List of Publications by Year in descending order

183 papers	16,219 citations	23500 58 h-index	16127 124 g-index
184 all docs	184 docs citations	184 times ranked	5881 citing authors

#	Article	IF	Citations
1	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.	1.2	2,168
2	HEAT: High accuracy extrapolatedab initiothermochemistry. Journal of Chemical Physics, 2004, 121, 11599-11613.	1.2	691
3	Analytic energy derivatives for ionized states described by the equationâ€ofâ€motion coupled cluster method. Journal of Chemical Physics, 1994, 101, 8938-8944.	1.2	534
4	The ACES II program system. International Journal of Quantum Chemistry, 1992, 44, 879-894.	1.0	404
5	Why CCSD(T) works: a different perspective. Chemical Physics Letters, 1997, 281, 130-134.	1.2	395
6	Coupled-cluster techniques for computational chemistry: The <scp>CFOUR</scp> program package. Journal of Chemical Physics, 2020, 152, 214108.	1.2	375
7	High-accuracy extrapolated ab initio thermochemistry. III. Additional improvements and overview. Journal of Chemical Physics, 2008, 128, 114111.	1.2	367
8	Perturbative treatment of triple excitations in coupledâ€cluster calculations of nuclear magnetic shielding constants. Journal of Chemical Physics, 1996, 104, 2574-2583.	1.2	359
9	The accurate determination of molecular equilibrium structures. Journal of Chemical Physics, 2001, 114, 6548-6556.	1.2	353
10	Coupled-cluster methods including noniterative corrections for quadruple excitations. Journal of Chemical Physics, 2005, 123, 054101.	1.2	344
11	Analytic CCSD(T) second derivatives. Chemical Physics Letters, 1997, 276, 70-77.	1.2	312
12	High-accuracy extrapolated ab initio thermochemistry. II. Minor improvements to the protocol and a vital simplification. Journal of Chemical Physics, 2006, 125, 064108.	1.2	312
13	Quantum-chemical calculation of spectroscopic parameters for rotational spectroscopy. International Reviews in Physical Chemistry, 2010, 29, 273-367.	0.9	288
14	IUPAC Critical Evaluation of Thermochemical Properties of Selected Radicals. Part I. Journal of Physical and Chemical Reference Data, 2005, 34, 573-656.	1.9	283
15	Coupledâ€cluster calculations of nuclear magnetic resonance chemical shifts. Journal of Chemical Physics, 1995, 103, 3561-3577.	1.2	257
16	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.	1.2	248
17	A direct product decomposition approach for symmetry exploitation in manyâ€body methods. I. Energy calculations. Journal of Chemical Physics, 1991, 94, 4334-4345.	1.2	246
18	Quantitative prediction of gas-phase 13C nuclear magnetic shielding constants. Journal of Chemical Physics, 2003, 118, 10407-10417.	1.2	246

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19	Molecular equilibrium structures from experimental rotational constants and calculated vibrationâ€“rotation interaction constants. Journal of Chemical Physics, 2002, 116, 6482-6496.	1.2	245
20	The equilibrium structure and fundamental vibrational frequencies of dioxirane. Journal of Chemical Physics, 1998, 108, 7190-7196.	1.2	244
21	Analytic second derivatives in high-order many-body perturbation and coupled-cluster theories: Computational considerations and applications. International Reviews in Physical Chemistry, 2000, 19, 61-95.	0.9	233
22	Many-body perturbation theory with a restricted open-shell Hartreeâ€”Fock reference. Chemical Physics Letters, 1991, 187, 21-28.	1.2	232
23	Perturbative treatment of the similarity transformed Hamiltonian in equationâ€ofâ€motion coupledâ€cluster approximations. Journal of Chemical Physics, 1995, 103, 1064-1076.	1.2	227
24	Analytic energy gradients for open-shell coupled-cluster singles and doubles (CCSD) calculations using restricted open-shell Hartreeâ€”Fock (ROHF) reference functions. Chemical Physics Letters, 1991, 182, 207-215.	1.2	209
25	On the extent of spin contamination in openâ€shell coupledâ€cluster wave functions. Journal of Chemical Physics, 1994, 101, 371-374.	1.2	205
26	Gaugeâ€invariant calculation of nuclear magnetic shielding constants at the coupledâ€“cluster singles and doubles level. Journal of Chemical Physics, 1995, 102, 251-253.	1.2	205
27	Analytic calculation of the diagonal Born-Oppenheimer correction within configuration-interaction and coupled-cluster theory. Journal of Chemical Physics, 2006, 125, 144111.	1.2	182
28	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.	1.2	176
29	On the choice of orbitals for symmetry breaking problems with application to NO3. Journal of Chemical Physics, 1992, 97, 5554-5559.	1.2	165
30	Calculation of Vibrational Transition Frequencies and Intensities in Water Dimer:â€‰ Comparison of Different Vibrational Approaches. Journal of Physical Chemistry A, 2008, 112, 4324-4335.	1.1	165
31	A simple scheme for the direct calculation of ionization potentials with coupled-cluster theory that exploits established excitation energy methods. Journal of Chemical Physics, 1999, 111, 8785-8788.	1.2	162
32	Problematic p-benzyne: Orbital instabilities, biradical character, and broken symmetry. Journal of Chemical Physics, 2001, 114, 10638-10650.	1.2	161
33	Analytic energy gradients for the equationâ€ofâ€motion coupledâ€cluster method: Implementation and application to the HCN/HNC system. Journal of Chemical Physics, 1994, 100, 4695-4698.	1.2	155
34	Hartreeâ€“Fock orbital instability envelopes in highly correlated single-reference wave functions. Journal of Chemical Physics, 1997, 107, 10626-10632.	1.2	142
35	Investigation of an asymmetric triple-excitation correction for coupled-cluster energies. International Journal of Quantum Chemistry, 1998, 70, 601-611.	1.0	139
36	On the vibronic level structure in the NO3 radical. I. The ground electronic state. Journal of Chemical Physics, 2007, 126, 134309.	1.2	133

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37	Simple(r) algebraic equation for transition moments of fundamental transitions in vibrational second-order perturbation theory. Molecular Physics, 2006, 104, 377-388.	0.8	122
38	Ab Initio Reaction Rate Constants Computed Using Semiclassical Transition-State Theory: HO + H₂ â† H₂O + H and Isotopologues. Journal of Physical Chemistry A, 2011, 115, 5118-5126.	1.1	109
39	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.	0.5	103
40	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.	1.2	96
41	A practical implementation of semi-classical transition state theory for polyatomics. Chemical Physics Letters, 2010, 499, 9-15.	1.2	92
42	Analytic gradients for the coupled-cluster singles, doubles, and triples (CCSDT) model. Journal of Chemical Physics, 2002, 116, 1773-1782.	1.2	83
43	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.	1.1	83
44	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
45	Quasidiabatic states described by coupled-cluster theory. Journal of Chemical Physics, 2009, 130, 174105.	1.2	81
46	Calculation of fundamental frequencies for small polyatomic molecules: a comparison between correlation consistent and atomic natural orbital basis sets. Molecular Physics, 2013, 111, 1492-1496.	0.8	80
47	Reaction of HO with CO: Tunneling Is Indeed Important. Journal of Physical Chemistry Letters, 2012, 3, 1549-1553.	2.1	79
48	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.	1.1	72
49	Non-orthogonal spin-adaptation of coupled cluster methods: A new implementation of methods including quadruple excitations. Journal of Chemical Physics, 2015, 142, 064108.	1.2	71
50	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.	0.9	70
51	A new approach to approximate equation-of-motion coupled cluster with triple excitations. Journal of Chemical Physics, 2016, 145, 124102.	1.2	70
52	Investigation of the electronic structure and spectroscopy of Jahnâ€"Teller distorted C+60. Chemical Physics Letters, 1992, 194, 467-471.	1.2	69
53	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.	1.2	68
54	Nonadiabatic effects in the photoelectron spectrum of the pyrazolide-d3 anion: Three-state interactions in the pyrazolyl-d3 radical. Journal of Chemical Physics, 2006, 125, 084312.	1.2	67

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55	Coupled-cluster theory, pseudo-Jahnâ€“Teller effects and conical intersections. Journal of Chemical Physics, 2001, 115, 10382.	1.2	65
56	On the vibronic level structure in the NO₃ radical: II. Adiabatic calculation of the infrared spectrum. Molecular Physics, 2009, 107, 1059-1075.	0.8	65
57	On the vertical excitation energy of cyclopentadiene. Journal of Chemical Physics, 2004, 121, 5236-5240.	1.2	64
58	The effect of triple excitations in coupled cluster calculations of frequency-dependent polarizabilities. Chemical Physics Letters, 1998, 292, 437-446.	1.2	61
59	HO + CO Reaction Rates and H/D Kinetic Isotope Effects: Master Equation Models with ab Initio SCTST Rate Constants. Journal of Physical Chemistry A, 2013, 117, 821-835.	1.1	61
60	Potential nonrigidity of the NO3 radical. Journal of Chemical Physics, 1991, 94, 4084-4087.	1.2	60
61	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.	1.2	59
62	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
63	High-accuracy extrapolated ab initio thermochemistry. IV. A modified recipe for computational efficiency. Journal of Chemical Physics, 2019, 150, 224102.	1.2	58
64	Triple excitation effects in coupled-cluster calculations of frequency-dependent hyperpolarizabilities. Chemical Physics Letters, 1998, 296, 117-124.	1.2	56
65	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.	1.3	56
66	Propargyl Radical:â€‰ Ab Initio Anharmonic Modes and the Polarized Infrared Absorption Spectra of Matrix-Isolated HCCCH2. Journal of Physical Chemistry A, 2005, 109, 3812-3821.	1.1	55
67	Structure and Energetics of Isomers of the Interstellar Molecule C5H. Journal of the American Chemical Society, 1999, 121, 1902-1911.	6.6	54
68	Some surprising failures of Brueckner coupled cluster theory. Journal of Chemical Physics, 2000, 112, 7873-7879.	1.2	54
69	Calculated stretching overtone levels and Darlingâ€“Dennison resonances in water: a triumph of simple theoretical approaches. Molecular Physics, 2007, 105, 2659-2666.	0.8	54
70	Chirped-pulse millimeter-wave spectroscopy for dynamics and kinetics studies of pyrolysis reactions. Physical Chemistry Chemical Physics, 2014, 16, 15739-15751.	1.3	54
71	The vibronic level structure of the cyclopentadienyl radical. Journal of Chemical Physics, 2008, 129, 084310.	1.2	52
72	Equilibrium geometries of cyclic SiC3 isomers. Journal of Chemical Physics, 2001, 114, 2993-2995.	1.2	50

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73	Perturbative triples correction for the equation-of-motion coupled-cluster wave functions with single and double substitutions for ionized states: Theory, implementation, and examples. Journal of Chemical Physics, 2009, 131, 114112.	1.2	50
74	Electron Affinities, Well Depths, and Vibrational Spectroscopy of cis- and trans-HOCO. Journal of the American Chemical Society, 2011, 133, 19606-19609.	6.6	45
75	Rotational spectroscopy of pyridazine and its isotopologs from 235â€“360â€‰GHz: Equilibrium structure and vibrational satellites. Journal of Chemical Physics, 2013, 139, 224304.	1.2	45
76	Spectroscopic characterization of isomerization transition states. Science, 2015, 350, 1338-1342.	6.0	45
77	Quantitative analysis of Fermi resonances by harmonic derivatives of perturbation theory corrections. Molecular Physics, 2009, 107, 213-222.	0.8	44
78	Towards highly accurate ab initio thermochemistry of larger systems: Benzene. Journal of Chemical Physics, 2011, 135, 044513.	1.2	44
79	A master equation simulation for the â€¢OH + CH3OH reaction. Journal of Chemical Physics, 2019, 150, 084105.	1.2	42
80	Geometric Energy Derivatives at the Complete Basis Set Limit: Application to the Equilibrium Structure and Molecular Force Field of Formaldehyde. Journal of Chemical Theory and Computation, 2018, 14, 1333-1350.	2.3	41
81	Molecular structure determination: Equilibrium structure of pyrimidine (m-C4H4N2) from rotational spectroscopy (r eSE) and high-level ab initio calculation (r) Tj ETQq1 1 0.784314 rgBT /Overlock 2020, 152, 104303.	1.2	41
82	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.	1.2	40
83	Triplet instability in doublet systems. Journal of Chemical Physics, 2004, 121, 7624.	1.2	38
84	Communication: Thermal unimolecular decomposition of syn-CH3CHOO: A kinetic study. Journal of Chemical Physics, 2016, 145, 131102.	1.2	38
85	Exhaustive Product Analysis of Three Benzene Discharges by Microwave Spectroscopy. Journal of Physical Chemistry A, 2020, 124, 5170-5181.	1.1	38
86	Ab Initio Thermal Rate Calculations of HO + HO = O(³P) + H₂O Reaction and Isotopologues. Journal of Physical Chemistry A, 2013, 117, 2678-2686.	1.1	37
87	A refined estimate of the bond length of methane. Molecular Physics, 1999, 97, 841-845.	0.8	36
88	Spectroscopy of the Free Phenalenyl Radical. Journal of the American Chemical Society, 2011, 133, 14554-14557.	6.6	36
89	Discovery of a Missing Link: Detection and Structure of the Elusive Disilicon Carbide Cluster. Journal of Physical Chemistry Letters, 2015, 6, 2107-2111.	2.1	36
90	A coupledâ€cluster study of the ground state of C+3. Journal of Chemical Physics, 1991, 94, 4320-4327.	1.2	35

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91	Interconversion of diborane (4) isomers. Journal of Chemical Physics, 1992, 97, 1211-1216.	1.2	33
92	The Î½₃ Fundamental in NO₃ Has Been Seen Near 1060 cm^{â€“1}, Albeit Some Time Ago. Journal of Physical Chemistry Letters, 2012, 3, 1946-1950.	2.1	33
93	A Steady-State Approximation to the Two-Dimensional Master Equation for Chemical Kinetics Calculations. Journal of Physical Chemistry A, 2015, 119, 7627-7636.	1.1	33
94	Active Thermochemical Tables: The Adiabatic Ionization Energy of Hydrogen Peroxide. Journal of Physical Chemistry A, 2017, 121, 8799-8806.	1.1	33
95	The Cì ƒâ€‰2A2 excited state of NO2: Evidence for a Cs equilibrium structure and a failure of some spin-restricted reference wavefunctions. Journal of Chemical Physics, 1997, 107, 2525-2528.	1.2	32
96	On the HCN â€“ HNC Energy Difference. Journal of Physical Chemistry A, 2015, 119, 10929-10934.	1.1	32
97	Fourth-order vibrational perturbation theory with the Watson Hamiltonian: Report of working equations and preliminary results. Journal of Chemical Physics, 2018, 149, 114102.	1.2	32
98	Precise equilibrium structure determination of hydrazoic acid (HN3) by millimeter-wave spectroscopy. Journal of Chemical Physics, 2015, 143, 104310.	1.2	31
99	Thermal Decomposition of Potential Ester Biofuels. Part I: Methyl Acetate and Methyl Butanoate. Journal of Physical Chemistry A, 2017, 121, 4658-4677.	1.1	31
100	New insights into the Jahnâ€“Teller effect in NO3via the dark Ãƒ2Eâ€³ state. Physica Scripta, 2006, 73, C64-C70.	1.2	29
101	Jet cooled cavity ringdown spectroscopy of the AËœ2Eâ€³â†ŽËœ2A2â€² transition of the NO3 radical. Journal of Chemical Physics, 2015, 142, 184305.	1.2	29
102	Quantitative vibronic coupling calculations: the formyloxyl radical. Theoretical Chemistry Accounts, 2011, 129, 527-543.	0.5	28
103	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.	1.3	27
104	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.	2.1	27
105	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.	1.2	24
106	Accuracy of Coupled Cluster Excited State Potential Energy Surfaces. Journal of Chemical Theory and Computation, 2018, 14, 5859-5869.	2.3	24
107	New vibrational assignments in the Ä€1Au-[Xtilde]1Î£+gelectronic transition of acetylene, C2H2: the vâ€²1frequency. Molecular Physics, 2003, 101, 663-673.	0.8	23
108	Accelerating the convergence of higher-order coupled cluster methods. Journal of Chemical Physics, 2015, 143, 204103.	1.2	23

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109	Rotational spectrum and theoretical structure of the carbene HC4N. Journal of Chemical Physics, 1999, 111, 6750-6754.	1.2	22
110	Theoretical Study of Reaction of Ketene with Water in the Gas Phase: Formation of Acetic Acid?. Journal of Physical Chemistry A, 2013, 117, 10997-11005.	1.1	22
111	Direct measurements of DOCO isomers in the kinetics of OD + CO. Science Advances, 2018, 4, eaao4777.	4.7	22
112	Factors Contributing to the Accuracy of Harmonic Force Field Calculations for Water. Journal of Chemical Theory and Computation, 2007, 3, 1267-1274.	2.3	21
113	Revisitation of Nonorthogonal Spin Adaptation in Coupled Cluster Theory. Journal of Chemical Theory and Computation, 2013, 9, 2567-2572.	2.3	21
114	Block diagonalization of the equation-of-motion coupled cluster effective Hamiltonian: Treatment of diabatic potential constants and triple excitations. Journal of Chemical Physics, 2014, 140, 214112.	1.2	21
115	Communication: The ground electronic state of Si2C: Rovibrational level structure, quantum monodromy, and astrophysical implications. Journal of Chemical Physics, 2015, 142, 231101.	1.2	21
116	Communication: An accurate calculation of the S1 C2H2â€ˆcis-trans isomerization barrier height. Journal of Chemical Physics, 2016, 144, 111102.	1.2	21
117	Isotopic studies of trans- and cis-HOCO using rotational spectroscopy: Formation, chemical bonding, and molecular structures. Journal of Chemical Physics, 2016, 144, 124304.	1.2	21
118	Semiclassical Transition-State Theory Based on Fourth-Order Vibrational Perturbation Theory: The Symmetrical Eckart Barrier. Journal of Physical Chemistry Letters, 2016, 7, 2708-2713.	2.1	21
119	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
120	Is the adiabatic approximation sufficient to account for the post-Bornâ€“Oppenheimer effects on molecular electric dipole moments?. Molecular Physics, 2009, 107, 1153-1159.	0.8	20
121	Unimolecular Reaction of Methyl Isocyanide to Acetonitrile: A High-Level Theoretical Study. Journal of Physical Chemistry Letters, 2018, 9, 2532-2538.	2.1	20
122	Ab initio thermal rate coefficients for H + NH₃ â‡Œ H₂ + NH₂. International Journal of Chemical Kinetics, 2019, 51, 321-328.	1.0	20
123	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.	1.2	20
124	Quantum-state-controlled reactions between molecular radicals and ions. Physical Review A, 2018, 98, .	1.0	19
125	Structures of Diethynyl Sulfide and Bis(phenylethynyl) Sulfide. Journal of Physical Chemistry A, 2002, 106, 12110-12116.	1.1	17
126	Pragmatic Solution for a Fully E,J-Resolved Master Equation. Journal of Physical Chemistry A, 2020, 124, 2907-2918.	1.1	17

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127	Theoretical prediction of magnetic exchange coupling constants from broken-symmetry coupled cluster calculations. Journal of Chemical Physics, 2020, 152, 234115.	1.2	17
128	Equation-of-motion coupled-cluster method with double electron-attaching operators: Theory, implementation, and benchmarks. Journal of Chemical Physics, 2021, 154, 114115.	1.2	17
129	Effects of vibrational averaging on coupled cluster calculations of spinâ€“spin coupling constants for hydrocarbons. Molecular Physics, 2012, 110, 2321-2327.	0.8	16
130	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.	1.1	16
131	The ionisation energy of cyclopentadienone: a photoelectronâ€“photoion coincidence study. Molecular Physics, 2015, 113, 2350-2358.	0.8	16
132	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, .	3.3	16
133	Inner-shell photoionization and core-hole decay of Xe and XeF2. Journal of Chemical Physics, 2015, 142, 224302.	1.2	15
134	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.	1.2	15
135	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.	1.1	15
136	Elaborated thermochemical treatment of HF, CO, N2, and H2O: Insight into HEAT and its extensions. Journal of Chemical Physics, 2021, 155, 184109.	1.2	15
137	Quantum Chemistry Common Driver and Databases (QCDB) and Quantum Chemistry Engine (QCE<scp>ngine</scp>): Automation and interoperability among computational chemistry programs. Journal of Chemical Physics, 2021, 155, 204801.	1.2	15
138	A Highly-Efficient Implementation of the Doktorov Recurrence Equations for Franckâ€“Condon Calculations. Journal of Chemical Theory and Computation, 2016, 12, 728-739.	2.3	14
139	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.	6.6	14
140	Precise equilibrium structure of thiazole (c-C3H3NS) from twenty-four isotopologues. Journal of Chemical Physics, 2021, 155, 054302.	1.2	14
141	Semiclassical transition state theory based on fourth order vibrational perturbation theory: Model system studies beyond symmetric Eckart barrier. Journal of Chemical Physics, 2018, 149, 134109.	1.2	13
142	Quantum-state-specific reaction rate measurements for the photo-induced reaction Ca⁺ + O₂ â†’ CaO⁺ + O. Molecular Physics, 2019, 117, 3036-3042.	0.8	13
143	High-Resolution Photoelectron Spectroscopy of Cryogenically Cooled NO₃Ì…. Journal of Physical Chemistry Letters, 2020, 11, 395-400.	2.1	13
144	Vibronically coupled states: computational considerations and characterisation of vibronic and rovibronic spectroscopic parameters. International Reviews in Physical Chemistry, 2021, 40, 165-298.	0.9	13

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145	A simple quasi-diabatization scheme suitable for spectroscopic problems based on one-electron properties of interacting states. Journal of Chemical Physics, 2016, 144, 054110.	1.2	12
146	Three-Dimensional Master Equation (3DME) Approach. Journal of Physical Chemistry A, 2018, 122, 7757-7767.	1.1	12
147	Gas-phase infrared spectrum of methyl nitrate. Journal of Molecular Spectroscopy, 2008, 251, 384-393.	0.4	11
148	Accurate ab Initio Thermal Rate Constants for Reaction of O(³P) with H₂ and Isotopic Analogues. Journal of Physical Chemistry A, 2014, 118, 4918-4928.	1.1	11
149	Pressure-Dependent Rate Constant Caused by Tunneling Effects: OH + HNO₃ as an Example. Journal of Physical Chemistry Letters, 2020, 11, 3712-3717.	2.1	11
150	Gas-Phase Optical Detection of 3-Ethynylcyclopentenyl: A Resonance-Stabilized C7H7 Radical with an Embedded 1-Vinylpropargyl Chromophore. Journal of the American Chemical Society, 2020, 142, 10400-10411.	6.6	10
151	Semi-Experimental Equilibrium (r_e^{SE}) and Theoretical Structures of Pyridazine (o-C₄H₄N₂). Journal of Physical Chemistry A, 2021, 125, 7976-7987.	1.1	10
152	Investigation of an asymmetric tripleâ€excitation correction for coupledâ€cluster energies. International Journal of Quantum Chemistry, 1998, 70, 601-611.	1.0	10
153	Quantifying the effects of higher order coupling terms on fits using a second order Jahn-Teller Hamiltonian. Journal of Molecular Spectroscopy, 2018, 343, 102-115.	0.4	9
154	Semiclassical transition state theory/master equation kinetics of HO + CO: Performance evaluation. International Journal of Chemical Kinetics, 2020, 52, 1022-1045.	1.0	9
155	Analysis of the potential atmospheric impact of the reaction of N2O with OH. Chemical Physics Letters, 2018, 708, 100-105.	1.2	8
156	Nonadiabatic Investigation of the Electronic Spectroscopy oftrans-1,3-Butadiene. Journal of Physical Chemistry A, 2019, 123, 3255-3271.	1.1	8
157	PAH Growth in Flames and Space: Formation of the Phenalenyl Radical. Journal of Physical Chemistry A, 2022, 126, 101-108.	1.1	8
158	Parallelization Strategy for Large-Scale Vibronic Coupling Calculations. Journal of Physical Chemistry A, 2014, 118, 12059-12068.	1.1	7
159	Simulation of laser excitation spectrum of CH3O and CD3O. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2014, 119, 90-99.	2.0	7
160	Atmospheric Reaction Rate Constants and Kinetic Isotope Effects Computed Using the HEAT Protocol and Semi-Classical Transition State Theory. , 2017, , 403-492.		7
161	Gasâ€Phase Formation of the Disilavinylidene (H 2 SiSi) Transient. Angewandte Chemie, 2017, 129, 1284-1288.	1.6	7
162	First-Principles Calculation of Jahnâ€“Teller Rotational Distortion Parameters. Journal of Physical Chemistry A, 2019, 123, 4990-5004.	1.1	7

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163	Structural Characterization of Phenoxy Radical with Mass-Correlated Broadband Microwave Spectroscopy. Journal of Physical Chemistry Letters, 2019, 10, 2919-2923.	2.1	7
164	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.	2.1	7
165	Directed Gas-Phase Formation of the Germaniumsilylene Butterfly Molecule (Ge(Î¼-H₂)Si). Journal of Physical Chemistry Letters, 2019, 10, 1264-1271.	2.1	6
166	Investigation of an asymmetric triple-excitation correction for coupled-cluster energies. , 1998, 70, 601.		6
167	Detection and structural characterization of nitrosamide H2NNO: A central intermediate in deNOxprocesses. Journal of Chemical Physics, 2017, 147, 134301.	1.2	5
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