Stephan P A Sauer

List of Publications by Year
in descending order

208	8,820	53794	53230
papers	citations	45 h-index	85 g-index

220	220	220	5270
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	The <scp>D</scp>alton quantum chemistry program system. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2014, 4, 269-284.	14.6	1,166
2	Benchmarks for electronically excited states: CASPT2, CC2, CCSD, and CC3. Journal of Chemical Physics, 2008, 128, 134110.	3.0	833
3	Benchmarks for electronically excited states: Time-dependent density functional theory and density functional theory based multireference configuration interaction. Journal of Chemical Physics, 2008, 129, 104103.	3.0	478
4	Correlated calculations of indirect nuclear spin-spin coupling constants using second-order polarization propagator approximations: SOPPA and SOPPA(CCSD). Theoretical Chemistry Accounts, 1998, 100, 275-284.	1.4	287
5	The effect of lone pairs and electronegativity on the indirect nuclear spinâ€“spin coupling constants in CH2X (X=CH2, NH, O, S):Ab initiocalculations using optimized contracted basis sets. Journal of Chemical Physics, 2001, 115, 1324-1334.	3.0	252
6	Benchmarks of electronically excited states: Basis set effects on CASPT2 results. Journal of Chemical Physics, 2010, 133, 174318.	3.0	201
7	Second-order polarization propagator approximation with coupled-cluster singles and doubles amplitudes - SOPPA(CCSD): the polarizability and hyperpolarizability of. Journal of Physics B: Atomic, Molecular and Optical Physics, 1997, 30, 3773-3780.	1.5	147
8	Basis set effects on coupled cluster benchmarks of electronically excited states: CC3, CCSDR(3) and CC2. Molecular Physics, 2010, 108, 453-465.	1.7	142
9	Atomic integral driven second order polarization propagator calculations of the excitation spectra of naphthalene and anthracene. Journal of Chemical Physics, 2000, 112, 4173-4185.	3.0	131
10	Benchmarks for Electronically Excited States: A Comparison of Noniterative and Iterative Triples Corrections in Linear Response Coupled Cluster Methods: CCSDR(3) versus CC3. Journal of Chemical Theory and Computation, 2009, 5, 555-564.	5.3	115
11	Ab Initio Calculation of the Electronic Spectrum of Azobenzene Dyes and Its Impact on the Design of Optical Data Storage Materials. Journal of the American Chemical Society, 2000, 122, 3482-3487.	13.7	114
12	Substituent Effects on Scalar 2J(19F,19F) and 3J(19F,19F) NMR Couplings:â€‰ A Comparison of SOPPA and DFT Methods. Journal of Physical Chemistry A, 2003, 107, 4748-4754.	2.5	103
13	Nuclear spinâ€“spin coupling in the acetylene isotopomers calculated fromab initiocorrelated surfaces for 1J(C,â€ŠH), 1J(C,â€ŠC), 2J(C,â€ŠH), and 3J(H,â€ŠH). Journal of Chemical Physics, 2000, 112, 3735-3746.	3.0	98
14	Calculated spin-spin coupling surfaces in the water molecule; prediction and analysis of J(O, H), J(O, D) and J(H, D) in water isotopomers. Molecular Physics, 1998, 94, 851-862.	1.7	88
15	The use of locally dense basis sets in the calculation of indirect nuclear spinâ€“spin coupling constants: The vicinal coupling constants in H3Câ€“CH2X (X=H, F, Cl, Br, I). Journal of Chemical Physics, 2000, 112, 6201-6208.	3.0	86
16	Optimized basis sets for the calculation of indirect nuclear spin-spin coupling constants involving the atoms B, Al, Si, P, and Cl. Journal of Chemical Physics, 2010, 133, 054308.	3.0	83
17	Failures of TDDFT in describing the lowest intramolecular charge-transfer excitation in para-nitroaniline. Molecular Physics, 2013, 111, 1235-1248.	1.7	79
18	Unexpected differential sensitivity of nuclear spinâ€“spin-coupling constants to bond stretching in BH4â^',â€‚NH4+, and SiH4. Journal of Chemical Physics, 2000, 113, 3121-3129.	3.0	78

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19	Optimized Basis Sets for Calculation of Electron Paramagnetic Resonance Hyperfine Coupling Constants: aug-cc-pVTZ-J for the 3d Atoms Scâ€“Zn. Journal of Chemical Theory and Computation, 2011, 7, 4077-4087.	5.3	78
20	Structural trends of ⁷⁷Seï£¿¹H spinâ€“spin coupling constants and conformational behavior of 2â€substituted selenophenes. Magnetic Resonance in Chemistry, 2010, 48, 44-52.	1.9	77
21	Anion binding by biotin[6]uril in water. Organic and Biomolecular Chemistry, 2015, 13, 369-373.	2.8	76
22	Benchmarking NMR indirect nuclear spin-spin coupling constants: SOPPA, SOPPA(CC2), and SOPPA(CCSD) versus CCSD. Journal of Chemical Physics, 2010, 133, 144106.	3.0	72
23	Nuclear spinâ€“spin coupling in silane and its isotopomers: Ab initio calculation and experimental investigation. Journal of Chemical Physics, 2001, 115, 5994-6006.	3.0	70
24	Non-empirical calculations of NMR indirect carbon-carbon coupling constants: 1. Three-membered rings. Magnetic Resonance in Chemistry, 2002, 40, 187-194.	1.9	69
25	On the Usage of Locally Dense Basis Sets in the Calculation of NMR Indirect Nuclear Spinâ€“Spin Coupling Constants: Vicinal Fluorineâ€“Fluorine Couplings. Advances in Quantum Chemistry, 2005, , 161-183.	0.8	65
26	Correlated, Static and Dynamic Polarizabilities of Small Molecules. Comparison of Four â€œBlack Boxâ€• Methods. Journal of Physical Chemistry A, 1998, 102, 5269-5274.	2.5	64
27	Correlated and gauge origin independent calculations of magnetic properties. Molecular Physics, 1994, 81, 87-118.	1.7	59
28	Theoretical Investigation of Steric and Electronic Effects in Coenzyme B12Models. Organometallics, 2001, 20, 550-556.	2.3	58
29	Five-membered rings as diazo components in optical data storage devices: an ab initio investigation of the lowest singlet excitation energies. Chemical Physics Letters, 2000, 325, 115-119.	2.6	57
30	Nuclear magnetic resonance shielding constants and chemical shifts in linear 199Hg compounds: A comparison of three relativistic computational methods. Journal of Chemical Physics, 2011, 135, 044306.	3.0	55
31	Calculations of the indirect nuclear spin-spin coupling constants of PbH 4. Theoretical Chemistry Accounts, 1999, 103, 146-153.	1.4	53
32	Interaction Energies and NMR Indirect Nuclear Spinâ^'Spin Coupling Constants in Linear HCN and HNC Complexes. Journal of Physical Chemistry A, 2005, 109, 6555-6564.	2.5	52
33	Pople Style Basis Sets for the Calculation of NMR Spinâ€“Spin Coupling Constants: the 6-31G-J and 6-311G-J Basis Sets. Journal of Chemical Theory and Computation, 2011, 7, 4070-4076.	5.3	52
34	Nuclear magnetic shielding in the acetylene isotopomers calculated from correlated shielding surfaces. Journal of Chemical Physics, 2000, 112, 736-746.	3.0	51
35	On the Accuracy of Density Functional Theory to Predict Shifts in Nuclear Magnetic Resonance Shielding Constants due to Hydrogen Bonding. Journal of Chemical Theory and Computation, 2008, 4, 267-277.	5.3	51
36	Benchmarking Second Order Methods for the Calculation of Vertical Electronic Excitation Energies: Valence and Rydberg States in Polycyclic Aromatic Hydrocarbons. Journal of Physical Chemistry A, 2009, 113, 11995-12012.	2.5	51

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37	Paramagnetism of closed shell diatomic hydrides with six valence electrons. Journal of Chemical Physics, 1993, 98, 9748-9757.	3.0	50
38	Non-empirical calculations of NMR indirect carbonâ€“carbon coupling constants. Part 8â€”Monocycloalkanes. Magnetic Resonance in Chemistry, 2004, 42, 671-686.	1.9	50
39	From CCSD(T)/augâ€ccâ€pVTZâ€) to CCSD(T) complete basis set limit isotropic nuclear magnetic shieldings via affordable DFT/CBS calculations. Magnetic Resonance in Chemistry, 2011, 49, 231-236.	1.9	50
40	The vibrational and temperature dependence of the indirect nuclear spinâ€“spin coupling constants of the oxonium (H3O+) and hydroxyl (OHâ^) ions. Chemical Physics, 1998, 238, 385-399.	1.9	49
41	Large Long-Range Fâ^'F Indirect Spinâ^'Spin Coupling Constants. Prediction of Measurable Fâ^'F Couplings over a Few Nanometers. Journal of Physical Chemistry A, 2004, 108, 5393-5398.	2.5	49
42	Prediction of spin-spin coupling constants in solution based on combined density functional theory/molecular mechanics. Journal of Chemical Physics, 2009, 130, 134508.	3.0	48
43	Correlated and gauge origin independent calculations of magnetic properties. Theoretica Chimica Acta, 1994, 88, 351-361.	0.8	47
44	Calculation, with the inclusion of vibrational corrections, of the dc-electric-field-induced second-harmonic-generation hyperpolarizability of methane. Journal of Chemical Physics, 1997, 107, 8502-8509.	3.0	46
45	Correlated and gauge invariant calculations of nuclear magnetic shielding constants using the continuous transformation of the origin of the current density approach. Journal of Chemical Physics, 2003, 118, 6830-6845.	3.0	46
46	Dalton Project: A Python platform for molecular- and electronic-structure simulations of complex systems. Journal of Chemical Physics, 2020, 152, 214115.	3.0	45
47	Correlated calculations of the rotationalg-tensor and origin independent magnetizability surface of BH. Molecular Physics, 1992, 76, 445-465.	1.7	44
48	Experimental and Theoretical Estimates of the Rotational g Factor of AlH in the Electronic Ground State X1.SIGMA.+. The Journal of Physical Chemistry, 1994, 98, 8617-8621.	2.9	44
49	Infrared spectra of CO in absorption and evaluation of radial functions for potential energy and electric dipolar moment. Theoretical Chemistry Accounts, 2002, 108, 85-97.	1.4	42
50	Importance of Triples Contributions to NMR Spinâ€“Spin Coupling Constants Computed at the CC3 and CCSDT Levels. Journal of Chemical Theory and Computation, 2017, 13, 696-709.	5.3	41
51	Calculation of the Verdet constants for H2, N2, CO, and FH. Journal of Chemical Physics, 1993, 98, 487-495.	3.0	40
52	Correlated polarization propagator calculations of static polarizabilities. International Journal of Quantum Chemistry, 1994, 50, 317-332.	2.0	40
53	Second-order polarization propagator calculations of dynamic dipole polarizabilities and C6 coefficients. International Journal of Quantum Chemistry, 1991, 39, 667-679.	2.0	39
54	A second-order doubles correction to excitation energies in the random-phase approximation. Chemical Physics Letters, 1998, 284, 47-55.	2.6	39

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55	On the importance of excited state dynamic response electron correlation in polarizable embedding methods. Journal of Computational Chemistry, 2012, 33, 2012-2022.	3.3	38
56	The magnetizability and g-factor surfaces of ammonia. Chemical Physics, 1991, 153, 189-200.	1.9	35
57	First principle calculations of 113Cd chemical shifts for proteins and model systems. Journal of Biological Inorganic Chemistry, 2004, 9, 591-599.	2.6	35
58	Gauge invariant calculations of nuclear magnetic shielding constants using the continuous transformation of the origin of the current density approach. II. Density functional and coupled cluster theory. Journal of Chemical Physics, 2007, 126, 154111.	3.0	34
59	Evaluation of adiabatic and nonadiabatic effects from vibrationâ€"rotational spectra of LiH X 1Î£+. Chemical Physics Letters, 1994, 228, 183-190.	2.6	33
60	Thermal averaging of the indirect nuclear spin-spin coupling constants of ammonia: The importance of the large amplitude inversion mode. Journal of Chemical Physics, 2010, 132, 114305.	3.0	33
61	Calculated molecular mean excitation energies for some small molecules. Nuclear Instruments & Methods in Physics Research B, 1995, 100, 458-463.	1.4	31
62	Benchmarking SOPPA(CC2) for the calculation of indirect nuclear spinâ€"spin coupling constants: Carbocycles. Chemical Physics, 2011, 381, 35-43.	1.9	31
63	Fully relativistic coupled cluster and DFT study of electric field gradients at Hg in 199Hg compounds. Physical Chemistry Chemical Physics, 2012, 14, 2651.	2.8	31
64	Improving the calculation of electron paramagnetic resonance hyperfine coupling tensors for d-block metals. Physical Chemistry Chemical Physics, 2012, 14, 10669.	2.8	31
65	Performance of SOPPA-based methods in the calculation of vertical excitation energies and oscillator strengths. Molecular Physics, 2015, 113, 2026-2045.	1.7	31
66	Correlated dipole oscillator sum rules. Journal of Chemical Physics, 1994, 100, 8969-8975.	3.0	30
67	Theoretical estimates of the rotational g-factor, magnetizability and electric dipole moment of GaH. Chemical Physics Letters, 1996, 260, 271-279.	2.6	30
68	Calculated nuclear shielding surfaces in the water molecule; prediction and analysis of Ïƒ(O), Ïƒ(H) and Ïƒ(D) in water isotopomers. Molecular Physics, 1999, 96, 1595-1607.	1.7	30
69	First example of a high-level correlated calculation of the indirect spinâ€"spin coupling constants involving tellurium: tellurophene and divinyl telluride. Physical Chemistry Chemical Physics, 2013, 15, 13101-13107.	2.8	30
70	A Physical Model of the Proton Radiation Belts of Jupiter inside Europa's Orbit. Journal of Geophysical Research: Space Physics, 2018, 123, 3512-3532.	2.4	30
71	A sumâ€overâ€states formulation of the diamagnetic contribution to the indirect nuclear spinâ€"spin coupling constant. Journal of Chemical Physics, 1993, 98, 9220-9221.	3.0	29
72	Validating and Analyzing EPR Hyperfine Coupling Constants with Density Functional Theory. Journal of Chemical Theory and Computation, 2013, 9, 2380-2388.	5.3	29

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73	Azadioxatriangulenium and Diazaoxatriangulenium: Quantum Yields and Fundamental Photophysical Properties. ACS Omega, 2017, 2, 193-203.	3.5	29
74	The computation of Karplus equation coefficients and their components using self-consistent field and second-order polarization propagator methods. Molecular Physics, 2000, 98, 1981-1990.	1.7	28
75	On the Angular Dependence of the Vicinal Fluorineâ^'Fluorine Coupling Constant in 1,2-Difluoroethane:â€‰ Deviation from a Karplus-like Shape. Journal of Chemical Theory and Computation, 2006, 2, 1019-1027.	5.3	28
76	The vibrational g-factor of dihydrogen from theoretical calculation and analysis of vibration-rotational spectra. Physical Chemistry Chemical Physics, 2005, 7, 1747.	2.8	27
77	Heterobimetallic Nitride Complexes from Terminal Chromium(V) Nitride Complexes: Hyperfine Coupling Increases with Distance. Angewandte Chemie - International Edition, 2011, 50, 4480-4483.	13.8	27
78	Halogen effect on structure and ¹³C NMR chemical shift of 3,6â€disubstitutedâ€Nâ€alkyl carbazoles. Magnetic Resonance in Chemistry, 2013, 51, 630-635.	1.9	27
79	The vibrational and temperature dependence of the magnetic properties of the oxonium ion (H3O+). Chemical Physics, 1994, 184, 1-11.	1.9	26
80	Correlated dipole polarizabilities and dipole moments of the halides HX and CH3X (X=F, Cl and Br). Theoretica Chimica Acta, 1994, 89, 323-333.	0.8	26
81	Directional Dependence of the Mean Excitation Energy and Spectral Moments of the Dipole Oscillator Strength Distribution of Glycine and Its Zwitterion. Journal of Physical Chemistry A, 2006, 110, 8811-8817.	2.5	26
82	On the aromaticity of tetrathiafulvalene cations. Chemical Physics Letters, 2008, 453, 136-139.	2.6	25
83	Calculations of magnetic hyperfine structure constants for the low-lying rovibrational levels of LiH, HF, CH+, and BH. Chemical Physics, 1995, 201, 405-425.	1.9	24
84	The Effect of Substituents on Indirect Nuclear Spin-Spin Coupling Constants: Methan- and Ethanimine, Methanal- and Ethanaloxime. International Journal of Molecular Sciences, 2003, 4, 231-248.	4.1	24
85	Estimation of isotropic nuclear magnetic shieldings in the CCSD(T) and MP2 complete basis set limit using affordable correlation calculations. Magnetic Resonance in Chemistry, 2013, 51, 482-489.	1.9	24
86	Two-photon absorption cross sections: An investigation of the accuracy of calculated absolute and relative values. Journal of Chemical Physics, 2006, 124, 114108.	3.0	23
87	Molecular Switching in Confined Spaces: Effects of Encapsulating the DHA/VHF Photoâ€Switch in Cucurbiturils. Chemistry - A European Journal, 2017, 23, 17010-17016.	3.3	23
88	Entropy/Enthalpy Compensation in Anion Binding: Biotin[6]uril and Biotin-<scp>l</scp>-sulfoxide[6]uril Reveal Strong Solvent Dependency. Journal of Organic Chemistry, 2019, 84, 2577-2584.	3.2	23
89	Rovibrational and Temperature Effects in Theoretical Studies of NMR Parameters. New Developments in NMR, 2016, , 218-266.	0.1	23
90	Development of polarization consistent basis sets for spin-spin coupling constant calculations for the atoms Li, Be, Na, and Mg. Journal of Chemical Physics, 2018, 149, 044117.	3.0	22

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91	Directional characteristics of the moments of the dipole-oscillator-strength distribution of molecules:H2andH2O. Physical Review A, 1993, 47, 1123-1129.	2.5	21
92	Kinetics and Thermodynamics of the Reaction between the ^{â€¢}OH Radical and Adenine: A Theoretical Investigation. Journal of Physical Chemistry A, 2015, 119, 6516-6527.	2.5	21
93	Quadrupole moments of Cd and Zn nuclei: When solid-state, molecular, atomic, and nuclear theory meet. Europhysics Letters, 2017, 117, 62001.	2.0	21
94	RPA(D) and HRPA(D): Two new models for calculations of NMR indirect nuclear spinâ€“spin coupling constants. Journal of Computational Chemistry, 2018, 39, 2647-2666.	3.3	21
95	A relation between the rotational g-factor and the electric dipole moment of a diatomic molecule. Chemical Physics Letters, 1998, 297, 475-483.	2.6	20
96	Relativistic calculations of the rotational g factor of the hydrogen halides and noble gas hydride cations. Journal of Chemical Physics, 2001, 114, 84.	3.0	20
97	Electric field gradients of water: A systematic investigation of basis set, electron correlation, and rovibrational effects. Journal of Chemical Physics, 2002, 116, 1424-1434.	3.0	20
98	The Effect of Solvation on the Mean Excitation Energy of Glycine. Journal of Physical Chemistry Letters, 2010, 1, 242-245.	4.6	20
99	Ligand Sphere Conversions in Terminal Carbide Complexes. Organometallics, 2016, 35, 100-105.	2.3	20
100	The vibrational dependence of the hydrogen and oxygen nuclear magnetic shielding constants in OHâ^' and OHâ^' Â· H2O. Chemical Physics, 1997, 214, 91-101.	1.9	19
101	On the discrepancy between theory and experiment for the Fâ€“F spinâ€“spin coupling constant of difluoroethyne. Physical Chemistry Chemical Physics, 2012, 14, 16440.	2.8	19
102	Effective potential energy curves of the ground electronic state of CH+. Journal of Chemical Physics, 2013, 138, 024315.	3.0	19
103	On the convergence of zero-point vibrational corrections to nuclear shieldings and shielding anisotropies towards the complete basis set limit in water. Molecular Physics, 2017, 115, 144-160.	1.7	19
104	Mean Excitation Energies for Biomolecules. Advances in Quantum Chemistry, 2011, 62, 215-242.	0.8	18
105	Electric field effects on nuclear spinâ€“spin coupling tensors and chiral discrimination via NMR spectroscopy. Theoretical Chemistry Accounts, 2011, 129, 359-366.	1.4	18
106	Insight into the Mechanism of the Initial Reaction of an OH Radical with DNA/RNA Nucleobases: A Computational Investigation of Radiation Damage. Chemistry - A European Journal, 2015, 21, 17786-17799.	3.3	18
107	Molecular modeling and experimental studies on structure and NMR parameters of 9-benzyl-3,6-diiodo-9H-carbazole. Structural Chemistry, 2015, 26, 997-1006.	2.0	18
108	Through-space spinâ€“spin coupling constants involving fluorine: benchmarking DFT functionals. Molecular Physics, 2019, 117, 1469-1480.	1.7	18

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109	Quantum-Chemical Calculations of Radial Functions for Rotational and Vibrational g Factors, Electric Dipolar Moment and Adiabatic Corrections to the Potential Energy for Analysis of Spectra of HeH+. Advances in Quantum Chemistry, 2005, , 319-334.	0.8	17
110	Analysis of isotope effects in NMR one-bond indirect nuclear spinâ€“spin coupling constants in terms of localized molecular orbitals. Physical Chemistry Chemical Physics, 2009, 11, 3987.	2.8	17
111	Symmetry, vibrational energy redistribution and vibronic coupling: The internal conversion processes of cycloketones. Journal of Chemical Physics, 2012, 137, 22A522.	3.0	17
112	Noniterative Doubles Corrections to the Random Phase and Higher Random Phase Approximations: Singlet and Triplet Excitation Energies. Journal of Computational Chemistry, 2020, 41, 43-55.	3.3	17
113	Mean Excitation Energies and Energy Deposition Characteristics of Bio-organic Molecules. Journal of Physical Chemistry B, 2010, 114, 633-637.	2.6	16
114	Definitive Benchmark Study of Ring Current Effects on Amide Proton Chemical Shifts. Journal of Chemical Theory and Computation, 2011, 7, 2078-2084.	5.3	16
115	Relativistic DFT Calculations of Hyperfine Coupling Constants in 5d Hexafluorido Complexes: [ReF₆]^{2â^'} and [IrF₆]^{2â^'}. Chemistry - A European Journal, 2018, 24, 5124-5133.	3.3	16
116	The role of explicit solvent molecules in the calculation of NMR chemical shifts of glycine in water. Theoretical Chemistry Accounts, 2018, 137, 1.	1.4	16
117	Determining short-lived solid forms during phase transformations using molecular dynamics. CrystEngComm, 2019, 21, 4020-4024.	2.6	16
118	The Second-Order-Polarization-Propagator-Approximation (SOPPA) in a four-component spinor basis. Journal of Chemical Physics, 2020, 152, 134113.	3.0	16
119	Response theory in the multipole reaction field model for equilibrium and nonequilibrium solvation: Exact theory and the second order polarization propagator approximation. Journal of Chemical Physics, 2003, 119, 3849-3870.	3.0	15
120	Calculations of Dipole and Quadrupole Polarizability Radial Functions for LiH and HF: A Comparison of Different Linear Response Methods. Advances in Quantum Chemistry, 2005, 48, 185-208.	0.8	15
121	The RotationalgFactor of Diatomic Molecules in State1Î£+or 0+. Advances in Chemical Physics, 2007, , 475-536.	0.3	15
122	The Anomalous Deuterium Isotope Effect in the NMR Spectrum of Methane: An Analysis in Localized Molecular Orbitals. ChemPhysChem, 2008, 9, 1259-1261.	2.1	15
123	Partial charges as reactivity descriptors for nitrido complexes. Computational and Theoretical Chemistry, 2009, 913, 1-7.	1.5	15
124	An Isofagomine Analogue with an Amidine at the Pseudoanomeric Position. Organic Letters, 2011, 13, 2908-2911.	4.6	15
125	Computational Prediction of ¹H and ¹³C NMR Chemical Shifts for Protonated Alkylpyrroles: Electron Correlation and Not Solvation is the Salvation. ChemPhysChem, 2019, 20, 78-91.	2.1	15
126	Free Molecule Studies by Perturbed <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mi>Î³</mml:mi><mml:mtext>â^'</mml:mtext><mml:mi>Î³</mml:mi></mml:mrow></mml:math> Angular Correlation: A New Path to Accurate Nuclear Quadrupole Moments. Physical Review Letters, 2021, 126, 103001.	7.8	15

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127	Mean Excitation Energies and Their Directional Characteristics for Energy Deposition by Swift Ions on the DNA and RNA Nucleobases. Journal of Physical Chemistry C, 2010, 114, 20335-20341.	3.1	14
128	Analysis of the interactions between difluoroacetylene and one or two hydrogen fluoride molecules based on calculated spinâ€“spin coupling constants. Computational and Theoretical Chemistry, 2012, 998, 98-105.	2.5	14
129	Theoretical study of the triplet excited state of PtPOP and the exciplexes M-PtPOP (M=Tl, Ag) in solution and comparison with ultrafast X-ray scattering results. Chemical Physics, 2012, 393, 117-122.	1.9	14
130	On the Determination of the Mean Excitation Energy of Water. Advances in Quantum Chemistry, 2013, 65, 63-77.	0.8	14
131	The Mean Excitation Energy of Atomic Ions. Advances in Quantum Chemistry, 2015, , 29-40.	0.8	14
132	Spinâ€orbit <scp>ZORA</scp> and fourâ€component <scp>D</scp>iracâ€“<scp>C</scp>oulomb estimation of relativistic corrections to isotropic nuclear shieldings and chemical shifts of noble gas dimers. Journal of Computational Chemistry, 2016, 37, 395-403.	3.3	14
133	On the convergence of the ccJ-pVXZ and pcJ-n basis sets in CCSD calculations of nuclear spinâ€“spin coupling constants: some difficult cases. Theoretical Chemistry Accounts, 2018, 137, 1.	1.4	14
134	A comparison of density functional theory and coupled cluster methods for the calculation of electric dipole polarizability gradients of methane. AIP Conference Proceedings, 2012, , .	0.4	13
135	Electric field gradients in Hg compounds: Molecular orbital (MO) analysis and comparison of 4-component and 2-component (ZORA) methods. Physical Chemistry Chemical Physics, 2012, 14, 16070.	2.8	13
136	Nuclear magnetic resonance J coupling constant polarizabilities of hydrogen peroxide: A basis set and correlation study. Journal of Computational Chemistry, 2012, 33, 1845-1853.	3.3	13
137	SOPPA and CCSD vibrational corrections to NMR indirect spin-spin coupling constants of small hydrocarbons. AIP Conference Proceedings, 2015, , .	0.4	13
138	Exploring the relationship between the conformation and pK_a: can a pK_avalue be used to determine the conformational equilibrium?. Organic and Biomolecular Chemistry, 2015, 13, 3116-3121.	2.8	13
139	Z-dependence of mean excitation energies for second and third row atoms and their ions. Journal of Chemical Physics, 2018, 148, 174307.	3.0	13
140	Ab initio calculations on 2-imidazolyl-2-thiazolyl azo compounds â€“ an investigation of potential near-infrared absorbing structures. Chemical Physics Letters, 2001, 343, 171-177.	2.6	12
141	Coupled cluster calculations of mean excitation energies of the noble gas atoms He, Ne and Ar and of the H2molecule. Molecular Physics, 2014, 112, 751-761.	1.7	12
142	DFT and experimental studies on structure and spectroscopic parameters of 3,6-diiodo-9-ethyl-9H-carbazole. Structural Chemistry, 2016, 27, 199-207.	2.0	12
143	Mean excitation energies for molecular ions. Nuclear Instruments & Methods in Physics Research B, 2017, 394, 73-80.	1.4	12
144	Direct observation of Mg²⁺complexes in ionic liquid solutions by³¹Mg Î²-NMR spectroscopy. Dalton Transactions, 2018, 47, 14431-14435.	3.3	12

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145	Enhancing NMR Quantum Computation by Exploring Heavy Metal Complexes as Multiqubit Systems: A Theoretical Investigation. Journal of Physical Chemistry A, 2020, 124, 4946-4955.	2.5	12
146	A multipole second order MÃ¸llerâ€“Plesset solvent reaction field method. Journal of Chemical Physics, 2001, 114, 7753-7760.	3.0	11
147	Comparison of the directional characteristics of swift ion excitation for two small biomolecules: glycine and alanine. European Physical Journal D, 2010, 60, 71-76.	1.3	11
148	Estimating the accuracy of calculated electron paramagnetic resonance hyperfine couplings for a lytic polysaccharide monooxygenase. Computational and Structural Biotechnology Journal, 2021, 19, 555-567.	4.1	11
149	A Comparison of MÃ¸ller-Plesset and Coupled Cluster Linear Response Theory Methods for the Calculation of Dipole Oscillator Strength Sum Rules and C6 Dispersion Coefficients. Collection of Czechoslovak Chemical Communications, 2008, 73, 1415-1436.	1.0	10
150	Atomic partition of the optical rotatory power of methylhydroperoxide. Journal of Chemical Physics, 2008, 128, 064318.	3.0	10
151	Communication: Rotational g-factor and spin-rotation constant of CH+. Journal of Chemical Physics, 2010, 133, 171101.	3.0	10
152	Estimating the carbonyl anharmonic vibrational frequency from affordable harmonic frequency calculations. Journal of Molecular Modeling, 2012, 18, 2471-2478.	1.8	10
153	Magnetic interactions in oxide-bridged dichromium(III) complexes. Computational determination of the importance of non-bridging ligands. Inorganica Chimica Acta, 2013, 396, 72-77.	2.4	10
154	Relation between properties of long-range diatomic bound states. Physical Review A, 2013, 87, .	2.5	10
155	Calculation of mean excitation energies. Advances in Quantum Chemistry, 2019, 80, 225-245.	0.8	10
156	NMR parameters of FNNF as a test for coupled-cluster methods: CCSDT shielding and CC3 spinâ€“spin coupling. Physical Chemistry Chemical Physics, 2020, 22, 21350-21359.	2.8	10
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