Kenneth Ruud

List of Publications by Year
in descending order

335 papers	16,495 citations	16791 66 h-index	26792 111 g-index
364 all docs	364 docs citations	364 times ranked	9253 citing authors

#	Article	IF	Citations
1	Ab Initio Methods for the Calculation of NMR Shielding and Indirect Spinâ"Spin Coupling Constants. Chemical Reviews, 1999, 99, 293-352.	23.0	1,318
2	The <scp>D</scp>alton quantum chemistry program system. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2014, 4, 269-284.	6.2	1,166
3	Recent Advances in Wave Function-Based Methods of Molecular-Property Calculations. Chemical Reviews, 2012, 112, 543-631.	23.0	549
4	Multiconfigurational selfâ€consistent field calculations of nuclear shieldings using London atomic orbitals. Journal of Chemical Physics, 1994, 100, 8178-8185.	1.2	229
5	Vibrational Raman optical activity calculations using London atomic orbitals. Faraday Discussions, 1994, 99, 165-180.	1.6	225
6	An efficient approach for calculating vibrational wave functions and zero-point vibrational corrections to molecular properties of polyatomic molecules. Journal of Chemical Physics, 2000, 112, 2668-2683.	1.2	209
7	Hartreeâ€"Fock limit magnetizabilities from London orbitals. Journal of Chemical Physics, 1993, 99, 3847-3859.	1.2	202
8	Perturbationâ€dependent atomic orbitals for the calculation of spinâ€rotation constants and rotational g tensors. Journal of Chemical Physics, 1996, 105, 2804-2812.	1.2	201
9	Optical rotation studied by density-functional and coupled-cluster methods. Chemical Physics Letters, 2002, 352, 533-539.	1.2	192
10	Gaugeâ€origin independent multiconfigurational selfâ€consistentâ€field theory for vibrational circular dichroism. Journal of Chemical Physics, 1993, 98, 8873-8887.	1.2	186
11	Basis-set dependence of nuclear spin-spin coupling constants. Theoretical Chemistry Accounts, 1998, 99, 175-182.	0.5	175
12	Arbitrary-Order Density Functional Response Theory from Automatic Differentiation. Journal of Chemical Theory and Computation, 2010, 6, 1971-1980.	2.3	174
13	Gauge-Origin Independent Density-Functional Theory Calculations of Vibrational Raman Optical Activity. Journal of Physical Chemistry A, 2002, 106, 7448-7455.	1.1	162
14	Benchmarking two-photon absorption cross sections: performance of CC2 and CAM-B3LYP. Physical Chemistry Chemical Physics, 2015, 17, 19306-19314.	1.3	160
15	Vibrational corrections to indirect nuclear spinâ€"spin coupling constants calculated by density-functional theory. Journal of Chemical Physics, 2003, 118, 9572-9581.	1.2	156
16	TDDFT diagnostic testing and functional assessment for triazene chromophores. Physical Chemistry Chemical Physics, 2009, 11, 4465.	1.3	145
17	Coupled-cluster calculations of optical rotation. Chemical Physics Letters, 2003, 373, 606-614.	1.2	138
18	Zero-Point Vibrational Effects on Proton Shieldings:Â Functional-Group Contributions from ab Initio Calculations. Journal of the American Chemical Society, 2001, 123, 4826-4833.	6.6	127

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19	Perturbationalab initiocalculations of relativistic contributions to nuclear magnetic resonance shielding tensors. Journal of Chemical Physics, 2003, 119, 2623-2637.	1.2	124
20	Density functional theory calculation of electronic circular dichroism using London orbitals. Chemical Physics Letters, 2004, 388, 110-119.	1.2	123
21	Excitation Energies in Solution: The Fully Polarizable QM/MM/PCM Method. Journal of Physical Chemistry B, 2011, 115, 3027-3037.	1.2	118
22	Rovibrational effects, temperature dependence, and isotope effects on the nuclear shielding tensors of water: A new 17O absolute shielding scale. Journal of Chemical Physics, 1998, 109, 8388-8397.	1.2	115
23	Multiconfigurational self-consistent field linear response for the polarizable continuum model: Theory and application to ground and excited-state polarizabilities of para-nitroaniline in solution. Journal of Chemical Physics, 2003, 119, 5818-5827.	1.2	113
24	Leading-order relativistic effects on nuclear magnetic resonance shielding tensors. Journal of Chemical Physics, 2005, 122, 114107.	1.2	113
25	The Ab Initio Calculation of Optical Rotation and Electronic Circular Dichroism. Advances in Quantum Chemistry, 2005, 50, 185-212.	0.4	109
26	Basis Set and Density Functional Dependence of Vibrational Raman Optical Activity Calculations. Journal of Physical Chemistry A, 2005, 109, 7567-7574.	1.1	105
27	Calculation of the vibrational wave function of polyatomic molecules. Journal of Chemical Physics, 2000, 112, 2655-2667.	1.2	104
28	Conformational Effects on the Optical Rotation of Alanine and Proline. Journal of Physical Chemistry A, 2004, 108, 4269-4276.	1.1	103
29	Density-functional-theory study of the electric-field-induced second harmonic generation (EFISHG) of pushâ€“pull phenylpolyenes in solution. Chemical Physics Letters, 2006, 425, 267-272.	1.2	99
30	A density matrix-based quasienergy formulation of the Kohnâ€“Sham density functional response theory using perturbation- and time-dependent basis sets. Journal of Chemical Physics, 2008, 129, 214108.	1.2	99
31	The Importance of Molecular Vibrations: The Sign Change of the Optical Rotation of Methyloxirane. Angewandte Chemie - International Edition, 2005, 44, 3594-3596.	7.2	98
32	Quadratic response calculations of the electronic spin-orbit contribution to nuclear shielding tensors. Journal of Chemical Physics, 1998, 109, 1212-1222.	1.2	97
33	Theoretical approaches to the calculation of Raman optical activity spectra. Chirality, 2009, 21, E54-67.	1.3	97
34	Zero-point vibrational effects on optical rotation. Chemical Physics Letters, 2001, 337, 217-223.	1.2	95
35	Electronically Excited States of Vitamin B₁₂: Benchmark Calculations Including Time-Dependent Density Functional Theory and Correlated ab Initio Methods. Journal of Physical Chemistry A, 2011, 115, 1280-1292.	1.1	94
36	Pyrrolo[3,2â€b]pyrrolesâ€”From Unprecedented Solvatofluorochromism to Twoâ€Photon Absorption. Chemistry - A European Journal, 2015, 21, 18364-18374.	1.7	93

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37	Explicit versus Implicit Solvent Modeling of Raman Optical Activity Spectra. Journal of Physical Chemistry B, 2011, 115, 4128-4137.	1.2	92
38	A Combined Atomic Force Microscopy and Computational Approach for the Structural Elucidation of Breitfussin A and B: Highly Modified Halogenated Dipeptides from Thuiaria breitfussi. Angewandte Chemie - International Edition, 2012, 51, 12238-12241.	7.2	92
39	Optical Rotation Calculation of a Highly Flexible Molecule:Â The Case of Paraconic Acid. Journal of Physical Chemistry A, 2005, 109, 1449-1453.	1.1	91
40	Ab initio calculations of zero-field splitting parameters. Chemical Physics, 2002, 279, 133-142.	0.9	90
41	All-Metal Aromaticity: Revisiting the Ring Current Model among Transition Metal Clusters. Journal of Chemical Theory and Computation, 2013, 9, 4789-4796.	2.3	90
42	ReSpect: Relativistic spectroscopy DFT program package. Journal of Chemical Physics, 2020, 152, 184101.	1.2	90
43	Electric field dependence of magnetic properties: Multiconfigurational selfâ€consistent field calculations of hypermagnetizabilities and nuclear shielding polarizabilities of N2, C2H2, HCN, and H2O. Journal of Chemical Physics, 1995, 102, 8953-8966.	1.2	89
44	Ab initio. Theoretica Chimica Acta, 1995, 90, 441.	0.9	86
45	On the Nature and Incidence of Î²-Agostic Interactions in Ethyl Derivatives of Early Transition Metals:Â Ethyltitanium Trichloride and Related Compounds. Journal of the American Chemical Society, 1998, 120, 3762-3772.	6.6	84
46	On the molecular electric quadrupole moment and the electric-field-gradient-induced birefringence of CO2 and CS2. Chemical Physics Letters, 2000, 326, 269-276.	1.2	83
47	Structure, solvent, and relativistic effects on the NMR chemical shifts in square-planar transition-metal complexes: assessment of DFT approaches. Physical Chemistry Chemical Physics, 2015, 17, 24944-24955.	1.3	82
48	Density-functional theory calculations of optical rotatory dispersion in the nonresonant and resonant frequency regions. Journal of Chemical Physics, 2004, 120, 5027-5035.	1.2	81
49	An analytical derivative procedure for the calculation of vibrational Raman optical activity spectra. Journal of Chemical Physics, 2007, 127, 204105.	1.2	79
50	Polarizable Density Embedding: A New QM/QM/MM-Based Computational Strategy. Journal of Physical Chemistry A, 2015, 119, 5344-5355.	1.1	78
51	Accurate magnetizabilities of the isoelectronic series BeHâº, BH, and CH+. The MCSCF-GIAO approach. Chemical Physics, 1995, 195, 157-169.	0.9	77
52	Calculation of two-photon absorption strengths with the approximate coupled cluster singles and doubles model CC2 using the resolution-of-identity approximation. Physical Chemistry Chemical Physics, 2012, 14, 1175-1184.	1.3	76
53	A combined quantum mechanics/molecular mechanics study of the one- and two-photon absorption in the green fluorescent protein. Physical Chemistry Chemical Physics, 2012, 14, 5440.	1.3	76
54	Coupled cluster response calculation of natural chiroptical spectra. Journal of Chemical Physics, 1999, 110, 2883-2892.	1.2	75

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55	Second- and third-order spin-orbit contributions to nuclear shielding tensors. Journal of Chemical Physics, 1999, 111, 2900-2909.	1.2	74
56	Solvent Effects on NMR Isotropic Shielding Constants. A Comparison between Explicit Polarizable Discrete and Continuum Approaches. Journal of Physical Chemistry A, 2007, 111, 4199-4210.	1.1	74
57	Magnetizability of Hydrocarbons. Journal of the American Chemical Society, 1994, 116, 10135-10140.	6.6	73
58	Excitation Energies from Real-Time Propagation of the Four-Component Diracâ€“Kohnâ€“Sham Equation. Journal of Chemical Theory and Computation, 2015, 11, 980-991.	2.3	72
59	A second-order, quadratically convergent multiconfigurational self-consistent field polarizable continuum model for equilibrium and nonequilibrium solvation. Journal of Chemical Physics, 2002, 117, 13-26.	1.2	71
60	Can Raman Optical Activity Separate Axial from Local Chirality? A Theoretical Study of Helical Deca-Alanine. ChemPhysChem, 2006, 7, 2189-2196.	1.0	71
61	Determining the Absolute Configuration of Two Marine Compounds Using Vibrational Chiroptical Spectroscopy. Journal of Organic Chemistry, 2012, 77, 858-869.	1.7	71
62	Electric and magnetic properties of fullerenes. Journal of Chemical Physics, 1998, 109, 572-577.	1.2	70
63	Solvent Effects on the Indirect Spinâ€“Spin Coupling Constants of Benzene: The DFT-PCM Approach. International Journal of Molecular Sciences, 2003, 4, 119-134.	1.8	68
64	Calculation of the first static hyperpolarizability tensor of three-dimensional periodic compounds with a local basis set: A comparison of LDA, PBE, PBE0, B3LYP, and HF results. Journal of Chemical Physics, 2010, 132, 244106.	1.2	68
65	Orbital connections for perturbation-dependent basis sets. Theoretica Chimica Acta, 1995, 90, 421-439.	0.9	67
66	Ab initio calculation of vibrational Raman optical activity. International Journal of Quantum Chemistry, 2005, 104, 816-829.	1.0	67
67	Ab initio determinations of magnetic circular dichroism. Chemical Physics Letters, 1999, 300, 61-68.	1.2	66
68	Internal and external heavy-atom effects on phosphorescence radiative lifetimes calculated using a mean-field spinâ€“orbit Hamiltonian. Chemical Physics Letters, 1999, 310, 215-221.	1.2	65
69	The Absolute Shielding Constants of Heavy Nuclei: Resolving the Enigma of the ¹¹⁹Sn Absolute Shielding. Journal of Physical Chemistry Letters, 2013, 4, 459-463.	2.1	64
70	Complex polarization propagator calculations of magnetic circular dichroism spectra. Journal of Chemical Physics, 2008, 128, 094103.	1.2	63
71	Relativistic effects on linear and nonlinear polarizabilities studied by effective-core potential, Douglasâ€“Kroll, and Diracâ€“Hartreeâ€“Fock response theory. Journal of Chemical Physics, 2002, 116, 6914-6923.	1.2	60
72	Ro-Vibrational Corrections to NMR Parameters. , 2004, , 153-173.		60

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73	Benchmarking density-functional-theory calculations of rotational g tensors and magnetizabilities using accurate coupled-cluster calculations. Journal of Chemical Physics, 2009, 131, 144104.	1.2	60
74	Transferability of Various Molecular Property Tensors in Vibrational Spectroscopy. Journal of Chemical Theory and Computation, 2012, 8, 977-985.	2.3	60
75	Four-Component Relativistic Density Functional Theory Calculations of NMR Shielding Tensors for Paramagnetic Systems. Journal of Physical Chemistry A, 2013, 117, 14209-14219.	1.1	60
76	Rovibrationally averaged magnetizability, rotational g factor, and indirect spinâ€“spin coupling of the hydrogen fluoride molecule. Journal of Chemical Physics, 1999, 110, 9463-9468.	1.2	59
77	Solvent Effects on Raman Optical Activity Spectra Calculated Using the Polarizable Continuum Model. Journal of Physical Chemistry A, 2006, 110, 2807-2815.	1.1	59
78	Nuclear magnetic shielding constants of liquid water: Insights from hybrid quantum mechanics/molecular mechanics models. Journal of Chemical Physics, 2007, 126, 034510.	1.2	59
79	Determination of Absolute Configuration and Conformation of a Cyclic Dipeptide by NMR and Chiral Spectroscopic Methods. Journal of Physical Chemistry A, 2013, 117, 1721-1736.	1.1	59
80	Chemical Control of Channel Interference in Two-Photon Absorption Processes. Accounts of Chemical Research, 2014, 47, 1604-1612.	7.6	59
81	Magnetizability and nuclear shielding constants of solvated water. Chemical Physics Letters, 1996, 253, 443-447.	1.2	58
82	Solvent effects on nuclear shieldings and spinâ€“spin couplings of hydrogen selenide. Journal of Chemical Physics, 1998, 108, 2528-2537.	1.2	58
83	Polarizable continuum model study of solvent effects on electronic circular dichroism parameters. Journal of Chemical Physics, 2005, 122, 024106.	1.2	58
84	The ab initio calculation of molecular electric, magnetic and geometric properties. Physical Chemistry Chemical Physics, 2011, 13, 2627-2651.	1.3	58
85	X-ray absorption resonances near L_{2,3}-edges from real-time propagation of the Diracâ€“Kohnâ€“Sham density matrix. Physical Chemistry Chemical Physics, 2015, 17, 22566-22570.	1.3	58
86	A multipole reaction-field model for gauge-origin independent magnetic properties of solvated molecules. Journal of Chemical Physics, 1997, 106, 1170-1180.	1.2	57
87	DFT as a Powerful Predictive Tool in Photoredox Catalysis: Redox Potentials and Mechanistic Analysis. Organometallics, 2015, 34, 4218-4228.	1.1	57
88	On the validity of the equivalent cores approximation for computing X-ray photoemission and photoabsorption spectral bands. Chemical Physics, 2000, 260, 11-28.	0.9	56
89	Benchmarking the Performance of Exchange-Correlation Functionals for Predicting Two-Photon Absorption Strengths. Journal of Chemical Theory and Computation, 2018, 14, 3677-3685.	2.3	56
90	The A and B Terms of Magnetic Circular Dichroism Revisited. Journal of Physical Chemistry A, 2008, 112, 9615-9618.	1.1	55

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91	Gauge-origin independent calculation of magnetizabilities and rotational g tensors at the coupled-cluster level. Journal of Chemical Physics, 2007, 127, 074101.	1.2	53
92	Molecular optical rotation: an evaluation of semiempirical models. Chemical Physics Letters, 2000, 319, 595-600.	1.2	52
93	Atomic Charges of the Water Molecule and the Water Dimer. Journal of Physical Chemistry A, 1998, 102, 7686-7691.	1.1	51
94	Solvent effects on zero-point vibrational corrections to optical rotations and nuclear magnetic resonance shielding constants. Chemical Physics Letters, 2008, 451, 226-232.	1.2	50
95	Ab initio study of the one- and two-photon circular dichroism of R-(+)-3-methyl-cyclopentanone. Journal of Chemical Physics, 2008, 128, 164312.	1.2	50
96	Calibration of the n-electron valence state perturbation theory approach. Journal of Chemical Physics, 2004, 120, 4619-4625.	1.2	49
97	Four-Component Relativistic Density Functional Theory Calculations of EPRg- and Hyperfine-Coupling Tensors Using Hybrid Functionals: Validation on Transition-Metal Complexes with Large Tensor Anisotropies and Higher-Order Spinâ€“Orbit Effects. Journal of Physical Chemistry A, 2015, 119, 12892-12905.	1.1	49
98	Correlated response calculations of the spin-orbit interaction contribution to nuclear spin-spin couplings. Journal of Computational Chemistry, 1999, 20, 1314-1327.	1.5	48
99	Ab initio calculations of zero-field splitting parameters in linear polyacenes. Chemical Physics, 2003, 286, 127-137.	0.9	48
100	Acceleration of Relativistic Electron Dynamics by Means of X2C Transformation: Application to the Calculation of Nonlinear Optical Properties. Journal of Chemical Theory and Computation, 2016, 12, 5823-5833.	2.3	48
101	Efficient parallel implementation of response theory: Calculations of the second hyperpolarizability of polyacenes. Chemical Physics Letters, 1996, 253, 1-7.	1.2	47
102	Charge-Transfer Excitations in Uranyl Tetrachloride ([UO₂Cl₄]^{2â€“}): How Reliable are Electronic Spectra from Relativistic Time-Dependent Density Functional Theory?. Journal of Physical Chemistry A, 2012, 116, 7397-7404.	1.1	47
103	Ab initio calculation of electronic circular dichroism fortrans-cyclooctene using London atomic orbitals. Theoretica Chimica Acta, 1995, 90, 441-458.	0.9	46
104	The magnetizability, rotational g tensor, and quadrupole moment of PF3 revisited. Chemical Physics Letters, 1997, 264, 17-23.	1.2	46
105	Large two-photon absorption cross section: molecular tweezer as a new promising class of compounds for nonlinear optics. Physical Chemistry Chemical Physics, 2009, 11, 2592.	1.3	46
106	Intermolecular charge transfer enhances two-photon absorption in yellow fluorescent protein. Physical Chemistry Chemical Physics, 2014, 16, 5958.	1.3	46
107	The effect of correlation on molecular magnetizabilities and rotational g tensors. Journal of Chemical Physics, 1997, 107, 10599-10606.	1.2	45
108	Computational Study of the One- and Two-Photon Absorption and Circular Dichroism of (<scp>l</scp>)-Tryptophan. Journal of Physical Chemistry B, 2010, 114, 6500-6512.	1.2	45

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109	The optical activity of Î²,Î³-enones in ground and excited states using circular dichroism and circularly polarized luminescence. Physical Chemistry Chemical Physics, 2011, 13, 643-650.	1.3	45
110	Dalton Project: A Python platform for molecular- and electronic-structure simulations of complex systems. Journal of Chemical Physics, 2020, 152, 214115.	1.2	45
111	A polarizable embedding DFT study of one-photon absorption in fluorescent proteins. Physical Chemistry Chemical Physics, 2013, 15, 4735.	1.3	44
112	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
113	Electronically Excited States of Vitamin B₁₂ and Methylcobalamin: Theoretical Analysis of Absorption, CD, and MCD Data. Journal of Physical Chemistry B, 2011, 115, 737-748.	1.2	43
114	GEN1INT: A unified procedure for the evaluation of one-electron integrals over Gaussian basis functions and their geometric derivatives. International Journal of Quantum Chemistry, 2011, 111, 858-872.	1.0	43
115	Second-harmonic generation of solvated molecules using multiconfigurational self-consistent-field quadratic response theory and the polarizable continuum model. Journal of Chemical Physics, 2005, 123, 144117.	1.2	42
116	Intermolecular Interaction-Controlled Tuning of the Two-Photon Absorption of Fullerene Bound in a Buckycatcher. Journal of Physical Chemistry A, 2009, 113, 5485-5488.	1.1	41
117	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.	2.3	41
118	Coupled cluster investigation of the electric-field-gradient-induced birefringence of H2, N2, C2H2, and CH4. Journal of Chemical Physics, 1998, 109, 7176-7184.	1.2	40
119	Electric field effects on the shielding constants of noble gases: A four-component relativistic Hartree-Fock study. Journal of Chemical Physics, 2004, 121, 3051-3057.	1.2	40
120	Magnetic properties with multiwavelets and DFT: the complete basis set limit achieved. Physical Chemistry Chemical Physics, 2016, 18, 21145-21161.	1.3	40
121	MCSCF calculations of hypermagnetizabilities and nuclear shielding polarizabilities of CO and CH₄. Molecular Physics, 1996, 88, 931-947.	0.8	39
122	The use of Coulomb-attenuated methods for the calculation of electronic circular dichroism spectra. Chemical Physics, 2008, 349, 234-243.	0.9	39
123	A modified variation-perturbation approach to zero-point vibrational motion. Theoretical Chemistry Accounts, 2000, 103, 365-373.	0.5	38
124	High-Polarity Solvents Decreasing the Two-Photon Transition Probability of Through-Space Charge-Transfer Systems â€" A Surprising In Silico Observation. Journal of Physical Chemistry Letters, 2012, 3, 961-966.	2.1	38
125	Analytic cubic and quartic force fields using density-functional theory. Journal of Chemical Physics, 2014, 140, 034103.	1.2	38
126	Fully adaptive algorithms for multivariate integral equations using the non-standard form and multiwavelets with applications to the Poisson and bound-state Helmholtz kernels in three dimensions. Molecular Physics, 2013, 111, 1143-1160.	0.8	37

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127	Convergence of environment polarization effects in multiscale modeling of excitation energies. Computational and Theoretical Chemistry, 2014, 1040-1041, 304-311.	1.1	36
128	NMR Shielding Tensors and Indirect Spin-Spin Coupling Tensors in HCN, HNC, CH3CN, and Ch3NC Molecules. Journal of Magnetic Resonance Series A, 1995, 114, 212-218.	1.6	35
129	The dispersion of the polarizability of C60: A confirmation of recent experimental results through theoretical calculations. Journal of Chemical Physics, 2001, 114, 4331-4332.	1.2	35
130	Plasmon resonances in linear noble-metal chains. Journal of Chemical Physics, 2012, 137, 194307.	1.2	35
131	Ab initio and relativistic DFT study of spinâ€“rotation and NMR shielding constants in XF6 molecules, X = S, Se, Te, Mo, and W. Journal of Chemical Physics, 2014, 140, 194308.	1.2	35
132	Open-Ended Recursive Approach for the Calculation of Multiphoton Absorption Matrix Elements. Journal of Chemical Theory and Computation, 2015, 11, 1129-1144.	2.3	35
133	Solvent effects on the NMR parameters of H2S and HCN. , 1999, 20, 1281-1291.		34
134	Coupledâ€Cluster Calculations of Vibrational Raman Optical Activity Spectra. ChemPhysChem, 2011, 12, 3442-3448.	1.0	34
135	Multiconfigurational Self-Consistent Field Calculations of the Magnetically Induced Current Density Using Gauge-Including Atomic Orbitals. Journal of Chemical Theory and Computation, 2013, 9, 2189-2198.	2.3	34
136	A general, recursive, and openâ€ended response code. Journal of Computational Chemistry, 2014, 35, 622-633.	1.5	34
137	Some recent developments of high-order response theory. International Journal of Quantum Chemistry, 1998, 70, 219-239.	1.0	33
138	Mercury Methylation by Cobalt Corrinoids: Relativistic Effects Dictate the Reaction Mechanism. Angewandte Chemie - International Edition, 2016, 55, 11503-11506.	7.2	33
139	Orbital connections for perturbation-dependent basis sets. Theoretica Chimica Acta, 1995, 90, 421.	0.9	33
140	Basis set convergence and correlation effects in vibrational circular dichroism calculations using London atomic orbitals. Faraday Discussions, 1994, 99, 121-129.	1.6	32
141	Energetics and Dynamics of Intermolecular Proton-Transfer Processes. 2. Ab Initio Direct Dynamics Calculations of the Reaction H3O++ NH3â†' NH4++ H2O. The Journal of Physical Chemistry, 1996, 100, 15388-15392.	2.9	32
142	Magnetizabilities and Nuclear Shielding Constants of the Fluoromethanes in the Gas Phase and Solution. The Journal of Physical Chemistry, 1996, 100, 19771-19782.	2.9	32
143	Internuclear distance dependence of the spinâ€“orbit coupling contributions to proton NMR chemical shifts. Chemical Physics Letters, 1998, 295, 455-461.	1.2	32
144	Solvent effects on the conformational distribution and optical rotation of Î³-methyl paraconic acids and esters. Chirality, 2006, 18, 357-369.	1.3	32

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145	Two-photon absorption of [2.2]paracyclophane derivatives in solution: A theoretical investigation. Journal of Chemical Physics, 2007, 127, 244103.	1.2	32
146	Importance of backbone angles versus amino acid configurations in peptide vibrational Raman optical activity spectra. Chemical Physics, 2008, 343, 200-209.	0.9	32
147	Porphyrin Protonation Studied by Magnetic Circular Dichroism. Journal of Physical Chemistry A, 2012, 116, 778-783.	1.1	32
148	Four-Component Relativistic Density-Functional Theory Calculations of Nuclear Spinâ€“Rotation Constants: Relativistic Effects in p-Block Hydrides. Journal of Chemical Theory and Computation, 2015, 11, 3729-3739.	2.3	32
149	Absolute Configuration of C76 from Optical Rotatory Dispersion. ChemPhysChem, 2005, 6, 2535-2540.	1.0	31
150	An IEF-PCM study of solvent effects on the Faraday $${mathcal{B}}$$ term of MCD. Theoretical Chemistry Accounts, 2008, 119, 231-244.	0.5	31
151	The First and Second Static Electronic Hyperpolarizabilities of Zigzag Boron Nitride Nanotubes. An ab Initio Approach through the Coupled Perturbed Kohnâ€“Sham Scheme. Journal of Physical Chemistry A, 2011, 115, 12631-12637.	1.1	31
152	Theoretical calculations of the magnetizability of some small fluorine-containing molecules using London atomic orbitals. Chemical Physics Letters, 1994, 223, 12-18.	1.2	30
153	Analytic Calculations of Vibrational Hyperpolarizabilities in the Atomic Orbital Basis. Journal of Physical Chemistry A, 2008, 112, 11942-11950.	1.1	30
154	Structure and NMR Spectra of Some [2.2]Paracyclophanes. The Dilemma of [2.2]Paracyclophane Symmetry. Journal of Physical Chemistry A, 2011, 115, 10638-10649.	1.1	30
155	Absolute Configuration of a Cyclic Dipeptide Reflected in Vibrational Optical Activity: Ab Initio and Experimental Investigation. Journal of Physical Chemistry A, 2012, 116, 2554-2563.	1.1	30
156	Rotational averaging of multiphoton absorption cross sections. Journal of Chemical Physics, 2014, 141, 204103.	1.2	30
157	MCSCF calculations of Verdet constants. Chemical Physics Letters, 1994, 222, 263-266.	1.2	29
158	Multiconfigurational selfâ€consistent field calculations of nuclear magnetic resonance indirect spinâ€“spin coupling constants. Journal of Chemical Physics, 1994, 101, 6822-6828.	1.2	29
159	Isotope and temperature effects on the 13C and 77Se nuclear shielding in carbon diselenide. Journal of Chemical Physics, 1997, 107, 1350-1361.	1.2	29
160	Cotton-Mouton effect and shielding polarizabilities of ethylene: An MCSCF study. Chemical Physics, 1997, 216, 53-66.	0.9	29
161	Spinâ€“spin coupling constants in C2H2. Chemical Physics Letters, 2001, 336, 473-478.	1.2	29
162	Basis set convergence of atomic axial tensors obtained from selfâ€consistent field calculations using London atomic orbitals. Journal of Chemical Physics, 1994, 100, 6620-6627.	1.2	28

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163	An Atomic-Orbital-Based Lagrangian Approach for Calculating Geometric Gradients of Linear Response Properties. Journal of Chemical Theory and Computation, 2010, 6, 1028-1047.	2.3	28
164	Strong Duschinsky Mixing Induced Breakdown of Kashaâ€™s Rule in an Organic Phosphor. Journal of Physical Chemistry Letters, 2019, 10, 369-374.	2.1	28
165	A numerically stable orbital connection for the calculation of analytical Hessians using perturbation-dependent basis sets. Chemical Physics Letters, 1995, 235, 47-52.	1.2	27
166	Ab initio calculation of the NMR shielding and indirect spin-spin coupling constants of fluoroethylene. Molecular Physics, 1997, 91, 881-890.	0.8	27
167	Zero-point vibrational contributions to fluorine shieldings in organic molecules. Physical Chemistry Chemical Physics, 2003, 5, 5015-5020.	1.3	27
168	Ab initio calculation of magnetic circular dichroism. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2012, 2, 443-455.	6.2	27
169	Communication: The absolute shielding scales of oxygen and sulfur revisited. Journal of Chemical Physics, 2015, 142, 091102.	1.2	27
170	Analytic calculations of anharmonic infrared and Raman vibrational spectra. Physical Chemistry Chemical Physics, 2016, 18, 4201-4215.	1.3	27
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