Stephan P A Sauer

List of Publications by Year in Descending Order

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	A tale of two vectors: A Lanczos algorithm for calculating RPA mean excitation energies.. *Journal of Chemical Physics*, **2022**, 156, 014102	3.9	
205	Extending NMR Quantum Computation Systems by Employing Compounds with Several Heavy Metals as Qubits. *Magnetochemistry*, **2022**, 8, 47	3.1	0
204	On the Unexpected Accuracy of the M06L Functional in the Calculation of Spin-Spin Coupling Constants. *Journal of Chemical Theory and Computation*, **2021**,	6.4	2
203	A Density Functional Theory Study of Optical Rotation in Some Aziridine and Oxirane Derivatives. *ChemPhysChem*, **2021**, 22, 764-774	3.2	0
202	Azo-hydrazone molecular switches: Synthesis and NMR conformational investigation. *Magnetic Resonance in Chemistry*, **2021**, 59, 1116-1125	2.1	1
201	A QM/MM study of the conformation stability and electronic structure of the photochromic switches derivatives of DHA/VHF in acetonitrile solution. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2021**, 251, 119434	4.4	3
200	Benchmarking Correlated Methods for Static and Dynamic Polarizabilities: The T145 Data Set Evaluated with RPA, RPA(D), HRPA, HRPA(D), SOPPA, SOPPA(CC2), SOPPA(CCSD), CC2, and CCSD. *Journal of Physical Chemistry A*, **2021**, 125, 3785-3792	2.8	0
199	The best density functional theory functional for the prediction of H and C chemical shifts of protonated alkylpyrroles. *Journal of Computational Chemistry*, **2021**, 42, 1248-1262	3.5	2
198	Importance of Relativistic Effects for Carbon as an NMR Reporter Nucleus in Carbide-Bridged [RuCPt] Complexes. *Organometallics*, **2021**, 40, 1443-1453	3.8	3
197	The aug-cc-pVTZ-J basis set for the p-block fourth-row elements Ga, Ge, As, Se, and Br. *Magnetic Resonance in Chemistry*, **2021**, 59, 1134-1145	2.1	3
196	Calculation of mean excitation energies of 3d-elements and their cations. *Molecular Physics*, **2021**, 119, e1823508	1.7	2
195	Estimating the accuracy of calculated electron paramagnetic resonance hyperfine couplings for a lytic polysaccharide monooxygenase. *Computational and Structural Biotechnology Journal*, **2021**, 19, 555-567	6.8	3
194	Free Molecule Studies by Perturbed □Angular Correlation: A New Path to Accurate Nuclear Quadrupole Moments. *Physical Review Letters*, **2021**, 126, 103001	7.4	3
193	Prediction of the standard potentials for one-electron oxidation of ,,',' tetrasubstituted -phenylenediamines by calculation. *Physical Chemistry Chemical Physics*, **2021**, 23, 20340-20351	3.6	1
192	Benchmarking anisotropic polarizabilities for 14 (hetero)-aromatic molecules at RPA, RPA(D), HRPA, HRPA(D), SOPPA, SOPPA(CC2), SOPPA(CCSD), CC2, CCSD and CC3 levels. *International Journal of Quantum Chemistry*, **2021**, 121, e26593	2.1	1
191	RPA(D) and HRPA(D): calculation of carbon□carbon spin□spin coupling constants for saturated cycloalkanes. *Molecular Physics*, **2020**, 118, e1757773	1.7	7
190	Interfacial tension in water/n-decane/naphthenic acid systems predicted by a combined COSMO-RS theory and pendant drop experimental study. *Molecular Physics*, **2020**, 118, e1764645	1.7	1

189	Dalton Project: A Python platform for molecular- and electronic-structure simulations of complex systems. *Journal of Chemical Physics*, **2020**, 152, 214115	3.9	24
188	Enhancing NMR Quantum Computation by Exploring Heavy Metal Complexes as Multiqubit Systems: A Theoretical Investigation. *Journal of Physical Chemistry A*, **2020**, 124, 4946-4955	2.8	5
187	On the relationship between bond correction factors and elemental mean excitation energies. *Nuclear Instruments & Methods in Physics Research B*, **2020**, 474, 6-9	1.2	
186	Bond correction factors and their applications to the calculation of molecular mean excitation energies. *Nuclear Instruments & Methods in Physics Research B*, **2020**, 468, 28-36	1.2	2
185	The Second-Order-Polarization-Propagator-Approximation (SOPPA) in a four-component spinor basis. *Journal of Chemical Physics*, **2020**, 152, 134113	3.9	11
184	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
183	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
182	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
181	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
180	Determining short-lived solid forms during phase transformations using molecular dynamics. *CrystEngComm*, **2019**, 21, 4020-4024	3.3	8
179	Test of the validity of Bragg rule for mean excitation energies of small molecules and ions. *Nuclear Instruments & Methods in Physics Research B*, **2019**, 444, 112-116	1.2	6
178	Mean excitation energies of singly charged atomic anions with Z 18. *Journal of Physics B: Atomic, Molecular and Optical Physics*, **2019**, 52, 095004	1.3	5
177	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
176	Bound and continuum state contributions to dipole oscillator strength sum rules: Total and orbital mean excitation energies for cations of C, F, Si, and Cl. *Advances in Quantum Chemistry*, **2019**, 80, 127-146	1.4	3
175	Calculation of mean excitation energies. *Advances in Quantum Chemistry*, **2019**, 80, 225-245	1.4	5
174	Through-space spin spin coupling constants involving fluorine: benchmarking DFT functionals. *Molecular Physics*, **2019**, 117, 1469-1480	1.7	12
173	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
172	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

171	Theoretical study of the NMR chemical shift of Xe in supercritical condition. *Journal of Molecular Modeling*, **2018**, 24, 62	2	3
170	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
169	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
168	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
167	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
166	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
165	Direct observation of Mg complexes in ionic liquid solutions by Mg NMR spectroscopy. *Dalton Transactions*, **2018**, 47, 14431-14435	4.3	8
164	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
163	The influence of relativistic effects on nuclear magnetic resonance spin-spin coupling constant polarizabilities of H O , H S , H Se , and H Te. *Journal of Computational Chemistry*, **2018**, 39, 2589-2600	3.5	5
162	Analysis of the interactions in FCCF:(H2O) and FCCF:(H2O)2 complexes through the study of their indirect spin spin coupling constants. *Molecular Physics*, **2018**, 116, 2396-2405	1.7	6
161	Azadioxatriangulenium and Diazaoxatriangulenium: Quantum Yields and Fundamental Photophysical Properties. *ACS Omega*, **2017**, 2, 193-203	3.9	23
160	Quadrupole moments of Cd and Zn nuclei: When solid-state, molecular, atomic, and nuclear theory meet. *Europhysics Letters*, **2017**, 117, 62001	1.6	16
159	Mean excitation energies for molecular ions. *Nuclear Instruments & Methods in Physics Research B*, **2017**, 394, 73-80	1.2	12
158	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
157	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
156	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
155	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
154	Ligand Sphere Conversions in Terminal Carbide Complexes. *Organometallics*, **2016**, 35, 100-105	3.8	18

153	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
152	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
151	Chapter 7:Rovibrational and Temperature Effects in Theoretical Studies of NMR Parameters. *New Developments in NMR*, **2016**, 218-266	0.9	16
150	Calculation of dipole polarizability derivatives of adamantane and their use in electron scattering computations. *European Physical Journal D*, **2016**, 70, 1	1.3	4
149	The Effect of Solvation on the Radiation Damage Rate Constants for Adenine. *ChemPhysChem*, **2016**, 17, 3086-3095	3.2	3
148	Performance of SOPPA-based methods in the calculation of vertical excitation energies and oscillator strengths. *Molecular Physics*, **2015**, 113, 2026-2045	1.7	27
147	Anion binding by biotin[6]uril in water. *Organic and Biomolecular Chemistry*, **2015**, 13, 369-73	3.9	62
146	On the truncation of the number of excited states in density functional theory sum-over-states calculations of indirect spin spin coupling constants. *Journal of Chemical Physics*, **2015**, 143, 244107	3.9	1
145	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
144	SOPPA and CCSD vibrational corrections to NMR indirect spin-spin coupling constants of small hydrocarbons **2015**,		10
143	The Mean Excitation Energy of Atomic Ions. *Advances in Quantum Chemistry*, **2015**, 29-40	1.4	12
142	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
141	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
140	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
139	The Dalton quantum chemistry program system. *Wiley Interdisciplinary Reviews: Computational Molecular Science*, **2014**, 4, 269-284	7.9	956
138	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
137	On the transferability of atomic contributions to the optical rotatory power of hydrogen peroxide, methyl hydroperoxide and dimethyl peroxide. *Molecular Physics*, **2014**, 112, 1624-1632	1.7	3
136	Optimizing the Structure of Tetracyanoplatinate (II): A Comparison of Relativistic Density Functional Theory Methods. *Current Inorganic Chemistry*, **2014**, 3, 213-219		5

135	On the Use of Locally Dense Basis Sets in the Calculation of EPR Hyperfine Couplings: A Study on Model Systems for Bio-Inorganic Fe and Co Complexes. *Current Inorganic Chemistry*, **2014**, 3, 270-283		4
134	Communication: Localized molecular orbital analysis of the effect of electron correlation on the anomalous isotope effect in the NMR spin-spin coupling constant in methane. *Journal of Chemical Physics*, **2014**, 141, 151101	3.9	6
133	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
132	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	36
131	Failures of TDDFT in describing the lowest intramolecular charge-transfer excitation in para-nitroaniline. *Molecular Physics*, **2013**, 111, 1235-1248	1.7	71
130	On the Determination of the Mean Excitation Energy of Water. *Advances in Quantum Chemistry*, **2013**, 65, 63-77	1.4	11
129	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
128	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
127	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
126	Validating and Analyzing EPR Hyperfine Coupling Constants with Density Functional Theory. *Journal of Chemical Theory and Computation*, **2013**, 9, 2380-8	6.4	23
125	Effective potential energy curves of the ground electronic state of CH+. *Journal of Chemical Physics*, **2013**, 138, 024315	3.9	14
124	Relation between properties of long-range diatomic bound states. *Physical Review A*, **2013**, 87,	2.6	7
123	Quantum-dynamical Modeling of the Rydberg to Valence Excited-State Internal Conversion in Cyclobutanone and Cyclopentanone. *EPJ Web of Conferences*, **2013**, 41, 02033	0.3	
122	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
121	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
120	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
119	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
118	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

117	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
116	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
115	Estimating the carbonyl anharmonic vibrational frequency from affordable harmonic frequency calculations. *Journal of Molecular Modeling*, **2012**, 18, 2471-8	2	10
114	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
113	Symmetry, vibrational energy redistribution and vibronic coupling: the internal conversion processes of cycloketones. *Journal of Chemical Physics*, **2012**, 137, 22A522	3.9	14
112	A comparison of density functional theory and coupled cluster methods for the calculation of electric dipole polarizability gradients of methane **2012**,		11
111	Theory and Calculation of Stopping Cross Sections of Nucleobases for Swift Ions **2012**, 191-200		
110	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
109	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
108	Mean Excitation Energies for Biomolecules: Glycine to DNA. *Advances in Quantum Chemistry*, **2011**, 62, 215-242	1.4	11
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	Calculated rotational and vibrational g factors of LiH X 1□ and evaluation of parameters in radial functions from rotational and vibration-rotational spectra. *International Journal of Quantum Chemistry*, **2011**, 111, 736-752	2.1	4
105	David M. Bishop: Esteemed colleague and dear friend. *International Journal of Quantum Chemistry*, **2011**, 111, 723-724	2.1	
104	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
103	The coupling constant polarizability and hyperpolarizabilty of 1J(NH) in N-methylacetamide, and its application for the multipole spin-spin coupling constant polarizability/reaction field approach to solvation. *Journal of Computational Chemistry*, **2011**, 32, 3168-74	3.5	4
102	Heterobimetallic Nitride Complexes from Terminal Chromium(V) Nitride Complexes: Hyperfine Coupling Increases with Distance. *Angewandte Chemie*, **2011**, 123, 4572-4575	3.6	2
101	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
100	Benchmarking SOPPA(CC2) for the calculation of indirect nuclear spin□pin coupling constants: Carbocycles. *Chemical Physics*, **2011**, 381, 35-43	2.3	28

99	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
98	An isofagomine analogue with an amidine at the pseudoanomeric position. *Organic Letters*, **2011**, 13, 2908-11	6.2	12
97	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
96	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
95	Molecular Electromagnetism **2011**,		63
94	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
93	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
92	Communication: Rotational g-factor and spin-rotation constant of CH+. *Journal of Chemical Physics*, **2010**, 133, 171101	3.9	8
91	Mean excitation energies and energy deposition characteristics of bio-organic molecules. *Journal of Physical Chemistry B*, **2010**, 114, 633-7	3.4	16
90	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
89	Stopping power of molecules for fast ions. *Molecular Physics*, **2010**, 108, 2891-2897	1.7	8
88	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
87	The Effect of Solvation on the Mean Excitation Energy of Glycine. *Journal of Physical Chemistry Letters*, **2010**, 1, 242-245	6.4	16
86	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
85	Benchmarks of electronically excited states: basis set effects on CASPT2 results. *Journal of Chemical Physics*, **2010**, 133, 174318	3.9	177
84	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
83	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
82	On the relation between the non-adiabatic vibrational reduced mass and the electric dipole moment gradient of a diatomic molecule. *Theoretical Chemistry Accounts*, **2009**, 122, 137-143	1.9	5

81	Partial charges as reactivity descriptors for nitrido complexes. *Computational and Theoretical Chemistry*, **2009**, 913, 1-7		11
80	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
79	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
78	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
77	Analysis of isotope effects in NMR one-bond indirect nuclear spin-spin coupling constants in terms of localized molecular orbitals. *Physical Chemistry Chemical Physics*, **2009**, 11, 3987-95	3.6	15
76	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
75	A Comparison of M□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		10
74	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
73	Benchmarks for electronically excited states: CASPT2, CC2, CCSD, and CC3. *Journal of Chemical Physics*, **2008**, 128, 134110	3.9	737
72	Amino Acid Mean Excitation Energies and Directional Dependencies from Core and Bond Calculations **2008**,		5
71	Atomic partition of the optical rotatory power of methylhydroperoxide. *Journal of Chemical Physics*, **2008**, 128, 064318	3.9	9
70	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
69	On the aromaticity of tetrathiafulvalene cations. *Chemical Physics Letters*, **2008**, 453, 136-139	2.5	23
68	Calculations of Polarizabilities and Their Gradients for Electron Energy-Loss Spectroscopy. *Collection of Czechoslovak Chemical Communications*, **2008**, 73, 1509-1524		5
67	The Rotational g Factor of Diatomic Molecules in State 1□ or 0+. *Advances in Chemical Physics*, **2007**, 475-536		11
66	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
65	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
64	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

63	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
62	The Rotational g Tensor of HF, H2O, NH3, and CH4: A Comparison of Correlated Ab Initio Methods. *Advances in Quantum Chemistry*, **2005**, 48, 469-490	1.4	4
61	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
60	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
59	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
58	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
57	Analysis of Pure Rotational and Vibration-rotational Spectra of NaCl X 1□ and Quantum-chemical Calculation of Related Molecular Properties. *Journal of the Chinese Chemical Society*, **2005**, 52, 631-639	1.5	3
56	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
55	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
54	Non-empirical calculations of NMR indirect carbon-carbon coupling constants. Part 8--monocycloalkanes. *Magnetic Resonance in Chemistry*, **2004**, 42, 671-86	2.1	49
53	Large Long-Range F□ Indirect Spin□Spin Coupling Constants. Prediction of Measurable F□ Couplings over a Few Nanometers. *Journal of Physical Chemistry A*, **2004**, 108, 5393-5398	2.8	46
52	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
51	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
50	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
49	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
48	Non-empirical calculations of NMR indirect carbon□arbon coupling constants: 1. Three-membered rings. *Magnetic Resonance in Chemistry*, **2002**, 40, 187-194	2.1	61
47	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
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