Stephan P A Sauer

List of Publications by Citations

206 papers	7,701 citations	43 h-index	80 g-index
220 ext. papers	8,232 ext. citations	3.2 avg, IF	6.06 L-index

#	Paper	IF	Citations
206	The Dalton quantum chemistry program system. *Wiley Interdisciplinary Reviews: Computational Molecular Science*, **2014**, 4, 269-284	7.9	956
205	Benchmarks for electronically excited states: CASPT2, CC2, CCSD, and CC3. *Journal of Chemical Physics*, **2008**, 128, 134110	3.9	737
204	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	3.9	433
203	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	1.9	260
202	The effect of lone pairs and electronegativity on the indirect nuclear spin□pin coupling constants in CH2X (X=CH2, NH, O, S): Ab initio calculations using optimized contracted basis sets. *Journal of Chemical Physics*, **2001**, 115, 1324-1334	3.9	232
201	Benchmarks of electronically excited states: basis set effects on CASPT2 results. *Journal of Chemical Physics*, **2010**, 133, 174318	3.9	177
200	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	1.3	134
199	Basis set effects on coupled cluster benchmarks of electronically excited states: CC3, CCSDR(3) and CC2. *Molecular Physics*, **2010**, 108, 453-465	1.7	123
198	Atomic integral driven second order polarization propagator calculations of the excitation spectra of naphthalene and anthracene. *Journal of Chemical Physics*, **2000**, 112, 4173-4185	3.9	122
197	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	16.4	103
196	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, 555-64	6.4	102
195	Substituent Effects on Scalar 2J(19F,19F) and 3J(19F,19F) NMR Couplings: A Comparison of SOPPA and DFT Methods. *Journal of Physical Chemistry A*, **2003**, 107, 4748-4754	2.8	93
194	Nuclear spin□pin coupling in the acetylene isotopomers calculated from ab initio correlated surfaces for 1J(C, H), 1J(C, C), 2J(C, H), and 3J(H, H). *Journal of Chemical Physics*, **2000**, 112, 3735-3746	3.9	92
193	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	82
192	The use of locally dense basis sets in the calculation of indirect nuclear spin□pin coupling constants: The vicinal coupling constants in H3C□CH2X (X=H, F, Cl, Br, I). *Journal of Chemical Physics*, **2000**, 112, 6201-6208	3.9	78
191	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	3.9	74
190	Failures of TDDFT in describing the lowest intramolecular charge-transfer excitation in para-nitroaniline. *Molecular Physics*, **2013**, 111, 1235-1248	1.7	71

189	Unexpected differential sensitivity of nuclear spin–spin-coupling constants to bond stretching in BH4−, NH4+, and SiH4. *Journal of Chemical Physics*, **2000**, 113, 3121-3129	3.9	71
188	Structural trends of 77Se-1H spin-spin coupling constants and conformational behavior of 2-substituted selenophenes. *Magnetic Resonance in Chemistry*, **2010**, 48, 44-52	2.1	69
187	Benchmarking NMR indirect nuclear spin-spin coupling constants: SOPPA, SOPPA(CC2), and SOPPA(CCSD) versus CCSD. *Journal of Chemical Physics*, **2010**, 133, 144106	3.9	64
186	Optimized Basis Sets for Calculation of Electron Paramagnetic Resonance Hyperfine Coupling Constants: aug-cc-pVTZ-J for the 3d Atoms Sc-Zn. *Journal of Chemical Theory and Computation*, **2011**, 7, 4077-87	6.4	64
185	Nuclear spin–spin coupling in silane and its isotopomers: Ab initio calculation and experimental investigation. *Journal of Chemical Physics*, **2001**, 115, 5994-6006	3.9	64
184	Correlated, Static and Dynamic Polarizabilities of Small Molecules. Comparison of Four "Black Box" Methods. *Journal of Physical Chemistry A*, **1998**, 102, 5269-5274	2.8	63
183	Molecular Electromagnetism **2011**,		63
182	Anion binding by biotin[6]uril in water. *Organic and Biomolecular Chemistry*, **2015**, 13, 369-73	3.9	62
181	Non-empirical calculations of NMR indirect carbon–carbon coupling constants: 1. Three-membered rings. *Magnetic Resonance in Chemistry*, **2002**, 40, 187-194	2.1	61
180	On the Usage of Locally Dense Basis Sets in the Calculation of NMR Indirect Nuclear Spin–Spin Coupling Constants: Vicinal Fluorine–Fluorine Couplings. *Advances in Quantum Chemistry*, **2005**, 161-183	1.4	58
179	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	2.5	56
178	Correlated and gauge origin independent calculations of magnetic properties. *Molecular Physics*, **1994**, 81, 87-118	1.7	56
177	Theoretical Investigation of Steric and Electronic Effects in Coenzyme B12 Models. *Organometallics* , **2001**, 20, 550-556	3.8	53
176	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, 267-77	6.4	51
175	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	3.9	50
174	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, 11995-2012	2.8	49
173	Non-empirical calculations of NMR indirect carbon-carbon coupling constants. Part 8--monocycloalkanes. *Magnetic Resonance in Chemistry*, **2004**, 42, 671-86	2.1	49
172	Calculations of the indirect nuclear spin–spin coupling constants of PbH4. *Theoretical Chemistry Accounts*, **1999**, 103, 146-153	1.9	49

171	Interaction energies and NMR indirect nuclear spin-spin coupling constants in linear HCN and HNC complexes. *Journal of Physical Chemistry A*, **2005**, 109, 6555-64	2.8	48
170	Nuclear magnetic shielding in the acetylene isotopomers calculated from correlated shielding surfaces. *Journal of Chemical Physics*, **2000**, 112, 736-746	3.9	48
169	Paramagnetism of closed shell diatomic hydrides with six valence electrons. *Journal of Chemical Physics*, **1993**, 98, 9748-9757	3.9	47
168	Prediction of spin-spin coupling constants in solution based on combined density functional theory/molecular mechanics. *Journal of Chemical Physics*, **2009**, 130, 134508	3.9	46
167	The vibrational and temperature dependence of the indirect nuclear spin□spin coupling constants of the oxonium (H3O+) and hydroxyl (OH□) ions. *Chemical Physics*, **1998**, 238, 385-399	2.3	46
166	Large Long-Range F□F Indirect Spin□Spin Coupling Constants. Prediction of Measurable F□F Couplings over a Few Nanometers. *Journal of Physical Chemistry A*, **2004**, 108, 5393-5398	2.8	46
165	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	3.9	45
164	Correlated calculations of the rotational g-tensor and origin independent magnetizability surface of BH. *Molecular Physics*, **1992**, 76, 445-465	1.7	44
163	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	3.9	43
162	Correlated and gauge origin independent calculations of magnetic properties. *Theoretica Chimica Acta*, **1994**, 88, 351-361		43
161	Pople Style Basis Sets for the Calculation of NMR Spin-Spin Coupling Constants: the 6-31G-J and 6-311G-J Basis Sets. *Journal of Chemical Theory and Computation*, **2011**, 7, 4070-6	6.4	42
160	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		42
159	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	1.9	41
158	Calculation of the Verdet constants for H2, N2, CO, and FH. *Journal of Chemical Physics*, **1993**, 98, 487-495	3.9	38
157	Correlated polarization propagator calculations of static polarizabilities. *International Journal of Quantum Chemistry*, **1994**, 50, 317-332	2.1	38
156	Second-order polarization propagator calculations of dynamic dipole polarizabilities and C6 coefficients. *International Journal of Quantum Chemistry*, **1991**, 39, 667-679	2.1	38
155	Importance of Triples Contributions to NMR Spin-Spin Coupling Constants Computed at the CC3 and CCSDT Levels. *Journal of Chemical Theory and Computation*, **2017**, 13, 696-709	6.4	37
154	From CCSD(T)/aug-cc-pVTZ-J to CCSD(T) complete basis set limit isotropic nuclear magnetic shieldings via affordable DFT/CBS calculations. *Magnetic Resonance in Chemistry*, **2011**, 49, 231-6	2.1	36

153	A second-order doubles correction to excitation energies in the random-phase approximation. *Chemical Physics Letters*, **1998**, 284, 47-55	2.5	36
152	The magnetizability and g-factor surfaces of ammonia. *Chemical Physics*, **1991**, 153, 189-200	2.3	35
151	First principle calculations of (113)Cd chemical shifts for proteins and model systems. *Journal of Biological Inorganic Chemistry*, **2004**, 9, 591-9	3.7	34
150	On the importance of excited state dynamic response electron correlation in polarizable embedding methods. *Journal of Computational Chemistry*, **2012**, 33, 2012-22	3.5	33
149	Evaluation of adiabatic and nonadiabatic effects from vibration□otational spectra of LiH X 1□. *Chemical Physics Letters*, **1994**, 228, 183-190	2.5	33
148	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	3.9	32
147	Calculated nuclear shielding surfaces in the water molecule; prediction and analysis of □O), □H) and □D) in water isotopomers. *Molecular Physics*, **1999**, 96, 1595-1607	1.7	30
146	Theoretical estimates of the rotational g-factor, magnetizability and electric dipole moment of GaH. *Chemical Physics Letters*, **1996**, 260, 271-279	2.5	30
145	Correlated dipole oscillator sum rules. *Journal of Chemical Physics*, **1994**, 100, 8969-8975	3.9	30
144	Benchmarking SOPPA(CC2) for the calculation of indirect nuclear spin□pin coupling constants: Carbocycles. *Chemical Physics*, **2011**, 381, 35-43	2.3	28
143	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	3.9	28
142	Calculated molecular mean excitation energies for some small molecules. *Nuclear Instruments & Methods in Physics Research B*, **1995**, 100, 458-463	1.2	28
141	Performance of SOPPA-based methods in the calculation of vertical excitation energies and oscillator strengths. *Molecular Physics*, **2015**, 113, 2026-2045	1.7	27
140	Improving the calculation of Electron Paramagnetic Resonance hyperfine coupling tensors for d-block metals. *Physical Chemistry Chemical Physics*, **2012**, 14, 10669-76	3.6	27
139	The vibrational g-factor of dihydrogen from theoretical calculation and analysis of vibration-rotational spectra. *Physical Chemistry Chemical Physics*, **2005**, 7, 1747-58	3.6	27
138	A sum-over-states formulation of the diamagnetic contribution to the indirect nuclear spin□pin coupling constant. *Journal of Chemical Physics*, **1993**, 98, 9220-9221	3.9	27
137	First example of a high-level correlated calculation of the indirect spin-spin coupling constants involving tellurium: tellurophene and divinyl telluride. *Physical Chemistry Chemical Physics*, **2013**, 15, 13101-13107	3.6	26
136	On the Angular Dependence of the Vicinal Fluorine-Fluorine Coupling Constant in 1,2-Difluoroethane: Deviation from a Karplus-like Shape. *Journal of Chemical Theory and Computation*, **2006**, 2, 1019-27	6.4	26

135	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	26
134	Correlated dipole polarizabilities and dipole moments of the halides HX and CH3X (X=F, Cl and Br). *Theoretica Chimica Acta*, **1994**, 89, 323-333		26
133	Fully relativistic coupled cluster and DFT study of electric field gradients at Hg in 199Hg compounds. *Physical Chemistry Chemical Physics*, **2012**, 14, 2651-7	3.6	25
132	The vibrational and temperature dependence of the magnetic properties of the oxonium ion (H3O+). *Chemical Physics*, **1994**, 184, 1-11	2.3	25
131	Dalton Project: A Python platform for molecular- and electronic-structure simulations of complex systems. *Journal of Chemical Physics*, **2020**, 152, 214115	3.9	24
130	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, 8811-7	2.8	24
129	Azadioxatriangulenium and Diazaoxatriangulenium: Quantum Yields and Fundamental Photophysical Properties. *ACS Omega*, **2017**, 2, 193-203	3.9	23
128	Validating and Analyzing EPR Hyperfine Coupling Constants with Density Functional Theory. *Journal of Chemical Theory and Computation*, **2013**, 9, 2380-8	6.4	23
127	On the aromaticity of tetrathiafulvalene cations. *Chemical Physics Letters*, **2008**, 453, 136-139	2.5	23
126	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	6.3	22
125	Calculations of magnetic hyperfine structure constants for the low-lying rovibrational levels of LiH, HF, CH+, and BH. *Chemical Physics*, **1995**, 201, 405-425	2.3	22
124	Halogen effect on structure and 13C NMR chemical shift of 3,6-disubstituted-N-alkyl carbazoles. *Magnetic Resonance in Chemistry*, **2013**, 51, 630-5	2.1	21
123	Two-photon absorption cross sections: an investigation of the accuracy of calculated absolute and relative values. *Journal of Chemical Physics*, **2006**, 124, 114108	3.9	21
122	Directional characteristics of the moments of the dipole-oscillator-strength distribution of molecules: H2 and H2O. *Physical Review A*, **1993**, 47, 1123-1129	2.6	21
121	A relation between the rotational g-factor and the electric dipole moment of a diatomic molecule. *Chemical Physics Letters*, **1998**, 297, 475-483	2.5	20
120	Electric field gradients of water: A systematic investigation of basis set, electron correlation, and rovibrational effects. *Journal of Chemical Physics*, **2002**, 116, 1424-1434	3.9	20
119	Heterobimetallic nitride complexes from terminal chromium(V) nitride complexes: hyperfine coupling increases with distance. *Angewandte Chemie - International Edition*, **2011**, 50, 4480-3	16.4	19
118	Relativistic calculations of the rotational g factor of the hydrogen halides and noble gas hydride cations. *Journal of Chemical Physics*, **2001**, 114, 84	3.9	19

117	Ligand Sphere Conversions in Terminal Carbide Complexes. *Organometallics*, **2016**, 35, 100-105	3.8	18
116	A Physical Model of the Proton Radiation Belts of Jupiter inside Europa's Orbit. *Journal of Geophysical Research: Space Physics*, **2018**, 123, 3512-3532	2.6	18
115	Kinetics and Thermodynamics of the Reaction between the (]OH Radical and Adenine: A Theoretical Investigation. *Journal of Physical Chemistry A*, **2015**, 119, 6516-27	2.8	18
114	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, 482-9	2.1	18
113	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	17
112	On the discrepancy between theory and experiment for the F-F spin-spin coupling constant of difluoroethyne. *Physical Chemistry Chemical Physics*, **2012**, 14, 16440-7	3.6	17
111	The vibrational dependence of the hydrogen and oxygen nuclear magnetic shielding constants in OH□and OH□H2O. *Chemical Physics*, **1997**, 214, 91-101	2.3	17
110	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	1.4	17
109	Quadrupole moments of Cd and Zn nuclei: When solid-state, molecular, atomic, and nuclear theory meet. *Europhysics Letters*, **2017**, 117, 62001	1.6	16
108	Molecular Switching in Confined Spaces: Effects of Encapsulating the DHA/VHF Photo-Switch in Cucurbiturils. *Chemistry - A European Journal*, **2017**, 23, 17010-17016	4.8	16
107	Electric field effects on nuclear spin□pin coupling tensors and chiral discrimination via NMR spectroscopy. *Theoretical Chemistry Accounts*, **2011**, 129, 359-366	1.9	16
106	Mean excitation energies and energy deposition characteristics of bio-organic molecules. *Journal of Physical Chemistry B*, **2010**, 114, 633-7	3.4	16
105	The Effect of Solvation on the Mean Excitation Energy of Glycine. *Journal of Physical Chemistry Letters*, **2010**, 1, 242-245	6.4	16
104	Definitive Benchmark Study of Ring Current Effects on Amide Proton Chemical Shifts. *Journal of Chemical Theory and Computation*, **2011**, 7, 2078-84	6.4	16
103	Chapter 7:Rovibrational and Temperature Effects in Theoretical Studies of NMR Parameters. *New Developments in NMR*, **2016**, 218-266	0.9	16
102	RPA(D) and HRPA(D): Two new models for calculations of NMR indirect nuclear spin-spin coupling constants. *Journal of Computational Chemistry*, **2018**, 39, 2647-2666	3.5	16
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100	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	3.9	15

99	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	1.4	15
98	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	3.5	15
97	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	3.9	14
96	Analysis of the interactions between difluoroacetylene and one or two hydrogen fluoride molecules based on calculated spin□spin coupling constants. *Computational and Theoretical Chemistry*, **2012**, 998, 98-105	2	14
95	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	2.3	14
94	Effective potential energy curves of the ground electronic state of CH+. *Journal of Chemical Physics*, **2013**, 138, 024315	3.9	14
93	Symmetry, vibrational energy redistribution and vibronic coupling: the internal conversion processes of cycloketones. *Journal of Chemical Physics*, **2012**, 137, 22A522	3.9	14
92	The anomalous deuterium isotope effect in the NMR spectrum of methane: an analysis in localized molecular orbitals. *ChemPhysChem*, **2008**, 9, 1259-61	3.2	14
91	Spin-orbit ZORA and four-component Dirac-Coulomb estimation of relativistic corrections to isotropic nuclear shieldings and chemical shifts of noble gas dimers. *Journal of Computational Chemistry*, **2016**, 37, 395-403	3.5	13
90	The role of explicit solvent molecules in the calculation of NMR chemical shifts of glycine in water. *Theoretical Chemistry Accounts*, **2018**, 137, 1	1.9	13
89	Molecular modeling and experimental studies on structure and NMR parameters of 9-benzyl-3,6-diiodo-9H-carbazole. *Structural Chemistry*, **2015**, 26, 997-1006	1.8	13
88	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	3.8	13
87	Relativistic DFT Calculations of Hyperfine Coupling Constants in 5d Hexafluorido Complexes: [ReF] and [IrF]. *Chemistry - A European Journal*, **2018**, 24, 5124-5133	4.8	13
86	Mean excitation energies for molecular ions. *Nuclear Instruments & Methods in Physics Research B*, **2017**, 394, 73-80	1.2	12
85	Entropy/Enthalpy Compensation in Anion Binding: Biotin[6]uril and Biotin-l-sulfoxide[6]uril Reveal Strong Solvent Dependency. *Journal of Organic Chemistry*, **2019**, 84, 2577-2584	4.2	12
84	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, 17786-99	4.8	12
83	The Mean Excitation Energy of Atomic Ions. *Advances in Quantum Chemistry*, **2015**, 29-40	1.4	12
82	Nuclear magnetic resonance J coupling constant polarizabilities of hydrogen peroxide: a basis set and correlation study. *Journal of Computational Chemistry*, **2012**, 33, 1845-53	3.5	12

81	An isofagomine analogue with an amidine at the pseudoanomeric position. *Organic Letters*, **2011**, 13, 2908-11	6.2	12
80	Ab initio calculations on 2-imidazolyl-2-thiazolyl azo compounds an investigation of potential near-infrared absorbing structures. *Chemical Physics Letters*, **2001**, 343, 171-177	2.5	12
79	Through-space spin–spin coupling constants involving fluorine: benchmarking DFT functionals. *Molecular Physics*, **2019**, 117, 1469-1480	1.7	12
78	The Second-Order-Polarization-Propagator-Approximation (SOPPA) in a four-component spinor basis. *Journal of Chemical Physics*, **2020**, 152, 134113	3.9	11
77	Coupled cluster calculations of mean excitation energies of the noble gas atoms He, Ne and Ar and of the H2 molecule. *Molecular Physics*, **2014**, 112, 751-761	1.7	11
76	On the Determination of the Mean Excitation Energy of Water. *Advances in Quantum Chemistry*, **2013**, 65, 63-77	1.4	11
75	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, 16070-9	3.6	11
74	Mean Excitation Energies for Biomolecules: Glycine to DNA. *Advances in Quantum Chemistry*, **2011**, 62, 215-242	1.4	11
73	Partial charges as reactivity descriptors for nitrido complexes. *Computational and Theoretical Chemistry*, **2009**, 913, 1-7		11
72	A comparison of density functional theory and coupled cluster methods for the calculation of electric dipole polarizability gradients of methane **2012**,		11
71	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
70	The Rotational g Factor of Diatomic Molecules in State 1 or 0+. *Advances in Chemical Physics*, **2007**, 475-536		11
69	On the convergence of the ccJ-pVXZ and pcJ-n basis sets in CCSD calculations of nuclear spin–spin coupling constants: some difficult cases. *Theoretical Chemistry Accounts*, **2018**, 137, 1	1.9	10
68	DFT and experimental studies on structure and spectroscopic parameters of 3,6-diiodo-9-ethyl-9H-carbazole. *Structural Chemistry*, **2016**, 27, 199-207	1.8	10
67	Z-dependence of mean excitation energies for second and third row atoms and their ions. *Journal of Chemical Physics*, **2018**, 148, 174307	3.9	10
66	SOPPA and CCSD vibrational corrections to NMR indirect spin-spin coupling constants of small hydrocarbons **2015**,		10
65	Exploring the relationship between the conformation and pKa: can a pKa value be used to determine the conformational equilibrium?. *Organic and Biomolecular Chemistry*, **2015**, 13, 3116-21	3.9	10
64	Estimating the carbonyl anharmonic vibrational frequency from affordable harmonic frequency calculations. *Journal of Molecular Modeling*, **2012**, 18, 2471-8	2	10

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62	A multipole second order Møller–Plesset solvent reaction field method. *Journal of Chemical Physics*, **2001**, 114, 7753-7760	3.9	10
61	Magnetic interactions in oxide-bridged dichromium(III) complexes. Computational determination of the importance of non-bridging ligands. *Inorganica Chimica Acta*, **2013**, 396, 72-77	2.7	9
60	Benchmarking the multipole shielding polarizability/reaction field approach to solvation against QM/MM: applications to the shielding constants of N-methylacetamide. *Journal of Chemical Physics*, **2011**, 134, 044514	3.9	9
59	Atomic partition of the optical rotatory power of methylhydroperoxide. *Journal of Chemical Physics*, **2008**, 128, 064318	3.9	9
58	Correlated and Gauge Invariant Calculations of Nuclear Shielding Constants **1993**, 351-365		9
57	Computational Prediction of H and C NMR Chemical Shifts for Protonated Alkylpyrroles: Electron Correlation and Not Solvation is the Salvation. *ChemPhysChem*, **2019**, 20, 78-91	3.2	9
56	Determining short-lived solid forms during phase transformations using molecular dynamics. *CrystEngComm*, **2019**, 21, 4020-4024	3.3	8
55	Benchmarking Correlated Methods for Frequency-Dependent Polarizabilities: Aromatic Molecules with the CC3, CCSD, CC2, SOPPA, SOPPA(CC2), and SOPPA(CCSD) Methods. *Journal of Chemical Theory and Computation*, **2020**, 16, 3006-3018	6.4	8
54	Continuum Contributions to Dipole Oscillator-Strength Sum Rules for Hydrogen in Finite Basis Sets. *Advances in Quantum Chemistry*, **2017**, 75, 229-241	1.4	8
53	The Second-Order Polarization Propagator Approximation (SOPPA) method coupled to the polarizable continuum model. *Computational and Theoretical Chemistry*, **2014**, 1040-1041, 54-60	2	8
52	Communication: Rotational g-factor and spin-rotation constant of CH+. *Journal of Chemical Physics*, **2010**, 133, 171101	3.9	8
51	Stopping power of molecules for fast ions. *Molecular Physics*, **2010**, 108, 2891-2897	1.7	8
50	The Bethe Sum Rule and Basis Set Selection in the Calculation of Generalized Oscillator Strengths. *Advances in Quantum Chemistry*, **1999**, 175-192	1.4	8
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48	RPA(D) and HRPA(D): calculation of carbon–carbon spin–spin coupling constants for saturated cycloalkanes. *Molecular Physics*, **2020**, 118, e1757773	1.7	7
47	Relation between properties of long-range diatomic bound states. *Physical Review A*, **2013**, 87,	2.6	7
46	NMR parameters of FNNF as a test for coupled-cluster methods: CCSDT shielding and CC3 spin-spin coupling. *Physical Chemistry Chemical Physics*, **2020**, 22, 21350-21359	3.6	7

45	Benchmarking doubles-corrected random-phase approximation methods for frequency dependent polarizabilities: Aromatic molecules calculated at the RPA, HRPA, RPA(D), HRPA(D), and SOPPA levels. *Journal of Chemical Physics*, **2020**, 152, 234101	3.9	7
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