List of Publications by Year in descending order

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605 papers	37,691 citations	3933 88 h-index	4432 172 g-index
609 all docs	609 docs citations	609 times ranked	15128 citing authors

#	Article	IF	Citations
1	Advances in methods and algorithms in a modern quantum chemistry program package. Physical Chemistry Chemical Physics, 2006, 8, 3172-3191.	2.8	2,597
2	Advances in molecular quantum chemistry contained in the Q-Chem 4 program package. Molecular Physics, 2015, 113, 184-215.	1.7	2,561
3	An efficient reformulation of the closedâ€shell coupled cluster single and double excitation (CCSD) equations. Journal of Chemical Physics, 1988, 89, 7382-7387.	3.0	1,519
4	Is coupled cluster singles and doubles (CCSD) more computationally intensive than quadratic configuration interaction (QCISD)?. Journal of Chemical Physics, 1989, 90, 3700-3703.	3.0	1,065
5	On the evaluation of analytic energy derivatives for correlated wave functions. Journal of Chemical Physics, 1984, 81, 5031-5033.	3.0	815
6	Extensive theoretical studies of the hydrogenâ€bonded complexes (H2O)2, (H2O)2H+, (HF)2, (HF)2H+, F2Hâ^, and (NH3)2. Journal of Chemical Physics, 1986, 84, 2279-2289.	3.0	666
7	In pursuit of theab initiolimit for conformational energy prototypes. Journal of Chemical Physics, 1998, 108, 9751-9764.	3.0	659
8	An Introduction to Coupled Cluster Theory for Computational Chemists. Reviews in Computational Chemistry, 2007, , 33-136.	1.5	531
9	P<scp>SI4</scp> 1.4: Open-source software for high-throughput quantum chemistry. Journal of Chemical Physics, 2020, 152, 184108.	3.0	440
10	The diagonal correction to the Bornâ€“Oppenheimer approximation: Its effect on the singletâ€“triplet splitting of CH2 and other molecular effects. Journal of Chemical Physics, 1986, 84, 4481-4484.	3.0	399
11	Analytic evaluation of energy gradients for the single and double excitation coupled cluster (CCSD) wave function: Theory and application. Journal of Chemical Physics, 1987, 87, 5361-5373.	3.0	378
12	The graphical unitary group approach to the electron correlation problem. Methods and preliminary applications. Journal of Chemical Physics, 1979, 70, 5092-5106.	3.0	351
13	Localized and Delocalized 1s Hole States of the O 2 + Molecular Ion. Journal of Chemical Physics, 1972, 56, 224-226.	3.0	323
14	Analytic Raman intensities from molecular electronic wave functions. Journal of Chemical Physics, 1986, 84, 531-532.	3.0	319
15	Toward subchemical accuracy in computational thermochemistry: Focal point analysis of the heat of formation of NCO and [H,N,C,O] isomers. Journal of Chemical Physics, 2004, 120, 11586-11599.	3.0	317
16	Electronic structure of homoleptic transition metal hydrides: TiH4, VH4, CrH4, MnH4, FeH4, CoH4, and NiH4. Journal of Chemical Physics, 1979, 71, 705-712.	3.0	316
17	The closedâ€shell coupled cluster single and double excitation (CCSD) model for the description of electron correlation. A comparison with configuration interaction (CISD) results. Journal of Chemical Physics, 1987, 86, 2881-2890.	3.0	316
18	Systematic study of molecular anions within the selfâ€consistentâ€field approximation: OHâ^, CNâ^, C2Hâ^, NHâ^'2, and CHâ^'3. Journal of Chemical Physics, 1985, 83, 1784-1794.	3.0	312

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19	Concerning zeroâ€point vibrational energy corrections to electronic energies. Journal of Chemical Physics, 1991, 95, 5128-5132.	3.0	284
20	Analytic gradients from correlated wave functions via the twoâ€particle density matrix and the unitary group approach. Journal of Chemical Physics, 1980, 72, 4652-4653.	3.0	279
21	Analytic evaluation and basis set dependence of intensities of infrared spectra. Journal of Chemical Physics, 1986, 84, 2262-2278.	3.0	279
22	Anchoring the water dimer potential energy surface with explicitly correlated computations and focal point analyses. Journal of Chemical Physics, 2002, 116, 690-701.	3.0	262
23	Coupling term derivation and general implementation of state-specific multireference coupled cluster theories. Journal of Chemical Physics, 2007, 127, 024102.	3.0	255
24	Homonuclear 3d transition-metal diatomics: A systematic density functional theory study. Journal of Chemical Physics, 2000, 113, 690-700.	3.0	249
25	The analytic configuration interaction gradient method: Application to the cyclic and open isomers of the S3 molecule. Journal of Chemical Physics, 1986, 85, 963-968.	3.0	245
26	Transition structures for the interchange of hydrogen atoms within the water dimer. Journal of Chemical Physics, 1990, 92, 1240-1247.	3.0	230
27	The shapeâ€driven graphical unitary group approach to the electron correlation problem. Application to the ethylene molecule. Journal of Chemical Physics, 1982, 77, 5584-5592.	3.0	222
28	Coupled cluster energy derivatives. Analytic Hessian for the closedâ€shell coupled cluster singles and doubles wave function: Theory and applications. Journal of Chemical Physics, 1990, 92, 4924-4940.	3.0	222
29	The balance between theoretical method and basis set quality: A systematic study of equilibrium geometries, dipole moments, harmonic vibrational frequencies, and infrared intensities. Journal of Chemical Physics, 1993, 99, 403-416.	3.0	213
30	High-order excitations in state-universal and state-specific multireference coupled cluster theories: Model systems. Journal of Chemical Physics, 2006, 125, 154113.	3.0	207
31	Definitive Ab Initio Studies of Model SN2 Reactions CH3X+F (X=F, Cl, CN, OH, SH, NH2, PH2). Chemistry - A European Journal, 2003, 9, 2173-2192.	3.3	196
32	Gradient techniques for openâ€shell restricted Hartreeâ€“Fock and multiconfiguration selfâ€consistentâ€field methods. Journal of Chemical Physics, 1979, 71, 1525-1530.	3.0	195
33	Concerning the applicability of density functional methods to atomic and molecular negative ions. Journal of Chemical Physics, 1996, 105, 862-864.	3.0	194
34	Interfacing Q-Chem and CHARMM to perform QM/MM reaction path calculations. Journal of Computational Chemistry, 2007, 28, 1485-1502.	3.3	190
35	The photodissociation of formaldehyde: Potential energy surface features. Journal of Chemical Physics, 1979, 70, 5117-5134.	3.0	184
36	Potential energy surface for the model unimolecular reaction HNC â† HCN. Journal of Chemical Physics, 1975, 62, 350.	3.0	181

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37	A systematic theoretical study of harmonic vibrational frequencies: The ammonium ion NH4+and other simple molecules. Journal of Chemical Physics, 1980, 73, 2310-2318.	3.0	181
38	CH+5: The neverâ€ending story or the final word?. Journal of Chemical Physics, 1993, 99, 3716-3720.	3.0	177
39	The protonated water dimer: Extensive theoretical studies of H5O+2. Journal of Chemical Physics, 1994, 101, 4878-4884.	3.0	174
40	Large-scale symmetry-adapted perturbation theory computations via density fitting and Laplace transformation techniques: Investigating the fundamental forces of DNA-intercalator interactions. Journal of Chemical Physics, 2011, 135, 174107.	3.0	174
41	Generalization of analytic configuration interaction (CI) gradient techniques for potential energy hypersurfaces, including a solution to the coupled perturbed Hartreeâ€“Fock equations for multiconfiguration SCF molecular wave functions. Journal of Chemical Physics, 1982, 77, 383-390.	3.0	169
42	Vinylidene: Potential energy surface and unimolecular reaction dynamics. Journal of Chemical Physics, 1984, 80, 4347-4354.	3.0	169
43	Analytic second derivatives in restricted Hartreeâ€“Fock theory. A method for highâ€spin openâ€shell molecular wave functions. Journal of Chemical Physics, 1982, 77, 5647-5654.	3.0	167
44	The torsional conformations of butane: Definitive energetics from ab initio methods. Journal of Chemical Physics, 1997, 106, 5143-5150.	3.0	159
45	Molecular Autoionization Lifetimes and Cross Sections for Penning Ionization: Numerical Results for He* (1s2sâ€‰3S) + H(1sâ€‰2S). Journal of Chemical Physics, 1972, 56, 1347-1358.	3.0	154
46	The weakly exothermic rearrangement of methoxy radical (CH3Oâ‹…) to the hydroxymethyl radical (CH2OHâ‹…). Journal of Chemical Physics, 1983, 78, 845-853.	3.0	147
47	Theoretical Treatment of Penning Ionizationâ€”He(1s2s 1S, 3S)â€‰+â€‰H(1s 2S). Journal of Chemical Physics, 1970, 53, 1421-1427.	3.0	144
48	Mechanism of the C2H5+O2 reaction. Journal of Chemical Physics, 1997, 107, 141-155.	3.0	142
49	Hartreeâ€“Fock orbital instability envelopes in highly correlated single-reference wave functions. Journal of Chemical Physics, 1997, 107, 10626-10632.	3.0	142
50	The malonaldehyde equilibrium geometry: A major structural shift due to the effects of electron correlation. Journal of Chemical Physics, 1985, 82, 4194-4198.	3.0	137
51	Ab Initio Calculations on 62 Lowâ€Lying States of the O2Molecule. Journal of Chemical Physics, 1968, 48, 4946-4955.	3.0	136
52	Potential energy surface for the Li+HFâ†’LiF+H reaction. Journal of Chemical Physics, 1980, 72, 4376-4393.	3.0	135
53	Carbene Rearrangements Unsurpassed:â€‰ Details of the C7H6 Potential Energy Surface Revealed. Journal of Organic Chemistry, 1996, 61, 7030-7039.	3.2	133
54	Interaction potential between two rigid HF molecules. Journal of Chemical Physics, 1974, 60, 855-865.	3.0	131

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55	An energetically lowâ€lying silacyclopropyne isomer of SiC2. Journal of Chemical Physics, 1984, 80, 3552-3555.	3.0	130
56	The remarkable monobridged structure of Si2H2. Journal of Chemical Physics, 1992, 97, 7990-7998.	3.0	129
57	Potential Energy Surface Including Electron Correlation for the Chemical F + H2 â†' FH + H I. Preliminary Surface. Journal of Chemical Physics, 1972, 56, 4626-4631.	3.0	127
58	Is Mo/llerâ€"Plesset perturbation theory a convergent ab initio method?. Journal of Chemical Physics, 2000, 112, 9213-9222.	3.0	125
59	A theory of selfâ€consistent electron pairs. Computational methods and preliminary applications. Journal of Chemical Physics, 1976, 65, 2740-2750.	3.0	124
60	Is the uniform electron gas limit important for small Ag clusters? Assessment of different density functionals for Agn (nâ©½4). Journal of Chemical Physics, 2006, 124, 184102.	3.0	124
61	Triple excitations in state-specific multireference coupled cluster theory: Application of Mk-MRCCSDT and Mk-MRCCSDT-n methods to model systems. Journal of Chemical Physics, 2008, 128, 124104.	3.0	123
62	Ab Initio Potential Curve for the X 3Î£gâ¯ State of O2. Journal of Chemical Physics, 1971, 54, 2207-2211.	3.0	122
63	The decarboxylation and dehydration reactions of monomeric formic acid. Journal of Chemical Physics, 1992, 96, 1158-1166.	3.0	119
64	Model studies of chemisorption. Interaction between atomic hydrogen and beryllium clusters. Journal of Chemical Physics, 1975, 62, 4815-4825.	3.0	118
65	Electron correlation in small metal clusters. Application of a theory of selfâ€consistent electron pairs to the Be4system. Journal of Chemical Physics, 1976, 65, 5141-5146.	3.0	118
66	Features of the H2CO potential energy hypersurface pertinent to formaldehyde photodissociation. Journal of Chemical Physics, 1981, 75, 3459-3465.	3.0	114
67	Predicting electron affinities with density functional theory: Some positive results for negative ions. Journal of Chemical Physics, 1997, 107, 2529-2541.	3.0	114
68	The Dichotomy of Dimetallocenes:Â Coaxial versus Perpendicular Dimetal Units in Sandwich Compounds. Journal of the American Chemical Society, 2005, 127, 2818-2819.	13.7	113
69	Analytic second derivatives for Rennerâ€"Teller potential energy surfaces. Examples of the five distinct cases. Journal of Chemical Physics, 1984, 81, 356-361.	3.0	111
70	The analytic evaluation of energy first derivatives for twoâ€configuration selfâ€consistentâ€field configuration interaction (TCSCFâ€CI) wave functions. Application to ozone and ethylene. Journal of Chemical Physics, 1987, 87, 7062-7075.	3.0	111
71	DNA Nucleosides and Their Radical Anions:Â Molecular Structures and Electron Affinities. Journal of the American Chemical Society, 2004, 126, 4404-4411.	13.7	109
72	The photodissociation of formaldehyde: A coupled cluster study including connected triple excitations of the transition state barrier height for H2COâ†'H2+CO. Journal of Chemical Physics, 1989, 90, 3629-3636.	3.0	108

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73	Multiple dâ€type basis functions for molecules containing second row atoms. Journal of Chemical Physics, 1985, 83, 5721-5726.	3.0	106
74	Metalâ€“Metal (MM) Bond Distances and Bond Orders in Binuclear Metal Complexes of the First Row Transition Metals Titanium Through Zinc. Chemical Reviews, 2018, 118, 11626-11706.	47.7	106
75	Valenceâ€Excited States of Carbon Monoxide. Journal of Chemical Physics, 1970, 53, 3994-4004.	3.0	105
76	A systematic theoretical study of harmonic vibrational frequencies: The single and double excitation coupled cluster (CCSD) method. Journal of Chemical Physics, 1988, 89, 360-366.	3.0	105
77	Quadratically convergent algorithm for orbital optimization in the orbital-optimized coupled-cluster doubles method and in orbital-optimized second-order MÃ¸ller-Plesset perturbation theory. Journal of Chemical Physics, 2011, 135, 104103.	3.0	104
78	The protonated water dimer: Brueckner methods remove the spurious C1 symmetry minimum. Journal of Chemical Physics, 1998, 108, 7197-7201.	3.0	102
79	Triplet electronic states of acetylene:cisandtransstructures and energetics. Journal of Chemical Physics, 1978, 69, 1648-1654.	3.0	100
80	Exploring the quantum mechanical/molecular mechanical replica path method: a pathway optimization of the chorismate to prephenate Claisen rearrangement catalyzed by chorismate mutase. Theoretical Chemistry Accounts, 2003, 109, 140-148.	1.4	100
81	Avoided intersection of potential energy surfaces: The (H+â€‰+â€‰H2,â€‰Hâ€‰+â€‰H2+) system. Journal of Chemical Physics, 1973, 59, 1286-1292.	3.0	99
82	Thermochemistry of CHn, SiHn(n=0â€“4), and the cations SiH+, SiH2+, and SiH3+: A converged quantum mechanical approach. Journal of Chemical Physics, 1992, 97, 8389-8406.	3.0	97
83	Perturbative triples corrections in state-specific multireference coupled cluster theory. Journal of Chemical Physics, 2010, 132, 074107.	3.0	96
84	Theoretical Potential Energy Curves for OH, HF+, HF, HFâ¯, NeH+, and NeH. Journal of Chemical Physics, 1972, 57, 1123-1128.	3.0	95
85	Structures and vibrational frequencies in the full configuration interaction limit: Predictions for four electronic states of methylene using a triple-zeta plus double polarization (TZ2P) basis. Journal of Chemical Physics, 1998, 108, 1040-1049.	3.0	93
86	Theoretical Study of SO2 Molecular Properties. Journal of Chemical Physics, 1970, 53, 3014-3019.	3.0	91
87	Electronic Structures and Potential Energy Curves for the Lowâ€Lying States of the CN Radical. Journal of Chemical Physics, 1971, 54, 2573-2580.	3.0	91
88	Geometrical structures and vibrational frequencies of the energetically lowâ€lying isomers of SiC3. Journal of Chemical Physics, 1990, 93, 5046-5052.	3.0	89
89	Hydrogen bonding between the water molecule and the hydroxyl radical (H2Oâ‹…HO): The global minimum. Journal of Chemical Physics, 1993, 98, 8829-8834.	3.0	89
90	A systematic theoretical study of the harmonic vibrational frequencies for polyatomic molecules: The single, double, and perturbative triple excitation coupledâ€cluster [CCSD(T)] method. Journal of Chemical Physics, 1993, 98, 1336-1344.	3.0	89

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91	Analytic configuration interaction (CI) gradient techniques for potential energy hypersurfaces. A method for openâ€shell molecular wave functions. Journal of Chemical Physics, 1981, 75, 2919-2922.	3.0	88
92	Direct Nearâ€Hartreeâ€“Fock Calculations on the 1s Hole States of NO+. Journal of Chemical Physics, 1971, 55, 1474-1475.	3.0	87
93	Analytic energy second derivatives for general MCSCF wave functions. Journal of Chemical Physics, 1984, 80, 2660-2668.	3.0	87
94	Analytic third derivatives for selfâ€consistentâ€field wave functions. Journal of Chemical Physics, 1984, 81, 6395-6396.	3.0	86
95	Electronic Splitting between the 2B1 and 2A1 States of the NH2 Radical. Journal of Chemical Physics, 1971, 55, 4798-4803.	3.0	85
96	C2Ï... Potential Energy Surfaces for Seven Lowâ€Lying States of CH2. Journal of Chemical Physics, 1971, 55, 162-169.	3.0	84
97	Electronic structure of the N4+molecular ion. Journal of Chemical Physics, 1981, 74, 550-558.	3.0	84
98	Potential energy surfaces related to the ionâ€molecule reaction C+ + H2. Journal of Chemical Physics, 1974, 61, 2507-2513.	3.0	81
99	The silicon analog of benzeneâ€“hexasilabenzene (Si6H6). Journal of Chemical Physics, 1986, 84, 1664-1669.	3.0	81
100	Use of 2h and 3hâ^'p-like coupled-cluster Tammâ€“Dancoff approaches for the equilibrium properties of ozone. Chemical Physics Letters, 2003, 378, 42-46.	2.6	81
101	Interpretation of excited state Hartreeâ€“Fock analytic derivative anomalies for NO2 and HCO2 using the molecular orbital Hessian. Journal of Chemical Physics, 1991, 95, 7466-7478.	3.0	80
102	Curve Crossing of theB3Î£uâ^' and 3Î u States of O2and Its Relation to Predissociation in the Schumannâ€"Runge Bands. Journal of Chemical Physics, 1971, 55, 4107-4113.	3.0	79
103	Ab initio calculation of reaction energies. III. Basis set dependence of relative energies on the FH2 and H2CO potential energy surfaces. Journal of Chemical Physics, 1984, 81, 1882-1893.	3.0	79
104	The H+5potential energy hypersurface: Characterization of ten distinct energetically lowâ€lying stationary points. Journal of Chemical Physics, 1987, 86, 5072-5081.	3.0	79
105	The convergence of the cluster model for the study of chemisorption: Be36H. Journal of Chemical Physics, 1983, 78, 1390-1395.	3.0	78
106	Molecular clustering about a positive ion. Structures, energetics, and vibrational frequencies of the protonated hydrogen clusters H+3, H+5, H+7, and H+9. Journal of Chemical Physics, 1983, 78, 4074-4085.	3.0	77
107	Diatomic sulfur: Low lying bound molecular electronic states of S2. Journal of Chemical Physics, 1979, 70, 947.	3.0	76
108	Carbon clusters: The structure of C10 studied with configuration interaction methods. Journal of Chemical Physics, 1990, 93, 8844-8849.	3.0	76

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109	The electron affinities of the silicon fluorides SiFn (n=1â€“5). Journal of Chemical Physics, 1996, 105, 6880-6886.	3.0	76
110	Structures, thermochemistry, and electron affinities of the PFn and PFâ¯n series, n=1â€“6. Journal of Chemical Physics, 1996, 104, 3676-3683.	3.0	76
111	A critical test of semiempirical FH2 potential energy sufaces: The barrier height for H + FH â† HF + H. Journal of Chemical Physics, 1975, 62, 1188-1189.	3.0	74
112	6â€311G is not of valence tripleâ€zeta quality. Journal of Chemical Physics, 1989, 91, 7305-7306.	3.0	74
113	Geometries of the excited electronic states of HCN. Journal of Chemical Physics, 1974, 60, 2787-2793.	3.0	73
114	The structure and stability of BH5. Does correlation make it a stable molecule? Qualitative changes at high levels of theory. Journal of Chemical Physics, 1994, 101, 7625-7632.	3.0	73
115	The barrier to linearity of water. Journal of Chemical Physics, 1999, 110, 11971-11981.	3.0	73
116	Unimolecular thermal fragmentation ofortho-benzyne. Journal of Chemical Physics, 2007, 126, 044312.	3.0	73
117	Large multiconfiguration selfâ€consistentâ€field wave functions for the ozone molecule. Journal of Chemical Physics, 1981, 74, 3411-3414.	3.0	72
118	Theoretical studies of oxygen rings: Cyclotetraoxygen, O4. Journal of Chemical Physics, 1988, 88, 7043-7049.	3.0	71
119	Equilibrium geometry of the HCCN triplet ground state: Carbene or allene? An openâ€shell coupled cluster study including connected triple excitations. Journal of Chemical Physics, 1992, 96, 4449-4452.	3.0	71
120	Molecular structures of the two most stable conformers of free glycine. Journal of Computational Chemistry, 2007, 28, 1373-1383.	3.3	71
121	On the accuracy limits of orbital expansion methods: Explicit effects ofr-functions on atomic and molecular energies. Journal of Chemical Physics, 2003, 118, 8594-8610.	3.0	70
122	Electron Correlation in the Lowest 1Î£+ State of Beryllium Oxide. Journal of Chemical Physics, 1971, 55, 176-181.	3.0	68
123	Generalization of the direct configuration interaction method to the Hartreeâ€“Fock interacting space for doublets, quartets, and openâ€shell singlets. Applications to NO2and NO2â¯. Journal of Chemical Physics, 1979, 71, 426-435.	3.0	68
124	Analytic gradients for the state-specific multireference coupled cluster singles and doubles model. Journal of Chemical Physics, 2009, 131, 064109.	3.0	68
125	Complete basis set limit studies of conventional and R12 correlation methods: The silicon dicarbide (SiC[sub 2]) barrier to linearity. Journal of Chemical Physics, 2003, 118, 7353.	3.0	67
126	Reaction paths for the dissociation alƒâ€‰3Aâ€˜ CH2COâ†'XÌƒâ€‰3B1 CH2â€‰+â€‰XÌƒâ€‰1Î£+ CO. Journal of Chemical Physics, 329-344.	3.0	66

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127	Thermochemistry of disputed soot formation intermediates C4H3 and C4H5. Journal of Chemical Physics, 2004, 121, 8800-8813.	3.0	66
128	A companion perturbation theory for state-specific multireference coupled cluster methods. Physical Chemistry Chemical Physics, 2009, 11, 4728.	2.8	65
129	Bending Frequency of the C3 Molecule. Journal of Chemical Physics, 1972, 56, 5075-5080.	3.0	64
130	An assessment for the full coupled cluster method including all single, double, and triple excitations: The diatomic molecules LiH, Li2, BH, LiF, C2, BeO, CN+, BF, NO+, and F2. Journal of Chemical Physics, 1990, 92, 568-573.	3.0	64
131	Generalization of analytic energy third derivatives for the RHF closedâ€shell wave function: Derivative energy and integral formalisms and the prediction of vibrationâ€“rotation interaction constants. Journal of Chemical Physics, 1986, 85, 5132-5142.	3.0	63
132	Hydrogen bonding between the water molecule and the hydroxyl radical (H2Oâ‹…OH): The 2Aâ€˜ and 2Aâ€™ minima. Journal of Chemical Physics, 1991, 94, 2057-2062.	3.0	63
133	Hydrogen bonding between the nitrate anion (conventional and peroxy forms) and the water molecule. Journal of Chemical Physics, 1990, 93, 3379-3388.	3.0	62
134	Symmetry breaking in the NO2 Ïƒ radical: Construction of the 2A1 and 2B2 states with Cs symmetry complete active space selfâ€consistentâ€field wave functions. Journal of Chemical Physics, 1990, 93, 8105-8109.	3.0	62
135	The highly anharmonic BH5 potential energy surface characterized in the ab initio limit. Journal of Chemical Physics, 2005, 122, 104302.	3.0	62
136	Firstâ€Order Wavefunctions, Orbital Correlation Energies, and Electron Affinities of Firstâ€Row Atoms. Journal of Chemical Physics, 1969, 51, 4643-4650.	3.0	61
137	Self-consistent-field wave functions, energies, multipole moments, diamagnetic susceptibility and shielding tensors, and electric field gradient tensors for nitrogen dioxide and ozone. Molecular Physics, 1971, 21, 317-327.	1.7	61
138	Infrared intensities of H3O+, H2DO+, HD2O+, and D3O+. Journal of Chemical Physics, 1983, 79, 1551-1552.	3.0	61
139	N(1Ag),T(3B1u), andV(1B1u) states of vertical ethylene. Journal of Chemical Physics, 1978, 68, 4839-4847.	3.0	60
140	A unimolecular reaction ABCâ†'A+B+C involving three product molecules and a single transition state. Photodissociation of glyoxal: HCOHCOâ†'H2+CO+CO. Journal of Chemical Physics, 1981, 75, 5828-5836.	3.0	60
141	Electrophile Affinity: A Reactivity Measure for Aromatic Substitution. Journal of the American Chemical Society, 2009, 131, 14722-14727.	13.7	60
142	On the H+F2â†'HF+F reaction. An ab initio potential energy surface. Journal of Chemical Physics, 1973, 58, 1126-1131.	3.0	59
143	The anharmonic force fields of HOF and F2O. Journal of Chemical Physics, 1988, 89, 4965-4975.	3.0	59
144	Geometrical structure and vibrational frequencies of several electronic states of Si2C. Journal of Chemical Physics, 1985, 82, 4126-4130.	3.0	58

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145	Abinitiostudies of the lowâ€lying electronic states of ketene. Journal of Chemical Physics, 1986, 84, 2212-2225.	3.0	58
146	Is there a transition state for the unimolecular dissociation of cyclotetraoxygen (O4)?. Journal of Chemical Physics, 1992, 96, 1176-1182.	3.0	58
147	Microsolvation effects on the electron capturing ability of thymine: Thymine-water clusters. Journal of Chemical Physics, 2006, 124, 204310.	3.0	58
148	A possible role for triplet H2CN+ isomers in the formation of HCN and HNC in interstellar clouds. Journal of Chemical Physics, 1980, 73, 3255-3263.	3.0	57
149	The classical and nonclassical forms of protonated acetylene, C2H+3. Structures, vibrational frequencies, and infrared intensities from explicitly correlated wave functions. Journal of Chemical Physics, 1986, 85, 3437-3443.	3.0	57
150	The valence isoelectronic molecules CCO, CNN, SiCO, and SiNN in their triplet ground states: Theoretical predictions of structures and infrared spectra. Journal of Chemical Physics, 1988, 89, 3016-3027.	3.0	57
151	Anharmonic force field, vibrational energies, and barrier to inversion of SiH3â^'. Journal of Chemical Physics, 2000, 112, 4053-4063.	3.0	57
152	Is there an absence of threefold symmetry at the equilibrium geometry of the ground electronic state for NO3?. Journal of Chemical Physics, 1989, 91, 4410-4411.	3.0	56
153	The known and unknown group 13 hydride molecules M2H6: Diborane(6), dialane(6), and digallane(6). Journal of Chemical Physics, 1992, 96, 2868-2876.	3.0	56
154	Spectroscopic constants and potential energy surfaces for the possible interstellar molecules A1NC and A1CN. Molecular Physics, 1995, 86, 1331-1337.	1.7	56
155	Multiconfiguration Wavefunctions for the Water Molecule. Journal of Chemical Physics, 1971, 55, 1720-1724.	3.0	55
156	Internal rotation barrier and transition state for glyoxal. Journal of Chemical Physics, 1981, 74, 4576-4580.	3.0	55
157	Is there a potential minimum corresponding to singlet methylnitrene? A study of the CH3N to CH2NH rearrangement on the lowest singlet state potential energy hypersurface. Journal of Chemical Physics, 1994, 100, 481-489.	3.0	55
158	Toward resolution of the silicon dicarbide (SiC2) saga:Ab initioexcursions in the web of polytopism. Journal of Chemical Physics, 1997, 107, 1195-1211.	3.0	55
159	Theab initiolimit quartic force field of BH3. Journal of Computational Chemistry, 2005, 26, 1106-1112.	3.3	54
160	The alkaline earth dimer cations (Be₂ ⁺, Mg₂ ⁺,) Tj ETQq0 0 0 rgBT /Overlock 10 Tf Coupled cluster and full configuration interaction studies^{â€}. Molecular Physics, 2013, 111, 2292-2298.	1.7	54
161	Is the oxywater radical cation more stable than neutral oxywater?. Journal of Chemical Physics, 1996, 104, 7615-7623.	3.0	53
162	The structures, electron affinities, and energetic stabilities of TiOn and TiOnâ^' (n=1â€“3). Journal of Chemical Physics, 1999, 110, 5224-5230.	3.0	53

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163	Binding energies of small lithium clusters (Lin) and hydrogenated lithium clusters (LinH). Journal of Chemical Physics, 2004, 120, 4683-4689.	3.0	53
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