixes at 4 K. Journal of the American Chemical Society, 1984, 106, 3700-3701.	6.6	122
49	Diradical Character of the Cope Rearrangement Transition State. Journal of the American Chemical Society, 2000, 122, 186-187.	6.6	121
50	Configuration interaction calculations on the planar 1(Ï€,Ï€*) state of ethylene. Journal of Chemical Physics, 1977, 66, 2959-2971.	1.2	119
51	The transition metal-carbonyl bond. Accounts of Chemical Research, 1993, 26, 628-635.	7.6	118
52	Theoretical Calculation of the Potential Curves of the Be2 Molecule. Journal of Chemical Physics, 1967, 47, 4972-4978.	1.2	117
53	Singleâ€Configuration Calculations on Excited States of Helium. II. Journal of Chemical Physics, 1965, 42, 4199-4200.	1.2	114
54	Configuration Interaction Description of Electron Correlation. , 1974, , 17-30.		114

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55	Validity of first-order perturbation theory for relativistic energy corrections. Chemical Physics Letters, 1981, 84, 226-227.	1.2	113
56	First Excited 1Î£g+ State of the Hydrogen Molecule. Journal of Chemical Physics, 1961, 35, 1189-1202.	1.2	112
57	Refinement of the Asymptotic Z Expansion for the Ground-State Correlation Energies of Atomic Ions. The Journal of Physical Chemistry, 1996, 100, 6167-6172.	2.9	110
58	The Cope Rearrangement Revisited with Multireference Perturbation Theory. Journal of the American Chemical Society, 1995, 117, 774-778.	6.6	109
59	Structure of ice Ih. Ab initio twoâ€•and threeâ€body waterâ€“water potentials and geometry optimization. Journal of Chemical Physics, 1985, 83, 1223-1231.	1.2	104
60	Zero kinetic energy photoelectron spectra of jetâ€cooled aniline. Journal of Chemical Physics, 1993, 99, 3224-3233.	1.2	103
61	Potential energy surfaces of CH+4. Journal of Chemical Physics, 1988, 88, 1775-1785.	1.2	100
62	Natural Orbitals for Hydrogenâ€Molecule Excited States. Journal of Chemical Physics, 1966, 45, 2560-2576.	1.2	99
63	The potential surfaces for the lowest singlet and triplet states of cyclobutadiene. Journal of the American Chemical Society, 1978, 100, 388-392.	6.6	99
64	Facile and Reversible Cleavage of Câ^'F Bonds. Contrasting Thermodynamic Selectivity for RuCF2H vs FOsCFH. Journal of the American Chemical Society, 2000, 122, 8916-8931.	6.6	99
65	MCSCF/CI investigation of the low-lying potential energy surfaces of the formyloxyl radical, HCO2.cntdot.. Journal of the American Chemical Society, 1983, 105, 1459-1466.	6.6	98
66	A multireference CI determination of the isotropic hyperfine constants for first row atoms Bâ€“F. Journal of Chemical Physics, 1988, 88, 7580-7587.	1.2	98
67	A configuration interaction study of the spin dipole-dipole parameters for formaldehyde and methylene. International Journal of Quantum Chemistry, 1973, 7, 999-1019.	1.0	97
68	A theoretical study on the potential surfaces of the lower electronic states of HCO. Journal of Chemical Physics, 1979, 70, 2904-2913.	1.2	97
69	Potential surfaces for the planar cyclopentadienyl radical and cation. Journal of the American Chemical Society, 1979, 101, 3771-3775.	6.6	95
70	A third isolated oxidation state for the Mn12 family of single-molecule magnets. Chemical Communications, 2000, , 2417-2418.	2.2	92
71	Applicability of selfâ€consistent field techniques based on the complex coordinate method to metastable electronic states. Journal of Chemical Physics, 1980, 73, 3268-3273.	1.2	91
72	ESR andabinitiotheoretical studies of the cation radicals14N+4and15N+4: The trapping of ionâ€“neutral reaction products in neon matrices at 4 K. Journal of Chemical Physics, 1987, 87, 885-897.	1.2	90

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73	Theoretical Study of the LiH Molecule. Journal of Chemical Physics, 1968, 49, 4222-4229.	1.2	89
74	Difficulties inab initio CI calculations of the hyperfine structure of small radicals. Theoretica Chimica Acta, 1985, 68, 57-67.	0.9	89
75	The Cope rearrangement revisited. Journal of the American Chemical Society, 1991, 113, 9756-9759.	6.6	89
76	Coordinated carbenes from electron-rich olefins on RuHCl(PPr3i)2. New Journal of Chemistry, 2000, 24, 9-26.	1.4	87
77	The water dimer: correlation energy calculations. The Journal of Physical Chemistry, 1993, 97, 6373-6383.	2.9	86
78	Correlation Energy and Molecular Properties of Hydrogen Fluoride. Journal of Chemical Physics, 1967, 47, 360-366.	1.2	84
79	A perturbation theory calculation on the 1Ï€Ï€* state of formamide. Journal of Chemical Physics, 1978, 68, 3103-3109.	1.2	82
80	Ab initio evaluation of the fine structure and radiative lifetime of the 3A2(nâ†'Ï€*) state of formaldehyde. Journal of Chemical Physics, 1976, 64, 4699-4710.	1.2	81
81	Effective local potentials for orbital-dependent density functionals. Journal of Chemical Physics, 2006, 125, 081104.	1.2	81
82	A theoretical investigation of some low-lying singlet states of 1,3-butadiene. The Journal of Physical Chemistry, 1987, 91, 4481-4490.	2.9	80
83	Quasidegenerate variational perturbation theory and the calculation of firstâ€order properties from variational perturbation theory wave functions. Journal of Chemical Physics, 1988, 89, 6798-6814.	1.2	80
84	Transition Regions in the Cope Rearrangement of 1,5-Hexadiene and Its Cyano Derivatives. Journal of the American Chemical Society, 2000, 122, 7377-7385.	6.6	80
85	Some Triplet States of the Hydrogen Molecule. Journal of Chemical Physics, 1965, 43, 834-839.	1.2	79
86	Electronic Structure of the B2 Molecule. Journal of Chemical Physics, 1967, 46, 3313-3319.	1.2	79
87	Ab initio study of m-benzoquinodimethane. Journal of the American Chemical Society, 1983, 105, 1791-1795.	6.6	79
88	Ab initio studies of [1.1.1]- and [2.2.2]propellane. Journal of the American Chemical Society, 1987, 109, 4133-4139.	6.6	77
89	Different forms of perturbation theory for the calculation of the correlation energy. International Journal of Quantum Chemistry, 1992, 43, 755-768.	1.0	77
90	Rotationally resolved laser photoelectron spectra of gas-phase NO: rotational propensity rules in photoionization. The Journal of Physical Chemistry, 1986, 90, 5078-5084.	2.9	76

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91	Local spin II. Molecular Physics, 2002, 100, 373-383.	0.8	76
92	Singlet-Triplet Energy Separations in Some Hydrocarbon Diradicals. Annual Review of Physical Chemistry, 1979, 30, 125-153.	4.8	72
93	How robust is present-day DFT?. International Journal of Quantum Chemistry, 1998, 69, 241-245.	1.0	72
94	Natural Expansions of Exact Wavefunctions. III. The Heliumâ€Atom Ground State. Journal of Chemical Physics, 1963, 39, 875-880.	1.2	71
95	Some aspects of the potential surface for singlet trimethylenemethane. Journal of the American Chemical Society, 1977, 99, 2053-2060.	6.6	70
96	Stereomutation of cyclopropane revisited. An ab initio investigation of the potential surface and calculation of secondary isotope effects. Journal of the American Chemical Society, 1992, 114, 2085-2093.	6.6	70
97	Population analyses that utilize projection operators. International Journal of Quantum Chemistry, 2003, 93, 384-394.	1.0	70
98	SCF methods for excited states. International Journal of Quantum Chemistry, 1976, 10, 21-31.	1.0	70
99	A study of the ground state wave function of carbon monoxide. International Journal of Quantum Chemistry, 1970, 4, 223-243.	1.0	69
100	Evaluation of a characteristic atomic radius by an ab initio method. International Journal of Quantum Chemistry, 1997, 62, 47-53.	1.0	69
101	Interaction Energy of Two Groundâ€State Helium Atoms at Small Internuclear Distances. Journal of Chemical Physics, 1967, 46, 402-403.	1.2	67
102	Fluorescence Analysis: A New Approach. Analytical Letters, 1975, 8, 665-681.	1.0	67
103	The electron affinity of oxygen: A systematic configuration interaction approach. Journal of Chemical Physics, 1989, 90, 1024-1030.	1.2	67
104	N-representability of the electron pair density. Chemical Physics Letters, 1995, 246, 209-213.	1.2	67
105	UDFT and MCSCF Descriptions of the Photochemical Bergman Cyclization of Enediynes. Journal of the American Chemical Society, 2001, 123, 2650-2657.	6.6	67
106	Energy partitioning of the selfâ€consistent field interaction energy of ScCO. Journal of Chemical Physics, 1989, 90, 5555-5562.	1.2	66
107	Linear Inequalities for Density Matrices. Journal of Mathematical Physics, 1969, 10, 725-734.	0.5	65
108	Linear Inequalities for Density Matrices. II. Journal of Mathematical Physics, 1972, 13, 1527-1538.	0.5	65

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109	Abinitiocalculation of extended x-ray-absorption fine structure inBr2. Physical Review B, 1987, 35, 2604-2614.	1.1	65
110	LÃ¶wdin population analysis with and without rotational invariance. International Journal of Quantum Chemistry, 2006, 106, 2065-2072.	1.0	65
111	RHF and two-configuration SCF calculations are inappropriate for conjugated diradicals. Tetrahedron, 1982, 38, 737-739.	1.0	64
112	A proposed antiferroelectric structure for proton ordered ice Ih. Journal of Chemical Physics, 1984, 81, 3741-3742.	1.2	64
113	Zero point corrections to vertical excitation energies. Chemical Physics Letters, 1998, 285, 155-159.	1.2	64
114	Laser sputtering generation of B2 for ESR matrix isolation studies: comparison with ab initio CI theoretical calculations. Journal of the American Chemical Society, 1987, 109, 3521-3525.	6.6	63
115	An electron spin resonance investigation of vanadium dioxide (51V16O2 and 51V17O2) and 51V17O in neon matrices with preliminary assignments for VO3 and V+2: Comparison with ab initio theoretical calculations. Journal of Chemical Physics, 1996, 105, 10237-10250.	1.2	63
116	Theoretical intensities for the transitions of H2. A study of the Franck-Condon principle. Journal of Molecular Spectroscopy, 1967, 22, 1-17.	0.4	62
117	Theory of the Hyperfine Splittings of Pâ€Electron Free Radicals. II. Nonempirical Calculations of Methyl Radical (Planar). Journal of Chemical Physics, 1970, 52, 1740-1754.	1.2	62
118	Natural Orbitals. Advances in Quantum Chemistry, 1972, 6, 235-266.	0.4	62
119	Calculational Evidence for Lack of Intermediates in the Thermal Unimolecular Vinylcyclopropane to Cyclopentene 1,3-Sigmatropic Shift. Journal of the American Chemical Society, 1997, 119, 10543-10544.	6.6	62
120	Potential surface for the methylenecyclopropane rearrangement. Journal of the American Chemical Society, 1982, 104, 967-972.	6.6	60
121	Electron spin resonance investigations of 11B12C, 11B13C, and 10B12C in neon, argon, and krypton matrices at 4 K:â€‰â€‰Comparison with theoretical results. Journal of Chemical Physics, 1989, 90, 690-699.	1.2	60
122	The Spatial Extent of the V State of Ethylene and Its Relation to Dynamic Correlation in the Cope Rearrangement. The Journal of Physical Chemistry, 1996, 100, 6161-6166.	2.9	60
123	Theoretical Study of the BeH Molecule. Journal of Chemical Physics, 1968, 49, 727-739.	1.2	59
124	Thermal Rearrangements of Norcaradiene. Journal of the American Chemical Society, 1999, 121, 6928-6935.	6.6	59
125	Structure of the exact wave function. II. Iterative configuration interaction method. Journal of Chemical Physics, 2001, 115, 2000-2006.	1.2	59
126	Methanolysis and Phenolysis Routes to Fe6, Fe8, and Fe10Complexes and Their Magnetic Properties:Â A New Type of Fe8Ferric Wheel. Inorganic Chemistry, 2003, 42, 7819-7829.	1.9	59

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127	Ab initio calculation of the transition state for the Cope rearrangement. Journal of the American Chemical Society, 1984, 106, 3362-3363.	6.6	58
128	Ab initio multireference CI determinations of the electron affinity of carbon and oxygen. Journal of Chemical Physics, 1985, 82, 4135-4141.	1.2	58
129	The generation and trapping of the high-temperature oxosilyliumyl cation radicals (28SiO+ and) Tj ETQq1 1 0.784314 rgBT /Overlock 10 American Chemical Society, 1985, 107, 2857-2864.	6.6	58
130	Singleâ€Configuration Calculations on Excited States of Helium. Journal of Chemical Physics, 1964, 41, 656-658.	1.2	57
131	Singlet Rydberg states of ethylene. Journal of Chemical Physics, 1977, 67, 5613-5618.	1.2	57
132	Halogen atomic and diatomic1shole states. Physical Review A, 1977, 16, 1341-1346.	1.0	57
133	First Excited1Î£g+State of H2. A Doubleâ€Minimum Problem. Journal of Chemical Physics, 1960, 33, 1577-1577.	1.2	55
134	A theoretical study of the acetaldehyde-derived radical. Journal of the American Chemical Society, 1982, 104, 2956-2959.	6.6	55
135	The Rayleighâ€"SchrÃ¶dinger BK method applied to the lower electronic states of pyrrole. Chemical Physics Letters, 1983, 98, 424-427.	1.2	55
136	Molecular properties of water. Chemical Physics Letters, 1984, 104, 54-58.	1.2	55
137	The Cope rearrangement in theoretical retrospect. Computational and Theoretical Chemistry, 2001, 573, 81-89.	1.5	55
138	AnAb Initio calculation of the spin dipole-dipole parameters for methylene. International Journal of Quantum Chemistry, 1973, 7, 759-777.	1.0	54
139	Theoretical investigations of the electronic states of porphyrins. II. Normal and hyper phosphorus porphyrins. International Journal of Quantum Chemistry, 1984, 26, 251-274.	1.0	54
140	Non-vertical excitation energies for low-lying singlet states of butadiene and hexatriene. Chemical Physics Letters, 1988, 148, 190-196.	1.2	54
141	Use of double cosets in constructing integrals over symmetry orbitals. Journal of Chemical Physics, 1975, 62, 400.	1.2	53
142	Polynuclear Manganese Complexes with the Dicarboxylate Ligand m-Phenylenedipropionate:â€‰ A Hexanuclear Mixed-Valence (3MnIII, 3MnIV) Complex. Inorganic Chemistry, 2004, 43, 101-115.	1.9	53
143	Perturbation theory for multiconfiguration reference states. Chemical Physics Letters, 1978, 59, 369-374.	1.2	52
144	Effect of carbon atom pyramidalization on the bonding in ethylene. Journal of the American Chemical Society, 1979, 101, 533-537.	6.6	52

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145	Dependence of the singlet-triplet splitting in heterosubstituted carbenes on the heteroatom electronegativity and conformation. Chemical Physics Letters, 1980, 71, 22-26.	1.2	52
146	ESR and ab initio theoretical studies of the cation radicals 12C2â€‰16O+2, 12,13C2â€‰16O+2, 13C2â€‰16O+2, 12C2â€‰16,17O+2, 12C2â€‰17O+2, and 12,13C2â€‰16,17O+2 isolated in neon matrices at 4 K. The use of matrix isolation for trapping ionâ€“neutral reaction products. Journal of Chemical Physics, 1984, 80, 4593-4604.	1.2	52
147	Theoretical investigation of several low-lying states of trans, trans-1, 3,5-hexatriene. The Journal of Physical Chemistry, 1988, 92, 614-620.	2.9	52
148	Electron correlation contribution to the hydrogen bond in hydrogen fluoride dimer. The Journal of Physical Chemistry, 1993, 97, 6367-6372.	2.9	52
149	Local Spin III:Â Wave Function Analysis along a Reaction Coordinate, H Atom Abstraction, and Addition Processes of Benzyne. Journal of Physical Chemistry A, 2002, 106, 6890-6896.	1.1	52
150	High-density limit of the Perdew-Burke-Ernzerhof generalized gradient approximation and related density functionals. Physical Review A, 2006, 74, .	1.0	52
151	Analysis of wave functions for open-shell molecules. Physical Chemistry Chemical Physics, 2007, 9, 1881.	1.3	52
152	Allylic resonance - when is it unimportant?. Journal of the American Chemical Society, 1984, 106, 2513-2519.	6.6	51
153	Relativistic corrections for methylene. Chemical Physics Letters, 1980, 76, 416-417.	1.2	49
154	The BK method: Application to methylene. Journal of Chemical Physics, 1981, 74, 5491-5496.	1.2	49
155	ESR investigation of matrix isolated Bâ€‰16O and Bâ€‰17O radicals: Comparison of nuclear hyperfine structure withabinitiocalculations. Journal of Chemical Physics, 1982, 76, 126-136.	1.2	49
156	Carbene Complexes from Olefins, Using RuHCl(PiPr3)2. Influence of the Olefin Substituent. Journal of the American Chemical Society, 1998, 120, 9388-9389.	6.6	49
157	Necessary conditions for theN-representability of pair distribution functions. International Journal of Quantum Chemistry, 2006, 106, 1487-1498.	1.0	49
158	Hydrogenâ€Molecule Excited States: 1Îu. Journal of Chemical Physics, 1966, 44, 730-737.	1.2	48
159	Theoretical Study of the MgH Molecule. Journal of Chemical Physics, 1970, 52, 4108-4121.	1.2	48
160	The potential surface for planar cyclopropenyl radical and anion. Journal of Chemical Physics, 1977, 67, 2191.	1.2	48
161	Ab initio theory of the polarizability and polarizability derivatives in H2S. Chemical Physics, 1979, 38, 341-348.	0.9	48
162	Semiempirical local spin: Theory and implementation of the ZILSH method for predicting Heisenberg exchange constants of polynuclear transition metal complexes. International Journal of Quantum Chemistry, 2003, 92, 294-325.	1.0	47

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163	Koopmansâ€™ Theorem in the Restricted Open-Shell Hartreeâ^'Fock Method. 1. A Variational Approach. Journal of Physical Chemistry A, 2009, 113, 12386-12395.	1.1	47
164	An ab initio study of formamide. Theoretica Chimica Acta, 1977, 44, 405-419.	0.9	46
165	The singlet and triplet state rotational potential surfaces for dihydroxycarbene. Journal of Chemical Physics, 1979, 71, 4987.	1.2	46
166	Hylleraas variational perturbation theory: Application to correlation problems in molecular systems. Journal of Chemical Physics, 1988, 88, 5770-5778.	1.2	46
167	Theory of the Hyperfine Splittings of Piâ€Electron Free Radicals. III. Methyl Radical in a Pyramidal Configuration: Temperature Dependence of the Hyperfine Splittings. Journal of Chemical Physics, 1970, 52, 5596-5606.	1.2	45
168	Dimerization paths of CH2 and SiH2 fragments to ethylene, disilene, and silaethylene: MCSCF and MRCI study of least- and non-least-motion paths. Journal of the American Chemical Society, 1985, 107, 3466-3471.	6.6	45
169	Correlation states of ethylene. Journal of Chemical Physics, 1995, 102, 6385-6399.	1.2	45
170	Ab initio calculations on urea. International Journal of Quantum Chemistry, 1974, 8, 857-892.	1.0	44
171	Ab initio studies of the 3nÏ€* states of glyoxal and methyl glyoxal. Chemical Physics Letters, 1978, 58, 171-174.	1.2	44
172	Molecular electron density distributions in position and momentum space. The Journal of Physical Chemistry, 1985, 89, 969-974.	2.9	44
173	Spin polarization and annihilation for radicals and diradicals. International Journal of Quantum Chemistry, 2005, 103, 1-9.	1.0	44
174	The potential surface for the cyclobutadiene radical cation. Journal of the American Chemical Society, 1981, 103, 5725-5729.	6.6	42
175	Neon matrix ESR and CI theoretical investigation of AlF+; photoionization of AlF from thermal and laser sputtering generation methods. Journal of the American Chemical Society, 1986, 108, 5065-5071.	6.6	42
176	Ab initio calculation of some vertical excitation energies of N-methylacetamide. Journal of the American Chemical Society, 1978, 100, 7201-7204.	6.6	41
177	Density functional theory calculations for Fâ^'. Chemical Physics Letters, 1999, 300, 44-52.	1.2	41
178	A systematic approach to vertically excited states of ethylene using configuration interaction and coupled cluster techniques. Journal of Chemical Physics, 2014, 141, 104302.	1.2	41
179	Electron spin resonance studies of 45Sc17O,â€Š89Y17O, and 139La17O in rare gas matrices: Comparison with ab initio electronic structure and nuclear hyperfine calculations. Journal of Chemical Physics, 1999, 110, 5658-5669.	1.2	40
180	Theoretical Study of Several Electronic States of the Hydrogen Fluoride Molecule. Journal of Chemical Physics, 1968, 49, 4989-4995.	1.2	39

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181	Selection of Proper Canonical Orbitals. II. Water. Journal of Chemical Physics, 1972, 57, 2005-2008.	1.2	39
182	A theoretical determination of the electron affinity of methylene. Journal of Chemical Physics, 1982, 77, 6134-6143.	1.2	39
183	Vibrational spectroscopy of hydrogen cyanide clusters. The Journal of Physical Chemistry, 1988, 92, 2913-2925.	2.9	39
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