Wesley D Allen

List of Publications by Year
in descending order

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139 papers	11,628 citations	26626 56 h-index	28296 105 g-index
143 all docs	143 docs citations	143 times ranked	6779 citing authors

#	Article	IF	Citations
1	Psi4: an openâ€source ab initio electronic structure program. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2012, 2, 556-565.	14.6	838
2	In pursuit of theab initiolimit for conformational energy prototypes. Journal of Chemical Physics, 1998, 108, 9751-9764.	3.0	659
3	A Hierarchy of Homodesmotic Reactions for Thermochemistry. Journal of the American Chemical Society, 2009, 131, 2547-2560.	13.7	508
4	The C2H5+ O2Reaction Mechanism:Â High-Level ab Initio Characterizations. Journal of Physical Chemistry A, 2000, 104, 9823-9840.	2.5	496
5	A systematic study of molecular vibrational anharmonicity and vibrationâ€"rotation interaction by self-consistent-field higher-derivative methods. Asymmetric top molecules. Chemical Physics, 1988, 123, 187-239.	1.9	476
6	The heat of formation of NCO. Journal of Chemical Physics, 1993, 99, 4638-4650.	3.0	365
7	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, 11586-11599.	3.0	317
8	Methylhydroxycarbene: Tunneling Control of a Chemical Reaction. Science, 2011, 332, 1300-1303.	12.6	274
9	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.	1.9	267
10	Capture of hydroxymethylene and its fast disappearance through tunnelling. Nature, 2008, 453, 906-909.	27.8	264
11	PSI3: An open-source Ab Initio electronic structure package. Journal of Computational Chemistry, 2007, 28, 1610-1616.	3.3	258
12	Coupling term derivation and general implementation of state-specific multireference coupled cluster theories. Journal of Chemical Physics, 2007, 127, 024102.	3.0	255
13	Popular Theoretical Methods Predict Benzene and Arenes To Be Nonplanar. Journal of the American Chemical Society, 2006, 128, 9342-9343.	13.7	238
14	High-order excitations in state-universal and state-specific multireference coupled cluster theories: Model systems. Journal of Chemical Physics, 2006, 125, 154113.	3.0	207
15	Definitive Ab Initio Studies of Model SN2 Reactions CH3X+F (X=F, Cl, CN, OH, SH, NH2, PH2). Chemistry - A European Journal, 2003, 9, 2173-2192.	3.3	196
16	On the ab initio determination of higherâ€order force constants at nonstationary reference geometries. Journal of Chemical Physics, 1993, 98, 2983-3015.	3.0	164
17	The torsional conformations of butane: Definitive energetics from ab initio methods. Journal of Chemical Physics, 1997, 106, 5143-5150.	3.0	159
18	Geometrical structures, force constants, and vibrational spectra of SiH, SiH2, SiH3, and SiH4. Chemical Physics, 1986, 108, 243-274.	1.9	148

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19	Mechanism of the C2H5+O2 reaction. Journal of Chemical Physics, 1997, 107, 141-155.	3.0	142
20	Hartreeâ€“Fock orbital instability envelopes in highly correlated single-reference wave functions. Journal of Chemical Physics, 1997, 107, 10626-10632.	3.0	142
21	Conformers of Gaseous Cysteine. Journal of Chemical Theory and Computation, 2009, 5, 1511-1523.	5.3	126
22	Characterization of theXÌƒâ€‰1Aâ€™ state of isocyanic acid. Journal of Chemical Physics, 1993, 98, 1299-1328.	3.0	125
23	Is Mo/llerâ€“Plesset perturbation theory a convergent ab initio method?. Journal of Chemical Physics, 2000, 112, 9213-9222.	3.0	125
24	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.	3.0	123
25	Assessment of Density Functional Theory for Model SN2 Reactions:Â CH3X + F-(X = F, Cl, CN, OH, SH, NH2,) Tj ETQq1 1 0.784314 rgBT	2.5	118
26	The lithium superoxide radical: Symmetry breaking phenomena and potential energy surfaces. Chemical Physics, 1989, 133, 11-45.	1.9	117
27	Exact ligand cone angles. Journal of Computational Chemistry, 2013, 34, 1189-1197.	3.3	112
28	The analytic evaluation of energy first derivatives for twoâ€configuration selfâ€consistentâ€field configuration interaction (TCSCFâ€CI) wave functions. Application to ozone and ethylene. Journal of Chemical Physics, 1987, 87, 7062-7075.	3.0	111
29	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.	13.7	109
30	The anharmonic force field and equilibrium molecular structure of ketene. Journal of Chemical Physics, 1995, 102, 8506-8532.	3.0	106
31	Ab Initio Anharmonic Vibrational Analyses of Non-Rigid Molecules. , 1993, , 343-373.		86
32	Reactions between Resonance-Stabilized Radicals: Propargyl + Allyl. Journal of Physical Chemistry A, 2010, 114, 4881-4890.	2.5	84
33	Ionization Thresholds of Small Carbon Clusters:â€‰ Tunable VUV Experiments and Theory. Journal of the American Chemical Society, 2007, 129, 10229-10243.	13.7	82
34	A high level ab initio map and direct statistical treatment of the fragmentation of singlet ketene. Journal of Chemical Physics, 1996, 105, 118-140.	3.0	81
35	Model Identity SN2 Reactions CH3X + X- (X = F, Cl, CN, OH, SH, NH2, PH2):â€‰ Marcus Theory Analyzed. Journal of Physical Chemistry A, 2005, 109, 10613-10628.	2.5	79
36	The SN2 identity exchange reaction ClCH2CN + Cl- .fwdarw. Cl- + ClCH2CN: experiment and theory. Journal of the American Chemical Society, 1992, 114, 9136-9153.	13.7	78

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37	Molecular Structure of Proline. Chemistry - A European Journal, 2004, 10, 4512-4517.	3.3	76
38	The effect of 1s correlation on De, re, and Ï‰e of firstâ€row diatomics. Journal of Chemical Physics, 1996, 104, 2746-2748.	3.0	74
39	The barrier to linearity of water. Journal of Chemical Physics, 1999, 110, 11971-11981.	3.0	73
40	Unimolecular thermal fragmentation ofortho-benzyne. Journal of Chemical Physics, 2007, 126, 044312.	3.0	73
41	Lowest-Lying Conformers of Alanine: Pushing Theory to Ascertain Precise Energetics and Semiexperimental R_e Structures. Journal of Chemical Theory and Computation, 2010, 6, 3066-3078.	5.3	73
42	Molecular structures of the two most stable conformers of free glycine. Journal of Computational Chemistry, 2007, 28, 1373-1383.	3.3	71
43	On the accuracy limits of orbital expansion methods: Explicit effects ofk-functions on atomic and molecular energies. Journal of Chemical Physics, 2003, 118, 8594-8610.	3.0	70
44	Probing the Delicate Balance between Pauli Repulsion and London Dispersion with Triphenylmethyl Derivatives. Journal of the American Chemical Society, 2018, 140, 14421-14432.	13.7	70
45	Analytic gradients for the state-specific multireference coupled cluster singles and doubles model. Journal of Chemical Physics, 2009, 131, 064109.	3.0	68
46	Complete basis set limit studies of conventional and R12 correlation methods: The silicon dicarbide (SiC[sub 2]) barrier to linearity. Journal of Chemical Physics, 2003, 118, 7353.	3.0	67
47	Origin of the S_N2 Benzylic Effect. Journal of the American Chemical Society, 2008, 130, 9887-9896.	13.7	67
48	Reaction paths for the dissociation alƒâ€‰3Aâ€˜ CH2COâ†’Xlƒâ€‰3B1 CH2â€‰+â€‰Xlƒâ€‰1Î£+ CO. Journal of Chemical Physics, 329-344.	3.0	66
49	Thermochemistry of disputed soot formation intermediates C4H3 and C4H5. Journal of Chemical Physics, 2004, 121, 8800-8813.	3.0	66
50	Downfield Proton Chemical Shifts Are Not Reliable Aromaticity Indicators. Organic Letters, 2005, 7, 1457-1460.	4.6	65
51	A companion perturbation theory for state-specific multireference coupled cluster methods. Physical Chemistry Chemical Physics, 2009, 11, 4728.	2.8	65
52	General derivative relations for anharmonic force fields. Molecular Physics, 1996, 89, 1213-1221.	1.7	62
53	The highly anharmonic BH5 potential energy surface characterized in the ab initio limit. Journal of Chemical Physics, 2005, 122, 104302.	3.0	62
54	Assigning quantum labels to variationally computed rotational-vibrational eigenstates of polyatomic molecules. Journal of Chemical Physics, 2010, 133, 034113.	3.0	61

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55	[5]Paracyclophane. An important example of ring strain and aromaticity in hydrocarbon compounds. Journal of the American Chemical Society, 1987, 109, 2902-2909.	13.7	59
56	The anharmonic force fields of HOF and F2O. Journal of Chemical Physics, 1988, 89, 4965-4975.	3.0	59
57	Abinitiostudies of the lowâ€lying electronic states of ketene. Journal of Chemical Physics, 1986, 84, 2212-2225.	3.0	58
58	Anharmonic force field, vibrational energies, and barrier to inversion of SiH3â^'. Journal of Chemical Physics, 2000, 112, 4053-4063.	3.0	57
59	Toward resolution of the silicon dicarbide (SiC2) saga:Ab initioexcursions in the web of polytopism. Journal of Chemical Physics, 1997, 107, 1195-1211.	3.0	55
60	Thermochemistry of Key Soot Formation Intermediates:Â C3H3Isomersâ€. Journal of Physical Chemistry A, 2007, 111, 3819-3830.	2.5	55
61	Theab initiolimit quartic force field of BH3. Journal of Computational Chemistry, 2005, 26, 1106-1112.	3.3	54
62	The SN2 Identity Exchange Reaction F- + CH3F .fwdarw. FCH3 + F-: Definitive ab Initio Predictions. The Journal of Physical Chemistry, 1994, 98, 13532-13540.	2.9	53
63	Is the oxywater radical cation more stable than neutral oxywater?. Journal of Chemical Physics, 1996, 104, 7615-7623.	3.0	53
64	Phenylhydroxycarbene. Journal of the American Chemical Society, 2010, 132, 7273-7275.	13.7	52
65	Dream or Reality: Complete Basis Set Full Configuration Interaction Potential Energy Hypersurfaces. , 2001, , 317-339.		51
66	The second-order MÃ¸llerâ€“Plesset limit for the barrier to linearity of water. Journal of Chemical Physics, 2001, 114, 2875-2878.	3.0	49
67	Establishment of the C2H5+O2 reaction mechanism: A combustion archetype. Journal of Chemical Physics, 2008, 128, 074308.	3.0	49
68	The infrared spectrum of the hydrogen bifluoride anion: unprecedented variation with level of theory. Chemical Physics Letters, 1986, 131, 352-358.	2.6	48
69	An examination of the 2â€‰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.	3.0	48
70	On apparent quantized transition-state thresholds in the photofragmentation of acetaldehyde. Journal of Chemical Physics, 2000, 112, 5585-5592.	3.0	46
71	Systematic Study of Selected Diagonalization Methods for Configuration Interaction Matrices. Journal of Computational Chemistry, 2001, 22, 1574-1589.	3.3	46
72	Domino Tunneling. Journal of the American Chemical Society, 2015, 137, 7828-7834.	13.7	46

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73	Taming the low-lying electronic states of FeH. Journal of Chemical Physics, 2012, 137, 234303.	3.0	44
74	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.	13.7	43
75	Anchoring the Absolute Proton Affinity Scale. Journal of Chemical Theory and Computation, 2008, 4, 1220-1229.	5.3	42
76	The Electronic Structure and Vibrational Spectrum oftrans-HNOOâ€. Journal of Physical Chemistry A, 2004, 108, 2893-2903.	2.5	41
77	Enthalpy of formation and anharmonic force field of diacetylene. Journal of Chemical Physics, 2009, 130, 044301.	3.0	41
78	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.	5.3	41
79	Benchmark configuration interaction spectroscopic constants for Xâ€‰1Î£g+â€‰C2 and Xâ€‰1Î£+â€‰CN+. Journal of Chemical Physics, 1998, 108, 6717-6721.	3.0	40
80	A combined crossed-beam, ab initio, and Riceâ€“Ramspergerâ€“Kasselâ€“ Marcus investigation of the reaction of carbon atoms C(3Pj) with benzene, C6H6(Xâ€Š1A1g) and d6-benzene, C6D6(Xâ€Š1A1g). Journal of Chemical Physics, 2002, 116, 3248-3262.	3.0	39
81	Low-lying electronic states of FeNC and FeCN: A theoretical journey into isomerization and quartet/sextet competition. Journal of Chemical Physics, 2004, 120, 4726-4741.	3.0	39
82	The sodium superoxide radical: Xì*f*2A2 and Ã*f* 2B2 potential energy surfaces. Chemical Physics Letters, 1991, 186, 346-355.	2.6	38
83	Polytwistane. Chemistry - A European Journal, 2014, 20, 1638-1645.	3.3	38
84	The [FHCl]â^'molecular anion: Structural aspects, global surface, and vibrational eigenspectrum. Journal of Chemical Physics, 1993, 99, 3865-3897.	3.0	35
85	Cyclopropyne and Silacyclopropyne:Â A World of Difference. Journal of the American Chemical Society, 1996, 118, 7158-7163.	13.7	35
86	Free Cyclooctatetraene Dianion: Planarity, Aromaticity, and Theoretical Challenges. Journal of Chemical Theory and Computation, 2013, 9, 4436-4443.	5.3	33
87	Ï€-Complexation in Nickel-Catalyzed Cross-Coupling Reactions. Journal of Organic Chemistry, 2014, 79, 1836-1841.	3.2	33
88	The experimental vibrational spectra, vibrational assignment, and normal coordinate analysis of thiiraneâ€h4and â€d4andcisâ€•andtransâ€1,2â€dideuteriothiirane:Abinitiotheoretical IR spectra of thiirane, thiirene, and isotopically substituted derivatives. Journal of Chemical Physics, 1986, 84, 4211-4227.	3.0	32
89	Variable reaction coordinate direct RRKM theory. Zeitschrift Fur Elektrotechnik Und Elektrochemie, 1997, 101, 423-437.	0.9	32
90	Fragmentation path for hydrogen atom dissociation from methoxy radical. Journal of Chemical Physics, 2002, 116, 10229-10237.	3.0	32

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91	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	32
92	Structureâ€“reactivity relationships for aromatic molecules: electrostatic potentials at nuclei and electrophile affinity indices. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2013, 3, 37-55.	14.6	31
93	Tunnelling in carbonic acid. Chemical Communications, 2016, 52, 7858-7861.	4.1	31
94	On the Role of Disproportionation Energy in Kumada Catalyst-Transfer Polycondensation. ACS Macro Letters, 2012, 1, 995-1000.	4.8	29
95	Adsorbing Colloid Flotation of Cu(II) with a Chelating Surfactant. Separation Science and Technology, 1979, 14, 769-776.	2.5	28
96	Adiabatic approximations to internal rotation. Journal of Chemical Physics, 2006, 124, 224310.	3.0	26
97	How bent can a benzene be? The molecular structure, infrared spectrum and energetics of [6]paracyclophane. Chemical Physics, 1988, 123, 1-25.	1.9	25
98	Nearly Degenerate Isomers of C(BH)₂: Cumulene, Carbene, or Carbone?. Chemistry - A European Journal, 2013, 19, 15941-15954.	3.3	25
99	The protonâ€transfer surface of CH3OHFâ¯. Journal of Chemical Physics, 1994, 100, 2058-2088.	3.0	24
100	On the nature of the MÃ¸ller-Plesset critical point. Journal of Chemical Physics, 2005, 123, 064105.	3.0	24
101	Exact Ligand Solid Angles. Journal of Chemical Theory and Computation, 2013, 9, 5734-5744.	5.3	24
102	Dipole Moment of the HOOO Radical: Resolution of a Structural Enigma. Journal of Physical Chemistry Letters, 2013, 4, 3584-3589.	4.6	23
103	Conformers of Gaseous Serine. Journal of Chemical Theory and Computation, 2016, 12, 3571-3582.	5.3	23
104	A first principles theoretical determination of the rate constant for the dissociation of singlet ketene. Journal of Chemical Physics, 1994, 101, 9198-9201.	3.0	22
105	Fragmentation surface of triplet ketene. Faraday Discussions, 1998, 110, 23-50.	3.2	22
106	Hâ¯Câ¯SiH3:Â Direct Generation and Spectroscopic Identification of Ethylidene's Cousin. Journal of the American Chemical Society, 2005, 127, 12156-12157.	13.7	22
107	Model Systems for Probing Metal Cation Hydration:Â The V+(H2O) and ArV+(H2O) Complexesâ€. Journal of Physical Chemistry A, 2007, 111, 7599-7610.	2.5	22
108	Triplet Hâ¯Câ¯SiHCl2:â€‰ Combined Matrix-IR and CCSD(T) Identification, and the Role of the Open-Shell Singlet State. Organic Letters, 2004, 6, 1163-1166.	4.6	21

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109	Do Ï€-Conjugative Effects Facilitate SN2 Reactions?. Journal of the American Chemical Society, 2014, 136, 3118-3126.	13.7	20
110	In search of definitive signatures of the elusive NCCO radical. Journal of Chemical Physics, 2007, 127, 014306.	3.0	19
111	Secondary Structures of Peptides and Proteins via NMR Chemical-Shielding Anisotropy (CSA) Parameters. Journal of the American Chemical Society, 2007, 129, 1568-1577.	13.7	19
112	Ring-Walking of Zerovalent Nickel on Aryl Halides. Journal of Chemical Theory and Computation, 2017, 13, 1706-1711.	5.3	19
113	Nucleophilic Influences and Origin of the S N 2 Allylic Effect. Chemistry - A European Journal, 2018, 24, 11637-11648.	3.3	17
114	On the convergence of Z-averaged perturbation theory. Journal of Chemical Physics, 2008, 128, 074107.	3.0	15
115	Interlocking Triplet Electronic States of Isocyanic Acid:Â Sources of Nonadiabatic Photofragmentation Dynamicsâ€. Journal of Physical Chemistry A, 2001, 105, 2716-2730.	2.5	14
116	The multichannel n-propyl + O2 reaction surface: Definitive theory on a model hydrocarbon oxidation mechanism. Journal of Chemical Physics, 2018, 148, .	3.0	14
117	Infrared signatures of the NCCO radical. Physical Chemistry Chemical Physics, 2009, 11, 10385.	2.8	13
118	Barrier To Linearity and Anharmonic Force Field of the Ketenyl Radical. Journal of Physical Chemistry A, 2009, 113, 11643-11650.	2.5	12
119	The electronic structure of vanadium monochloride cation (VCl+): Tackling the complexities of transition metal species. Journal of Chemical Physics, 2014, 141, 204302.	3.0	12
120	Chemistry as a function of the fine-structure constant and the electron-proton mass ratio. Physical Review A, 2010, 81, .	2.5	11
121	Tunneling Isomerizations on the Potential Energy Surfaces of Formaldehyde and Methanol Radical Cations. ACS Earth and Space Chemistry, 2017, 1, 361-367.	2.7	11
122	Intricate Conformational Tunneling in Carbonic Acid Monomethyl Ester. Journal of Physical Chemistry Letters, 2018, 9, 1663-1667.	4.6	11
123	Riddles of the structure and vibrational dynamics of HO3 resolved near the ab initio limit. Journal of Chemical Physics, 2019, 151, 094304.	3.0	11
124	The problematic C2H4+F2 reaction barrier. Journal of Chemical Physics, 2010, 132, 094304.	3.0	10
125	Intricate Internal Rotation Surface and Fundamental Infrared Transitions of the n-Propyl Radical. Journal of Physical Chemistry B, 2015, 119, 728-735.	2.6	10
126	Reaction Profiles and Kinetics for Radicalâ€“Radical Hydrogen Abstraction via Multireference Coupled Cluster Theory. Journal of Chemical Theory and Computation, 2020, 16, 1511-1525.	5.3	8

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127	Systematic Study of Selected Diagonalization Methods for Configuration Interaction Matrices. Journal of Computational Chemistry, 2001, 22, 1574-1589.	3.3	7
128	Sub-Doppler infrared spectroscopy and formation dynamics of triacetylene in a slit supersonic expansion. Journal of Chemical Physics, 2016, 144, 074301.	3.0	6
129	Polytriangulane. Journal of Chemical Theory and Computation, 2016, 12, 4707-4716.	5.3	6
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.	2.8	6
131	Ligand Steric Descriptors. Annual Reports in Computational Chemistry, 2013, , 3-23.	1.7	5
132	Identification and Reactivity of s-cis,s-cis-Dihydroxycarbene, a New [CH₂O₂] Intermediate. Journal of the American Chemical Society, 2020, 142, 19457-19461.	13.7	5
133	Ïƒ Bond activation through tunneling: formation of the boron hydride cations BH_n⁺ (n = 2, 4, 6). Physical Chemistry Chemical Physics, 2016, 18, 4063-4070.	2.8	4
134	The LiÂ·Â·Â·HF van der Waals minimum and the barrier to the deep HFâ€“Li potential well. Molecular Physics, 2014, 112, 770-773.	1.7	3
135	General derivative relations for anharmonic force fields. Molecular Physics, 1996, 89, 1213-1221.	1.7	3
136	Bond Angles around a Tetravalent Atom. Journal of Physical Chemistry A, 2015, 119, 1534-1538.	2.5	1
137	A Universal Integrated Rate Equation for Chemical Kinetics. Journal of Physical Chemistry A, 2018, 122, 4009-4014.	2.5	1
138	Wigner numbers. Journal of Chemical Physics, 2019, 151, 244122.	3.0	1
139	Counterfactual Quantum Chemistry of Water. , 2010, , 119-134.		0