John F Stanton

List of Publications by Citations

155 papers	10,643 citations	48 h-index	101 g-index
163 ext. papers	11,521 ext. citations	4.4 avg, IF	6.41 L-index

#	Paper	IF	Citations
155	The equation of motion coupled-cluster method. A systematic biorthogonal approach to molecular excitation energies, transition probabilities, and excited state properties. *Journal of Chemical Physics*, **1993**, 98, 7029-7039	3.9	1895
154	HEAT: High accuracy extrapolated ab initio thermochemistry. *Journal of Chemical Physics*, **2004**, 121, 11599-613	3.9	606
153	The ACES II program system. *International Journal of Quantum Chemistry*, **1992**, 44, 879-894	2.1	390
152	Perturbative treatment of triple excitations in coupled-cluster calculations of nuclear magnetic shielding constants. *Journal of Chemical Physics*, **1996**, 104, 2574-2583	3.9	323
151	The accurate determination of molecular equilibrium structures. *Journal of Chemical Physics*, **2001**, 114, 6548-6556	3.9	322
150	High-accuracy extrapolated ab initio thermochemistry. III. Additional improvements and overview. *Journal of Chemical Physics*, **2008**, 128, 114111	3.9	315
149	High-accuracy extrapolated ab initio thermochemistry. II. Minor improvements to the protocol and a vital simplification. *Journal of Chemical Physics*, **2006**, 125, 64108	3.9	277
148	IUPAC Critical Evaluation of Thermochemical Properties of Selected Radicals. Part I. *Journal of Physical and Chemical Reference Data*, **2005**, 34, 573-656	4.3	275
147	Quantum-chemical calculation of spectroscopic parameters for rotational spectroscopy. *International Reviews in Physical Chemistry*, **2010**, 29, 273-367	7	237
146	Coupled-cluster calculations of nuclear magnetic resonance chemical shifts. *Journal of Chemical Physics*, **1995**, 103, 3561-3577	3.9	233
145	Applications of Post-Hartree□ock Methods: A Tutorial. *Reviews in Computational Chemistry*, **2007**, 65-169		230
144	Quantitative prediction of gas-phase 13C nuclear magnetic shielding constants. *Journal of Chemical Physics*, **2003**, 118, 10407-10417	3.9	229
143	Coupled-cluster open-shell analytic gradients: Implementation of the direct product decomposition approach in energy gradient calculations. *Journal of Chemical Physics*, **1991**, 95, 2623-2638	3.9	229
142	Molecular equilibrium structures from experimental rotational constants and calculated vibration□otation interaction constants. *Journal of Chemical Physics*, **2002**, 116, 6482-6496	3.9	222
141	A direct product decomposition approach for symmetry exploitation in many-body methods. I. Energy calculations. *Journal of Chemical Physics*, **1991**, 94, 4334-4345	3.9	220
140	Gauge-invariant calculation of nuclear magnetic shielding constants at the coupled□luster singles and doubles level. *Journal of Chemical Physics*, **1995**, 102, 251-253	3.9	189
139	On the extent of spin contamination in open-shell coupled-cluster wave functions. *Journal of Chemical Physics*, **1994**, 101, 371-374	3.9	184

138	The Equilibrium Structure of Benzene. *Journal of Physical Chemistry A*, **2000**, 104, 2865-2868	2.8	164
137	Many-body methods for excited state potential energy surfaces. I. General theory of energy gradients for the equation-of-motion coupled-cluster method. *Journal of Chemical Physics*, **1993**, 99, 8840-8847	3.9	160
136	Coupled-cluster techniques for computational chemistry: The CFOUR program package. *Journal of Chemical Physics*, **2020**, 152, 214108	3.9	156
135	On the choice of orbitals for symmetry breaking problems with application to NO3. *Journal of Chemical Physics*, **1992**, 97, 5554-5559	3.9	150
134	On the vibronic level structure in the NO3 radical. I. The ground electronic state. *Journal of Chemical Physics*, **2007**, 126, 134309	3.9	127
133	Structures, Automerizations, and Isomerizations of C3H2Isomers. *Journal of the American Chemical Society*, **1997**, 119, 5847-5856	16.4	126
132	Simple(r) algebraic equation for transition moments of fundamental transitions in vibrational second-order perturbation theory. *Molecular Physics*, **2006**, 104, 377-388	1.7	114
131	Photoelectron wave function in photoionization: plane wave or Coulomb wave?. *Journal of Physical Chemistry Letters*, **2015**, 6, 4532-40	6.4	97
130	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	1.9	97
129	A coupled-cluster based effective Hamiltonian method for dynamic electric polarizabilities. *Journal of Chemical Physics*, **1993**, 99, 5178-5183	3.9	95
128	Analytic evaluation of energy gradients at the coupled-cluster singles and doubles level using quasi-restricted Hartree□Fock open-shell reference functions. *Journal of Chemical Physics*, **1991**, 95, 2639-2645	3.9	90
127	Highly correlated single-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	3.9	87
126	The Simplest Criegee Intermediate (H2C?OO): Isotopic Spectroscopy, Equilibrium Structure, and Possible Formation from Atmospheric Lightning. *Journal of Physical Chemistry Letters*, **2013**, 4, 4133-4139	6.4	83
125	Analytic gradients for the coupled-cluster singles, doubles, and triples (CCSDT) model. *Journal of Chemical Physics*, **2002**, 116, 1773-1782	3.9	77
124	Linear and cyclic isomers of C4. A theoretical study with coupled-cluster methods and large basis sets. *Journal of Chemical Physics*, **1992**, 97, 8372-8381	3.9	75
123	Treatment of Fermi resonance effects on transition moments in vibrational perturbation theory. *Molecular Physics*, **2007**, 105, 101-109	1.7	65
122	Restricted open-shell Hartree□Fock-based many-body perturbation theory: Theory and application of energy and gradient calculations. *Journal of Chemical Physics*, **1992**, 97, 6606-6620	3.9	65
121	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, 5524-33	2.8	64

120	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		62
119	On the vibronic level structure in the NO3 radical: II. Adiabatic calculation of the infrared spectrum. *Molecular Physics*, **2009**, 107, 1059-1075	1.7	61
118	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	6.4	60
117	Correlated studies of infrared intensities. *Journal of Chemical Physics*, **1989**, 90, 3241-3249	3.9	57
116	Quantifying Hydrogen-Bond Populations in Dimethyl Sulfoxide/Water Mixtures. *Angewandte Chemie - International Edition*, **2017**, 56, 11375-11379	16.4	56
115	Electron-Correlated Approaches for the Calculation of NMR Chemical Shifts. *Advances in Chemical Physics*, **2003**, 355-422		55
114	Potential nonrigidity of the NO3 radical. *Journal of Chemical Physics*, **1991**, 94, 4084-4087	3.9	55
113	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	3.9	54
112	Spontaneous and Selective Formation of HSNO, a Crucial Intermediate Linking H2S and Nitroso Chemistries. *Journal of the American Chemical Society*, **2016**, 138, 11441-4	16.4	53
111	Non-orthogonal spin-adaptation of coupled cluster methods: A new implementation of methods including quadruple excitations. *Journal of Chemical Physics*, **2015**, 142, 064108	3.9	51
110	Analytic first and second derivatives for the CCSDT-n (n=1□) models: a first step towards the efficient calculation of CCSDT properties. *Physical Chemistry Chemical Physics*, **2000**, 2, 2047-2060	3.6	50
109	Does chlorine peroxide exhibit a strong ultraviolet absorption near 250 nm?. *Journal of Chemical Physics*, **1993**, 98, 9335-9339	3.9	50
108	A new approach to approximate equation-of-motion coupled cluster with triple excitations. *Journal of Chemical Physics*, **2016**, 145, 124102	3.9	49
107	A Discussion of Some Problems Associated with the Quantum Mechanical Treatment of Open-Shell Molecules. *Advances in Chemical Physics*, **2003**, 101-146		47
106	Chirped-Pulse millimeter-Wave spectroscopy for dynamics and kinetics studies of pyrolysis reactions. *Physical Chemistry Chemical Physics*, **2014**, 16, 15739-15751	3.6	43
105	Anharmonic force fields from analytic CCSD(T) second derivatives: HOF and F2O. *Journal of Chemical Physics*, **1999**, 110, 3687-3696	3.9	43
104	Quantitative analysis of Fermi resonances by harmonic derivatives of perturbation theory corrections. *Molecular Physics*, **2009**, 107, 213-222	1.7	41
103	Towards highly accurate ab initio thermochemistry of larger systems: benzene. *Journal of Chemical Physics*, **2011**, 135, 044513	3.9	40

102	Harmonic vibrational frequencies and infrared intensities from analytic fourth-order many-body perturbation theory gradients. *Journal of Chemical Physics*, **1991**, 94, 404-413	3.9	39
101	High-accuracy extrapolated ab initio thermochemistry of the propargyl radical and the singlet C(3)H(2) carbenes. *Journal of Physical Chemistry A*, **2009**, 113, 12447-53	2.8	37
100	Analytic ROHF/MBPT(2) second derivatives. *Journal of Chemical Physics*, **1992**, 97, 7825-7828	3.9	37
99	Rotational spectroscopy of pyridazine and its isotopologs from 235-360 GHz: equilibrium structure and vibrational satellites. *Journal of Chemical Physics*, **2013**, 139, 224304	3.9	34
98	The Molecular Structure of gauche-1,3-Butadiene: Experimental Establishment of Non-planarity. *Angewandte Chemie - International Edition*, **2018**, 57, 1821-1825	16.4	34
97	Separability properties of reduced and effective density matrices in the equation-of-motion coupled cluster method. *Journal of Chemical Physics*, **1994**, 101, 8928-8937	3.9	33
96	Ab initio determination of the heat of formation of ketenyl (HCCO) and ethynyl (CCH) radicals. *Molecular Physics*, **2005**, 103, 2159-2168	1.7	32
95	A coupled-cluster study of the ground state of C+3. *Journal of Chemical Physics*, **1991**, 94, 4320-4327	3.9	32
94	Communication: Thermal unimolecular decomposition of syn-CHCHOO: A kinetic study. *Journal of Chemical Physics*, **2016**, 145, 131102	3.9	32
93	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	3.9	28
92	Discovery of a Missing Link: Detection and Structure of the Elusive Disilicon Carbide Cluster. *Journal of Physical Chemistry Letters*, **2015**, 6, 2107-11	6.4	28
91	Quantitative vibronic coupling calculations: the formyloxyl radical. *Theoretical Chemistry Accounts*, **2011**, 129, 527-543	1.9	27
90	Thermal Decomposition of Potential Ester Biofuels. Part I: Methyl Acetate and Methyl Butanoate. *Journal of Physical Chemistry A*, **2017**, 121, 4658-4677	2.8	26
89	On the HCN - HNC Energy Difference. *Journal of Physical Chemistry A*, **2015**, 119, 10929-34	2.8	26
88	Jet cooled cavity ringdown spectroscopy of the □(2)E(?)<-X(2)A2 (0)transition of the NO3 radical. *Journal of Chemical Physics*, **2015**, 142, 184305	3.9	26
87	A master equation simulation for the OH + CHOH reaction. *Journal of Chemical Physics*, **2019**, 150, 084105	3.9	26
86	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, 4742-4	3.6	25
85	Structural and Thermodynamic Analysis of a Three-Component Assembly Forming ortho-Iminophenylboronate Esters. *Journal of Organic Chemistry*, **2016**, 81, 8319-30	4.2	23

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, 2201-7	6.4	23
83	Electron-Correlated Methods for the Calculation of NMR Chemical Shifts **2004**, 123-139		23
82	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	2.8	23
81	A Steady-State Approximation to the Two-Dimensional Master Equation for Chemical Kinetics Calculations. *Journal of Physical Chemistry A*, **2015**, 119, 7627-36	2.8	22
80	Photoelectron Spectroscopy of the Methide Anion: Electron Affinities of ^{1}CH3 and ^{1}CD3 and Inversion Splittings of CH3(-) and CD3(-). *Journal of the American Chemical Society*, **2015**, 137, 12939-45	16.4	22
79	An unusually large nonadiabatic error in the BNB molecule. *Journal of Chemical Physics*, **2010**, 133, 174309	3.9	22
78	The global minimum structure of SiC3: The controversy continues. *Journal of Chemical Physics*, **2002**, 116, 9151-9153	3.9	22
77	Active Thermochemical Tables: The Adiabatic Ionization Energy of Hydrogen Peroxide. *Journal of Physical Chemistry A*, **2017**, 121, 8799-8806	2.8	21
76	Pyrolysis of Cyclopentadienone: Mechanistic Insights from a Direct Measurement of Product Branching Ratios. *Journal of Physical Chemistry A*, **2015**, 119, 7222-34	2.8	21
75	Precise equilibrium structure determination of hydrazoic acid (HN3) by millimeter-wave spectroscopy. *Journal of Chemical Physics*, **2015**, 143, 104310	3.9	20
74	Factors Contributing to the Accuracy of Harmonic Force Field Calculations for Water. *Journal of Chemical Theory and Computation*, **2007**, 3, 1267-74	6.4	19
73	Accuracy of Coupled Cluster Excited State Potential Energy Surfaces. *Journal of Chemical Theory and Computation*, **2018**, 14, 5859-5869	6.4	19
72	Direct measurements of DOCO isomers in the kinetics of OD + CO. *Science Advances*, **2018**, 4, eaao4777	14.3	18
71	Unimolecular Reaction of Methyl Isocyanide to Acetonitrile: A High-Level Theoretical Study. *Journal of Physical Chemistry Letters*, **2018**, 9, 2532-2538	6.4	18
70	Semiclassical Transition-State Theory Based on Fourth-Order Vibrational Perturbation Theory: The Symmetrical Eckart Barrier. *Journal of Physical Chemistry Letters*, **2016**, 7, 2708-13	6.4	18
69	Revisitation of Nonorthogonal Spin Adaptation in Coupled Cluster Theory. *Journal of Chemical Theory and Computation*, **2013**, 9, 2567-72	6.4	18
68	Vibrational Energy Levels via Finite-Basis Calculations Using a Quasi-Analytic Form of the Kinetic Energy. *Journal of Chemical Theory and Computation*, **2011**, 7, 1428-42	6.4	18
67	Exhaustive Product Analysis of Three Benzene Discharges by Microwave Spectroscopy. *Journal of Physical Chemistry A*, **2020**, 124, 5170-5181	2.8	17

66	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	3.9	17
65	Ground and low-lying excited states of propadienylidene (H2C=C=C:) obtained by negative ion photoelectron spectroscopy. *Journal of Chemical Physics*, **2012**, 136, 134312	3.9	17
64	Molecular structure determination: Equilibrium structure of pyrimidine (m-CHN) from rotational spectroscopy (r) and high-level ab initio calculation (r) agree within the uncertainty of experimental measurement. *Journal of Chemical Physics*, **2020**, 152, 104303	3.9	16
63	Communication: The ground electronic state of Si2C: Rovibrational level structure, quantum monodromy, and astrophysical implications. *Journal of Chemical Physics*, **2015**, 142, 231101	3.9	16
62	Laser spectroscopy of Si3C. *Journal of Chemical Physics*, **2005**, 122, 124314	3.9	16
61	On the equilibrium bond length of ammonia in the first excited singlet state. *Journal of Chemical Physics*, **1995**, 102, 1096-1097	3.9	16
60	Quantum-state-controlled reactions between molecular radicals and ions. *Physical Review A*, **2018**, 98,	2.6	16
59	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, 7197-204	2.8	15
58	Analytic Evaluation of Second Derivatives of the Energy: Computational Strategies for the CCSD and CCSD(T) Approximations. *Recent Advances in Computational*, **1997**, 49-79		15
57	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		15
56	Point group symmetry and cartesian force constant redundancy. *International Journal of Quantum Chemistry*, **1991**, 39, 19-29	2.1	15
55	Quantifying Hydrogen-Bond Populations in Dimethyl Sulfoxide/Water Mixtures. *Angewandte Chemie*, **2017**, 129, 11533-11537	3.6	14
54	The ionisation energy of cyclopentadienone: a photoelectron–photoion coincidence study. *Molecular Physics*, **2015**, 113, 2350-2358	1.7	14
53	Barrier to Methyl Internal Rotation of Cis- and Trans-2-Methylvinoxy Radicals in the X (2A″) and B (2A′) States: Experiment and Theory. *Journal of Physical Chemistry A*, **2000**, 104, 9906-9913	2.8	14
52	Quantitative vibronic coupling calculations. The visible spectrum of propadienylidene. *Faraday Discussions*, **2011**, 150, 331-43; discussion 391-418	3.6	13
51	Structure, energetics, and vibrational spectra of beryllium borohydride isomers. *Journal of Chemical Physics*, **1988**, 88, 5726-5734	3.9	13
50	Low-lying vibronic level structure of the ground state of the methoxy radical: Slow electron velocity-map imaging (SEVI) spectra and Köppel-Domcke-Cederbaum (KDC) vibronic Hamiltonian calculations. *Journal of Chemical Physics*, **2017**, 146, 224309	3.9	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	2.8	12

48	Gas-Phase Formation of the Disilavinylidene (H SiSi) Transient. *Angewandte Chemie - International Edition*, **2017**, 56, 1264-1268	16.4	11
47	Ab initio thermal rate coefficients for H + NH3 ? H2 + NH2. *International Journal of Chemical Kinetics* , **2019**, 51, 321-328	1.4	11
46	The equilibrium structure of the ammonium radical Rydberg ground state. *Journal of Chemical Physics*, **2001**, 114, 9863-9865	3.9	11
45	Electron-Withdrawing Effects in the Photodissociation of CHICl To Form CHCl Radical, Simultaneously Viewed Through the Carbon K and Chlorine L X-ray Edges. *Journal of the American Chemical Society*, **2018**, 140, 13360-13366	16.4	11
44	A Highly-Efficient Implementation of the Doktorov Recurrence Equations for Franck-Condon Calculations. *Journal of Chemical Theory and Computation*, **2016**, 12, 728-39	6.4	10
43	Isomerization and Fragmentation of Cyclohexanone in a Heated Micro-Reactor. *Journal of Physical Chemistry A*, **2015**, 119, 12635-47	2.8	10
42	The gas-phase structure of the asymmetric, trans-dinitrogen tetroxide (NO), formed by dimerization of nitrogen dioxide (NO), from rotational spectroscopy and ab initio quantum chemistry. *Journal of Chemical Physics*, **2017**, 146, 134305	3.9	9
41	Quantum-state-specific reaction rate measurements for the photo-induced reaction Ca+ + O2 -o CaO+ + O. *Molecular Physics*, **2019**, 117, 3036-3042	1.7	9
40	Spectroscopy of Ethylenedione and Ethynediolide: A Reinvestigation. *Angewandte Chemie - International Edition*, **2018**, 57, 5394-5397	16.4	9
39	Reduced dimension rovibrational variational calculations of the S(1) state of C2H2. II. The S(1) rovibrational manifold and the effects of isomerization. *Journal of Chemical Physics*, **2014**, 140, 024313	3.9	9
38	Communication: Helium nanodroplet isolation and rovibrational spectroscopy of hydroxymethylene. *Journal of Chemical Physics*, **2014**, 140, 171102	3.9	9
37	Equation-of-motion coupled-cluster method with double electron-attaching operators: Theory, implementation, and benchmarks. *Journal of Chemical Physics*, **2021**, 154, 114115	3.9	9
36	Relativistic coupled-cluster calculations on XeF6: Delicate interplay between electron-correlation and basis-set effects. *Journal of Chemical Physics*, **2015**, 142, 224309	3.9	8
35	High-Resolution Photoelectron Spectroscopy of Cryogenically Cooled NO . *Journal of Physical Chemistry Letters*, **2020**, 11, 395-400	6.4	8
34	Pyrolysis of the Simplest Carbohydrate, Glycolaldehyde (CHO-CH2OH), and Glyoxal in a Heated Microreactor. *Journal of Physical Chemistry A*, **2016**, 120, 2161-72	2.8	8
33	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	3.5	8
32	Pragmatic Solution for a Fully ,-Resolved Master Equation. *Journal of Physical Chemistry A*, **2020**, 124, 2907-2918	2.8	7
31	The Molecular Structure of gauche-1,3-Butadiene: Experimental Establishment of Non-planarity. *Angewandte Chemie*, **2018**, 130, 1839-1843	3.6	7

30	Spectroscopy of Ethylenedione and Ethynediolide: A Reinvestigation. *Angewandte Chemie*, **2018**, 130, 5492-5495	3.6	7
29	Equilibrium structure of LiCCH. *International Journal of Quantum Chemistry*, **2000**, 77, 305-310	2.1	7
28	Three-Dimensional Master Equation (3DME) Approach. *Journal of Physical Chemistry A*, **2018**, 122, 7757-7767	2.8	7
27	First-Principles Calculation of Jahn-Teller Rotational Distortion Parameters. *Journal of Physical Chemistry A*, **2019**, 123, 4990-5004	2.8	6
26	Structural Characterization of Phenoxy Radical with Mass-Correlated Broadband Microwave Spectroscopy. *Journal of Physical Chemistry Letters*, **2019**, 10, 2919-2923	6.4	6
25	Reactive intermediates in (4)He nanodroplets: infrared laser Stark spectroscopy of dihydroxycarbene. *Journal of Chemical Physics*, **2015**, 142, 144309	3.9	6
24	Computation of quadratic electric dipole moment functions. *Journal of Chemical Physics*, **1988**, 88, 7650-7652	3.9	6
23	Pressure-Dependent Rate Constant Caused by Tunneling Effects: OH + HNO as an Example. *Journal of Physical Chemistry Letters*, **2020**, 11, 3712-3717	6.4	5
22	Coupled-cluster studies of singlet propynylidene. *Molecular Physics*, **1999**, 96, 505-509	1.7	5
21	Semiclassical transition state theory/master equation kinetics of HO + CO: Performance evaluation. *International Journal of Chemical Kinetics*, **2020**, 52, 1022-1045	1.4	5
20	Vibronically coupled states: computational considerations and characterisation of vibronic and rovibronic spectroscopic parameters. *International Reviews in Physical Chemistry*, **2021**, 40, 165-298	7	5
19	Precise equilibrium structure determination of thiophene (c-CHS) by rotational spectroscopy-Structure of a five-membered heterocycle containing a third-row atom. *Journal of Chemical Physics*, **2021**, 154, 244310	3.9	5
18	Spectral analyses of trans- and cis-DOCO transients via comb spectroscopy. *Molecular Physics*, **2018**, 116, 3710-3717	1.7	5
17	The Hunt for Elusive Molecules: Insights from Joint Theoretical and Experimental Investigations. *Chemistry - A European Journal*, **2019**, 25, 7243-7258	4.8	4
16	Theoretical prediction of magnetic exchange coupling constants from broken-symmetry coupled cluster calculations. *Journal of Chemical Physics*, **2020**, 152, 234115	3.9	4
15	An Accurate Molecular Structure of Phenyl, the Simplest Aryl Radical. *Angewandte Chemie*, **2015**, 127, 1828-1831	3.6	4
14	A simple correction to final state energies of doublet radicals described by equation-of-motion coupled cluster theory in the singles and doubles approximation **1996**, 93, 303		4
13	Directed Gas-Phase Formation of the Germaniumsilylene Butterfly Molecule (Ge(□H)Si). *Journal of Physical Chemistry Letters*, **2019**, 10, 1264-1271	6.4	4

12	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,	11.5	3
11	Atomic isotropic hyperfine properties for first row elements (B-F) revisited.. *Journal of Chemical Physics*, **2022**, 156, 034304	3.9	2
10	Precise equilibrium structure of thiazole (c-CHNS) from twenty-four isotopologues. *Journal of Chemical Physics*, **2021**, 155, 054302	3.9	2
9	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) **1997**, 95, 97		1
8	Using isotopologues to probe the potential energy surface of reactions of CH +CH. *Journal of Chemical Physics*, **2021**, 154, 124310	3.9	1
7	Semi-Experimental Equilibrium () and Theoretical Structures of Pyridazine (-CHN). *Journal of Physical Chemistry A*, **2021**, 125, 7976-7987	2.8	0
6	Probing the Exit Channel of the OH + CHOH -ϕHO + CHO Reaction by Photodetachment of CHO(HO).. *Journal of Physical Chemistry Letters*, **2021**, 142-148	6.4	0
5	A VSEPR-inspired force field for determining molecular properties of PF5. *Molecular Physics*, **2019**, 117, 1344-1350	1.7	
4	Innentitelbild: Spectroscopy of Ethylenedione and Ethynediolide: A Reinvestigation (Angew. Chem. 19/2018). *Angewandte Chemie*, **2018**, 130, 5276-5276	3.6	
3	Titelbild: Quantifying Hydrogen-Bond Populations in Dimethyl Sulfoxide/Water Mixtures (Angew. Chem. 38/2017). *Angewandte Chemie*, **2017**, 129, 11429-11429	3.6	
2	Equilibrium Structure of the Silicon Trimer. *ACS Symposium Series*, **2007**, 193-200	0.4	
1	Thermal Decomposition of CHO: A Curious Case of Pressure-Dependent Tunneling Effects. *Journal of Physical Chemistry A*, **2021**, 125, 6761-6771	2.8	