

# Juha Vaara

## List of Publications by Year in descending order

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139  
papers

4,953  
citations

94381

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144  
docs citations

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times ranked

2715  
citing authors

#	ARTICLE	IF	CITATIONS
1	Energetics and exchange of xenon and water in a prototypic cryptophane-A biosensor structure. <i>Physical Chemistry Chemical Physics</i> , 2022, 24, 17946-17950.	1.3	5
2	Direct enantiomeric discrimination through antisymmetric hyperfine coupling. <i>Chemical Communications</i> , 2021, 57, 8264-8267.	2.2	0
3	Polarization transfer in a spin-exchange optical-pumping experiment. <i>Physical Review A</i> , 2020, 102, .	1.0	1
4	Paramagnetic Pyrazolylborate Complexes $Tp^{2+}M$ and $Tp^{2+}M$ : $^{13}C$ , $^{11}B$ , and $^{14}N$ NMR Spectra and First-Principles Studies of Chemical Shifts. <i>Inorganic Chemistry</i> , 2020, 59, 9294-9307.	1.9	10
5	Remarkable reversal of $^{13}C$ -NMR assignment in $d^{1+}$ , $d^{2+}$ compared to $d^{8+}$ , $d^{9+}$ acetylacetonate complexes: analysis and explanation based on solid-state MAS NMR and computations. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 8048-8059.	1.3	12
6	Direct magnetic-field dependence of NMR chemical shift. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 8485-8490.	1.3	4
7	Calculation of scalar nuclear spin-spin coupling in a noble-gas mixture. <i>Physical Review A</i> , 2019, 99, .	1.0	8
8	Brownian Translational Dynamics on a Flexible Surface: Nuclear Spin Relaxation of Fluid Membrane Phases. <i>Langmuir</i> , 2018, 34, 3755-3766.	1.6	2
9	Chemical shift extremum of $^{129}Xe(aq)$ reveals details of hydrophobic solvation. <i>Scientific Reports</i> , 2018, 8, 7023.	1.6	9
10	Ab initio paramagnetic NMR shifts via point-dipole approximation in a large magnetic-anisotropy $Co(ii)$ complex. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 22547-22555.	1.3	14
11	Paramagnetic Enhancement of Nuclear Spin-Spin Coupling. <i>Journal of Chemical Theory and Computation</i> , 2017, 13, 1275-1283.	2.3	8
12	Characterization of pore structures of hydrated cements and natural shales by $^{129}Xe$ NMR spectroscopy. <i>Microporous and Mesoporous Materials</i> , 2017, 253, 49-54.	2.2	15
13	Relativistic Approximations to Paramagnetic NMR Chemical Shift and Shielding Anisotropy in Transition Metal Systems. <i>Journal of Chemical Theory and Computation</i> , 2017, 13, 3731-3745.	2.3	26
14	Electron and nuclear spin polarization in Rb-Xe spin-exchange optical hyperpolarization. <i>Physical Review A</i> , 2017, 95, .	1.0	6
15	Ratcheting rotation or speedy spinning: EPR and dynamics of $Sc^{3+}C^{2+}@C^{80}$ . <i>Chemical Communications</i> , 2017, 53, 8992-8995.	2.2	6
16	Assignment of solid-state $^{13}C$ and $^1H$ NMR spectra of paramagnetic $Ni(II)$ acetylacetonate complexes aided by first-principles computations. <i>Solid State Nuclear Magnetic Resonance</i> , 2017, 87, 29-37.	1.5	17
17	Relation between molecular electronic structure and nuclear spin-induced circular dichroism. <i>Scientific Reports</i> , 2017, 7, 46617.	1.6	6
18	Experimental and First-Principles NMR Analysis of $Pt(II)$ Complexes With $\alpha$ -Dialkyldithiophosphate Ligands. <i>Journal of Physical Chemistry A</i> , 2016, 120, 8326-8338.	1.1	8

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19	Pseudo-Contact NMR Shifts over the Paramagnetic Metalloprotein CoMMP-12 from First Principles. <i>Angewandte Chemie - International Edition</i> , 2016, 55, 14713-14717.	7.2	51
20	Pseudo-Contact NMR Shifts over the Paramagnetic Metalloprotein CoMMP-12 from First Principles. <i>Angewandte Chemie</i> , 2016, 128, 14933-14937.	1.6	14
21	Liquid-state paramagnetic relaxation from first principles. <i>Physical Review A</i> , 2016, 94, .	1.0	8
22	Magnetic Couplings in the Chemical Shift of Paramagnetic NMR. <i>Journal of Chemical Theory and Computation</i> , 2015, 11, 4840-4849.	2.3	69
23	Spin Doublet Point Defects in Graphenes: Predictions for ESR and NMR Spectral Parameters. <i>Journal of Chemical Theory and Computation</i> , 2015, 11, 3746-3754.	2.3	12
24	Xenon NMR of liquid crystals confined to cylindrical nanocavities: a simulation study. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 7158-7171.	1.3	14
25	<sup>1</sup> H Chemical Shifts in Paramagnetic Co(II) Pyrazolylborate Complexes: A First-Principles Study. <i>Journal of Chemical Theory and Computation</i> , 2015, 11, 1683-1691.	2.3	52
26	Nuclear spin circular dichroism in fullerenes: a computational study. <i>Chemical Communications</i> , 2014, 50, 15228-15231.	2.2	9
27	Spin dynamics simulation of electron spin relaxation in Ni <sup>2+</sup> (aq). <i>Journal of Chemical Physics</i> , 2014, 141, 014109.	1.2	12
28	Nuclear spin circular dichroism. <i>Journal of Chemical Physics</i> , 2014, 140, 134103.	1.2	20
29	Nuclear quadrupole moment-induced Cotton-Mouton effect in molecules. <i>Journal of Chemical Physics</i> , 2014, 140, 024103.	1.2	11
30	Nuclear Spin-Induced Cotton-Mouton Effect in a Strong External Magnetic Field. <i>ChemPhysChem</i> , 2014, 15, 2337-2350.	1.0	10
31	Curie-type paramagnetic NMR relaxation in the aqueous solution of Ni <sup>2+</sup> . <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 6916-6924.	1.3	13
32	Solvation chemical shifts of perylenic antenna molecules from molecular dynamics simulations. <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 22309-22320.	1.3	7
33	Characteristic Spectral Patterns in the Carbon-13 Nuclear Magnetic Resonance Spectra of Hexagonal and Crenellated Graphene Fragments. <i>ChemPhysChem</i> , 2014, 15, 1799-1808.	1.0	11
34	Faraday Rotation in Graphene Quantum Dots: Interplay of Size, Perimeter Type, and Functionalization. <i>Journal of Physical Chemistry C</i> , 2014, 118, 23996-24005.	1.5	17
35	Solvation structure and dynamics of Ni <sup>2+</sup> (aq) from a polarizable force field. <i>Chemical Physics</i> , 2014, 443, 112-122.	0.9	1
36	Chemical Shift in Paramagnetic Systems. <i>Science and Technology of Atomic, Molecular, Condensed Matter and Biological Systems</i> , 2013, , 41-67.	0.6	7

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37	Toward Reproducing Sequence Trends in Phosphorus Chemical Shifts for Nucleic Acids by MD/DFT Calculations. <i>Journal of Chemical Theory and Computation</i> , 2013, 9, 1641-1656.	2.3	26
38	Observation of Optical Chemical Shift by Precision Nuclear Spin Optical Rotation Measurements and Calculations. <i>Journal of Physical Chemistry Letters</i> , 2013, 4, 437-441.	2.1	30
39	Electron correlation and relativistic effects in the secondary NMR isotope shifts of CSe <sub>2</sub> . <i>Physical Chemistry Chemical Physics</i> , 2013, 15, 17468.	1.3	6
40	Nuclear spin-induced Cotton-Mouton effect in molecules. <i>Journal of Chemical Physics</i> , 2013, 138, 204110.	1.2	19
41	Constant-pressure simulations of Gay-Berne liquid-crystalline phases in cylindrical nanocavities. <i>Physical Chemistry Chemical Physics</i> , 2013, 15, 14047.	1.3	14
42	Nuclear spin-spin coupling anisotropy in the van der Waals-bonded <sup>129</sup> Xe dimer. <i>Physical Chemistry Chemical Physics</i> , 2013, 15, 11427.	1.3	6
43	Nuclear magnetic resonance predictions for graphenes: concentric finite models and extrapolation to large systems. <i>Physical Chemistry Chemical Physics</i> , 2013, 15, 4634.	1.3	26
44	Magnetic field-induced nuclear quadrupole coupling in atomic <sup>131</sup> Xe. <i>Molecular Physics</i> , 2013, 111, 1390-1400.	0.8	7
45	Nuclear spin-spin coupling in a van der Waals-bonded system: Xenon dimer. <i>Journal of Chemical Physics</i> , 2013, 138, 104313.	1.2	13
46	Communication: Nuclear quadrupole moment-induced Cotton-Mouton effect in noble gas atoms. <i>Journal of Chemical Physics</i> , 2013, 139, 181102.	1.2	13
47	Nuclear spin optical rotation and Faraday effect in gaseous and liquid water. <i>Journal of Chemical Physics</i> , 2012, 136, 184502.	1.2	21
48	Rovibrational effects on NMR shieldings in a heavy-element system: XeF <sub>2</sub> . <i>Journal of Chemical Physics</i> , 2012, 137, 214309.	1.2	8
49	Fully Relativistic Calculations of Faraday and Nuclear Spin-Induced Optical Rotation in Xenon. <i>Journal of Chemical Theory and Computation</i> , 2012, 8, 91-98.	2.3	23
50	Exploring new <sup>129</sup> Xe chemical shift ranges in HXeY compounds: hydrogen more relativistic than xenon. <i>Physical Chemistry Chemical Physics</i> , 2012, 14, 10944.	1.3	32
51	Relativistic effects on group-12 metal nuclear shieldings. <i>Physical Chemistry Chemical Physics</i> , 2011, 13, 21016.	1.3	35
52	Calculation of isotropic Compton profiles with Gaussian basis sets. <i>Physical Chemistry Chemical Physics</i> , 2011, 13, 5630.	1.3	16
53	Nuclear spin relaxation due to chemical shift anisotropy of gas-phase <sup>129</sup> Xe. <i>Physical Chemistry Chemical Physics</i> , 2011, 13, 13704.	1.3	17
54	Solvation Structure and Dynamics of Ni <sup>2+</sup> (aq) from First Principles. <i>Journal of Chemical Theory and Computation</i> , 2011, 7, 2937-2946.	2.3	11

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55	Magnetic Properties of Ni <sup>2+</sup> (aq) from First Principles. Journal of Chemical Theory and Computation, 2011, 7, 3248-3260.	2.3	19
56	Nuclear magnetic resonance parameters in water dimer. Theoretical Chemistry Accounts, 2011, 129, 313-324.	0.5	6
57	Understanding the NMR chemical shifts for 6-halopurines: role of structure, solvent and relativistic effects. Physical Chemistry Chemical Physics, 2010, 12, 5126.	1.3	44
58	Electron spin resonance parameters of bulk oxygen vacancy in semiconducting tin dioxide. Physical Review B, 2010, 81, .	1.1	21
59	Chemical Distinction by Nuclear Spin Optical Rotation. Physical Review Letters, 2010, 105, 153001.	2.9	39
60	Ferrocene-like iron bis(dicarbollide), [3-FeIII-(1,2-C <sub>2</sub> B <sub>9</sub> H <sub>11</sub> ) <sub>2</sub> ] <sup>+</sup> . The first experimental and theoretical refinement of a paramagnetic <sup>11</sup> B NMR spectrum. Physical Chemistry Chemical Physics, 2010, 12, 7018.	1.3	25
61	Carbon and proton shielding tensors in methyl halides. Physical Chemistry Chemical Physics, 2010, 12, 2679.	1.3	52
62	Charge localization in alcohol isomers studied by Compton scattering. Journal of Chemical Physics, 2009, 130, 034506.	1.2	17
63	Characteristic Spin-Orbit Induced <sup>1</sup> H(CH <sub>2</sub> ) Chemical Shifts upon Deprotonation of Group 9 Polyamine Aqua and Alcohol Complexes. Journal of the American Chemical Society, 2009, 131, 11909-11918.	6.6	25
64	NMR tensors in planar hydrocarbons of increasing size. Physical Chemistry Chemical Physics, 2009, 11, 11404.	1.3	27
65	Pairwise additivity in the nuclear magnetic resonance interactions of atomic xenon. Physical Chemistry Chemical Physics, 2009, 11, 2485.	1.3	23
66	<sup>19</sup> F spin-spin coupling in peri-difluoronaphthalene. Physical Chemistry Chemical Physics, 2009, 11, 4136.	1.3	8
67	Effect of molecular size on the parity-non-conserving contributions to the nuclear magnetic resonance shielding constant. Theoretical Chemistry Accounts, 2008, 121, 53-57.	0.5	5
68	Nuclear Magnetic Resonance Chemical Shift in an Arbitrary Electronic Spin State. Physical Review Letters, 2008, 100, 133002.	2.9	111
69	Laser-induced nuclear magnetic resonance splitting in hydrocarbons. Journal of Chemical Physics, 2008, 129, 124102.	1.2	26
70	Dynamics and magnetic resonance properties of Sc <sub>3</sub> C <sub>2</sub> @C <sub>80</sub> and its monoanion. Physical Chemistry Chemical Physics, 2008, 10, 7158.	1.3	31
71	Toward Calculations of the <sup>129</sup> Xe Chemical Shift in Xe@C <sub>60</sub> at Experimental Conditions: Relativity, Correlation, and Dynamics. Journal of Physical Chemistry A, 2008, 112, 2658-2668.	1.1	60
72	Exploring the Stability of Golden Fullerenes. Journal of Physical Chemistry C, 2008, 112, 19311-19315.	1.5	37

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73	Methodological aspects in the calculation of parity-violating effects in nuclear magnetic resonance parameters. <i>Journal of Chemical Physics</i> , 2007, 126, 074107.	1.2	18
74	Xe129 chemical shift by the perturbational relativistic method: Xenon fluorides. <i>Journal of Chemical Physics</i> , 2007, 127, 084312.	1.2	33
75	Relativistic effects in the intermolecular interaction-induced nuclear magnetic resonance parameters of xenon dimer. <i>Journal of Chemical Physics</i> , 2007, 127, 164313.	1.2	36
76	Theoretical predictions of nuclear magnetic resonance parameters in a novel organo-xenon species: Chemical shifts and nuclear quadrupole couplings in HXeCCH. <i>Journal of Chemical Physics</i> , 2007, 127, 234314.	1.2	36
77	Nuclear magnetic resonance parameters of atomic xenon dissolved in Gay-Berne model liquid crystal. <i>Physical Review E</i> , 2007, 75, 031707.	0.8	11
78	A London-type formula for the dispersion interactions of endohedral A@B systems. <i>Physical Chemistry Chemical Physics</i> , 2007, 9, 2954.	1.3	48
79	Experimental and quantum-chemical determination of the <sup>2</sup> H quadrupole coupling tensor in deuterated benzenes. <i>Physical Chemistry Chemical Physics</i> , 2007, 9, 481-490.	1.3	13
80	Nuclear Magnetic Resonance Chemical Shifts and Quadrupole Couplings for Different Hydrogen-Bonding Cases Occurring in Liquid Water: A Computational Study. <i>Journal of Physical Chemistry A</i> , 2007, 111, 182-192.	1.1	26
81	Theory and computation of nuclear magnetic resonance parameters. <i>Physical Chemistry Chemical Physics</i> , 2007, 9, 5399.	1.3	226
82	Relativistic heavy-atom effects on heavy-atom nuclear shieldings. <i>Journal of Chemical Physics</i> , 2006, 125, 184113.	1.2	48
83	Density Functional Calculations of <sup>3</sup> He Chemical Shift in Endohedral Helium Fullerenes: Neutral, Anionic, and Di-Helium Species. <i>Journal of Physical Chemistry A</i> , 2006, 110, 12338-12341.	1.1	29
84	Systematic Gaussian basis-set limit using completeness-optimized primitive sets. A case for magnetic properties. <i>Journal of Computational Chemistry</i> , 2006, 27, 434-445.	1.5	75
85	Comment on "Calculation of nuclear magnetic shieldings using an analytically differentiated relativistic shielding formula" [J. Chem. Phys. 123, 114102 (2005)]. <i>Journal of Chemical Physics</i> , 2006, 124, 137101.	1.2	15
86	Calculations of nuclear quadrupole coupling in noble gas noble metal fluorides: Interplay of relativistic and electron correlation effects. <i>Journal of Chemical Physics</i> , 2006, 125, 174315.	1.2	22
87	Leading-order relativistic effects on nuclear magnetic resonance shielding tensors. <i>Journal of Chemical Physics</i> , 2005, 122, 114107.	1.2	113
88	Perturbational calculations of parity-violating effects in nuclear-magnetic-resonance parameters. <i>Journal of Chemical Physics</i> , 2005, 123, 054501.	1.2	35
89	Density-functional calculations of relativistic spin-orbit effects on nuclear magnetic shielding in paramagnetic molecules. <i>Journal of Chemical Physics</i> , 2005, 123, 174102.	1.2	50
90	Magnetic-field dependence of <sup>59</sup> Co nuclear magnetic shielding in Co(III) complexes. <i>Physical Review A</i> , 2004, 69, .	1.0	19

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91	Perturbational and ECP Calculation of Relativistic Effects in NMR Shielding and Spin-Spin Coupling. , 2004, , 209-226.		54
92	Calculation of binary magnetic properties and potential energy curve in xenon dimer: Second virial coefficient of <sup>129</sup> Xe nuclear shielding. Journal of Chemical Physics, 2004, 121, 5908-5919.	1.2	40
93	Relativistic spin-orbit effects on hyperfine coupling tensors by density-functional theory. Journal of Chemical Physics, 2004, 120, 2127-2139.	1.2	89
94	Magnetic-field-induced quadrupole coupling in the nuclear magnetic resonance of noble-gas atoms and molecules. Physical Review A, 2004, 70, .	1.0	5
95	Perturbational relativistic theory of electron spin resonance g-tensor. Journal of Chemical Physics, 2004, 121, 1258-1265.	1.2	17
96	Au <sub>32</sub> : A 24-Carat Golden Fullerene. Angewandte Chemie - International Edition, 2004, 43, 2678-2681.	7.2	285
97	Au <sub>32</sub> : A 24-Carat Golden Fullerene.. ChemInform, 2004, 35, no.	0.1	0
98	Laser-induced splittings in the nuclear magnetic resonance spectra of the rare gas atoms. Chemical Physics Letters, 2004, 400, 226-230.	1.2	15
99	Influence of Hydrogen Bonding in the Paramagnetic NMR Shieldings of NitronylNitroxide Derivative Molecules. Journal of Physical Chemistry B, 2004, 108, 1197-1206.	1.2	8
100	Spin-Orbit Effects on Hyperfine Coupling Tensors in Transition Metal Complexes Using Hybrid Density Functionals and Accurate Spin-Orbit Operators. Journal of Physical Chemistry A, 2004, 108, 5026-5033.	1.1	62
101	Nuclear Magnetic Shielding and Quadrupole Coupling Tensors in Liquid Water: A Combined Molecular Dynamics Simulation and Quantum Chemical Study. Journal of the American Chemical Society, 2004, 126, 11093-11102.	6.6	60
102	Magnetic field dependence of nuclear magnetic shielding in closed-shell atomic systems. Chemical Physics Letters, 2003, 372, 750-757.	1.2	22
103	Relativistic, nearly basis-set-limit nuclear magnetic shielding constants of the rare gases He-Rn: A way to absolute nuclear magnetic resonance shielding scales. Journal of Chemical Physics, 2003, 118, 2973-2976.	1.2	109
104	Calculations of nuclear magnetic shielding in paramagnetic molecules. Journal of Chemical Physics, 2003, 118, 2550.	1.2	71
105	Perturbationalab initio calculations of relativistic contributions to nuclear magnetic resonance shielding tensors. Journal of Chemical Physics, 2003, 119, 2623-2637.	1.2	124
106	Relativistic Spin-Orbit Coupling Effects on Secondary Isotope Shifts of <sup>13</sup> C Nuclear Shielding in CX <sub>2</sub> (X) Tj ETQq0 0.0 rgBT / Overlock 10	8.6	25
107	Density Functional Calculations of Electronic g-Tensors for Semiquinone Radical Anions. The Role of Hydrogen Bonding and Substituent Effects. Journal of the American Chemical Society, 2002, 124, 2709-2722.	6.6	94
108	Spin-spin coupling tensors by density-functional linear response theory. Journal of Chemical Physics, 2002, 117, 5998-6009.	1.2	70

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109	Density Functional Theory Calculations of Electron Paramagnetic Resonance Parameters of a Nitroxide Spin Label in Tissue Factor and Factor VIIa Protein Complex. <i>Journal of Physical Chemistry B</i> , 2002, 106, 12354-12360.	1.2	19
110	Spin-spin coupling tensors as determined by experiment and computational chemistry. <i>Progress in Nuclear Magnetic Resonance Spectroscopy</i> , 2002, 41, 233-304.	3.9	169
111	Study of relativistic effects on nuclear shieldings using density-functional theory and spin-orbit pseudopotentials. <i>Journal of Chemical Physics</i> , 2001, 114, 61.	1.2	101
112	Application of Self-Organizing Maps in Conformational Analysis of Lipids. <i>Journal of the American Chemical Society</i> , 2001, 123, 810-816.	6.6	33
113	Effect of correlating core orbitals in calculations of nuclear spin-spin couplings. <i>Journal of Chemical Physics</i> , 2001, 114, 5482-5490.	1.2	20
114	Magnetic-Field-Induced Quadrupole Splitting in Gaseous and Liquid $^{13}\text{C}$ NMR: Quadratic and Quartic Field Dependence. <i>Physical Review Letters</i> , 2001, 86, 3268-3271.	2.9	18
115	Spin-Spin Coupling Tensors in Fluoromethanes. <i>Chemistry - A European Journal</i> , 2000, 6, 1395-1406.	1.7	25
116	Density Functional Calculations of Electronic Spin-Orbit Pseudopotentials and Mean-Field All-Electron Spin-Orbit Operators. <i>Journal of the American Chemical Society</i> , 2000, 122, 9206-9218.	6.6	222
117	Second- and third-order spin-orbit contributions to nuclear shielding tensors. <i>Journal of Chemical Physics</i> , 1999, 111, 2900-2909.	1.2	74
118	Correlated response calculations of the spin-orbit interaction contribution to nuclear spin-spin couplings. <i>Journal of Computational Chemistry</i> , 1999, 20, 1314-1327.	1.5	48
119	Experimental and Theoretical Study of the Spin-Spin Coupling Tensors in Methylsilane. <i>Journal of Physical Chemistry A</i> , 1999, 103, 9669-9677.	1.1	11
120	Indirect Fluorine Coupling Anisotropies in <i>p</i> -Difluorobenzene: Implications to Orientation and Structure Determination of Fluorinated Liquid Crystals. <i>Journal of Physical Chemistry A</i> , 1999, 103, 5675-5684.	1.1	28
121	Internuclear distance dependence of the spin-orbit coupling contributions to proton NMR chemical shifts. <i>Chemical Physics Letters</i> , 1998, 295, 455-461.	1.2	32
122	Vibrationally averaged magnetizabilities and rotational $g$ tensors of the water molecule. <i>Chemical Physics Letters</i> , 1998, 297, 467-474.	1.2	25
123	Vibrationally Averaged Nuclear Shielding Constants in OCS. <i>Journal of Magnetic Resonance</i> , 1998, 135, 444-453.	1.2	24
124	Experimental and Theoretical Study of the $^{13}\text{C}$ Spin-Spin Coupling and $^1\text{H}$ and $^{13}\text{C}$ Shielding Tensors in Ethane, Ethene, and Ethyne. <i>Journal of the American Chemical Society</i> , 1998, 120, 3993-4005.	6.6	86
125	Quadratic response calculations of the electronic spin-orbit contribution to nuclear shielding tensors. <i>Journal of Chemical Physics</i> , 1998, 109, 1212-1222.	1.2	97
126	$^{13}\text{C}$ NMR of methane in an $\text{AlPO}_4$ molecular sieve: Exchange effects and shielding anisotropy. <i>Physical Review B</i> , 1998, 58, 14833-14836.	1.1	9



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127	Rovibrational effects, temperature dependence, and isotope effects on the nuclear shielding tensors of water: A new $^{17}\text{O}$ absolute shielding scale. <i>Journal of Chemical Physics</i> , 1998, 109, 8388-8397.	1.2	115
128	Xe129 adsorbed in AlPO <sub>4</sub> -11 molecular sieve: Molecular dynamics simulation of adsorbate dynamics and NMR chemical shift. <i>Journal of Chemical Physics</i> , 1997, 107, 6470-6478.	1.2	23
129	Deuterium quadrupole coupling tensors in methyl halides: Ab initio effective core potential and liquid crystal nuclear magnetic resonance study. <i>Journal of Chemical Physics</i> , 1997, 107, 1744-1752.	1.2	11
130	NMR Properties of Formamide: A First Principles and Experimental Study. <i>Journal of Physical Chemistry A</i> , 1997, 101, 5069-5081.	1.1	48
131	$^{14}\text{N}$ and $^2\text{H}$ NMR Study of the Mesophases of Cetyltrimethylammonium Bromide in Formamide. <i>Journal of Physical Chemistry B</i> , 1997, 101, 32-38.	1.2	27
132	Isotope and temperature effects on the $^{13}\text{C}$ and $^{77}\text{Se}$ nuclear shielding in carbon diselenide. <i>Journal of Chemical Physics</i> , 1997, 107, 1350-1361.	1.2	29
133	Inequivalence of single $\text{CH}_a$ and $\text{CH}_b$ methylene bonds in the interior of a diunsaturated lipid bilayer from a molecular dynamics simulation. <i>Chemical Physics Letters</i> , 1997, 268, 55-60.	1.2	7
134	Surface relaxation of the (100) face of wurtzite CdS. <i>Surface Science</i> , 1996, 352-354, 77-82.	0.8	14
135	$^{13}\text{C}$ Spin-Spin Coupling Tensors in Benzene As Determined Experimentally by Liquid Crystal NMR and Theoretically by Ab Initio Calculations. <i>Journal of the American Chemical Society</i> , 1996, 118, 8879-8886.	6.6	56
136	Anisotropy of the $^1\text{H}$ and $^{13}\text{C}$ shielding tensors in chloroform. <i>Chemical Physics Letters</i> , 1996, 253, 340-348.	1.2	15
137	$^{13}\text{C}$ NMR spectroscopy of methane adsorbed in SAPO-11 molecular sieve. <i>Chemical Physics Letters</i> , 1996, 261, 425-430.	1.2	17
138	Effects of two double bonds on the hydrocarbon interior of a phospholipid bilayer. <i>Chemical Physics Letters</i> , 1995, 246, 300-306.	1.2	7
139	Computational and experimental study of NMR relaxation of quadrupolar noble gas nuclei in organic solvents. <i>Molecular Physics</i> , 1994, 82, 13-27.	0.8	11