John F Stanton

List of Publications by Year
in descending order

159 papers	12,516 citations	36303 51 h-index	25787 108 g-index
163 all docs	163 docs citations	163 times ranked	5827 citing authors

#	Article	IF	Citations
1	Atomic isotropic hyperfine properties for first row elements (Bâ€“F) revisited. Journal of Chemical Physics, 2022, 156, 034304.	3.0	3
2	PAH Growth in Flames and Space: Formation of the Phenalenyl Radical. Journal of Physical Chemistry A, 2022, 126, 101-108.	2.5	8
3	Probing the Exit Channel of the OH + CH₃OH â†' H₂O + CH₃O Reaction by Photodetachment of CH₃O^{â€“}(H₂O). Journal of Physical Chemistry Letters, 2022, 13, 142-148.	4.6	7
4	Theoretical Rovibrational Spectroscopy of Magnesium Tricarbideâ€“Multireference Character Thwarts a Full Analysis of All Isomers. Journal of Physical Chemistry A, 2022, 126, 4132-4146.	2.5	5
5	Semi-experimental equilibrium (r eSE) and theoretical structures of hydrazoic acid (HN3). Journal of Chemical Physics, 2022, 157, .	3.0	3
6	How to VPT2: Accurate and Intuitive Simulations of CH Stretching Infrared Spectra Using VPT2+K with Large Effective Hamiltonian Resonance Treatments. Journal of Physical Chemistry A, 2021, 125, 1301-1324.	2.5	72
7	Using isotopologues to probe the potential energy surface of reactions of C2H2++C3H4. Journal of Chemical Physics, 2021, 154, 124310.	3.0	4
8	Vibronically coupled states: computational considerations and characterisation of vibronic and rovibronic spectroscopic parameters. International Reviews in Physical Chemistry, 2021, 40, 165-298.	2.3	13
9	Equation-of-motion coupled-cluster method with double electron-attaching operators: Theory, implementation, and benchmarks. Journal of Chemical Physics, 2021, 154, 114115.	3.0	17
10	Bob Cave Memorial. Journal of Physical Chemistry A, 2021, 125, 4037-4038.	2.5	0
11	Precise equilibrium structure determination of thiophene (c-C4H4S) by rotational spectroscopyâ€"Structure of a five-membered heterocycle containing a third-row atom. Journal of Chemical Physics, 2021, 154, 244310.	3.0	20
12	Precise equilibrium structure of thiazole (c-C3H3NS) from twenty-four isotopologues. Journal of Chemical Physics, 2021, 155, 054302.	3.0	14
13	Thermal Decomposition of CH3O: A Curious Case of Pressure-Dependent Tunneling Effects. Journal of Physical Chemistry A, 2021, 125, 6761-6771.	2.5	0
14	Semi-Experimental Equilibrium (r_e^{SE}) and Theoretical Structures of Pyridazine (o-C₄H₄N₂). Journal of Physical Chemistry A, 2021, 125, 7976-7987.	2.5	10
15	Photodissociation of dicarbon: How nature breaks an unusual multiple bond. Proceedings of the National Academy of Sciences of the United States of America, 2021, 118, .	7.1	16
16	High-Resolution Photoelectron Spectroscopy of Cryogenically Cooled NO₃Ì.... Journal of Physical Chemistry Letters, 2020, 11, 395-400.	4.6	13
17	Semiclassical transition state theory/master equation kinetics of HO + CO: Performance evaluation. International Journal of Chemical Kinetics, 2020, 52, 1022-1045.	1.6	9
18	Exhaustive Product Analysis of Three Benzene Discharges by Microwave Spectroscopy. Journal of Physical Chemistry A, 2020, 124, 5170-5181.	2.5	38

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19	Coupled-cluster techniques for computational chemistry: The <scp>CFOUR</scp> program package. Journal of Chemical Physics, 2020, 152, 214108.	3.0	375
20	Molecular structure determination: Equilibrium structure of pyrimidine (m-C4H4N2) from rotational spectroscopy (r eSE) and high-level ab initio calculation (r) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50 7 2020, 152, 104303.	3.0	41
21	Pragmatic Solution for a Fully E,J-Resolved Master Equation. Journal of Physical Chemistry A, 2020, 124, 2907-2918.	2.5	17
22	Theoretical prediction of magnetic exchange coupling constants from broken-symmetry coupled cluster calculations. Journal of Chemical Physics, 2020, 152, 234115.	3.0	17
23	Pressure-Dependent Rate Constant Caused by Tunneling Effects: OH + HNO₃ as an Example. Journal of Physical Chemistry Letters, 2020, 11, 3712-3717.	4.6	11
24	Frontispiece: The Hunt for Elusive Molecules: Insights from Joint Theoretical and Experimental Investigations. Chemistry - A European Journal, 2019, 25, .	3.3	0
25	The Hunt for Elusive Molecules: Insights from Joint Theoretical and Experimental Investigations. Chemistry - A European Journal, 2019, 25, 7243-7258.	3.3	8
26	Ab initio thermal rate coefficients for H + NH₃ â‡Œ H₂ + NH₂. International Journal of Chemical Kinetics, 2019, 51, 321-328.	1.6	20
27	Quantum-state-specific reaction rate measurements for the photo-induced reaction Ca⁺ + O₂ â†’ CaO⁺ + O. Molecular Physics, 2019, 117, 3036-3042.	1.7	13
28	A VSEPR-inspired force field for determining molecular properties of PF₅. Molecular Physics, 2019, 117, 1344-1350.	1.7	0
29	First-Principles Calculation of Jahnâ€“Teller Rotational Distortion Parameters. Journal of Physical Chemistry A, 2019, 123, 4990-5004.	2.5	7
30	Structural Characterization of Phenoxy Radical with Mass-Correlated Broadband Microwave Spectroscopy. Journal of Physical Chemistry Letters, 2019, 10, 2919-2923.	4.6	7
31	Directed Gas-Phase Formation of the Germaniumsilylene Butterfly Molecule (Ge(Î¼-H₂)Si). Journal of Physical Chemistry Letters, 2019, 10, 1264-1271.	4.6	6
32	A master equation simulation for the â€¢OH + CH3OH reaction. Journal of Chemical Physics, 2019, 150, 084105.	3.0	42
33	Spectroscopy of Ethylenedione and Ethynediolide: A Reinvestigation. Angewandte Chemie - International Edition, 2018, 57, 5394-5397.	13.8	13
34	Perturbative treatment of spin-orbit-coupling within spin-free exact two-component theory using equation-of-motion coupled-cluster methods. Journal of Chemical Physics, 2018, 148, 044108.	3.0	40
35	Direct measurements of DOCO isomers in the kinetics of OD + CO. Science Advances, 2018, 4, eaao4777.	10.3	22
36	The Molecular Structure of gauche â€1,3â€Butadiene: Experimental Establishment of Nonâ€planarity. Angewandte Chemie, 2018, 130, 1839-1843.	2.0	10

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37	Spectroscopy of Ethylenedione and Ethynediolide: A Reinvestigation. Angewandte Chemie, 2018, 130, 5492-5495.	2.0	8
38	Innentitelbild: Spectroscopy of Ethylenedione and Ethynediolide: A Reinvestigation (Angew. Chem.) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 5	2.0	0
39	Unimolecular Reaction of Methyl Isocyanide to Acetonitrile: A High-Level Theoretical Study. Journal of Physical Chemistry Letters, 2018, 9, 2532-2538.	4.6	20
40	The Molecular Structure of gaucheâ€1,3â€Butadiene: Experimental Establishment of Nonâ€planarity. Angewandte Chemie - International Edition, 2018, 57, 1821-1825.	13.8	46
41	Electron-Withdrawing Effects in the Photodissociation of CH₂ICl To Form CH₂Cl Radical, Simultaneously Viewed Through the Carbon K and Chlorine L_{2,3} X-ray Edges. Journal of the American Chemical Society, 2018, 140, 13360-13366.	13.7	14
42	Accuracy of Coupled Cluster Excited State Potential Energy Surfaces. Journal of Chemical Theory and Computation, 2018, 14, 5859-5869.	5.3	24
43	Quantum-state-controlled reactions between molecular radicals and ions. Physical Review A, 2018, 98, .	2.5	19
44	Three-Dimensional Master Equation (3DME) Approach. Journal of Physical Chemistry A, 2018, 122, 7757-7767.	2.5	12
45	Radical Rearrangement Chemistry in Ultraviolet Photodissociation of Iodotyrosine Systems: Insights from Metastable Dissociation, Infrared Ion Spectroscopy, and Reaction Pathway Calculations. Journal of the American Society for Mass Spectrometry, 2018, 29, 1791-1801.	2.8	10
46	Spectral analyses of trans- and cis-DOCO transients via comb spectroscopy. Molecular Physics, 2018, 116, 3710-3717.	1.7	7
47	Broadband Microwave Spectroscopy of 2-Furanyloxy Radical: Primary Pyrolysis Product of the Second-Generation Biofuel 2-Methoxyfuran. Journal of Physical Chemistry A, 2018, 122, 6879-6885.	2.5	15
48	Bond Dissociation Energies for Diatomic Molecules Containing 3d Transition Metals: Benchmark Scalar-Relativistic Coupled-Cluster Calculations for 20 Molecules. Journal of Chemical Theory and Computation, 2017, 13, 1044-1056.	5.3	81
49	The gas-phase structure of the asymmetric, trans-dinitrogen tetroxide (N2O4), formed by dimerization of nitrogen dioxide (NO2), from rotational spectroscopy and ab initio quantum chemistry. Journal of Chemical Physics, 2017, 146, 134305.	3.0	13
50	Quantifying Hydrogenâ€Bond Populations in Dimethyl Sulfoxide/Water Mixtures. Angewandte Chemie - International Edition, 2017, 56, 11375-11379.	13.8	94
51	Thermal Decomposition of Potential Ester Biofuels. Part I: Methyl Acetate and Methyl Butanoate. Journal of Physical Chemistry A, 2017, 121, 4658-4677.	2.5	31
52	Quantifying Hydrogenâ€Bond Populations in Dimethyl Sulfoxide/Water Mixtures. Angewandte Chemie, 2017, 129, 11533-11537.	2.0	25
53	Low-lying vibronic level structure of the ground state of the methoxy radical: Slow electron velocity-map imaging (SEVI) spectra and KÃ¶ppel-Domcke-Cederbaum (KDC) vibronic Hamiltonian calculations. Journal of Chemical Physics, 2017, 146, 224309.	3.0	15
54	Gasâ€Phase Formation of the Disilavinylidene (H₂SiSi) Transient. Angewandte Chemie - International Edition, 2017, 56, 1264-1268.	13.8	17

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55	Active Thermochemical Tables: The Adiabatic Ionization Energy of Hydrogen Peroxide. Journal of Physical Chemistry A, 2017, 121, 8799-8806.	2.5	33
56	Titelbild: Quantifying Hydrogenâ€Bond Populations in Dimethyl Sulfoxide/Water Mixtures (Angew.) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 5	2.0	0
57	High-level theoretical study of the reaction between hydroxyl and ammonia: Accurate rate constants from 200 to 2500 K. Journal of Chemical Physics, 2017, 147, 152704.	3.0	24
58	Communication: Thermal unimolecular decomposition of syn-CH3CHOO: A kinetic study. Journal of Chemical Physics, 2016, 145, 131102.	3.0	38
59	A new approach to approximate equation-of-motion coupled cluster with triple excitations. Journal of Chemical Physics, 2016, 145, 124102.	3.0	70
60	Pyrolysis of the Simplest Carbohydrate, Glycolaldehyde (CHOâ^'CH₂OH), and Glyoxal in a Heated Microreactor. Journal of Physical Chemistry A, 2016, 120, 2161-2172.	2.5	13
61	Structural and Thermodynamic Analysis of a Three-Component Assembly Forming ortho-Iminophenylboronate Esters. Journal of Organic Chemistry, 2016, 81, 8319-8330.	3.2	30
62	Spontaneous and Selective Formation of HSNO, a Crucial Intermediate Linking H₂S and Nitroso Chemistries. Journal of the American Chemical Society, 2016, 138, 11441-11444.	13.7	60
63	Semiclassical Transition-State Theory Based on Fourth-Order Vibrational Perturbation Theory: The Symmetrical Eckart Barrier. Journal of Physical Chemistry Letters, 2016, 7, 2708-2713.	4.6	21
64	A Highly-Efficient Implementation of the Doktorov Recurrence Equations for Franckâ€“Condon Calculations. Journal of Chemical Theory and Computation, 2016, 12, 728-739.	5.3	14
65	Precise equilibrium structure determination of hydrazoic acid (HN3) by millimeter-wave spectroscopy. Journal of Chemical Physics, 2015, 143, 104310.	3.0	31
66	Communication: The ground electronic state of Si2C: Rovibrational level structure, quantum monodromy, and astrophysical implications. Journal of Chemical Physics, 2015, 142, 231101.	3.0	21
67	Stabilization of the Simplest Criegee Intermediate from the Reaction between Ozone and Ethylene: A High-Level Quantum Chemical and Kinetic Analysis of Ozonolysis. Journal of Physical Chemistry A, 2015, 119, 5524-5533.	2.5	83
68	Discovery of a Missing Link: Detection and Structure of the Elusive Disilicon Carbide Cluster. Journal of Physical Chemistry Letters, 2015, 6, 2107-2111.	4.6	36
69	Isomerization and Fragmentation of Cyclohexanone in a Heated Micro-Reactor. Journal of Physical Chemistry A, 2015, 119, 12635-12647.	2.5	11
70	Pyrolysis of Cyclopentadienone: Mechanistic Insights from a Direct Measurement of Product Branching Ratios. Journal of Physical Chemistry A, 2015, 119, 7222-7234.	2.5	23
71	Relatively Selective Production of the Simplest Criegee Intermediate in a CH₄/O₂ Electric Discharge: Kinetic Analysis of a Plausible Mechanism. Journal of Physical Chemistry A, 2015, 119, 7197-7204.	2.5	16
72	The ionisation energy of cyclopentadienone: a photoelectronâ€“photoion coincidence study. Molecular Physics, 2015, 113, 2350-2358.	1.7	16

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73	A Steady-State Approximation to the Two-Dimensional Master Equation for Chemical Kinetics Calculations. Journal of Physical Chemistry A, 2015, 119, 7627-7636.	2.5	33
74	Photoelectron Spectroscopy of the Methide Anion: Electron Affinities of ^{â€¢}CH₃ and ^{â€¢}CD₃ and Inversion Splittings of CH₃^{â€“} and CD₃^{â€“}. Journal of the American Chemical Society, 2015, 137, 12939-12945.	13.7	25
75	Photoelectron Wave Function in Photoionization: Plane Wave or Coulomb Wave?. Journal of Physical Chemistry Letters, 2015, 6, 4532-4540.	4.6	115
76	On the HCN â€“ HNC Energy Difference. Journal of Physical Chemistry A, 2015, 119, 10929-10934.	2.5	32
77	Non-orthogonal spin-adaptation of coupled cluster methods: A new implementation of methods including quadruple excitations. Journal of Chemical Physics, 2015, 142, 064108.	3.0	71
78	Jet cooled cavity ringdown spectroscopy of the AËœ2Eâ€³â†XËœ2A2â€² transition of the NO3 radical. Journal of Chemical Physics, 2015, 142, 184305.	3.0	29
79	Relativistic coupled-cluster calculations on XeF6: Delicate interplay between electron-correlation and basis-set effects. Journal of Chemical Physics, 2015, 142, 224309.	3.0	13
80	Reactive intermediates in 4He nanodroplets: Infrared laser Stark spectroscopy of dihydroxycarbene. Journal of Chemical Physics, 2015, 142, 144309.	3.0	6
81	Chirped-pulse millimeter-wave spectroscopy for dynamics and kinetics studies of pyrolysis reactions. Physical Chemistry Chemical Physics, 2014, 16, 15739-15751.	2.8	54
82	Reduced dimension rovibrational variational calculations of the S1 state of C2H2. II. The S1 rovibrational manifold and the effects of isomerization. Journal of Chemical Physics, 2014, 140, 024313.	3.0	9
83	Communication: Helium nanodroplet isolation and rovibrational spectroscopy of hydroxymethylene. Journal of Chemical Physics, 2014, 140, 171102.	3.0	9
84	Chirped-Pulse Fourier Transform Microwave Spectroscopy Coupled with a Flash Pyrolysis Microreactor: Structural Determination of the Reactive Intermediate Cyclopentadienone. Journal of Physical Chemistry Letters, 2014, 5, 2201-2207.	4.6	27
85	Rotational spectroscopy of pyridazine and its isotopologs from 235â€“360â€‰GHz: Equilibrium structure and vibrational satellites. Journal of Chemical Physics, 2013, 139, 224304.	3.0	45
86	Revisitation of Nonorthogonal Spin Adaptation in Coupled Cluster Theory. Journal of Chemical Theory and Computation, 2013, 9, 2567-2572.	5.3	21
87	The Simplest Criegee Intermediate (H₂Câ•Oâ€“O): Isotopic Spectroscopy, Equilibrium Structure, and Possible Formation from Atmospheric Lightning. Journal of Physical Chemistry Letters, 2013, 4, 4133-4139.	4.6	88
88	Ground and low-lying excited states of propadienylidene (H2C=C=C:) obtained by negative ion photoelectron spectroscopy. Journal of Chemical Physics, 2012, 136, 134312.	3.0	18
89	Quantitative vibronic coupling calculations. The visible spectrum of propadienylidene. Faraday Discussions, 2011, 150, 331.	3.2	15
90	Vibrational Energy Levels via Finite-Basis Calculations Using a Quasi-Analytic Form of the Kinetic Energy. Journal of Chemical Theory and Computation, 2011, 7, 1428-1442.	5.3	20

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91	Quantitative vibronic coupling calculations: the formyloxyl radical. Theoretical Chemistry Accounts, 2011, 129, 527-543.	1.4	28
92	Towards highly accurate ab initio thermochemistry of larger systems: Benzene. Journal of Chemical Physics, 2011, 135, 044513.	3.0	44
93	Quantum-chemical calculation of spectroscopic parameters for rotational spectroscopy. International Reviews in Physical Chemistry, 2010, 29, 273-367.	2.3	288
94	An unusually large nonadiabatic error in the BNB molecule. Journal of Chemical Physics, 2010, 133, 174309.	3.0	27
95	Quantitative analysis of Fermi resonances by harmonic derivatives of perturbation theory corrections. Molecular Physics, 2009, 107, 213-222.	1.7	44
96	On the vibronic level structure in the NO₃ radical: II. Adiabatic calculation of the infrared spectrum. Molecular Physics, 2009, 107, 1059-1075.	1.7	65
97	High-Accuracy Extrapolated ab Initio Thermochemistry of the Propargyl Radical and the Singlet C₃H₂ Carbenes. Journal of Physical Chemistry A, 2009, 113, 12447-12453.	2.5	39
98	On the vibronic level structure in the NO3 radical : Part III. Observation of intensity borrowing via ground state mixing. Physical Chemistry Chemical Physics, 2009, 11, 4742.	2.8	27
99	High-accuracy extrapolated ab initio thermochemistry. III. Additional improvements and overview. Journal of Chemical Physics, 2008, 128, 114111.	3.0	367
100	Applications of Post-Hartree-Fock Methods: A Tutorial. Reviews in Computational Chemistry, 2007, , 65-169.	1.5	273
101	Equilibrium Structure of the Silicon Trimer. ACS Symposium Series, 2007, , 193-200.	0.5	0
102	Treatment of Fermi resonance effects on transition moments in vibrational perturbation theory. Molecular Physics, 2007, 105, 101-109.	1.7	74
103	Factors Contributing to the Accuracy of Harmonic Force Field Calculations for Water. Journal of Chemical Theory and Computation, 2007, 3, 1267-1274.	5.3	21
104	On the vibronic level structure in the NO3 radical. I. The ground electronic state. Journal of Chemical Physics, 2007, 126, 134309.	3.0	133
105	Simple(r) algebraic equation for transition moments of fundamental transitions in vibrational second-order perturbation theory. Molecular Physics, 2006, 104, 377-388.	1.7	122
106	High-accuracy extrapolated ab initio thermochemistry. II. Minor improvements to the protocol and a vital simplification. Journal of Chemical Physics, 2006, 125, 064108.	3.0	312
107	Laser spectroscopy of Si3C. Journal of Chemical Physics, 2005, 122, 124314.	3.0	19
108	IUPAC Critical Evaluation of Thermochemical Properties of Selected Radicals. Part I. Journal of Physical and Chemical Reference Data, 2005, 34, 573-656.	4.2	283

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109	Ab initiodetermination of the heat of formation of ketenyl (HCCO) and ethynyl (CCH) radicals. Molecular Physics, 2005, 103, 2159-2168.	1.7	33
110	Electron-Correlated Methods for the Calculation of NMR Chemical Shifts. , 2004, , 123-139.		25
111	HEAT: High accuracy extrapolatedab initiothermochemistry. Journal of Chemical Physics, 2004, 121, 11599-11613.	3.0	691
112	Electron-Correlated Approaches for the Calculation of NMR Chemical Shifts. Advances in Chemical Physics, 2003, , 355-422.	0.3	79
113	Quantitative prediction of gas-phase 13C nuclear magnetic shielding constants. Journal of Chemical Physics, 2003, 118, 10407-10417.	3.0	246
114	A Discussion of Some Problems Associated with the Quantum Mechanical Treatment of Open-Shell Molecules. Advances in Chemical Physics, 2003, , 101-146.	0.3	58
115	The global minimum structure of SiC3: The controversy continues. Journal of Chemical Physics, 2002, 116, 9151-9153.	3.0	23
116	Analytic gradients for the coupled-cluster singles, doubles, and triples (CCSDT) model. Journal of Chemical Physics, 2002, 116, 1773-1782.	3.0	83
117	Molecular equilibrium structures from experimental rotational constants and calculated vibrationâ€“rotation interaction constants. Journal of Chemical Physics, 2002, 116, 6482-6496.	3.0	245
118	The equilibrium structure of the ammonium radical Rydberg ground state. Journal of Chemical Physics, 2001, 114, 9863-9865.	3.0	11
119	The accurate determination of molecular equilibrium structures. Journal of Chemical Physics, 2001, 114, 6548-6556.	3.0	353
120	Equilibrium structure of LiCCH. International Journal of Quantum Chemistry, 2000, 77, 305-310.	2.0	7
121	Analytic first and second derivatives for the CCSDT-n (n = 1â€“3) models: a first step towards the efficient calculation of CCSDT properties. Physical Chemistry Chemical Physics, 2000, 2, 2047-2060.	2.8	56
122	Barrier to Methyl Internal Rotation of Cis- andTrans-2-Methylvinoxy Radicals in the XÌƒ(2Aâ€˜Ââ€˜) and BÌƒ(2Aâ€˜Ââ€˜) States:Â Experiment and Theory. Journal of Physical Chemistry A, 2000, 104, 9906-9913.	2.5	14
123	The Equilibrium Structure of Benzene. Journal of Physical Chemistry A, 2000, 104, 2865-2868.	2.5	177
124	Coupled-cluster studies of singlet propynylidene. Molecular Physics, 1999, 96, 505-509.	1.7	6
125	Anharmonic force fields from analytic CCSD(T) second derivatives: HOF and F2O. Journal of Chemical Physics, 1999, 110, 3687-3696.	3.0	45
126	Application of an equation-of-motion coupled cluster method including higher-order corrections to potential energy surfaces of radicals. Journal of Chemical Physics, 1999, 111, 8275-8285.	3.0	59

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127	Analytic UHF-CCSD(T) second derivatives: implementation and application to the calculation of the vibration-rotation interaction constants of NCO and NCS. Theoretical Chemistry Accounts, 1998, 100, 5-11.	1.4	103
128	Analytic Evaluation of Second Derivatives of the Energy: Computational Strategies for the CCSD and CCSD(T) Approximations. Recent Advances in Computational, 1997, , 49-79.	0.8	20
129	Structures, Automerizations, and Isomerizations of C3H2Isomers. Journal of the American Chemical Society, 1997, 119, 5847-5856.	13.7	141
130	A simple correction to final state energies of doublet radicals described by equation-of-motion coupled cluster theory in the singles and doubles approximation (Erratum). Theoretica Chimica Acta, 1997, 95, 97-98.	0.8	15
131	A simple correction to final state energies of doublet radicals described by equation-of-motion coupled cluster theory in the singles and doubles approximation (Erratum). Theoretica Chimica Acta, 1997, 95, 97.	0.8	3
132	A simple correction to final state energies of doublet radicals described by equation-of-motion coupled cluster theory in the singles and doubles approximation. Theoretica Chimica Acta, 1996, 93, 303-313.	0.8	70
133	Perturbative treatment of triple excitations in coupledâ€cluster calculations of nuclear magnetic shielding constants. Journal of Chemical Physics, 1996, 104, 2574-2583.	3.0	359
134	A simple correction to final state energies of doublet radicals described by equation-of-motion coupled cluster theory in the singles and doubles approximation. Theoretica Chimica Acta, 1996, 93, 303.	0.8	4
135	Gaugeâ€invariant calculation of nuclear magnetic shielding constants at the coupledâ€“cluster singles and doubles level. Journal of Chemical Physics, 1995, 102, 251-253.	3.0	205
136	Coupledâ€cluster calculations of nuclear magnetic resonance chemical shifts. Journal of Chemical Physics, 1995, 103, 3561-3577.	3.0	257
137	On the equilibrium bond length of ammonia in the first excited singlet state. Journal of Chemical Physics, 1995, 102, 1096-1097.	3.0	17
138	On the extent of spin contamination in openâ€shell coupledâ€cluster wave functions. Journal of Chemical Physics, 1994, 101, 371-374.	3.0	205
139	Separability properties of reduced and effective density matrices in the equationâ€ofâ€motion coupled cluster method. Journal of Chemical Physics, 1994, 101, 8928-8937.	3.0	37
140	The equation of motion coupledâ€cluster method. A systematic biorthogonal approach to molecular excitation energies, transition probabilities, and excited state properties. Journal of Chemical Physics, 1993, 98, 7029-7039.	3.0	2,168
141	Manyâ€body methods for excited state potential energy surfaces. I. General theory of energy gradients for the equationâ€ofâ€motion coupledâ€cluster method. Journal of Chemical Physics, 1993, 99, 8840-8847.	3.0	176
142	A coupledâ€cluster based effective Hamiltonian method for dynamic electric polarizabilities. Journal of Chemical Physics, 1993, 99, 5178-5183.	3.0	103
143	Does chlorine peroxide exhibit a strong ultraviolet absorption near 250 nm?. Journal of Chemical Physics, 1993, 98, 9335-9339.	3.0	53
144	Restricted openâ€shell Hartreeâ€“Fockâ€based manyâ€body perturbation theory: Theory and application of energy and gradient calculations. Journal of Chemical Physics, 1992, 97, 6606-6620.	3.0	68

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145	Linear and cyclic isomers of C4. A theoretical study with coupledâ€cluster methods and large basis sets. Journal of Chemical Physics, 1992, 97, 8372-8381.	3.0	85
146	Analytic ROHFâ€“MBPT(2) second derivatives. Journal of Chemical Physics, 1992, 97, 7825-7828.	3.0	39
147	On the choice of orbitals for symmetry breaking problems with application to NO3. Journal of Chemical Physics, 1992, 97, 5554-5559.	3.0	165
148	The ACES II program system. International Journal of Quantum Chemistry, 1992, 44, 879-894.	2.0	404
149	A direct product decomposition approach for symmetry exploitation in manyâ€body methods. I. Energy calculations. Journal of Chemical Physics, 1991, 94, 4334-4345.	3.0	246
150	A coupledâ€cluster study of the ground state of C+3. Journal of Chemical Physics, 1991, 94, 4320-4327.	3.0	35
151	Point group symmetry and cartesian force constant redundancy. International Journal of Quantum Chemistry, 1991, 39, 19-29.	2.0	15
152	Analytic evaluation of energy gradients at the coupledâ€cluster singles and doubles level using quasiâ€restricted Hartreeâ€“Fock openâ€shell reference functions. Journal of Chemical Physics, 1991, 95, 2639-2645.	3.0	96
153	Potential nonrigidity of the NO3 radical. Journal of Chemical Physics, 1991, 94, 4084-4087.	3.0	60
154	Harmonic vibrational frequencies and infrared intensities from analytic fourthâ€order manyâ€body perturbation theory gradients. Journal of Chemical Physics, 1991, 94, 404-413.	3.0	42
155	Coupledâ€cluster openâ€shell analytic gradients: Implementation of the direct product decomposition approach in energy gradient calculations. Journal of Chemical Physics, 1991, 95, 2623-2638.	3.0	248
156	Highly correlated singleâ€reference studies of the O3 potential surface. I. Effects of high order excitations on the equilibrium structure and harmonic force field of ozone. Journal of Chemical Physics, 1989, 90, 1077-1082.	3.0	92
157	Correlated studies of infrared intensities. Journal of Chemical Physics, 1989, 90, 3241-3249.	3.0	58
158	Structure, energetics, and vibrational spectra of beryllium borohydride isomers. Journal of Chemical Physics, 1988, 88, 5726-5734.	3.0	16
159	Computation of quadratic electric dipole moment functions. Journal of Chemical Physics, 1988, 88, 7650-7652.	3.0	7