# T Daniel Crawford

List of Publications by Year
in descending order



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|---|---|---|---|
| 150 papers | 8,514 citations | 71061 41 h-index | 46771 89 g-index |
| 154 all docs | 154 docs citations | 154 times ranked | 6035 citing authors |

| # | Article | IF | Citations |
|---|---|---|---|
| 1 | <scp>Psi4</scp> 1.1: An Open-Source Electronic Structure Program Emphasizing Automation, Advanced Libraries, and Interoperability. Journal of Chemical Theory and Computation, 2017, 13, 3185-3197. | 2.3 | 961 |
| 2 | Psi4: an openâ€source ab initio electronic structure program. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2012, 2, 556-565. | 6.2 | 838 |
| 3 | An Introduction to Coupled Cluster Theory for Computational Chemists. Reviews in Computational Chemistry, 2007, , 33-136. | 1.5 | 531 |
| 4 | P<scp>SI4</scp> 1.4: Open-source software for high-throughput quantum chemistry. Journal of Chemical Physics, 2020, 152, 184108. | 1.2 | 440 |
| 5 | Ab initio calculation of molecular chiroptical properties. Theoretical Chemistry Accounts, 2006, 115, 227-245. | 0.5 | 362 |
| 6 | PSI3: An open-source Ab Initio electronic structure package. Journal of Computational Chemistry, 2007, 28, 1610-1616. | 1.5 | 258 |
| 7 | The Current State of Ab Initio Calculations of Optical Rotation and Electronic Circular Dichroism Spectra. Journal of Physical Chemistry A, 2007, 111, 12057-12068. | 1.1 | 251 |
| 8 | The balance between theoretical method and basis set quality: A systematic study of equilibrium geometries, dipole moments, harmonic vibrational frequencies, and infrared intensities. Journal of Chemical Physics, 1993, 99, 403-416. | 1.2 | 213 |
| 9 | Sources of error in electronic structure calculations on small chemical systems. Journal of Chemical Physics, 2006, 124, 054107. | 1.2 | 183 |
| 10 | Problematic p-benzyne: Orbital instabilities, biradical character, and broken symmetry. Journal of Chemical Physics, 2001, 114, 10638-10650. | 1.2 | 161 |
| 11 | M<sub>2</sub>@C<sub>79</sub>N (M = Y, Tb): Isolation and Characterization of Stable Endohedral Metallofullerenes Exhibiting Mâ‹¯M Bonding Interactions inside Aza[80]fullerene Cages. Journal of the American Chemical Society, 2008, 130, 12992-12997. | 6.6 | 155 |
| 12 | Hartreeâ€“Fock orbital instability envelopes in highly correlated single-reference wave functions. Journal of Chemical Physics, 1997, 107, 10626-10632. | 1.2 | 142 |
| 13 | Investigation of an asymmetric triple-excitation correction for coupled-cluster energies. International Journal of Quantum Chemistry, 1998, 70, 601-611. | 1.0 | 139 |
| 14 | Coupled cluster calculations of optical rotatory dispersion of (S)-methyloxirane. Journal of Chemical Physics, 2004, 121, 3550-3557. | 1.2 | 128 |
| 15 | The trans-HOCO radical: Quartic force fields, vibrational frequencies, and spectroscopic constants. Journal of Chemical Physics, 2011, 135, 134301. | 1.2 | 116 |
| 16 | Simple coupled-cluster singles and doubles method with perturbative inclusion of triples and explicitly correlated geminals: The CCSD(T)R12Â model. Journal of Chemical Physics, 2008, 128, 244113. | 1.2 | 113 |
| 17 | P<scp>si</scp>4N<scp>um</scp>P<scp>y</scp>: An Interactive Quantum Chemistry Programming Environment for Reference Implementations and Rapid Development. Journal of Chemical Theory and Computation, 2018, 14, 3504-3511. | 2.3 | 106 |
| 18 | Quartic force field predictions of the fundamental vibrational frequencies and spectroscopic constants of the cations HOCO+ and DOCO+. Journal of Chemical Physics, 2012, 136, 234309. | 1.2 | 105 |

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| 19 | Conformations of [10]Annulene:â€‰ More Bad News for Density Functional Theory and Second-Order Perturbation Theory. Journal of the American Chemical Society, 1999, 121, 10788-10793. | 6.6 | 98 |
| 20 | Locally correlated equation-of-motion coupled cluster theory for the excited states of large molecules. Chemical Physics Letters, 2002, 366, 611-622. | 1.2 | 98 |
| 21 | Comparison of Time-Dependent Density-Functional Theory and Coupled Cluster Theory for the Calculation of the Optical Rotations of Chiral Molecules. Journal of Physical Chemistry A, 2008, 112, 1339-1345. | 1.1 | 98 |
| 22 | Structure, Anharmonic Vibrational Frequencies, and Intensities of NNHNN<sup>+</sup>. Journal of Physical Chemistry A, 2015, 119, 11623-11631. | 1.1 | 81 |
| 23 | A new diagnostic for open-shell coupled-cluster theory. Chemical Physics Letters, 2000, 328, 431-436. | 1.2 | 79 |
| 24 | Local correlation in coupled cluster calculations of molecular response properties. Chemical Physics Letters, 2004, 400, 104-111. | 1.2 | 77 |
| 25 | Ab Initio Calculation of Optical Rotation in (P)-(+)-[4]Triangulane. Journal of the American Chemical Society, 2005, 127, 1368-1369. | 6.6 | 75 |
| 26 | Quartic Force Field Rovibrational Analysis of Protonated Acetylene, C<sub>2</sub>H<sub>3</sub><sup>+</sup>, and Its Isotopologues. Journal of Physical Chemistry A, 2014, 118, 7034-7043. | 1.1 | 75 |
| 27 | Perspective: Computational chemistry software and its advancement as illustrated through three grand challenge cases for molecular science. Journal of Chemical Physics, 2018, 149, 180901. | 1.2 | 72 |
| 28 | Fundamental Vibrational Frequencies and Spectroscopic Constants of HOCS<sup>+</sup>, HSCO<sup>+</sup>, and Isotopologues via Quartic Force Fields. Journal of Physical Chemistry A, 2012, 116, 9582-9590. | 1.1 | 70 |
| 29 | Real versus artifactual symmetry-breaking effects in Hartreeâ€“Fock, density-functional, and coupled-cluster methods. Journal of Chemical Physics, 2004, 120, 7298-7306. | 1.2 | 68 |
| 30 | Potential energy surface discontinuities in local correlation methods. Journal of Chemical Physics, 2004, 121, 691-696. | 1.2 | 66 |
| 31 | Coupled cluster methods including triple excitations for excited states of radicals. Journal of Chemical Physics, 2005, 122, 054110. | 1.2 | 64 |
| 32 | HIGH-ACCURACY QUARTIC FORCE FIELD CALCULATIONS FOR THE SPECTROSCOPIC CONSTANTS AND VIBRATIONAL FREQUENCIES OF 1<sup>1</sup>Aâ€²l-C<sub>3</sub>H<sup>â€“</sup>: A POSSIBLE LINK TO LINES OBSERVED IN THE HORSEHEAD NEBULA PHOTODISSOCIATION REGION. Astrophysical Journal, 2013, 772, 39. | 1.6 | 63 |
| 33 | Vibrational frequencies and spectroscopic constants from quartic force fields for cis-HOCO: The radical and the anion. Journal of Chemical Physics, 2011, 135, 214303. | 1.2 | 62 |
| 34 | Structure and Energetics of Isomers of the Interstellar Molecule C5H. Journal of the American Chemical Society, 1999, 121, 1902-1911. | 6.6 | 54 |
| 35 | Some surprising failures of Brueckner coupled cluster theory. Journal of Chemical Physics, 2000, 112, 7873-7879. | 1.2 | 54 |
| 36 | The structures of m-benzyne and tetrafluoro-m-benzyne. Journal of Chemical Physics, 2005, 122, 174309. | 1.2 | 48 |

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| 37 | Theoretical prediction of new dipole-bound singlet states for anions of interstellar interest. Journal of Chemical Physics, 2011, 134, 154304. | 1.2 | 48 |
| 38 | Electronic structure of the two isomers of the anionic form of p-coumaric acid chromophore. Journal of Chemical Physics, 2011, 134, 034310. | 1.2 | 47 |
| 39 | Large Solvation Effect in the Optical Rotatory Dispersion of Norbornenone. Angewandte Chemie - International Edition, 2014, 53, 1386-1389. | 7.2 | 46 |
| 40 | On the importance of vibrational contributions to small-angle optical rotation: Fluoro-oxirane in gas phase and solution. Journal of Chemical Physics, 2009, 130, 034310. | 1.2 | 43 |
| 41 | Communication: Spectroscopic consequences of proton delocalization in OCHCO+. Journal of Chemical Physics, 2015, 143, 071102. | 1.2 | 42 |
| 42 | The <scp>MolSSI</scp> QCA<scp>rchive</scp> project: An openâ€source platform to compute, organize, and share quantum chemistry data. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2021, 11, e1491. | 6.2 | 42 |
| 43 | Optical Rotatory Dispersion of 2,3-Hexadiene and 2,3-Pentadiene. Journal of Physical Chemistry A, 2008, 112, 2415-2422. | 1.1 | 41 |
| 44 | A benchmark study of the vertical electronic spectra of the linear chain radicals C2H and C4H. Journal of Chemical Physics, 2010, 132, 144303. | 1.2 | 40 |
| 45 | Frozen Virtual Natural Orbitals for Coupled-Cluster Linear-Response Theory. Journal of Physical Chemistry A, 2017, 121, 708-716. | 1.1 | 40 |
| 46 | Ab Initio Optical Rotatory Dispersion and Electronic Circular Dichroism Spectra of (S)-2-Chloropropionitrile. Journal of Physical Chemistry A, 2006, 110, 7649-7654. | 1.1 | 39 |
| 47 | Local correlation domains for coupled cluster theory: optical rotation and magnetic-field perturbations. Physical Chemistry Chemical Physics, 2008, 10, 3345. | 1.3 | 39 |
| 48 | THE POSSIBLE INTERSTELLAR ANION CH<sub>2</sub>CN<sup>â€“</sup>: SPECTROSCOPIC CONSTANTS, VIBRATIONAL FREQUENCIES, AND OTHER CONSIDERATIONS. Astrophysical Journal, 2013, 762, 121. | 1.6 | 38 |
| 49 | Gas phase optical rotation calculated from coupled cluster theory with zeroâ€point vibrational corrections from density functional theory. Chirality, 2009, 21, E68-75. | 1.3 | 37 |
| 50 | Basis Set Dependence of Coupled Cluster Optical Rotation Computations. Journal of Physical Chemistry A, 2011, 115, 10045-10051. | 1.1 | 37 |
| 51 | Ab Initio Determination of Optical Rotatory Dispersion in the Conformationally Flexible Molecule (R)-Epichlorohydrin. Journal of Physical Chemistry A, 2006, 110, 2290-2298. | 1.1 | 36 |
| 52 | Protonated 2-Methyl-1,2-epoxypropane:Â A Challenging Problem for Density Functional Theory. Journal of Organic Chemistry, 2006, 71, 1592-1597. | 1.7 | 35 |
| 53 | Experimental Bond Critical Point and Local Energy Density Properties Determined for Mnâ”O, Feâ”O, and Coâ”O Bonded Interactions for Tephroite, Mn2SiO4, Fayalite, Fe2SiO4, and Co2SiO4 Olivine and Selected Organic Metal Complexes: Comparison with Properties Calculated for Non-Transition and Transition Metal Mâ”O Bonded Interactions for Silicates and Oxides. Journal of Physical Chemistry A, 2008, 112, 8811-8823. | 1.1 | 35 |
| 54 | Coupledâ€Cluster Calculations of Vibrational Raman Optical Activity Spectra. ChemPhysChem, 2011, 12, 3442-3448. | 1.0 | 34 |

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| 55 | The problematic case of ( S )-methylthiirane: electronic circular dichroism spectra and optical rotatory dispersion. Molecular Physics, 2007, 105, 2607-2617. | 0.8 | 33 |
| 56 | The Cl̀ƒâ€‰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 |
| 57 | Optical activity in conformationally flexible molecules: a theoretical study of large-amplitude vibrational averaging in (R)-3-chloro-1-butene. Molecular Physics, 2009, 107, 1041-1057. | 0.8 | 32 |
| 58 | A comparison of two approaches to perturbation triple excitation corrections to the coupledâ€cluster singles and doubles method for highâ€spin openâ€shell systems. Journal of Chemical Physics, 1996, 104, 6259-6264. | 1.2 | 31 |
| 59 | On the energy invariance of openâ€shell perturbation theory with respect to unitary transformations of molecular orbitals. Journal of Chemical Physics, 1996, 105, 1060-1069. | 1.2 | 31 |
| 60 | Spin-restricted Brueckner orbitals for coupled-cluster wavefunctions. Journal of Chemical Physics, 1997, 107, 9980-9984. | 1.2 | 31 |
| 61 | Insights on the Origin of the Unusually Large Specific Rotation of (1S,4S)-Norbornenone. Journal of Physical Chemistry A, 2014, 118, 4863-4871. | 1.1 | 31 |
| 62 | Dipole Surface and Infrared Intensities for the cis- and trans-HOCO and DOCO Radicals. Journal of Physical Chemistry A, 2013, 117, 6932-6939. | 1.1 | 30 |
| 63 | The lowest Aâ€²2 excited state of the water-hydroxyl complex. Journal of Chemical Physics, 2006, 125, 204302. | 1.2 | 29 |
| 64 | Singlet Excited States of Silicon-Containing Anions Relevant to Interstellar Chemistry. Journal of Physical Chemistry A, 2011, 115, 8119-8124. | 1.1 | 28 |
| 65 | The weakly bound dinitrogen tetroxide molecule: High level single reference wavefunctions are good enough. Journal of Chemical Physics, 1997, 106, 7178-7184. | 1.2 | 27 |
| 66 | A new spin-restricted triple excitation correction for coupled cluster theory. Journal of Chemical Physics, 1997, 107, 7943-7950. | 1.2 | 27 |
| 67 | A Family of Decamethylmetallocene Charge-Transfer Salt Magnets Using Methyl Tricyanoethylenecarboxylate (MTCE) as the Electron Acceptor. Journal of the American Chemical Society, 2004, 126, 16890-16895. | 6.6 | 27 |
| 68 | Localized optimized orbitals, coupled cluster theory, and chiroptical response properties. Physical Chemistry Chemical Physics, 2012, 14, 7830. | 1.3 | 26 |
| 69 | Simulation of circularly polarized luminescence spectra using coupled cluster theory. Journal of Chemical Physics, 2015, 142, 154101. | 1.2 | 26 |
| 70 | Reducedâ€scaling coupled cluster response theory: Challenges and opportunities. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2019, 9, e1406. | 6.2 | 26 |
| 71 | A contribution to the understanding of the structure of xenon hexafluoride. Journal of Chemical Physics, 1995, 102, 3307-3311. | 1.2 | 25 |
| 72 | The optical activity of carvone: A theoretical and experimental investigation. Journal of Chemical Physics, 2012, 136, 114512. | 1.2 | 25 |

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| 73 | Room-Temperature and Near-Room-Temperature Molecule-Based Magnets. Inorganic Chemistry, 2008, 47, 5649-5655. | 1.9 | 24 |
| 74 | A Comparison of Three Approaches to the Reduced-Scaling Coupled Cluster Treatment of Non-Resonant Molecular Response Properties. Journal of Chemical Theory and Computation, 2016, 12, 209-222. | 2.3 | 24 |
| 75 | The 1 <sup>3</sup>Aâ€² HCN and 1 <sup>3</sup>Aâ€² HCO<sup>+</sup> Vibrational Frequencies and Spectroscopic Constants from Quartic Force Fields. Journal of Physical Chemistry A, 2013, 117, 9324-9330. | 1.1 | 23 |
| 76 | Antiplasmodial Sesquiterpenoid Lactones from Trichospira verticillata: Structure Elucidation by Spectroscopic Methods and Comparison of Experimental and Calculated ECD Data. Journal of Natural Products, 2017, 80, 1639-1647. | 1.5 | 23 |
| 77 | Rotational spectrum and theoretical structure of the carbene HC4N. Journal of Chemical Physics, 1999, 111, 6750-6754. | 1.2 | 22 |
| 78 | Chiroptical Properties of (R)-3-Chloro-1-butene and (R)-2-Chlorobutane. Journal of Physical Chemistry A, 2007, 111, 11232-11241. | 1.1 | 22 |
| 79 | Machine-Learning Coupled Cluster Properties through a Density Tensor Representation. Journal of Physical Chemistry A, 2020, 124, 4861-4871. | 1.1 | 21 |
| 80 | Aluminum monocarbonyl and aluminum isocarbonyl. Journal of Chemical Physics, 1996, 104, 3672-3675. | 1.2 | 20 |
| 81 | Comparison of the Electron Localization Function and Deformation Electron Density Maps for Selected Earth Materials. Journal of Physical Chemistry A, 2005, 109, 10022-10027. | 1.1 | 20 |
| 82 | Role of Long-Range Intermolecular Forces in the Formation of Inorganic Nanoparticle Clusters. Journal of Physical Chemistry A, 2011, 115, 12933-12940. | 1.1 | 20 |
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| 84 | A mapping of the electron localization function for the silica polymorphs: evidence for domains of electron pairs and sites of potential electrophilic attack. Physics and Chemistry of Minerals, 2002, 29, 307-318. | 0.3 | 19 |
| 85 | A mapping of the electron localization function for earth materials. Physics and Chemistry of Minerals, 2005, 32, 208-221. | 0.3 | 19 |
| 86 | The Equilibrium Geometry, Harmonic Vibrational Frequencies, and Estimated ab Initio Limit for the Barrier to Planarity of the Ethylene Radical Cation. Journal of Physical Chemistry A, 2002, 106, 2671-2675. | 1.1 | 18 |
| 87 | Lowâ€lying singlet excited states of isocyanogen. International Journal of Quantum Chemistry, 2008, 108, 1137-1140. | 1.0 | 17 |
| 88 | A Coupled Cluster Benchmark Study of the Electronic Spectrum of the Allyl Radical<sup>â€</sup>. Journal of Physical Chemistry A, 2010, 114, 8852-8857. | 1.1 | 17 |
| 89 | Symmetry breaking in the cyclic C3C2H radical. Physical Chemistry Chemical Physics, 2010, 12, 15459. | 1.3 | 17 |
| 90 | QUANTUM CHEMICAL ROVIBRATIONAL DATA FOR THE INTERSTELLAR DETECTION OFc-C<sub>3</sub>H<sup>â€“</sup>. Astrophysical Journal, 2014, 796, 139. | 1.6 | 17 |

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| 91 | Fundamental Vibrational Frequencies and Spectroscopic Constants of cis- and trans-HOCS, HSCO, and Isotopologues via Quartic Force Fields. Journal of Physical Chemistry B, 2014, 118, 6498-6510. | 1.2 | 16 |
| 92 | Frozen-Density Embedding Potentials and Chiroptical Properties. Journal of Chemical Theory and Computation, 2015, 11, 5305-5315. | 2.3 | 16 |
| 93 | Phloroglucinols from the Roots of Garcinia dauphinensis and Their Antiproliferative and Antiplasmodial Activities. Journal of Natural Products, 2019, 82, 431-439. | 1.5 | 16 |
| 94 | Performance of Property-Optimized Basis Sets for Optical Rotation with Coupled Cluster Theory. Journal of Physical Chemistry A, 2018, 122, 5962-5969. | 1.1 | 15 |
| 95 | Definitive ab initio structure for the XÌƒâ€‰2Aâ€²H2PO radical and resolution of the Pâ€“O stretching mode assignment. Journal of Chemical Physics, 1998, 109, 2694-2699. | 1.2 | 14 |
| 96 | Thermokinetic Proton Transfer and Ab Initio Studies of the [2H,S,O]+ System. The Proton Affinity of HSO. Journal of Physical Chemistry A, 2000, 104, 4636-4647. | 1.1 | 14 |
| 97 | Reduced-Scaling Coupled-Cluster Theory for Response Properties of Large Molecules. Challenges and Advances in Computational Chemistry and Physics, 2010, , 37-55. | 0.6 | 14 |
| 98 | Computing optical rotation via an N-body approach. Theoretical Chemistry Accounts, 2014, 133, 1. | 0.5 | 14 |
| 99 | Diagrammatic Coupled Cluster Monte Carlo. Journal of Physical Chemistry Letters, 2019, 10, 925-935. | 2.1 | 14 |
| 100 | Incremental evaluation of coupled cluster dipole polarizabilities. Physical Chemistry Chemical Physics, 2015, 17, 14284-14296. | 1.3 | 13 |
| 101 | Modeling Complex Solvent Effects on the Optical Rotation of Chiral Molecules: A Combined Molecular Dynamics and Density Functional Theory Study. Journal of Physical Chemistry A, 2021, 125, 3095-3108. | 1.1 | 13 |
| 102 | Hartreeâ^'Fock Orbital Instabilities and Symmetry-Breaking in ScO2:Â Is aCsEquilibrium Structure Viable?â€. Journal of Physical Chemistry A, 2004, 108, 3097-3102. | 1.1 | 12 |
| 103 | Properties of atoms under pressure: Bonded interactions of the atoms in three perovskites. Journal of Chemical Physics, 2012, 137, 164313. | 1.2 | 12 |
| 104 | The optimized orbital coupled cluster doubles method and optical rotation. Chemical Physics, 2012, 401, 125-129. | 0.9 | 12 |
| 105 | Basis Set Superposition Errors in the Many-Body Expansion of Molecular Properties. Journal of Physical Chemistry A, 2019, 123, 4500-4511. | 1.1 | 11 |
| 106 | The MolSSI Driver Interface Project: A framework for standardized, on-the-fly interoperability between computational molecular sciences codes. Computer Physics Communications, 2021, 261, 107688. | 3.0 | 11 |
| 107 | Rotational constants for the CÌƒâ€‰2A2 state of NO2. Journal of Chemical Physics, 1993, 99, 7926-7928. | 1.2 | 10 |
| 108 | The aminoboranylideneâ€“iminoborane isomerization. Journal of Chemical Physics, 2003, 119, 10647-10652. | 1.2 | 10 |

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| 109 | Vibrational Frequencies and Spectroscopic Constants for 1 <sup>3</sup>Aâ€² HNC and 1 <sup>3</sup>Aâ€² HOC<sup>+</sup> from High-Accuracy Quartic Force Fields. Journal of Physical Chemistry A, 2013, 117, 11339-11345. | 1.1 | 10 |
| 110 | Electronically Excited States in Solution via a Smooth Dielectric Model Combined with Equation-of-Motion Coupled Cluster Theory. Journal of Chemical Theory and Computation, 2017, 13, 5572-5581. | 2.3 | 10 |
| 111 | Investigation of an asymmetric tripleâ€excitation correction for coupledâ€cluster energies. International Journal of Quantum Chemistry, 1998, 70, 601-611. | 1.0 | 10 |
| 112 | Potential curves and spectroscopic properties for the ground state of ClO and for the ground and various excited states of ClOâ^. Journal of Chemical Physics, 2002, 117, 9703-9709. | 1.2 | 9 |
| 113 | Ab initio and analytic intermolecular potentials for Arâ€“CH3OH. Physical Chemistry Chemical Physics, 2006, 8, 4678-4684. | 1.3 | 9 |
| 114 | Electronically Excited States in Interstellar Chemistry. Annual Reports in Computational Chemistry, 2011, 7, 195-214. | 0.9 | 9 |
| 115 | Building capacity for undergraduate education and training in computational molecular science: A collaboration between the MERCURY consortium and the Molecular Sciences Software Institute. International Journal of Quantum Chemistry, 2020, 120, e26359. | 1.0 | 9 |
| 116 | On the Performance of a Size-Extensive Variant of Equation-of-Motion Coupled Cluster Theory for Optical Rotation in Chiral Molecules. Progress in Theoretical Chemistry and Physics, 2009, , 225-239. | 0.2 | 9 |
| 117 | Monofluorinated hydrogen sulfide (HFS): A definitive theoretical prediction of the infrared spectrum. Journal of Chemical Physics, 1992, 96, 2044-2047. | 1.2 | 8 |
| 118 | Application of equation-of-motion coupled-cluster methods to low-lying singlet and triplet electronic states of HBO and BOH. Journal of Chemical Physics, 2005, 122, 234316. | 1.2 | 7 |
| 119 | PNO++: Perturbed Pair Natural Orbitals for Coupled Cluster Linear Response Theory. Journal of Chemical Theory and Computation, 2021, 17, 290-301. | 2.3 | 7 |
| 120 | The electron cusp condition and the virial ratio as indicators of basis set quality. Journal of Chemical Physics, 2003, 118, 2491. | 1.2 | 6 |
| 121 | â€œNew Physical Insightsâ€•in Theoretical and Computational Studies. Journal of Physical Chemistry A, 2017, 121, 4850-4850. | 1.1 | 6 |
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| 123 | Investigation of an asymmetric triple-excitation correction for coupled-cluster energies. , 1998, 70, 601. | | 6 |
| 124 | Bornâ^'Oppenheimer Symmetry Breaking in the CÌƒ State of NO<sub>2</sub>:â€‰ Importance of Static and Dynamic Correlation Effects. Journal of Physical Chemistry A, 2008, 112, 2669-2676. | 1.1 | 4 |
| 125 | The Hartley basis functions and transform: alternatives to plane waves and the Fourier transform. Chemical Physics Letters, 1992, 192, 45-48. | 1.2 | 3 |
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| 128 | Theory and implementation of a novel stochastic approach to coupled cluster. Journal of Chemical Physics, 2020, 153, 144117. | 1.2 | 3 |
| 129 | Characteristics of Impactful Computational Contributions to The Journal of Physical Chemistry A. Journal of Physical Chemistry A, 2020, 124, 5059-5060. | 1.1 | 3 |
| 130 | Evolving Sections of The Journal of Physical Chemistry to Reflect an Ever-Changing Field. Journal of Physical Chemistry B, 2021, 125, 2465-2466. | 1.2 | 3 |
| 131 | A special issue of Molecular Physics honoring Prof. Henry F. Schaefer III. Molecular Physics, 2009, 107, 711-711. | 0.8 | 2 |
| 132 | The JPC Periodic Table. Journal of Physical Chemistry A, 2019, 123, 5837-5848. | 1.1 | 2 |
| 133 | The JPC Periodic Table. Journal of Physical Chemistry Letters, 2019, 10, 4051-4062. | 2.1 | 2 |
| 134 | Structure Elucidation and Confirmation of Phloroglucinols from the Roots of Garcinia dauphinensis by Comparison of Experimental and Calculated ECD Spectra and Specific Rotations. Journal of Natural Products, 2021, 84, 1163-1174. | 1.5 | 2 |
| 135 | The JPC Periodic Table. Journal of Physical Chemistry B, 2019, 123, 5973-5984. | 1.2 | 1 |
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| 137 | Tensor representations and symmetry in many-electron wave functions. Annual Reports in Computational Chemistry, 2019, 15, 79-101. | 0.9 | 1 |
| 138 | Celebrating the 125th Anniversary of The Journal of Physical Chemistry. Journal of Physical Chemistry C, 2021, 125, 1-2. | 1.5 | 1 |
| 139 | Introduction to proceedings of Molecular Quantum Mechanics 2010: from methylene to DNA and beyond. Molecular Physics, 2010, 108, 2437-2438. | 0.8 | 0 |
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| 142 | Evolving Sections of The Journal of Physical Chemistry to Reflect an Ever-Changing Field. Journal of Physical Chemistry C, 2021, 125, 5425-5426. | 1.5 | 0 |
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| 144 | The Journal of Physical Chemistry: Looking Back on Our 125th Anniversary and Looking Ahead to 2022. Journal of Physical Chemistry C, 2022, 126, 1-2. | 1.5 | 0 |

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| 147 | The Journal of Physical Chemistry: Looking Back on Our 125th Anniversary and Looking Ahead to 2022. Journal of Physical Chemistry B, 2022, 126, 1-2. | 1.2 | 0 |
| 148 | 50 and 100 Years Ago in The Journal of Physical Chemistry. Journal of Physical Chemistry C, 2022, 126, 6093-6095. | 1.5 | 0 |
| 149 | 50 and 100 Years Ago in The Journal of Physical Chemistry. Journal of Physical Chemistry B, 2022, 126, 2609-2611. | 1.2 | 0 |
| 150 | 50 and 100 Years Ago in The Journal of Physical Chemistry. Journal of Physical Chemistry A, 2022, 126, 2149-2151. | 1.1 | 0 |