Stephan P A Sauer

List of Publications by Year
in descending order

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207 papers	8,820 citations	66250 44 h-index	60403 85 g-index
220 all docs	220 docs citations	220 times ranked	5857 citing authors

#	Article	IF	Citations
1	A tale of two vectors: A Lanczos algorithm for calculating RPA mean excitation energies. Journal of Chemical Physics, 2022, 156, 014102.	1.2	1
2	Extending NMR Quantum Computation Systems by Employing Compounds with Several Heavy Metals as Qubits. Magnetochemistry, 2022, 8, 47.	1.0	5
3	Calculation of mean excitation energies of 3d-elements and their cations. Molecular Physics, 2021, 119, e1823508.	0.8	4
4	Estimating the accuracy of calculated electron paramagnetic resonance hyperfine couplings for a lytic polysaccharide monooxygenase. Computational and Structural Biotechnology Journal, 2021, 19, 555-567.	1.9	11
5	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.	2.9	15
6	A Density Functional Theory Study of Optical Rotation in Some Aziridine and Oxirane Derivatives. ChemPhysChem, 2021, 22, 764-774.	1.0	2
7	Azoâ€hydrazone molecular switches: Synthesis and NMR conformational investigation. Magnetic Resonance in Chemistry, 2021, 59, 1116-1125.	1.1	5
8	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.	2.0	10
9	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.	1.1	5
10	The best <scp>density functional theory</scp> functional for the prediction of ¹H and ¹³C chemical shifts of protonated alkylpyrroles. Journal of Computational Chemistry, 2021, 42, 1248-1262.	1.5	5
11	Importance of Relativistic Effects for Carbon as an NMR Reporter Nucleus in Carbide-Bridged [RuCPt] Complexes. Organometallics, 2021, 40, 1443-1453.	1.1	4
12	The augâ€ccâ€pVTZâ€J basis set for the pâ€block fourthâ€row elements Ga, Ge, As, Se, and Br. Magnetic Resonance in Chemistry, 2021, 59, 1134-1145.	1.1	6
13	Prediction of the standard potentials for one-electron oxidation ofN,N,Nâ€²,Nâ€² tetrasubstitutedp-phenylenediamines by calculation. Physical Chemistry Chemical Physics, 2021, 23, 20340-20351.	1.3	3
14	Benchmarking anisotropic polarizabilities for 14 (hetero)â€aromatic molecules at <scp>RPA</scp>, <scp>RPA</scp>(D), <scp>HRPA</scp>, <scp>HRPA</scp>(D), <scp>SOPPA</scp>, <scp>SOPPA</scp>(<scp>CC2</scp>), <scp>SOPPA</scp>(<scp>CCSD</scp>), <scp>CC2</scp>, <scp>CCSD</scp> and <scp>CC3</scp> levels. International Journal of Quantum Chemistry, 2021, 121, e26593.	1.0	3
15	On the Unexpected Accuracy of the M06L Functional in the Calculation of ¹J_{FC} Spinâ€“Spin Coupling Constants. Journal of Chemical Theory and Computation, 2021, 17, 7712-7723.	2.3	10
16	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.	1.5	17
17	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.	1.3	10
18	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.	1.2	10

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19	RPA(D) and HRPA(D): calculation of carbonâ€“carbon spinâ€“spin coupling constants for saturated cycloalkanes. Molecular Physics, 2020, 118, .	0.8	9
20	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.	0.8	3
21	Dalton Project: A Python platform for molecular- and electronic-structure simulations of complex systems. Journal of Chemical Physics, 2020, 152, 214115.	1.2	45
22	Enhancing NMR Quantum Computation by Exploring Heavy Metal Complexes as Multiqubit Systems: A Theoretical Investigation. Journal of Physical Chemistry A, 2020, 124, 4946-4955.	1.1	12
23	On the relationship between bond correction factors and elemental mean excitation energies. Nuclear Instruments & Methods in Physics Research B, 2020, 474, 6-9.	0.6	0
24	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.	0.6	2
25	The Second-Order-Polarization-Propagator-Approximation (SOPPA) in a four-component spinor basis. Journal of Chemical Physics, 2020, 152, 134113.	1.2	16
26	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.	2.3	10
27	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.	1.0	15
28	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.	0.4	3
29	Calculation of mean excitation energies. Advances in Quantum Chemistry, 2019, 80, 225-245.	0.4	10
30	Determining short-lived solid forms during phase transformations using molecular dynamics. CrystEngComm, 2019, 21, 4020-4024.	1.3	16
31	Test of the validity of Braggâ€™s rule for mean excitation energies of small molecules and ions. Nuclear Instruments & Methods in Physics Research B, 2019, 444, 112-116.	0.6	6
32	Mean excitation energies of singly charged atomic anions with Z â‰¥ 18. Journal of Physics B: Atomic, Molecular and Optical Physics, 2019, 52, 095004.	0.6	5
33	Entropy/Enthalpy Compensation in Anion Binding: Biotin[6]uril and Biotin-<scp>I</scp>-sulfoxide[6]uril Reveal Strong Solvent Dependency. Journal of Organic Chemistry, 2019, 84, 2577-2584.	1.7	23
34	Through-space spinâ€“spin coupling constants involving fluorine: benchmarking DFT functionals. Molecular Physics, 2019, 117, 1469-1480.	0.8	18
35	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.	0.5	14
36	Theoretical study of the NMR chemical shift of Xe in supercritical condition. Journal of Molecular Modeling, 2018, 24, 62.	0.8	3

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37	Frontispiece: Relativistic DFT Calculations of Hyperfine Coupling Constants in 5d Hexafluorido Complexes: [ReF6]2â^' and [IrF6]2â^'. Chemistry - A European Journal, 2018, 24, .	1.7	1
38	Relativistic DFT Calculations of Hyperfine Coupling Constants in 5d Hexafluorido Complexes: [ReF₆]^{2â^'} and [IrF₆]^{2â^'}. Chemistry - A European Journal, 2018, 24, 5124-5133.	1.7	16
39	Direct observation of Mg²⁺complexes in ionic liquid solutions by³¹Mg Î²-NMR spectroscopy. Dalton Transactions, 2018, 47, 14431-14435.	1.6	12
40	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.	1.5	21
41	The influence of relativistic effects on nuclear magnetic resonance spinâ€"spin coupling constant polarizabilities of H₂O₂, H₂S₂, H₂Se₂, and H₂Te₂. Journal of Computational Chemistry, 2018, 39, 2589-2600.	1.5	7
42	Analysis of the interactions in FCCF:(H2O) and FCCF:(H2O)2 complexes through the study of their indirect spinâ€"spin coupling constants. Molecular Physics, 2018, 116, 2396-2405.	0.8	8
43	A Physical Model of the Proton Radiation Belts of Jupiter inside Europa's Orbit. Journal of Geophysical Research: Space Physics, 2018, 123, 3512-3532.	0.8	30
44	Z-dependence of mean excitation energies for second and third row atoms and their ions. Journal of Chemical Physics, 2018, 148, 174307.	1.2	13
45	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.	1.2	22
46	The role of explicit solvent molecules in the calculation of NMR chemical shifts of glycine in water. Theoretical Chemistry Accounts, 2018, 137, 1.	0.5	16
47	Azadioxatriangulenium and Diazaoxatriangulenium: Quantum Yields and Fundamental Photophysical Properties. ACS Omega, 2017, 2, 193-203.	1.6	29
48	Quadrupole moments of Cd and Zn nuclei: When solid-state, molecular, atomic, and nuclear theory meet. Europhysics Letters, 2017, 117, 62001.	0.7	21
49	Mean excitation energies for molecular ions. Nuclear Instruments & Methods in Physics Research B, 2017, 394, 73-80.	0.6	12
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.	2.3	41
51	Molecular Switching in Confined Spaces: Effects of Encapsulating the DHA/VHF Photoâ€Switch in Cucurbiturils. Chemistry - A European Journal, 2017, 23, 17010-17016.	1.7	23
52	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.	0.8	19
53	Continuum Contributions to Dipole Oscillator-Strength Sum Rules for Hydrogen in Finite Basis Sets. Advances in Quantum Chemistry, 2017, 75, 229-241.	0.4	8
54	Calculation of dipole polarizability derivatives of adamantane and their use in electron scattering computations. European Physical Journal D, 2016, 70, 1.	0.6	5

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55	The Effect of Solvation on the Radiation Damage Rate Constants for Adenine. ChemPhysChem, 2016, 17, 3086-3095.	1.0	5
56	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.	1.5	14
57	DFT and experimental studies on structure and spectroscopic parameters of 3,6-diiodo-9-ethyl-9H-carbazole. Structural Chemistry, 2016, 27, 199-207.	1.0	12
58	Ligand Sphere Conversions in Terminal Carbide Complexes. Organometallics, 2016, 35, 100-105.	1.1	20
59	Rovibrational and Temperature Effects in Theoretical Studies of NMR Parameters. New Developments in NMR, 2016, , 218-266.	0.1	23
60	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.	1.2	3
61	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.	1.7	18
62	SOPPA and CCSD vibrational corrections to NMR indirect spin-spin coupling constants of small hydrocarbons. AIP Conference Proceedings, 2015, , .	0.3	13
63	The Mean Excitation Energy of Atomic Ions. Advances in Quantum Chemistry, 2015, , 29-40.	0.4	14
64	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.	1.1	21
65	Molecular modeling and experimental studies on structure and NMR parameters of 9-benzyl-3,6-diiodo-9H-carbazole. Structural Chemistry, 2015, 26, 997-1006.	1.0	18
66	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.	1.5	13
67	Performance of SOPPA-based methods in the calculation of vertical excitation energies and oscillator strengths. Molecular Physics, 2015, 113, 2026-2045.	0.8	31
68	Anion binding by biotin[6]uril in water. Organic and Biomolecular Chemistry, 2015, 13, 369-373.	1.5	76
69	Optimizing the Structure of Tetracyanoplatinate (II): A Comparison of Relativistic Density Functional Theory Methods. Current Inorganic Chemistry, 2014, 3, 213-219.	0.2	7
70	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.	0.2	6
71	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.	1.2	8
72	The Second-Order Polarization Propagator Approximation (SOPPA) method coupled to the polarizable continuum model. Computational and Theoretical Chemistry, 2014, 1040-1041, 54-60.	1.1	9

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73	The <scp>D</scp>alton quantum chemistry program system. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2014, 4, 269-284.	6.2	1,166
74	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.	0.8	12
75	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.	0.8	3
76	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.	1.3	30
77	Failures of TDDFT in describing the lowest intramolecular charge-transfer excitation in para-nitroaniline. Molecular Physics, 2013, 111, 1235-1248.	0.8	79
78	On the Determination of the Mean Excitation Energy of Water. Advances in Quantum Chemistry, 2013, 65, 63-77.	0.4	14
79	Halogen effect on structure and ¹³C NMR chemical shift of 3,6â€disubstitutedâ€Nâ€alkyl carbazoles. Magnetic Resonance in Chemistry, 2013, 51, 630-635.	1.1	27
80	Magnetic interactions in oxide-bridged dichromium(III) complexes. Computational determination of the importance of non-bridging ligands. Inorganica Chimica Acta, 2013, 396, 72-77.	1.2	10
81	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.	1.1	24
82	Validating and Analyzing EPR Hyperfine Coupling Constants with Density Functional Theory. Journal of Chemical Theory and Computation, 2013, 9, 2380-2388.	2.3	29
83	Effective potential energy curves of the ground electronic state of CH+. Journal of Chemical Physics, 2013, 138, 024315.	1.2	19
84	Relation between properties of long-range diatomic bound states. Physical Review A, 2013, 87, .	1.0	10
85	Quantum-dynamical Modeling of the Rydberg to Valence Excited-State Internal Conversion in Cyclobutanone and Cyclopentanone. EPJ Web of Conferences, 2013, 41, 02033.	0.1	0
86	Symmetry, vibrational energy redistribution and vibronic coupling: The internal conversion processes of cycloketones. Journal of Chemical Physics, 2012, 137, 22A522.	1.2	17
87	A comparison of density functional theory and coupled cluster methods for the calculation of electric dipole polarizability gradients of methane. AIP Conference Proceedings, 2012, , .	0.3	13
88	Fully relativistic coupled cluster and DFT study of electric field gradients at Hg in 199Hg compounds. Physical Chemistry Chemical Physics, 2012, 14, 2651.	1.3	31
89	On the discrepancy between theory and experiment for the Fâ€“F spinâ€“spin coupling constant of difluoroethyne. Physical Chemistry Chemical Physics, 2012, 14, 16440.	1.3	19
90	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.	1.3	13

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91	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.	1.1	14
92	Improving the calculation of electron paramagnetic resonance hyperfine coupling tensors for d-block metals. Physical Chemistry Chemical Physics, 2012, 14, 10669.	1.3	31
93	Nuclear magnetic resonance J coupling constant polarizabilities of hydrogen peroxide: A basis set and correlation study. Journal of Computational Chemistry, 2012, 33, 1845-1853.	1.5	13
94	On the importance of excited state dynamic response electron correlation in polarizable embedding methods. Journal of Computational Chemistry, 2012, 33, 2012-2022.	1.5	38
95	Estimating the carbonyl anharmonic vibrational frequency from affordable harmonic frequency calculations. Journal of Molecular Modeling, 2012, 18, 2471-2478.	0.8	10
96	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.	0.9	14
97	Definitive Benchmark Study of Ring Current Effects on Amide Proton Chemical Shifts. Journal of Chemical Theory and Computation, 2011, 7, 2078-2084.	2.3	16
98	An Isofagomine Analogue with an Amidine at the Pseudoanomeric Position. Organic Letters, 2011, 13, 2908-2911.	2.4	15
99	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.	2.3	78
100	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.	1.2	55
101	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.	2.3	52
102	Mean Excitation Energies for Biomolecules. Advances in Quantum Chemistry, 2011, 62, 215-242.	0.4	18
103	Electric field effects on nuclear spinâ€“spin coupling tensors and chiral discrimination via NMR spectroscopy. Theoretical Chemistry Accounts, 2011, 129, 359-366.	0.5	18
104	Calculated rotational and vibrational g factors of LiH X ¹Î£⁺ and evaluation of parameters in radial functions from rotational and vibrationâ€rotational spectra. International Journal of Quantum Chemistry, 2011, 111, 736-752.	1.0	4
105	David M. Bishop: Esteemed colleague and dear friend. International Journal of Quantum Chemistry, 2011, 111, 723-724.	1.0	0
106	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.	1.1	50
107	The coupling constant polarizability and hyperpolarizabilty of ¹J(NH) in Nâ€methylacetamide, and its application for the multipole spinâ€“spin coupling constant polarizability/reaction field approach to solvation. Journal of Computational Chemistry, 2011, 32, 3168-3174.	1.5	4
108	Heterobimetallic Nitride Complexes from Terminal Chromium(V) Nitride Complexes: Hyperfine Coupling Increases with Distance. Angewandte Chemie - International Edition, 2011, 50, 4480-4483.	7.2	27

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109	Benchmarking SOPPA(CC2) for the calculation of indirect nuclear spinâ€“spin coupling constants: Carbocycles. Chemical Physics, 2011, 381, 35-43.	0.9	31
110	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.	1.2	9
111	Comparison of the directional characteristics of swift ion excitation for two small biomolecules: glycine and alanine. European Physical Journal D, 2010, 60, 71-76.	0.6	11
112	Structural trends of ⁷⁷Seï£¿¹H spinâ€“spin coupling constants and conformational behavior of 2â€substituted selenophenes. Magnetic Resonance in Chemistry, 2010, 48, 44-52.	1.1	77
113	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.	1.2	33
114	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.	1.2	83
115	Communication: Rotational g-factor and spin-rotation constant of CH+. Journal of Chemical Physics, 2010, 133, 171101.	1.2	10
116	Mean Excitation Energies and Energy Deposition Characteristics of Bio-organic Molecules. Journal of Physical Chemistry B, 2010, 114, 633-637.	1.2	16
117	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.	1.5	14
118	Stopping power of molecules for fast ions. Molecular Physics, 2010, 108, 2891-2897.	0.8	8
119	Basis set effects on coupled cluster benchmarks of electronically excited states: CC3, CCSDR(3) and CC2. Molecular Physics, 2010, 108, 453-465.	0.8	142
120	The Effect of Solvation on the Mean Excitation Energy of Glycine. Journal of Physical Chemistry Letters, 2010, 1, 242-245.	2.1	20
121	Benchmarking NMR indirect nuclear spin-spin coupling constants: SOPPA, SOPPA(CC2), and SOPPA(CCSD) versus CCSD. Journal of Chemical Physics, 2010, 133, 144106.	1.2	72
122	Benchmarks of electronically excited states: Basis set effects on CASPT2 results. Journal of Chemical Physics, 2010, 133, 174318.	1.2	201
123	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.	0.5	5
124	Partial charges as reactivity descriptors for nitrido complexes. Computational and Theoretical Chemistry, 2009, 913, 1-7.	1.5	15
125	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.	1.1	51
126	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.	2.3	115

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127	Prediction of spin-spin coupling constants in solution based on combined density functional theory/molecular mechanics. Journal of Chemical Physics, 2009, 130, 134508.	1.2	48
128	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.	1.3	17
129	The Anomalous Deuterium Isotope Effect in the NMR Spectrum of Methane: An Analysis in Localized Molecular Orbitals. ChemPhysChem, 2008, 9, 1259-1261.	1.0	15
130	On the aromaticity of tetrathiafulvalene cations. Chemical Physics Letters, 2008, 453, 136-139.	1.2	25
131	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.	2.3	51
132	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
133	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.	1.2	478
134	Benchmarks for electronically excited states: CASPT2, CC2, CCSD, and CC3. Journal of Chemical Physics, 2008, 128, 134110.	1.2	833
135	Amino Acid Mean Excitation Energies and Directional Dependencies from Core and Bond Calculations. , 2008, , .		5
136	Atomic partition of the optical rotatory power of methylhydroperoxide. Journal of Chemical Physics, 2008, 128, 064318.	1.2	10
137	Calculations of Polarizabilities and Their Gradients for Electron Energy-Loss Spectroscopy. Collection of Czechoslovak Chemical Communications, 2008, 73, 1509-1524.	1.0	5
138	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.	1.2	34
139	The RotationalgFactor of Diatomic Molecules in State1Î£+or 0+. Advances in Chemical Physics, 2007, , 475-536.	0.3	15
140	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.	2.3	28
141	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.	1.1	26
142	Two-photon absorption cross sections: An investigation of the accuracy of calculated absolute and relative values. Journal of Chemical Physics, 2006, 124, 114108.	1.2	23
143	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.	0.4	17
144	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.	0.4	65

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145	Analysis of Pure Rotational and Vibration-rotational Spectra of NaCl X1Î£+and Quantum-chemical Calculation of Related Molecular Properties. Journal of the Chinese Chemical Society, 2005, 52, 631-639.	0.8	4
146	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.	0.4	15
147	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.	0.4	5
148	The vibrational g-factor of dihydrogen from theoretical calculation and analysis of vibration-rotational spectra. Physical Chemistry Chemical Physics, 2005, 7, 1747.	1.3	27
149	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.	1.1	52
150	First principle calculations of 113Cd chemical shifts for proteins and model systems. Journal of Biological Inorganic Chemistry, 2004, 9, 591-599.	1.1	35
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