# John F Stanton

List of Publications by Year
in descending order



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|---|---|---|---|
| 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 | 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 |
| 2 | HEAT: High accuracy extrapolatedab initiothermochemistry. Journal of Chemical Physics, 2004, 121, 11599-11613. | 3.0 | 691 |
| 3 | The ACES II program system. International Journal of Quantum Chemistry, 1992, 44, 879-894. | 2.0 | 404 |
| 4 | Coupled-cluster techniques for computational chemistry: The <scp>CFOUR</scp> program package. Journal of Chemical Physics, 2020, 152, 214108. | 3.0 | 375 |
| 5 | High-accuracy extrapolated ab initio thermochemistry. III. Additional improvements and overview. Journal of Chemical Physics, 2008, 128, 114111. | 3.0 | 367 |
| 6 | 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 |
| 7 | The accurate determination of molecular equilibrium structures. Journal of Chemical Physics, 2001, 114, 6548-6556. | 3.0 | 353 |
| 8 | 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 |
| 9 | Quantum-chemical calculation of spectroscopic parameters for rotational spectroscopy. International Reviews in Physical Chemistry, 2010, 29, 273-367. | 2.3 | 288 |
| 10 | 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 |
| 11 | Applications of Post-Hartree-Fock Methods: A Tutorial. Reviews in Computational Chemistry, 2007, , 65-169. | 1.5 | 273 |
| 12 | Coupledâ€cluster calculations of nuclear magnetic resonance chemical shifts. Journal of Chemical Physics, 1995, 103, 3561-3577. | 3.0 | 257 |
| 13 | 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 |
| 14 | 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 |
| 15 | Quantitative prediction of gas-phase 13C nuclear magnetic shielding constants. Journal of Chemical Physics, 2003, 118, 10407-10417. | 3.0 | 246 |
| 16 | Molecular equilibrium structures from experimental rotational constants and calculated vibrationâ€“rotation interaction constants. Journal of Chemical Physics, 2002, 116, 6482-6496. | 3.0 | 245 |
| 17 | On the extent of spin contamination in openâ€shell coupledâ€cluster wave functions. Journal of Chemical Physics, 1994, 101, 371-374. | 3.0 | 205 |
| 18 | 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 |

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| 19 | The Equilibrium Structure of Benzene. Journal of Physical Chemistry A, 2000, 104, 2865-2868. | 2.5 | 177 |
| 20 | 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 |
| 21 | On the choice of orbitals for symmetry breaking problems with application to NO3. Journal of Chemical Physics, 1992, 97, 5554-5559. | 3.0 | 165 |
| 22 | Structures, Automerizations, and Isomerizations of C3H2Isomers. Journal of the American Chemical Society, 1997, 119, 5847-5856. | 13.7 | 141 |
| 23 | On the vibronic level structure in the NO3 radical. I. The ground electronic state. Journal of Chemical Physics, 2007, 126, 134309. | 3.0 | 133 |
| 24 | 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 |
| 25 | Photoelectron Wave Function in Photoionization: Plane Wave or Coulomb Wave?. Journal of Physical Chemistry Letters, 2015, 6, 4532-4540. | 4.6 | 115 |
| 26 | A coupledâ€cluster based effective Hamiltonian method for dynamic electric polarizabilities. Journal of Chemical Physics, 1993, 99, 5178-5183. | 3.0 | 103 |
| 27 | 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 |
| 28 | 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 |
| 29 | Quantifying Hydrogenâ€Bond Populations in Dimethyl Sulfoxide/Water Mixtures. Angewandte Chemie - International Edition, 2017, 56, 11375-11379. | 13.8 | 94 |
| 30 | 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 |
| 31 | The Simplest Criegee Intermediate (H<sub>2</sub>Câ•Oâ€“O): Isotopic Spectroscopy, Equilibrium Structure, and Possible Formation from Atmospheric Lightning. Journal of Physical Chemistry Letters, 2013, 4, 4133-4139. | 4.6 | 88 |
| 32 | 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 |
| 33 | Analytic gradients for the coupled-cluster singles, doubles, and triples (CCSDT) model. Journal of Chemical Physics, 2002, 116, 1773-1782. | 3.0 | 83 |
| 34 | 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 |
| 35 | 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 |
| 36 | Electron-Correlated Approaches for the Calculation of NMR Chemical Shifts. Advances in Chemical Physics, 2003, , 355-422. | 0.3 | 79 |

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| 37 | Treatment of Fermi resonance effects on transition moments in vibrational perturbation theory. Molecular Physics, 2007, 105, 101-109. | 1.7 | 74 |
| 38 | 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 |
| 39 | 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 |
| 40 | 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 |
| 41 | A new approach to approximate equation-of-motion coupled cluster with triple excitations. Journal of Chemical Physics, 2016, 145, 124102. | 3.0 | 70 |
| 42 | 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 |
| 43 | On the vibronic level structure in the NO<sub>3</sub> radical: II. Adiabatic calculation of the infrared spectrum. Molecular Physics, 2009, 107, 1059-1075. | 1.7 | 65 |
| 44 | Potential nonrigidity of the NO3 radical. Journal of Chemical Physics, 1991, 94, 4084-4087. | 3.0 | 60 |
| 45 | Spontaneous and Selective Formation of HSNO, a Crucial Intermediate Linking H<sub>2</sub>S and Nitroso Chemistries. Journal of the American Chemical Society, 2016, 138, 11441-11444. | 13.7 | 60 |
| 46 | 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 |
| 47 | Correlated studies of infrared intensities. Journal of Chemical Physics, 1989, 90, 3241-3249. | 3.0 | 58 |
| 48 | 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 |
| 49 | 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 |
| 50 | Chirped-pulse millimeter-wave spectroscopy for dynamics and kinetics studies of pyrolysis reactions. Physical Chemistry Chemical Physics, 2014, 16, 15739-15751. | 2.8 | 54 |
| 51 | Does chlorine peroxide exhibit a strong ultraviolet absorption near 250 nm?. Journal of Chemical Physics, 1993, 98, 9335-9339. | 3.0 | 53 |
| 52 | The Molecular Structure of gaucheâ€1,3â€Butadiene: Experimental Establishment of Nonâ€planarity. Angewandte Chemie - International Edition, 2018, 57, 1821-1825. | 13.8 | 46 |
| 53 | Anharmonic force fields from analytic CCSD(T) second derivatives: HOF and F2O. Journal of Chemical Physics, 1999, 110, 3687-3696. | 3.0 | 45 |
| 54 | 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 |

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| 55 | Quantitative analysis of Fermi resonances by harmonic derivatives of perturbation theory corrections. Molecular Physics, 2009, 107, 213-222. | 1.7 | 44 |
| 56 | Towards highly accurate ab initio thermochemistry of larger systems: Benzene. Journal of Chemical Physics, 2011, 135, 044513. | 3.0 | 44 |
| 57 | 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 |
| 58 | A master equation simulation for the â€¢OH + CH3OH reaction. Journal of Chemical Physics, 2019, 150, 084105. | 3.0 | 42 |
| 59 | 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. | 3.0 | 41 |
| 60 | 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 |
| 61 | Analytic ROHFâ€“MBPT(2) second derivatives. Journal of Chemical Physics, 1992, 97, 7825-7828. | 3.0 | 39 |
| 62 | High-Accuracy Extrapolated ab Initio Thermochemistry of the Propargyl Radical and the Singlet C<sub>3</sub>H<sub>2</sub> Carbenes. Journal of Physical Chemistry A, 2009, 113, 12447-12453. | 2.5 | 39 |
| 63 | Communication: Thermal unimolecular decomposition of syn-CH3CHOO: A kinetic study. Journal of Chemical Physics, 2016, 145, 131102. | 3.0 | 38 |
| 64 | Exhaustive Product Analysis of Three Benzene Discharges by Microwave Spectroscopy. Journal of Physical Chemistry A, 2020, 124, 5170-5181. | 2.5 | 38 |
| 65 | 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 |
| 66 | 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 |
| 67 | A coupledâ€cluster study of the ground state of C+3. Journal of Chemical Physics, 1991, 94, 4320-4327. | 3.0 | 35 |
| 68 | Ab initiodetermination of the heat of formation of ketenyl (HCCO) and ethynyl (CCH) radicals. Molecular Physics, 2005, 103, 2159-2168. | 1.7 | 33 |
| 69 | 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 |
| 70 | Active Thermochemical Tables: The Adiabatic Ionization Energy of Hydrogen Peroxide. Journal of Physical Chemistry A, 2017, 121, 8799-8806. | 2.5 | 33 |
| 71 | On the HCN â€“ HNC Energy Difference. Journal of Physical Chemistry A, 2015, 119, 10929-10934. | 2.5 | 32 |
| 72 | Precise equilibrium structure determination of hydrazoic acid (HN3) by millimeter-wave spectroscopy. Journal of Chemical Physics, 2015, 143, 104310. | 3.0 | 31 |

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| 73 | 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 |
| 74 | Structural and Thermodynamic Analysis of a Three-Component Assembly Forming ortho-Iminophenylboronate Esters. Journal of Organic Chemistry, 2016, 81, 8319-8330. | 3.2 | 30 |
| 75 | 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 |
| 76 | Quantitative vibronic coupling calculations: the formyloxyl radical. Theoretical Chemistry Accounts, 2011, 129, 527-543. | 1.4 | 28 |
| 77 | 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 |
| 78 | An unusually large nonadiabatic error in the BNB molecule. Journal of Chemical Physics, 2010, 133, 174309. | 3.0 | 27 |
| 79 | 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 |
| 80 | Electron-Correlated Methods for the Calculation of NMR Chemical Shifts. , 2004, , 123-139. | | 25 |
| 81 | Photoelectron Spectroscopy of the Methide Anion: Electron Affinities of <sup>â€¢</sup>CH<sub>3</sub> and <sup>â€¢</sup>CD<sub>3</sub> and Inversion Splittings of CH<sub>3</sub><sup>â€“</sup> and CD<sub>3</sub><sup>â€“</sup>. Journal of the American Chemical Society, 2015, 137, 12939-12945. | 13.7 | 25 |
| 82 | Quantifying Hydrogenâ€Bond Populations in Dimethyl Sulfoxide/Water Mixtures. Angewandte Chemie, 2017, 129, 11533-11537. | 2.0 | 25 |
| 83 | 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 |
| 84 | Accuracy of Coupled Cluster Excited State Potential Energy Surfaces. Journal of Chemical Theory and Computation, 2018, 14, 5859-5869. | 5.3 | 24 |
| 85 | The global minimum structure of SiC3: The controversy continues. Journal of Chemical Physics, 2002, 116, 9151-9153. | 3.0 | 23 |
| 86 | 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 |
| 87 | Direct measurements of DOCO isomers in the kinetics of OD + CO. Science Advances, 2018, 4, eaao4777. | 10.3 | 22 |
| 88 | 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 |
| 89 | Revisitation of Nonorthogonal Spin Adaptation in Coupled Cluster Theory. Journal of Chemical Theory and Computation, 2013, 9, 2567-2572. | 5.3 | 21 |
| 90 | 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 |

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| 91 | 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 |
| 92 | 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 |
| 93 | 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 |
| 94 | Unimolecular Reaction of Methyl Isocyanide to Acetonitrile: A High-Level Theoretical Study. Journal of Physical Chemistry Letters, 2018, 9, 2532-2538. | 4.6 | 20 |
| 95 | Ab initio thermal rate coefficients for H + NH<sub>3</sub> â‡Œ H<sub>2</sub> + NH<sub>2</sub>. International Journal of Chemical Kinetics, 2019, 51, 321-328. | 1.6 | 20 |
| 96 | 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 |
| 97 | Laser spectroscopy of Si3C. Journal of Chemical Physics, 2005, 122, 124314. | 3.0 | 19 |
| 98 | Quantum-state-controlled reactions between molecular radicals and ions. Physical Review A, 2018, 98, . | 2.5 | 19 |
| 99 | 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 |
| 100 | On the equilibrium bond length of ammonia in the first excited singlet state. Journal of Chemical Physics, 1995, 102, 1096-1097. | 3.0 | 17 |
| 101 | Gasâ€Phase Formation of the Disilavinylidene (H<sub>2</sub>SiSi) Transient. Angewandte Chemie - International Edition, 2017, 56, 1264-1268. | 13.8 | 17 |
| 102 | Pragmatic Solution for a Fully E,J-Resolved Master Equation. Journal of Physical Chemistry A, 2020, 124, 2907-2918. | 2.5 | 17 |
| 103 | Theoretical prediction of magnetic exchange coupling constants from broken-symmetry coupled cluster calculations. Journal of Chemical Physics, 2020, 152, 234115. | 3.0 | 17 |
| 104 | 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 |
| 105 | Structure, energetics, and vibrational spectra of beryllium borohydride isomers. Journal of Chemical Physics, 1988, 88, 5726-5734. | 3.0 | 16 |
| 106 | Relatively Selective Production of the Simplest Criegee Intermediate in a CH<sub>4</sub>/O<sub>2</sub> Electric Discharge: Kinetic Analysis of a Plausible Mechanism. Journal of Physical Chemistry A, 2015, 119, 7197-7204. | 2.5 | 16 |
| 107 | The ionisation energy of cyclopentadienone: a photoelectronâ€"photoion coincidence study. Molecular Physics, 2015, 113, 2350-2358. | 1.7 | 16 |
| 108 | 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 |

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| 109 | Point group symmetry and cartesian force constant redundancy. International Journal of Quantum Chemistry, 1991, 39, 19-29. | 2.0 | 15 |
| 110 | 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 |
| 111 | Quantitative vibronic coupling calculations. The visible spectrum of propadienylidene. Faraday Discussions, 2011, 150, 331. | 3.2 | 15 |
| 112 | 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 |
| 113 | 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 |
| 114 | Barrier to Methyl Internal Rotation of Cis- andTrans-2-Methylvinoxy Radicals in the XÌƒ(2Aâ€²Âˆ) and BÌƒ(2Aâ€²Âˆ) States:Â Experiment and Theory. Journal of Physical Chemistry A, 2000, 104, 9906-9913. | 2.5 | 14 |
| 115 | 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 |
| 116 | Electron-Withdrawing Effects in the Photodissociation of CH<sub>2</sub>ICl To Form CH<sub>2</sub>Cl Radical, Simultaneously Viewed Through the Carbon K and Chlorine L<sub>2,3</sub> X-ray Edges. Journal of the American Chemical Society, 2018, 140, 13360-13366. | 13.7 | 14 |
| 117 | Precise equilibrium structure of thiazole (c-C3H3NS) from twenty-four isotopologues. Journal of Chemical Physics, 2021, 155, 054302. | 3.0 | 14 |
| 118 | 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 |
| 119 | Pyrolysis of the Simplest Carbohydrate, Glycolaldehyde (CHOâ^'CH<sub>2</sub>OH), and Glyoxal in a Heated Microreactor. Journal of Physical Chemistry A, 2016, 120, 2161-2172. | 2.5 | 13 |
| 120 | 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 |
| 121 | Spectroscopy of Ethylenedione and Ethynediolide: A Reinvestigation. Angewandte Chemie - International Edition, 2018, 57, 5394-5397. | 13.8 | 13 |
| 122 | Quantum-state-specific reaction rate measurements for the photo-induced reaction Ca<sup>+</sup> + O<sub>2</sub> â†' CaO<sup>+</sup> + O. Molecular Physics, 2019, 117, 3036-3042. | 1.7 | 13 |
| 123 | High-Resolution Photoelectron Spectroscopy of Cryogenically Cooled NO<sub>3</sub>Ì…. Journal of Physical Chemistry Letters, 2020, 11, 395-400. | 4.6 | 13 |
| 124 | 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 |
| 125 | Three-Dimensional Master Equation (3DME) Approach. Journal of Physical Chemistry A, 2018, 122, 7757-7767. | 2.5 | 12 |
| 126 | The equilibrium structure of the ammonium radical Rydberg ground state. Journal of Chemical Physics, 2001, 114, 9863-9865. | 3.0 | 11 |

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| 127 | Isomerization and Fragmentation of Cyclohexanone in a Heated Micro-Reactor. Journal of Physical Chemistry A, 2015, 119, 12635-12647. | 2.5 | 11 |
| 128 | Pressure-Dependent Rate Constant Caused by Tunneling Effects: OH + HNO<sub>3</sub> as an Example. Journal of Physical Chemistry Letters, 2020, 11, 3712-3717. | 4.6 | 11 |
| 129 | The Molecular Structure of gauche â€1,3â€Butadiene: Experimental Establishment of Nonâ€planarity. Angewandte Chemie, 2018, 130, 1839-1843. | 2.0 | 10 |
| 130 | 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 |
| 131 | Semi-Experimental Equilibrium (r<sub>e</sub><sup>SE</sup>) and Theoretical Structures of Pyridazine (o-C<sub>4</sub>H<sub>4</sub>N<sub>2</sub>). Journal of Physical Chemistry A, 2021, 125, 7976-7987. | 2.5 | 10 |
| 132 | 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 |
| 133 | Communication: Helium nanodroplet isolation and rovibrational spectroscopy of hydroxymethylene. Journal of Chemical Physics, 2014, 140, 171102. | 3.0 | 9 |
| 134 | Semiclassical transition state theory/master equation kinetics of HO + CO: Performance evaluation. International Journal of Chemical Kinetics, 2020, 52, 1022-1045. | 1.6 | 9 |
| 135 | Spectroscopy of Ethylenedione and Ethynediolide: A Reinvestigation. Angewandte Chemie, 2018, 130, 5492-5495. | 2.0 | 8 |
| 136 | The Hunt for Elusive Molecules: Insights from Joint Theoretical and Experimental Investigations. Chemistry - A European Journal, 2019, 25, 7243-7258. | 3.3 | 8 |
| 137 | PAH Growth in Flames and Space: Formation of the Phenalenyl Radical. Journal of Physical Chemistry A, 2022, 126, 101-108. | 2.5 | 8 |
| 138 | Computation of quadratic electric dipole moment functions. Journal of Chemical Physics, 1988, 88, 7650-7652. | 3.0 | 7 |
| 139 | Equilibrium structure of LiCCH. International Journal of Quantum Chemistry, 2000, 77, 305-310. | 2.0 | 7 |
| 140 | Spectral analyses of trans- and cis-DOCO transients via comb spectroscopy. Molecular Physics, 2018, 116, 3710-3717. | 1.7 | 7 |
| 141 | First-Principles Calculation of Jahnâ€“Teller Rotational Distortion Parameters. Journal of Physical Chemistry A, 2019, 123, 4990-5004. | 2.5 | 7 |
| 142 | Structural Characterization of Phenoxy Radical with Mass-Correlated Broadband Microwave Spectroscopy. Journal of Physical Chemistry Letters, 2019, 10, 2919-2923. | 4.6 | 7 |
| 143 | Probing the Exit Channel of the OH + CH<sub>3</sub>OH â†’ H<sub>2</sub>O + CH<sub>3</sub>O Reaction by Photodetachment of CH<sub>3</sub>O<sup>â€“</sup>(H<sub>2</sub>O). Journal of Physical Chemistry Letters, 2022, 13, 142-148. | 4.6 | 7 |
| 144 | Coupled-cluster studies of singlet propynylidene. Molecular Physics, 1999, 96, 505-509. | 1.7 | 6 |

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| 145 | Reactive intermediates in 4He nanodroplets: Infrared laser Stark spectroscopy of dihydroxycarbene. Journal of Chemical Physics, 2015, 142, 144309. | 3.0 | 6 |
| 146 | Directed Gas-Phase Formation of the Germaniumsilylene Butterfly Molecule (Ge(Î¼-H<sub>2</sub>)Si). Journal of Physical Chemistry Letters, 2019, 10, 1264-1271. | 4.6 | 6 |
| 147 | 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 |
| 148 | Using isotopologues to probe the potential energy surface of reactions of C2H2++C3H4. Journal of Chemical Physics, 2021, 154, 124310. | 3.0 | 4 |
| 149 | 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 |
| 150 | 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 |
| 151 | Atomic isotropic hyperfine properties for first row elements (Bâ€“F) revisited. Journal of Chemical Physics, 2022, 156, 034304. | 3.0 | 3 |
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| 153 | Equilibrium Structure of the Silicon Trimer. ACS Symposium Series, 2007, , 193-200. | 0.5 | 0 |
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