Henry F Schaefer

List of Publications by Year
in descending order

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1,011 papers	56,131 citations	1606 105 h-index	2323 199 g-index
1026 all docs	1026 docs citations	1026 times ranked	21258 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.	1.3	2,597
2	Advances in molecular quantum chemistry contained in the Q-Chem 4 program package. Molecular Physics, 2015, 113, 184-215.	0.8	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.	1.2	1,519
4	Atomic and Molecular Electron Affinities:â€‰ Photoelectron Experiments and Theoretical Computations. Chemical Reviews, 2002, 102, 231-282.	23.0	1,152
5	Is coupled cluster singles and doubles (CCSD) more computationally intensive than quadratic configuration interaction (QCISD)?. Journal of Chemical Physics, 1989, 90, 3700-3703.	1.2	1,065
6	<scp>Psi4</scp> 1.1: An Open-Source Electronic Structure Program Emphasizing Automation, Advanced Libraries, and Interoperability. Journal of Chemical Theory and Computation, 2017, 13, 3185-3197.	2.3	961
7	Psi4: an openâ€source ab initio electronic structure program. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2012, 2, 556-565.	6.2	838
8	On the evaluation of analytic energy derivatives for correlated wave functions. Journal of Chemical Physics, 1984, 81, 5031-5033.	1.2	815
9	A Stable Silicon(0) Compound with a Si=Si Double Bond. Science, 2008, 321, 1069-1071.	6.0	680
10	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.	1.2	666
11	In pursuit of theab initiolimit for conformational energy prototypes. Journal of Chemical Physics, 1998, 108, 9751-9764.	1.2	659
12	A new implementation of the full CCSDT model for molecular electronic structure. Chemical Physics Letters, 1988, 152, 382-386.	1.2	579
13	An Introduction to Coupled Cluster Theory for Computational Chemists. Reviews in Computational Chemistry, 2007, , 33-136.	1.5	531
14	A Stable Neutral Diborene Containing a BB Double Bond. Journal of the American Chemical Society, 2007, 129, 12412-12413.	6.6	508
15	The C2H5+ O2Reaction Mechanism:Â High-Level ab Initio Characterizations. Journal of Physical Chemistry A, 2000, 104, 9823-9840.	1.1	496
16	A systematic study of molecular vibrational anharmonicity and vibrationâ€"rotation interaction by self-consistent-field higher-derivative methods. Asymmetric top molecules. Chemical Physics, 1988, 123, 187-239.	0.9	476
17	P<scp>SI4</scp> 1.4: Open-source software for high-throughput quantum chemistry. Journal of Chemical Physics, 2020, 152, 184108.	1.2	440
18	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.	1.2	399

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19	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.	1.2	378
20	The graphical unitary group approach to the electron correlation problem. Methods and preliminary applications. Journal of Chemical Physics, 1979, 70, 5092-5106.	1.2	351
21	Localized and Delocalized 1s Hole States of the O 2 + Molecular Ion. Journal of Chemical Physics, 1972, 56, 224-226.	1.2	323
22	Analytic Raman intensities from molecular electronic wave functions. Journal of Chemical Physics, 1986, 84, 531-532.	1.2	319
23	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.	1.2	317
24	Electronic structure of homoleptic transition metal hydrides: TiH4, VH4, CrH4, MnH4, FeH4, CoH4, and NiH4. Journal of Chemical Physics, 1979, 71, 705-712.	1.2	316
25	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.	1.2	316
26	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.	1.2	312
27	The Configuration Interaction Method: Advances in Highly Correlated Approaches. Advances in Quantum Chemistry, 1999, , 143-269.	0.4	294
28	Concerning zeroâ€point vibrational energy corrections to electronic energies. Journal of Chemical Physics, 1991, 95, 5128-5132.	1.2	284
29	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.	1.2	279
30	Analytic evaluation and basis set dependence of intensities of infrared spectra. Journal of Chemical Physics, 1986, 84, 2262-2278.	1.2	279
31	A systematic study of molecular vibrational anharmonicity and vibration-rotation interaction by self-consistent-field higher-derivative methods. Linear polyatomic molecules. Chemical Physics, 1990, 145, 427-466.	0.9	267
32	Anchoring the water dimer potential energy surface with explicitly correlated computations and focal point analyses. Journal of Chemical Physics, 2002, 116, 690-701.	1.2	262
33	Coupling term derivation and general implementation of state-specific multireference coupled cluster theories. Journal of Chemical Physics, 2007, 127, 024102.	1.2	255
34	Homonuclear 3d transition-metal diatomics: A systematic density functional theory study. Journal of Chemical Physics, 2000, 113, 690-700.	1.2	249
35	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.	1.2	245
36	Electron Affinities of the DNA and RNA Bases. Journal of the American Chemical Society, 2001, 123, 4023-4028.	6.6	236

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37	Transition structures for the interchange of hydrogen atoms within the water dimer. Journal of Chemical Physics, 1990, 92, 1240-1247.	1.2	230
38	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.	1.2	222
39	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.	1.2	222
40	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.	1.2	213
41	High-order excitations in state-universal and state-specific multireference coupled cluster theories: Model systems. Journal of Chemical Physics, 2006, 125, 154113.	1.2	207
42	A Viable Anionic N-Heterocyclic Dicarbene. Journal of the American Chemical Society, 2010, 132, 14370-14372.	6.6	206
43	Concerning the precision of standard density functional programs: Gaussian, Molpro, NWChem, Q-Chem, and Gamess. Computational and Theoretical Chemistry, 2006, 768, 175-181.	1.5	197
44	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.	1.7	196
45	Gradient techniques for openâ€shell restricted Hartreeâ€“Fock and multiconfiguration selfâ€consistentâ€field methods. Journal of Chemical Physics, 1979, 71, 1525-1530.	1.2	195
46	Concerning the applicability of density functional methods to atomic and molecular negative ions. Journal of Chemical Physics, 1996, 105, 862-864.	1.2	194
47	Interfacing Q-Chem and CHARMM to perform QM/MM reaction path calculations. Journal of Computational Chemistry, 2007, 28, 1485-1502.	1.5	190
48	The photodissociation of formaldehyde: Potential energy surface features. Journal of Chemical Physics, 1979, 70, 5117-5134.	1.2	184
49	Vinylidene: the final chapter?. Journal of the American Chemical Society, 1990, 112, 8714-8719.	6.6	184
50	Potential energy surface for the model unimolecular reaction HNC â†' HCN. Journal of Chemical Physics, 1975, 62, 350.	1.2	181
51	A systematic theoretical study of harmonic vibrational frequencies: The ammonium ion NH4+and other simple molecules. Journal of Chemical Physics, 1980, 73, 2310-2318.	1.2	181
52	Remarkable Aspects of Unsaturation in Trinuclear Metal Carbonyl Clusters:Â The Triiron Species Fe3(CO)n(n= 12, 11, 10, 9). Journal of the American Chemical Society, 2006, 128, 11376-11384.	6.6	181
53	CH+5: The neverâ€ending story or the final word?. Journal of Chemical Physics, 1993, 99, 3716-3720.	1.2	177
54	Structures and stability of hydrated clusters of hydrogen chloride, HCl(H2O)n, n=1â€“5. Journal of Chemical Physics, 1998, 109, 973-977.	1.2	176

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55	The protonated water dimer: Extensive theoretical studies of H5O+2. Journal of Chemical Physics, 1994, 101, 4878-4884.	1.2	174
56	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.	1.2	174
57	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.	1.2	169
58	Vinylidene: Potential energy surface and unimolecular reaction dynamics. Journal of Chemical Physics, 1984, 80, 4347-4354.	1.2	169
59	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.	1.2	167
60	Mindless Chemistry. Journal of Physical Chemistry A, 2006, 110, 4287-4290.	1.1	165
61	Design of a Catalytic Active Site for Electrochemical CO₂ Reduction with Mn(I)-Tricarbonyl Species. Inorganic Chemistry, 2015, 54, 5285-5294.	1.9	163
62	The torsional conformations of butane: Definitive energetics from ab initio methods. Journal of Chemical Physics, 1997, 106, 5143-5150.	1.2	159
63	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.	1.2	154
64	The automated solution of second quantization equations with applications to the coupled cluster approach. Theoretica Chimica Acta, 1991, 79, 1-42.	0.9	151
65	The weakly exothermic rearrangement of methoxy radical (CH3Oâ‹…) to the hydroxymethyl radical (CH2OHâ‹…). Journal of Chemical Physics, 1983, 78, 845-853.	1.2	147
66	Theoretical Treatment of Penning Ionizationâ€”He(1s2s 1S, 3S)â€‰+â€‰H(1s 2S). Journal of Chemical Physics, 1970, 53, 1421-1427.	1.2	144
67	The optimization of molecular orbitals for coupled cluster wavefunctions. Chemical Physics Letters, 1987, 142, 354-358.	1.2	144
68	Accelerating the convergence of the coupled-cluster approach. Chemical Physics Letters, 1986, 130, 236-239.	1.2	143
69	Mechanism of the C2H5+O2 reaction. Journal of Chemical Physics, 1997, 107, 141-155.	1.2	142
70	Hartreeâ€“Fock orbital instability envelopes in highly correlated single-reference wave functions. Journal of Chemical Physics, 1997, 107, 10626-10632.	1.2	142
71	The malonaldehyde equilibrium geometry: A major structural shift due to the effects of electron correlation. Journal of Chemical Physics, 1985, 82, 4194-4198.	1.2	137
72	Ab Initio Calculations on 62 Lowâ€Lying States of the O2Molecule. Journal of Chemical Physics, 1968, 48, 4946-4955.	1.2	136

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73	Potential energy surface for the Li+HFâ†'LiF+H reaction. Journal of Chemical Physics, 1980, 72, 4376-4393.	1.2	135
74	Carbene Rearrangements Unsurpassed:â€‰ Details of the C7H6 Potential Energy Surface Revealed. Journal of Organic Chemistry, 1996, 61, 7030-7039.	1.7	133
75	Interaction potential between two rigid HF molecules. Journal of Chemical Physics, 1974, 60, 855-865.	1.2	131
76	Binuclear Homoleptic Iron Carbonyls:Â Incorporation of Formal Ironâ€'Iron Single, Double, Triple, and Quadruple Bonds, Fe2(CO)x(x= 9, 8, 7, 6). Journal of the American Chemical Society, 2000, 122, 8746-8761.	6.6	131
77	An energetically lowâ€lying silacyclopropyne isomer of SiC2. Journal of Chemical Physics, 1984, 80, 3552-3555.	1.2	130
78	Infrared cavity ringdown spectroscopy of methanol clusters: Single donor hydrogen bonding. Journal of Chemical Physics, 1999, 110, 4258-4267.	1.2	130
79	The remarkable monobridged structure of Si2H2. Journal of Chemical Physics, 1992, 97, 7990-7998.	1.2	129
80	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.	1.2	127
81	The silicon-carbon double bond: a healthy rivalry between theory and experiment. Accounts of Chemical Research, 1982, 15, 283-290.	7.6	126
82	Conformers of Gaseous Cysteine. Journal of Chemical Theory and Computation, 2009, 5, 1511-1523.	2.3	126
83	Is Mo/llerâ€"Plesset perturbation theory a convergent ab initio method?. Journal of Chemical Physics, 2000, 112, 9213-9222.	1.2	125
84	Electron Affinity of the Guanineâ€'Cytosine Base Pair and Structural Perturbations upon Anion Formation. Journal of the American Chemical Society, 2002, 124, 10163-10170.	6.6	125
85	A theory of selfâ€consistent electron pairs. Computational methods and preliminary applications. Journal of Chemical Physics, 1976, 65, 2740-2750.	1.2	124
86	The Nature of the Galliumâ€'Gallium Triple Bond. Journal of the American Chemical Society, 1998, 120, 3773-3780.	6.6	124
87	Electron Affinities of Polycyclic Aromatic Hydrocarbons. Journal of Physical Chemistry A, 2001, 105, 524-528.	1.1	124
88	Characteristics of novel sandwiched beryllium, magnesium, and calcium dimers: C5H5BeBeC5H5, C5H5MgMgC5H5, and C5H5CaCaC5H5. Chemical Physics Letters, 2005, 402, 414-421.	1.2	124
89	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.	1.2	124
90	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.	1.2	123

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91	Electrophilic Aromatic Substitution: New Insights into an Old Class of Reactions. Accounts of Chemical Research, 2016, 49, 1191-1199.	7.6	123
92	Ab Initio Potential Curve for the X 3Î£gâ¯ State of O2. Journal of Chemical Physics, 1971, 54, 2207-2211.	1.2	122
93	The decarboxylation and dehydration reactions of monomeric formic acid. Journal of Chemical Physics, 1992, 96, 1158-1166.	1.2	119
94	Non-innocent Additives in a Palladium(II)-Catalyzed Câ€“H Bond Activation Reaction: Insights into Multimetallic Active Catalysts. Journal of the American Chemical Society, 2014, 136, 5535-5538.	6.6	119
95	Model studies of chemisorption. Interaction between atomic hydrogen and beryllium clusters. Journal of Chemical Physics, 1975, 62, 4815-4825.	1.2	118
96	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.	1.2	118
97	Assessment of Density Functional Theory for Model SN2 Reactions:Â CH3X + F-(X = F, Cl, CN, OH, SH, NH2,) Tj ETQq1 1 0.784314 rgBT	1.1	118
98	Features of the H2CO potential energy hypersurface pertinent to formaldehyde photodissociation. Journal of Chemical Physics, 1981, 75, 3459-3465.	1.2	114
99	Predicting electron affinities with density functional theory: Some positive results for negative ions. Journal of Chemical Physics, 1997, 107, 2529-2541.	1.2	114
100	The Dichotomy of Dimetallocenes:Â Coaxial versus Perpendicular Dimetal Units in Sandwich Compounds. Journal of the American Chemical Society, 2005, 127, 2818-2819.	6.6	113
101	Analytic second derivatives for Rennerâ€“Teller potential energy surfaces. Examples of the five distinct cases. Journal of Chemical Physics, 1984, 81, 356-361.	1.2	111
102	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.	1.2	111
103	DNA Nucleosides and Their Radical Anions:Â Molecular Structures and Electron Affinities. Journal of the American Chemical Society, 2004, 126, 4404-4411.	6.6	109
104	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.	1.2	108
105	Multiple dâ€type basis functions for molecules containing second row atoms. Journal of Chemical Physics, 1985, 83, 5721-5726.	1.2	106
106	The Adenineâ¯Thymine Base Pair Radical Anion:â€‰ Adding an Electron Results in a Major Structural Change. Journal of Physical Chemistry B, 2003, 107, 848-853.	1.2	106
107	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.	23.0	106
108	P<scp>si</scp>4N<scp>um</scp>P<scp>y</scp>: An Interactive Quantum Chemistry Programming Environment for Reference Implementations and Rapid Development. Journal of Chemical Theory and Computation, 2018, 14, 3504-3511.	2.3	106

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109	Valenceâ€Excited States of Carbon Monoxide. Journal of Chemical Physics, 1970, 53, 3994-4004.	1.2	105
110	Calculation of the Attractive He Pair Potential. Physical Review Letters, 1970, 25, 988-990.	2.9	105
111	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.	1.2	105
112	An Efficient Computational Approach for the Evaluation of Substituent Constants. Journal of Organic Chemistry, 2006, 71, 6382-6387.	1.7	105
113	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.	1.2	104
114	Stabilization of elusive silicon oxides. Nature Chemistry, 2015, 7, 509-513.	6.6	104
115	Negative Ion Thermochemistry:â€‰ The Sulfur Fluorides SFn/SFn- (n = 1â^'7). The Journal of Physical Chemistry, 1996, 100, 6061-6068.	2.9	102
116	The protonated water dimer: Brueckner methods remove the spurious C1 symmetry minimum. Journal of Chemical Physics, 1998, 108, 7197-7201.	1.2	102
117	Theoretical Studies of the Potential Energy Surfaces and Compositions of thed-Aldo-andd-Ketohexoses. Journal of the American Chemical Society, 1998, 120, 3411-3422.	6.6	101
118	Triplet electronic states of acetylene:cisandtransstructures and energetics. Journal of Chemical Physics, 1978, 69, 1648-1654.	1.2	100
119	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.	0.5	100
120	Binuclear Cyclopentadienylcobalt Carbonyls:Â Comparison with Binuclear Iron Carbonyls. Journal of the American Chemical Society, 2005, 127, 11646-11651.	6.6	100
121	Avoided intersection of potential energy surfaces: The (H+â€‰+â€‰H2,â€‰Hâ€‰+â€‰H2+) system. Journal of Chemical Physics, 1973, 59, 1286-1292.	1.2	99
122	Cleavage of Carbene-Stabilized Disilicon. Journal of the American Chemical Society, 2011, 133, 8874-8876.	6.6	98
123	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.	1.2	97
124	A new zincâ€“zinc-bonded compound with a dianionic Î±-diimine ligand: synthesis and structure of [Na(THF)2]2Â·[LZnâ€“ZnL] (L = [(2,6-iPr2C6H3)N(Me)C]22â^). Chemical Communications, 2007, , 2363-2365.	2.2	97
125	New theoretical evidence for the nonlinearity of the triplet ground state of methylene. Journal of the American Chemical Society, 1970, 92, 4984-4985.	6.6	96
126	Perturbative triples corrections in state-specific multireference coupled cluster theory. Journal of Chemical Physics, 2010, 132, 074107.	1.2	96

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127	Theoretical Potential Energy Curves for OH, HF+, HF, HFâˆ', NeH+, and NeH. Journal of Chemical Physics, 1972, 57, 1123-1128.	1.2	95
128	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.	1.2	93
129	The existence of secondary orbital interactions. Journal of Computational Chemistry, 2007, 28, 344-361.	1.5	92
130	Theoretical Study of SO2 Molecular Properties. Journal of Chemical Physics, 1970, 53, 3014-3019.	1.2	91
131	Electronic Structures and Potential Energy Curves for the Lowâ€Lying States of the CN Radical. Journal of Chemical Physics, 1971, 54, 2573-2580.	1.2	91
132	A combined crossed molecular beam and ab initio investigation of C2 and C3 elementary reactions with unsaturated hydrocarbonsÃ¢â‚¬â€pathways to hydrogen deficient hydrocarbon radicals in combustion flames. Faraday Discussions, 2001, 119, 51-66.	1.6	91
133	Relativistic and correlation effects in CuH, AgH, and AuH: Comparison of various relativistic methods. Journal of Chemical Physics, 1995, 102, 2024-2031.	1.2	90
134	Theoretical study of the H+O3â†'OH+O2â†'O+HO2 system. Journal of Chemical Physics, 1986, 84, 2691-2697.	1.2	89
135	Geometrical structures and vibrational frequencies of the energetically lowâ€lying isomers of SiC3. Journal of Chemical Physics, 1990, 93, 5046-5052.	1.2	89
136	Hydrogen bonding between the water molecule and the hydroxyl radical (H2Oâ‹…HO): The global minimum. Journal of Chemical Physics, 1993, 98, 8829-8834.	1.2	89
137	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.	1.2	89
138	Crossed beam reaction of cyano radicals with hydrocarbon molecules. I. Chemical dynamics of cyanobenzene (C6H5CN; Xâ€Š1A1) and perdeutero cyanobenzene (C6D5CN; Xâ€Š1A1) formation from reaction of CN(Xâ€Š2Î£+) with benzene C6H6(Xâ€Š1A1g), and d6-benzene C6D6(Xâ€Š1A1g). Journal of Chemical Physics, 1999, 111, 7457-7471.	1.2	89
139	NHCâ€Containing Manganese(I) Electrocatalysts for the Twoâ€Electron Reduction of CO₂. Angewandte Chemie - International Edition, 2014, 53, 5152-5155.	7.2	89
140	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.	1.2	88
141	The Chemical Vapor Deposition of Aluminum Nitride:Â Unusual Cluster Formation in the Gas Phase. Journal of the American Chemical Society, 1997, 119, 5668-5678.	6.6	88
142	Direct Nearâ€Hartreeâ€"Fock Calculations on the 1s Hole States of NO+. Journal of Chemical Physics, 1971, 55, 1474-1475.	1.2	87
143	Analytic energy second derivatives for general MCSCF wave functions. Journal of Chemical Physics, 1984, 80, 2660-2668.	1.2	87
144	Analytic third derivatives for selfâ€consistentâ€field wave functions. Journal of Chemical Physics, 1984, 81, 6395-6396.	1.2	86

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145	A Systematic Application of Density Functional Theory to Some Carbon-Containing Molecules and Their Anions. Journal of Physical Chemistry A, 1999, 103, 4065-4077.	1.1	86
146	Electronic Splitting between the 2B1 and 2A1 States of the NH2 Radical. Journal of Chemical Physics, 1971, 55, 4798-4803.	1.2	85
147	C2Ï... Potential Energy Surfaces for Seven Lowâ€Lying States of CH2. Journal of Chemical Physics, 1971, 55, 162-169.	1.2	84
148	Electronic structure of the N4+molecular ion. Journal of Chemical Physics, 1981, 74, 550-558.	1.2	84
149	Potential energy surfaces related to the ionâ€molecule reaction C+ + H2. Journal of Chemical Physics, 1974, 61, 2507-2513.	1.2	81
150	The silicon analog of benzeneâ€“hexasilabenzene (Si6H6). Journal of Chemical Physics, 1986, 84, 1664-1669.	1.2	81
151	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.	1.2	81
152	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.	1.2	80
153	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.	1.2	79
154	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.	1.2	79
155	The H+5potential energy hypersurface: Characterization of ten distinct energetically lowâ€lying stationary points. Journal of Chemical Physics, 1987, 86, 5072-5081.	1.2	79
156	The convergence of the cluster model for the study of chemisorption: Be36H. Journal of Chemical Physics, 1983, 78, 1390-1395.	1.2	78
157	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.	1.2	77
158	Re(I) NHC Complexes for Electrocatalytic Conversion of CO₂. Inorganic Chemistry, 2016, 55, 3136-3144.	1.9	77
159	Methane as a Numerical Experiment for Polarization Basis Function Selection. Journal of Chemical Physics, 1971, 54, 2764-2766.	1.2	76
160	Diatomic sulfur: Low lying bound molecular electronic states of S2. Journal of Chemical Physics, 1979, 70, 947.	1.2	76
161	Carbon clusters: The structure of C10 studied with configuration interaction methods. Journal of Chemical Physics, 1990, 93, 8844-8849.	1.2	76
162	Protonated Ethane. A Theoretical Investigation of C2H7+ Structures and Energies. Journal of the American Chemical Society, 1994, 116, 3483-3493.	6.6	76

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