# Wesley D Allen

## List of Publications by Year in Descending Order



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|---|---|---|---|
| 139 papers | 10,424 citations | 54 h-index | 100 g-index |
| 143 ext. papers | 11,008 ext. citations | 5.9 avg, IF | 5.94 L-index |

| # | Paper | IF | Citations |
|---|---|---|---|
| 139 | Identification and Reactivity of -,--Dihydroxycarbene, a New [CHO] Intermediate. *Journal of the American Chemical Society*, **2020**, 142, 19457-19461 | 16.4 | 3 |
| 138 | Reaction Profiles and Kinetics for Radical-Radical Hydrogen Abstraction via Multireference Coupled Cluster Theory. *Journal of Chemical Theory and Computation*, **2020**, 16, 1511-1525 | 6.4 | 2 |
| 137 | Riddles of the structure and vibrational dynamics of HO resolved near the ab initio limit. *Journal of Chemical Physics*, **2019**, 151, 094304 | 3.9 | 8 |
| 136 | Wigner numbers. *Journal of Chemical Physics*, **2019**, 151, 244122 | 3.9 | 1 |
| 135 | The multichannel n-propyl + O2 reaction surface: Definitive theory on a model hydrocarbon oxidation mechanism. *Journal of Chemical Physics*, **2018**, 148, 094303 | 3.9 | 11 |
| 134 | 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 | 6.4 | 25 |
| 133 | Intricate Conformational Tunneling in Carbonic Acid Monomethyl Ester. *Journal of Physical Chemistry Letters*, **2018**, 9, 1663-1667 | 6.4 | 8 |
| 132 | A Universal Integrated Rate Equation for Chemical Kinetics. *Journal of Physical Chemistry A*, **2018**, 122, 4009-4014 | 2.8 | |
| 131 | Probing the Delicate Balance between Pauli Repulsion and London Dispersion with Triphenylmethyl Derivatives. *Journal of the American Chemical Society*, **2018**, 140, 14421-14432 | 16.4 | 43 |
| 130 | Most favorable cumulenic structures in iron-capped linear carbon chains are short singlet odd-carbon dications: a theoretical view. *Physical Chemistry Chemical Physics*, **2018**, 20, 15496-15506 | 3.6 | 5 |
| 129 | Nucleophilic Influences and Origin of the S 2 Allylic Effect. *Chemistry - A European Journal*, **2018**, 24, 11637-11648 | 4.8 | 11 |
| 128 | Ring-Walking of Zerovalent Nickel on Aryl Halides. *Journal of Chemical Theory and Computation*, **2017**, 13, 1706-1711 | 6.4 | 15 |
| 127 | Tunneling Isomerizations on the Potential Energy Surfaces of Formaldehyde and Methanol Radical Cations. *ACS Earth and Space Chemistry*, **2017**, 1, 361-367 | 3.2 | 9 |
| 126 | Tunnelling in carbonic acid. *Chemical Communications*, **2016**, 52, 7858-61 | 5.8 | 24 |
| 125 | Conformers of Gaseous Serine. *Journal of Chemical Theory and Computation*, **2016**, 12, 3571-82 | 6.4 | 20 |
| 124 | Bond activation through tunneling: formation of the boron hydride cations BHn(+) (n = 2, 4, 6). *Physical Chemistry Chemical Physics*, **2016**, 18, 4063-70 | 3.6 | 4 |
| 123 | Sub-Doppler infrared spectroscopy and formation dynamics of triacetylene in a slit supersonic expansion. *Journal of Chemical Physics*, **2016**, 144, 074301 | 3.9 | 6 |

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| 122 | Polytriangulane. *Journal of Chemical Theory and Computation*, **2016**, 12, 4707-16 | 6.4 | 4 |
| 121 | Domino Tunneling. *Journal of the American Chemical Society*, **2015**, 137, 7828-34 | 16.4 | 36 |
| 120 | Bond angles around a tetravalent atom. *Journal of Physical Chemistry A*, **2015**, 119, 1534-8 | 2.8 | 1 |
| 119 | Intricate internal rotation surface and fundamental infrared transitions of the n-propyl radical. *Journal of Physical Chemistry B*, **2015**, 119, 728-35 | 3.4 | 9 |
| 118 | Polytwistane. *Chemistry - A European Journal*, **2014**, 20, 1638-45 | 4.8 | 30 |
| 117 | Complexation in nickel-catalyzed cross-coupling reactions. *Journal of Organic Chemistry*, **2014**, 79, 1836-41 | 4.2 | 30 |
| 116 | Do conjugative effects facilitate SN2 reactions?. *Journal of the American Chemical Society*, **2014**, 136, 3118-26 | 16.4 | 17 |
| 115 | The Li HF van der Waals minimum and the barrier to the deep HFLi potential well Special Issue of Molecular Physics: Seventh Molecular Quantum Mechanics Conference, Lugano, Switzerland, 2 June 2013.View all notes. *Molecular Physics*, **2014**, 112, 770-773 | 1.7 | 2 |
| 114 | The electronic structure of vanadium monochloride cation (VCl(+)): tackling the complexities of transition metal species. *Journal of Chemical Physics*, **2014**, 141, 204302 | 3.9 | 12 |
| 113 | Free Cyclooctatetraene Dianion: Planarity, Aromaticity, and Theoretical Challenges. *Journal of Chemical Theory and Computation*, **2013**, 9, 4436-43 | 6.4 | 28 |
| 112 | Exact Ligand Solid Angles. *Journal of Chemical Theory and Computation*, **2013**, 9, 5734-44 | 6.4 | 19 |
| 111 | Ligand Steric Descriptors. *Annual Reports in Computational Chemistry*, **2013**, 3-23 | 1.8 | 4 |
| 110 | Nearly degenerate isomers of C(BH)2: cumulene, carbene, or carbone?. *Chemistry - A European Journal*, **2013**, 19, 15941-54 | 4.8 | 22 |
| 109 | Exact ligand cone angles. *Journal of Computational Chemistry*, **2013**, 34, 1189-97 | 3.5 | 89 |
| 108 | Dipole Moment of the HOOO Radical: Resolution of a Structural Enigma. *Journal of Physical Chemistry Letters*, **2013**, 4, 3584-3589 | 6.4 | 22 |
| 107 | Structureeactivity relationships for aromatic molecules: electrostatic potentials at nuclei and electrophile affinity indices. *Wiley Interdisciplinary Reviews: Computational Molecular Science*, **2013**, 3, 37-55 | 7.9 | 24 |
| 106 | On the Role of Disproportionation Energy in Kumada Catalyst-Transfer Polycondensation. *ACS Macro Letters*, **2012**, 1, 995-1000 | 6.6 | 28 |
| 105 | Taming the low-lying electronic states of FeH. *Journal of Chemical Physics*, **2012**, 137, 234303 | 3.9 | 37 |

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| 104 | Psi4: an open-source ab initio electronic structure program. *Wiley Interdisciplinary Reviews: Computational Molecular Science*, **2012**, 2, 556-565 | 7.9 | 678 |
| 103 | Methylhydroxycarbene: tunneling control of a chemical reaction. *Science*, **2011**, 332, 1300-3 | 33.3 | 226 |
| 102 | Chemistry as a function of the fine-structure constant and the electron-proton mass ratio. *Physical Review A*, **2010**, 81, | 2.6 | 10 |
| 101 | Assigning quantum labels to variationally computed rotational-vibrational eigenstates of polyatomic molecules. *Journal of Chemical Physics*, **2010**, 133, 034113 | 3.9 | 54 |
| 100 | The problematic C2H4+F2 reaction barrier. *Journal of Chemical Physics*, **2010**, 132, 094304 | 3.9 | 10 |
| 99 | Reactions between resonance-stabilized radicals: propargyl + allyl. *Journal of Physical Chemistry A*, **2010**, 114, 4881-90 | 2.8 | 64 |
| 98 | Phenylhydroxycarbene. *Journal of the American Chemical Society*, **2010**, 132, 7273-5 | 16.4 | 48 |
| 97 | Lowest-Lying Conformers of Alanine: Pushing Theory to Ascertain Precise Energetics and Semiexperimental Re Structures. *Journal of Chemical Theory and Computation*, **2010**, 6, 3066-78 | 6.4 | 63 |
| 96 | Counterfactual Quantum Chemistry of Water **2010**, 119-134 | | |
| 95 | 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 | 1.7 | 30 |
| 94 | Analytic gradients for the state-specific multireference coupled cluster singles and doubles model. *Journal of Chemical Physics*, **2009**, 131, 064109 | 3.9 | 68 |
| 93 | Conformers of Gaseous Cysteine. *Journal of Chemical Theory and Computation*, **2009**, 5, 1511-23 | 6.4 | 111 |
| 92 | Barrier to linearity and anharmonic force field of the ketenyl radical. *Journal of Physical Chemistry A*, **2009**, 113, 11643-50 | 2.8 | 9 |
| 91 | Enthalpy of formation and anharmonic force field of diacetylene. *Journal of Chemical Physics*, **2009**, 130, 044301 | 3.9 | 39 |
| 90 | A companion perturbation theory for state-specific multireference coupled cluster methods. *Physical Chemistry Chemical Physics*, **2009**, 11, 4728-41 | 3.6 | 60 |
| 89 | Infrared signatures of the NCCO radical. *Physical Chemistry Chemical Physics*, **2009**, 11, 10385-90 | 3.6 | 11 |
| 88 | A hierarchy of homodesmotic reactions for thermochemistry. *Journal of the American Chemical Society*, **2009**, 131, 2547-60 | 16.4 | 418 |
| 87 | Capture of hydroxymethylene and its fast disappearance through tunnelling. *Nature*, **2008**, 453, 906-9 | 50.4 | 233 |

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| 86 | Anchoring the Absolute Proton Affinity Scale. *Journal of Chemical Theory and Computation*, **2008**, 4, 1220-9 | 6.4 | 39 |
| 85 | Origin of the SN2 benzylic effect. *Journal of the American Chemical Society*, **2008**, 130, 9887-96 | 16.4 | 63 |
| 84 | Establishment of the C(2)H(5)+O(2) reaction mechanism: a combustion archetype. *Journal of Chemical Physics*, **2008**, 128, 074308 | 3.9 | 45 |
| 83 | Triple excitations in state-specific multireference coupled cluster theory: application of Mk-MRCCSDT and Mk-MRCCSDT-n methods to model systems. *Journal of Chemical Physics*, **2008**, 128, 124104 | 3.9 | 119 |
| 82 | On the convergence of Z-averaged perturbation theory. *Journal of Chemical Physics*, **2008**, 128, 074107 | 3.9 | 15 |
| 81 | Thermochemistry of key soot formation intermediates: C3H3 isomers. *Journal of Physical Chemistry A*, **2007**, 111, 3819-30 | 2.8 | 54 |
| 80 | Ionization thresholds of small carbon clusters: tunable VUV experiments and theory. *Journal of the American Chemical Society*, **2007**, 129, 10229-43 | 16.4 | 69 |
| 79 | Model systems for probing metal cation hydration: the V+(H2O) and ArV+(H2O) complexes. *Journal of Physical Chemistry A*, **2007**, 111, 7599-610 | 2.8 | 21 |
| 78 | PSI3: an open-source Ab Initio electronic structure package. *Journal of Computational Chemistry*, **2007**, 28, 1610-1616 | 3.5 | 249 |
| 77 | Molecular structures of the two most stable conformers of free glycine. *Journal of Computational Chemistry*, **2007**, 28, 1373-83 | 3.5 | 68 |
| 76 | In search of definitive signatures of the elusive NCCO radical. *Journal of Chemical Physics*, **2007**, 127, 014306 | 3.9 | 19 |
| 75 | Unimolecular thermal fragmentation of ortho-benzyne. *Journal of Chemical Physics*, **2007**, 126, 044312 | 3.9 | 70 |
| 74 | Coupling term derivation and general implementation of state-specific multireference coupled cluster theories. *Journal of Chemical Physics*, **2007**, 127, 024102 | 3.9 | 242 |
| 73 | Secondary structures of peptides and proteins via NMR chemical-shielding anisotropy (CSA) parameters. *Journal of the American Chemical Society*, **2007**, 129, 1568-77 | 16.4 | 18 |
| 72 | High-order excitations in state-universal and state-specific multireference coupled cluster theories: model systems. *Journal of Chemical Physics*, **2006**, 125, 154113 | 3.9 | 199 |
| 71 | Adiabatic approximations to internal rotation. *Journal of Chemical Physics*, **2006**, 124, 224310 | 3.9 | 24 |
| 70 | Popular theoretical methods predict benzene and arenes to be nonplanar. *Journal of the American Chemical Society*, **2006**, 128, 9342-3 | 16.4 | 205 |
| 69 | On the nature of the M□ller-Plesset critical point. *Journal of Chemical Physics*, **2005**, 123, 64105 | 3.9 | 21 |

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| 68 | Downfield proton chemical shifts are not reliable aromaticity indicators. *Organic Letters*, **2005**, 7, 1457-60 | 6.2 | 62 |
| 67 | H-C-SiH3: direct generation and spectroscopic identification of ethylidene's cousin. *Journal of the American Chemical Society*, **2005**, 127, 12156-7 | 16.4 | 20 |
| 66 | Model identity SN2 reactions CH3X + X- (X = F, Cl, CN, OH, SH, NH2, PH2): Marcus theory analyzed. *Journal of Physical Chemistry A*, **2005**, 109, 10613-28 | 2.8 | 72 |
| 65 | The ab initio limit quartic force field of BH3. *Journal of Computational Chemistry*, **2005**, 26, 1106-12 | 3.5 | 49 |
| 64 | The highly anharmonic BH5 potential energy surface characterized in the ab initio limit. *Journal of Chemical Physics*, **2005**, 122, 104302 | 3.9 | 58 |
| 63 | Low-lying electronic states of FeNC and FeCN: a theoretical journey into isomerization and quartet/sextet competition. *Journal of Chemical Physics*, **2004**, 120, 4726-41 | 3.9 | 38 |
| 62 | Toward subchemical accuracy in computational thermochemistry: focal point analysis of the heat of formation of NCO and [H,N,C,O] isomers. *Journal of Chemical Physics*, **2004**, 120, 11586-99 | 3.9 | 285 |
| 61 | Molecular structure of proline. *Chemistry - A European Journal*, **2004**, 10, 4512-7 | 4.8 | 71 |
| 60 | Thermochemistry of disputed soot formation intermediates C4H3 and C4H5. *Journal of Chemical Physics*, **2004**, 121, 8800-13 | 3.9 | 64 |
| 59 | The Electronic Structure and Vibrational Spectrum oftrans-HNOO *Journal of Physical Chemistry A*, **2004**, 108, 2893-2903 | 2.8 | 40 |
| 58 | Triplet H-C-SiHCl(2): combined matrix-IR and CCSD(T) identification, and the role of the open-shell singlet state. *Organic Letters*, **2004**, 6, 1163-6 | 6.2 | 19 |
| 57 | Definitive ab initio studies of model SN2 reactions CH(3)X+F- (X=F, Cl, CN, OH, SH, NH(2), PH(2)). *Chemistry - A European Journal*, **2003**, 9, 2173-92 | 4.8 | 185 |
| 56 | Complete basis set limit studies of conventional and R12 correlation methods: The silicon dicarbide (SiC2) barrier to linearity. *Journal of Chemical Physics*, **2003**, 118, 7353 | 3.9 | 62 |
| 55 | On the accuracy limits of orbital expansion methods: Explicit effects of k-functions on atomic and molecular energies. *Journal of Chemical Physics*, **2003**, 118, 8594-8610 | 3.9 | 68 |
| 54 | A combined crossed-beam, ab initio, and RiceRamspergerKasselMarcus investigation of the reaction of carbon atoms C(3Pj) with benzene, C6H6(X 1A1g) and d6-benzene, C6D6(X 1A1g). *Journal of Chemical Physics*, **2002**, 116, 3248-3262 | 3.9 | 36 |
| 53 | Fragmentation path for hydrogen atom dissociation from methoxy radical. *Journal of Chemical Physics*, **2002**, 116, 10229-10237 | 3.9 | 32 |
| 52 | Systematic Study of Selected Diagonalization Methods for Configuration Interaction Matrices. *Journal of Computational Chemistry*, **2001**, 22, 1574-1589 | 3.5 | 40 |
| 51 | The second-order MllerPlesset limit for the barrier to linearity of water. *Journal of Chemical Physics*, **2001**, 114, 2875-2878 | 3.9 | 47 |

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| 50 | Dream or Reality: Complete Basis Set Full Configuration Interaction Potential Energy Hypersurfaces **2001**, 317-339 | | 47 |
| 49 | Interlocking Triplet Electronic States of Isocyanic Acid: Sources of Nonadiabatic Photofragmentation Dynamics *Journal of Physical Chemistry A*, **2001**, 105, 2716-2730 | 2.8 | 14 |
| 48 | Assessment of Density Functional Theory for Model SN2 Reactions: CH3X + F-(X = F, Cl, CN, OH, SH, NH2, PH2). *Journal of Physical Chemistry A*, **2001**, 105, 11327-11346 | 2.8 | 107 |
| 47 | Systematic Study of Selected Diagonalization Methods for Configuration Interaction Matrices **2001**, 22, 1574 | | 7 |
| 46 | Is Mo/ller Plesset perturbation theory a convergent ab initio method?. *Journal of Chemical Physics*, **2000**, 112, 9213-9222 | 3.9 | 117 |
| 45 | On apparent quantized transition-state thresholds in the photofragmentation of acetaldehyde. *Journal of Chemical Physics*, **2000**, 112, 5585-5592 | 3.9 | 44 |
| 44 | Anharmonic force field, vibrational energies, and barrier to inversion of SiH3 *Journal of Chemical Physics*, **2000**, 112, 4053-4063 | 3.9 | 52 |
| 43 | The C2H5 + O2 Reaction Mechanism: High-Level ab Initio Characterizations. *Journal of Physical Chemistry A*, **2000**, 104, 9823-9840 | 2.8 | 436 |
| 42 | The barrier to linearity of water. *Journal of Chemical Physics*, **1999**, 110, 11971-11981 | 3.9 | 65 |
| 41 | In pursuit of the ab initio limit for conformational energy prototypes. *Journal of Chemical Physics*, **1998**, 108, 9751-9764 | 3.9 | 606 |
| 40 | Fragmentation surface of triplet ketene. *Faraday Discussions*, **1998**, 110, 23-50 | 3.6 | 20 |
| 39 | Benchmark configuration interaction spectroscopic constants for X 1 + C2 and X 1 CN+. *Journal of Chemical Physics*, **1998**, 108, 6717-6721 | 3.9 | 36 |
| 38 | Mechanism of the C2H5+O2 reaction. *Journal of Chemical Physics*, **1997**, 107, 141-155 | 3.9 | 137 |
| 37 | Toward resolution of the silicon dicarbide (SiC2) saga: Ab initio excursions in the web of polytopism. *Journal of Chemical Physics*, **1997**, 107, 1195-1211 | 3.9 | 51 |
| 36 | The torsional conformations of butane: Definitive energetics from ab initio methods. *Journal of Chemical Physics*, **1997**, 106, 5143-5150 | 3.9 | 145 |
| 35 | Hartree Fock orbital instability envelopes in highly correlated single-reference wave functions. *Journal of Chemical Physics*, **1997**, 107, 10626-10632 | 3.9 | 128 |
| 34 | Variable reaction coordinate direct RRKM theory. *Zeitschrift Fur Elektrotechnik Und Elektrochemie*, **1997**, 101, 423-437 | | 30 |
| 33 | Cyclopropyne and Silacyclopropyne: A World of Difference. *Journal of the American Chemical Society*, **1996**, 118, 7158-7163 | 16.4 | 30 |

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| 32 | The effect of 1s correlation on De, re, and ω of first-row diatomics. *Journal of Chemical Physics*, **1996**, 104, 2746-2748 | 3.9 | 67 |
| 31 | Is the oxywater radical cation more stable than neutral oxywater?. *Journal of Chemical Physics*, **1996**, 104, 7615-7623 | 3.9 | 49 |
| 30 | A high level ab initio map and direct statistical treatment of the fragmentation of singlet ketene. *Journal of Chemical Physics*, **1996**, 105, 118-140 | 3.9 | 72 |
| 29 | General derivative relations for anharmonic force fields. *Molecular Physics*, **1996**, 89, 1213-1221 | 1.7 | 58 |
| 28 | The anharmonic force field and equilibrium molecular structure of ketene. *Journal of Chemical Physics*, **1995**, 102, 8506-8532 | 3.9 | 96 |
| 27 | The SN2 Identity Exchange Reaction F- + CH3F .fwdarw. FCH3 + F-: Definitive ab Initio Predictions. *The Journal of Physical Chemistry*, **1994**, 98, 13532-13540 | | 50 |
| 26 | A first principles theoretical determination of the rate constant for the dissociation of singlet ketene. *Journal of Chemical Physics*, **1994**, 101, 9198-9201 | 3.9 | 18 |
| 25 | The proton-transfer surface of CH3OHF+. *Journal of Chemical Physics*, **1994**, 100, 2058-2088 | 3.9 | 22 |
| 24 | The [FHCl]- molecular anion: Structural aspects, global surface, and vibrational eigenspectrum. *Journal of Chemical Physics*, **1993**, 99, 3865-3897 | 3.9 | 28 |
| 23 | Ab Initio Anharmonic Vibrational Analyses of Non-Rigid Molecules **1993**, 343-373 | | 80 |
| 22 | On the ab initio determination of higher-order force constants at nonstationary reference geometries. *Journal of Chemical Physics*, **1993**, 98, 2983-3015 | 3.9 | 151 |
| 21 | The heat of formation of NCO. *Journal of Chemical Physics*, **1993**, 99, 4638-4650 | 3.9 | 335 |
| 20 | Characterization of the X 1A' state of isocyanic acid. *Journal of Chemical Physics*, **1993**, 98, 1299-1328 | 3.9 | 116 |
| 19 | The puckering inversion barrier and vibrational spectrum of cyclopentene. A scaled quantum mechanical force field algorithm. *Journal of the American Chemical Society*, **1992**, 114, 6834-6849 | 16.4 | 103 |
| 18 | The SN2 identity exchange reaction ClCH2CN + Cl- .fwdarw. Cl- + ClCH2CN: experiment and theory. *Journal of the American Chemical Society*, **1992**, 114, 9136-9153 | 16.4 | 71 |
| 17 | The sodium superoxide radical: X 2A2 and ⍺ 2B2 potential energy surfaces. *Chemical Physics Letters*, **1991**, 186, 346-355 | 2.5 | 36 |
| 16 | A systematic study of molecular vibrational anharmonicity and vibration-rotation interaction by self-consistent-field higher-derivative methods. Linear polyatomic molecules. *Chemical Physics*, **1990**, 145, 427-466 | 2.3 | 250 |
| 15 | The lithium superoxide radical: Symmetry breaking phenomena and potential energy surfaces. *Chemical Physics*, **1989**, 133, 11-45 | 2.3 | 111 |

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|---|---|---|---|
| 14 | How bent can a benzene be? The molecular structure, infrared spectrum and energetics of [6]paracyclophane. *Chemical Physics*, **1988**, 123, 1-25 | 2.3 | 20 |
| 13 | A systematic study of molecular vibrational anharmonicity and vibration□otation interaction by self-consistent-field higher-derivative methods. Asymmetric top molecules. *Chemical Physics*, **1988**, 123, 187-239 | 2.3 | 443 |
| 12 | Reaction paths for the dissociation a 3A□CH2CO-¥n 3B1 CH2 + X 1⊞ CO. *Journal of Chemical Physics*, **1988**, 89, 329-344 | 3.9 | 61 |
| 11 | The anharmonic force fields of HOF and F2O. *Journal of Chemical Physics*, **1988**, 89, 4965-4975 | 3.9 | 57 |
| 10 | An examination of the 2 1A1 states of formaldehyde and ketene including analytic configuration interaction energy first derivatives for singlet excited electronic states of the same symmetry as the ground state. *Journal of Chemical Physics*, **1987**, 87, 7076-7095 | 3.9 | 43 |
| 9 | The analytic evaluation of energy first derivatives for two-configuration self-consistent-field configuration interaction (TCSCF-CI) wave functions. Application to ozone and ethylene. *Journal of Chemical Physics*, **1987**, 87, 7062-7075 | 3.9 | 102 |
| 8 | [5]Paracyclophane. An important example of ring strain and aromaticity in hydrocarbon compounds. *Journal of the American Chemical Society*, **1987**, 109, 2902-2909 | 16.4 | 49 |
| 7 | An ab initio study of the vibrational spectrum of bicyclo[1.1.0]but-1(3)-ene. *Journal of the American Chemical Society*, **1987**, 109, 1615-1621 | 16.4 | 42 |
| 6 | The infrared spectrum of the hydrogen bifluoride anion: unprecedented variation with level of theory. *Chemical Physics Letters*, **1986**, 131, 352-358 | 2.5 | 47 |
| 5 | Geometrical structures, force constants, and vibrational spectra of SiH, SiH2, SiH3, and SiH4. *Chemical Physics*, **1986**, 108, 243-274 | 2.3 | 142 |
| 4 | The experimental vibrational spectra, vibrational assignment, and normal coordinate analysis of thiirane-h4 and -d4 and cis- and trans-1,2-dideuteriothiirane: Ab initio theoretical IR spectra of thiirane, thiirene, and isotopically substituted derivatives. *Journal of Chemical Physics*, **1986**, 84, 4211-4227 | 3.9 | 25 |
| 3 | Ab initio studies of the low-lying electronic states of ketene. *Journal of Chemical Physics*, **1986**, 84, 2212-2225 | 3.9 | 51 |
| 2 | Adsorbing Colloid Flotation of Cu(II) with a Chelating Surfactant. *Separation Science and Technology*, **1979**, 14, 769-776 | 2.5 | 25 |
| 1 | General derivative relations for anharmonic force fields | | 3 |