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	Atomic isotropic hyperfine properties for first row elements (Bâ€“F) revisited. Journal of Chemical Physics, 2022, 156, 034304.	1.2	3
2	PAH Growth in Flames and Space: Formation of the Phenalenyl Radical. Journal of Physical Chemistry A, 2022, 126, 101-108.	1.1	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.	2.1	7
4	Semi-experimental equilibrium (r eSE) and theoretical structures of hydrazoic acid (HN3). Journal of Chemical Physics, 2022, 157, .	1.2	3
5	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
6	Using isotopologues to probe the potential energy surface of reactions of C2H2++C3H4. Journal of Chemical Physics, 2021, 154, 124310.	1.2	4
7	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
8	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
9	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
10	Why the CC Stretch in HCC Is So Anharmonic. Journal of Physical Chemistry A, 2021, 125, 7694-7698.	1.1	1
11	Precise equilibrium structure of thiazole (c-C3H3NS) from twenty-four isotopologues. Journal of Chemical Physics, 2021, 155, 054302.	1.2	14
12	Thermal Decomposition of CH3O: A Curious Case of Pressure-Dependent Tunneling Effects. Journal of Physical Chemistry A, 2021, 125, 6761-6771.	1.1	0
13	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
14	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
15	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
16	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
17	High-Resolution Photoelectron Spectroscopy of Cryogenically Cooled NO₃Ì…. Journal of Physical Chemistry Letters, 2020, 11, 395-400.	2.1	13
18	Semiclassical transition state theory/master equation kinetics of HO + CO: Performance evaluation. International Journal of Chemical Kinetics, 2020, 52, 1022-1045.	1.0	9

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19	Reaction of N2O with the prototype singlet biradical CH2: A theoretical study. Chemical Physics Letters, 2020, 749, 137446.	1.2	2
20	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
21	Exhaustive Product Analysis of Three Benzene Discharges by Microwave Spectroscopy. Journal of Physical Chemistry A, 2020, 124, 5170-5181.	1.1	38
22	Coupled-cluster techniques for computational chemistry: The <scp>CFOUR</scp> program package. Journal of Chemical Physics, 2020, 152, 214108.	1.2	375
23	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
24	Pragmatic Solution for a Fully E,J-Resolved Master Equation. Journal of Physical Chemistry A, 2020, 124, 2907-2918.	1.1	17
25	Theoretical prediction of magnetic exchange coupling constants from broken-symmetry coupled cluster calculations. Journal of Chemical Physics, 2020, 152, 234115.	1.2	17
26	Hartree-Fock instabilities and the diagonal Born-Oppenheimer correction. Molecular Physics, 2020, 118, e1742936.	0.8	3
27	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
28	The atmospheric impact of the reaction of N2O with NO3: A theoretical study. Chemical Physics Letters, 2019, 731, 136605.	1.2	4
29	Ab initio thermal rate coefficients for H + NH₃ â‡Œ H₂ + NH₂. International Journal of Chemical Kinetics, 2019, 51, 321-328.	1.0	20
30	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
31	High-accuracy extrapolated ab initio thermochemistry. IV. A modified recipe for computational efficiency. Journal of Chemical Physics, 2019, 150, 224102.	1.2	58
32	First-Principles Calculation of Jahnâ€“Teller Rotational Distortion Parameters. Journal of Physical Chemistry A, 2019, 123, 4990-5004.	1.1	7
33	Structural Characterization of Phenoxy Radical with Mass-Correlated Broadband Microwave Spectroscopy. Journal of Physical Chemistry Letters, 2019, 10, 2919-2923.	2.1	7
34	Nonadiabatic Investigation of the Electronic Spectroscopy oftrans-1,3-Butadiene. Journal of Physical Chemistry A, 2019, 123, 3255-3271.	1.1	8
35	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
36	A master equation simulation for the â€¢OH + CH3OH reaction. Journal of Chemical Physics, 2019, 150, 084105.	1.2	42

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37	Diagrams in coupled-cluster theory: Algebraic derivation of a new diagrammatic method for closed shells. , 2019, , 327-375.		3
38	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
39	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
40	Direct measurements of DOCO isomers in the kinetics of OD + CO. Science Advances, 2018, 4, eaao4777.	4.7	22
41	Unimolecular Reaction of Methyl Isocyanide to Acetonitrile: A High-Level Theoretical Study. Journal of Physical Chemistry Letters, 2018, 9, 2532-2538.	2.1	20
42	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
43	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
44	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
45	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
46	Accuracy of Coupled Cluster Excited State Potential Energy Surfaces. Journal of Chemical Theory and Computation, 2018, 14, 5859-5869.	2.3	24
47	Quantum-state-controlled reactions between molecular radicals and ions. Physical Review A, 2018, 98, .	1.0	19
48	Three-Dimensional Master Equation (3DME) Approach. Journal of Physical Chemistry A, 2018, 122, 7757-7767.	1.1	12
49	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
50	Analysis of the potential atmospheric impact of the reaction of N2O with OH. Chemical Physics Letters, 2018, 708, 100-105.	1.2	8
51	Atmospheric Reaction Rate Constants and Kinetic Isotope Effects Computed Using the HEAT Protocol and Semi-Classical Transition State Theory. , 2017, , 403-492.		7
52	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
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.	1.2	15
54	Gasâ€Phase Formation of the Disilavinylidene (H 2 SiSi) Transient. Angewandte Chemie, 2017, 129, 1284-1288.	1.6	7

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56	Active Thermochemical Tables: The Adiabatic Ionization Energy of Hydrogen Peroxide. Journal of Physical Chemistry A, 2017, 121, 8799-8806.	1.1	33
57	Oxygen-18 Isotopic Studies of HOOO and DOOO. Journal of Physical Chemistry A, 2017, 121, 6296-6303.	1.1	4
58	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
59	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
60	Communication: Thermal unimolecular decomposition of syn-CH3CHOO: A kinetic study. Journal of Chemical Physics, 2016, 145, 131102.	1.2	38
61	Communication: An accurate calculation of the S1 C2H2â€ˆcis-trans isomerization barrier height. Journal of Chemical Physics, 2016, 144, 111102.	1.2	21
62	A new approach to approximate equation-of-motion coupled cluster with triple excitations. Journal of Chemical Physics, 2016, 145, 124102.	1.2	70
63	Cation States of Ethane: HEAT Calculations and Vibronic Simulations of the Photoelectron Spectrum of Ethane. Journal of Physical Chemistry A, 2016, 120, 7548-7553.	1.1	4
64	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
65	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
66	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
67	Precise equilibrium structure determination of hydrazoic acid (HN3) by millimeter-wave spectroscopy. Journal of Chemical Physics, 2015, 143, 104310.	1.2	31
68	Accelerating the convergence of higher-order coupled cluster methods. Journal of Chemical Physics, 2015, 143, 204103.	1.2	23
69	Heavy atom vibrational modes and low-energy vibrational autodetachment in nitromethane anions. Journal of Chemical Physics, 2015, 142, 234304.	1.2	2
70	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
71	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
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74	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
75	The ionisation energy of cyclopentadienone: a photoelectronâ€“photoion coincidence study. Molecular Physics, 2015, 113, 2350-2358.	0.8	16
76	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
77	On the HCN â€“ HNC Energy Difference. Journal of Physical Chemistry A, 2015, 119, 10929-10934.	1.1	32
78	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
79	Jet cooled cavity ringdown spectroscopy of the AËœ2Eâ€³â†XËœ2A2â€² transition of the NO3 radical. Journal of Chemical Physics, 2015, 142, 184305.	1.2	29
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81	The permanent electric dipole moment of gold chloride, AuCl. Molecular Physics, 2015, 113, 2073-2080.	0.8	3
82	Chirped-pulse millimeter-wave spectroscopy for dynamics and kinetics studies of pyrolysis reactions. Physical Chemistry Chemical Physics, 2014, 16, 15739-15751.	1.3	54
83	Parallelization Strategy for Large-Scale Vibronic Coupling Calculations. Journal of Physical Chemistry A, 2014, 118, 12059-12068.	1.1	7
84	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
85	Scientific Achievements of Rodney J. Bartlett. Molecular Physics, 2014, 112, 560-561.	0.8	0
86	Introduction to proceedings of Molecular Quantum Mechanics 2013: electron correlation: theÂmany-body problem at the heart of chemistry. Molecular Physics, 2014, 112, 557-558.	0.8	0
87	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
88	Simulation of laser excitation spectrum of CH3O and CD3O. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2014, 119, 90-99.	2.0	7
89	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
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93	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
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96	Effects of vibrational averaging on coupled cluster calculations of spinâ€“spin coupling constants for hydrocarbons. Molecular Physics, 2012, 110, 2321-2327.	0.8	16
97	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
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99	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
100	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
101	Spectroscopy of the Free Phenalenyl Radical. Journal of the American Chemical Society, 2011, 133, 14554-14557.	6.6	36
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104	A practical implementation of semi-classical transition state theory for polyatomics. Chemical Physics Letters, 2010, 499, 9-15.	1.2	92
105	Quantum-chemical calculation of spectroscopic parameters for rotational spectroscopy. International Reviews in Physical Chemistry, 2010, 29, 273-367.	0.9	288
106	Quantitative analysis of Fermi resonances by harmonic derivatives of perturbation theory corrections. Molecular Physics, 2009, 107, 213-222.	0.8	44
107	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
108	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

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111	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
112	Gas-phase infrared spectrum of methyl nitrate. Journal of Molecular Spectroscopy, 2008, 251, 384-393.	0.4	11
113	The vibronic level structure of the cyclopentadienyl radical. Journal of Chemical Physics, 2008, 129, 084310.	1.2	52
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115	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
116	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
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119	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
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121	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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124	Coupled-cluster methods including noniterative corrections for quadruple excitations. Journal of Chemical Physics, 2005, 123, 054101.	1.2	344
125	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
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136	Molecular equilibrium structures from experimental rotational constants and calculated vibrationâ€"rotation interaction constants. Journal of Chemical Physics, 2002, 116, 6482-6496.	1.2	245
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