

Juha Vaara

List of Publications by Year in descending order

Source: <https://exaly.com/author-pdf/2959682/publications.pdf>

Version: 2024-02-01

139
papers

4,953
citations

94269

37
h-index

114278

63
g-index

144
all docs

144
docs citations

144
times ranked

2715
citing authors

#	ARTICLE	IF	CITATIONS
1	Au32: A 24-Carat Golden Fullerene. <i>Angewandte Chemie - International Edition</i> , 2004, 43, 2678-2681.	7.2	285
2	Theory and computation of nuclear magnetic resonance parameters. <i>Physical Chemistry Chemical Physics</i> , 2007, 9, 5399.	1.3	226
3	Density Functional Calculations of Electronic g-Tensors Using 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
4	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
5	Perturbational ab initio calculations of relativistic contributions to nuclear magnetic resonance shielding tensors. <i>Journal of Chemical Physics</i> , 2003, 119, 2623-2637.	1.2	124
6	Rovibrational effects, temperature dependence, and isotope effects on the nuclear shielding tensors of water: A new ¹⁷ O absolute shielding scale. <i>Journal of Chemical Physics</i> , 1998, 109, 8388-8397.	1.2	115
7	Leading-order relativistic effects on nuclear magnetic resonance shielding tensors. <i>Journal of Chemical Physics</i> , 2005, 122, 114107.	1.2	113
8	Nuclear Magnetic Resonance Chemical Shift in an Arbitrary Electronic Spin State. <i>Physical Review Letters</i> , 2008, 100, 133002.	2.9	111
9	Relativistic, nearly basis-set-limit nuclear magnetic shielding constants of the rare gases He-Rn: A way to absolute nuclear magnetic resonance shielding scales. <i>Journal of Chemical Physics</i> , 2003, 118, 2973-2976.	1.2	109
10	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
11	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
12	Density Functional Calculations of Electronic g-Tensors for Semiquinone Radical Anions. The Role of Hydrogen Bonding and Substituent Effects. <i>Journal of the American Chemical Society</i> , 2002, 124, 2709-2722.	6.6	94
13	Relativistic spin-orbit effects on hyperfine coupling tensors by density-functional theory. <i>Journal of Chemical Physics</i> , 2004, 120, 2127-2139.	1.2	89
14	Experimental and Theoretical ab Initio Study of the ¹³ C- ¹³ C Spin-Spin Coupling and ¹ H and ¹³ C Shielding Tensors in Ethane, Ethene, and Ethyne. <i>Journal of the American Chemical Society</i> , 1998, 120, 3993-4005.	6.6	86
15	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
16	Second- and third-order spin-orbit contributions to nuclear shielding tensors. <i>Journal of Chemical Physics</i> , 1999, 111, 2900-2909.	1.2	74
17	Calculations of nuclear magnetic shielding in paramagnetic molecules. <i>Journal of Chemical Physics</i> , 2003, 118, 2550.	1.2	71
18	Spin-spin coupling tensors by density-functional linear response theory. <i>Journal of Chemical Physics</i> , 2002, 117, 5998-6009.	1.2	70

#	ARTICLE	IF	CITATIONS
19	Magnetic Couplings in the Chemical Shift of Paramagnetic NMR. Journal of Chemical Theory and Computation, 2015, 11, 4840-4849.	2.3	69
20	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
21	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
22	Toward Calculations of the ¹²⁹ Xe Chemical Shift in Xe@C ₆₀ at Experimental Conditions: Relativity, Correlation, and Dynamics. Journal of Physical Chemistry A, 2008, 112, 2658-2668.	1.1	60
23	¹³ C- ¹³ C Spin-Spin Coupling Tensors in Benzene As Determined Experimentally by Liquid Crystal NMR and Theoretically by ab Initio Calculations. Journal of the American Chemical Society, 1996, 118, 8879-8886.	6.6	56
24	Perturbational and ECP Calculation of Relativistic Effects in NMR Shielding and Spin-Spin Coupling. , 2004, , 209-226.		54
25	Carbon and proton shielding tensors in methyl halides. Physical Chemistry Chemical Physics, 2010, 12, 2679.	1.3	52
26	¹ H Chemical Shifts in Paramagnetic Co(II) Pyrazolylborate Complexes: A First-Principles Study. Journal of Chemical Theory and Computation, 2015, 11, 1683-1691.	2.3	52
27	Pseudo-Contact NMR Shifts over the Paramagnetic Metalloprotein CoMMP-12 from First Principles. Angewandte Chemie - International Edition, 2016, 55, 14713-14717.	7.2	51
28	Density-functional calculations of relativistic spin-orbit effects on nuclear magnetic shielding in paramagnetic molecules. Journal of Chemical Physics, 2005, 123, 174102.	1.2	50
29	NMR Properties of Formamide: A First Principles and Experimental Study. Journal of Physical Chemistry A, 1997, 101, 5069-5081.	1.1	48
30	Correlated response calculations of the spin-orbit interaction contribution to nuclear spin-spin couplings. Journal of Computational Chemistry, 1999, 20, 1314-1327.	1.5	48
31	Relativistic heavy-atom effects on heavy-atom nuclear shieldings. Journal of Chemical Physics, 2006, 125, 184113.	1.2	48
32	A London-type formula for the dispersion interactions of endohedral A@B systems. Physical Chemistry Chemical Physics, 2007, 9, 2954.	1.3	48
33	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
34	Calculation of binary magnetic properties and potential energy curve in xenon dimer: Second virial coefficient of ¹²⁹ Xe nuclear shielding. Journal of Chemical Physics, 2004, 121, 5908-5919.	1.2	40
35	Chemical Distinction by Nuclear Spin Optical Rotation. Physical Review Letters, 2010, 105, 153001.	2.9	39
36	Exploring the Stability of Golden Fullerenes. Journal of Physical Chemistry C, 2008, 112, 19311-19315.	1.5	37

#	ARTICLE	IF	CITATIONS
37	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
38	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
39	Perturbational calculations of parity-violating effects in nuclear-magnetic-resonance parameters. <i>Journal of Chemical Physics</i> , 2005, 123, 054501.	1.2	35
40	Relativistic effects on group-12 metal nuclear shieldings. <i>Physical Chemistry Chemical Physics</i> , 2011, 13, 21016.	1.3	35
41	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
42	Xe129 chemical shift by the perturbational relativistic method: Xenon fluorides. <i>Journal of Chemical Physics</i> , 2007, 127, 084312.	1.2	33
43	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
44	Exploring new 129Xe chemical shift ranges in HXeY compounds: hydrogen more relativistic than xenon. <i>Physical Chemistry Chemical Physics</i> , 2012, 14, 10944.	1.3	32
45	Dynamics and magnetic resonance properties of Sc3C2@C80 and its monoanion. <i>Physical Chemistry Chemical Physics</i> , 2008, 10, 7158.	1.3	31
46	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
47	Isotope and temperature effects on the 13C and 77Se nuclear shielding in carbon diselenide. <i>Journal of Chemical Physics</i> , 1997, 107, 1350-1361.	1.2	29
48	Density Functional Calculations of 3He 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
49	Indirect Fluorine Coupling Anisotropies in p-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
50	14N and 2H NMR Study of the Mesophases of Cetyltrimethylammonium Bromide in Formamide. <i>Journal of Physical Chemistry B</i> , 1997, 101, 32-38.	1.2	27
51	NMR tensors in planar hydrocarbons of increasing size. <i>Physical Chemistry Chemical Physics</i> , 2009, 11, 11404.	1.3	27
52	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
53	Laser-induced nuclear magnetic resonance splitting in hydrocarbons. <i>Journal of Chemical Physics</i> , 2008, 129, 124102.	1.2	26
54	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

#	ARTICLE	IF	CITATIONS
55	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
56	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
57	Vibrationally averaged magnetizabilities and rotational g tensors of the water molecule. <i>Chemical Physics Letters</i> , 1998, 297, 467-474.	1.2	25
58	Spin-Spin Coupling Tensors in Fluoromethanes. <i>Chemistry - A European Journal</i> , 2000, 6, 1395-1406.	1.7	25
59	Relativistic Spin-Orbit Coupling Effects on Secondary Isotope Shifts of ¹³ C Nuclear Shielding in CX ₂ (X) Tj ETQq1 1.0.784314 rgBT /Qv	6.6	25
60	Characteristic Spin-Orbit Induced ¹ H(CH ₂) Chemical Shifts upon Deprotonation of Group 9 Polyamine Aqua and Alcohol Complexes. <i>Journal of the American Chemical Society</i> , 2009, 131, 11909-11918.	6.6	25
61	Ferrocene-like iron bis(dicarbollide), [3-FeIII-(1,2-C ₂ B ₉ H ₁₁) ₂] ⁺ . The first experimental and theoretical refinement of a paramagnetic ¹¹ B NMR spectrum. <i>Physical Chemistry Chemical Physics</i> , 2010, 12, 7018.	1.3	25
62	Rovibrationally Averaged Nuclear Shielding Constants in OCS. <i>Journal of Magnetic Resonance</i> , 1998, 135, 444-453.	1.2	24
63	Xe ¹²⁹ adsorbed in AlPO ₄ -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
64	Pairwise additivity in the nuclear magnetic resonance interactions of atomic xenon. <i>Physical Chemistry Chemical Physics</i> , 2009, 11, 2485.	1.3	23
65	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
66	Magnetic field dependence of nuclear magnetic shielding in closed-shell atomic systems. <i>Chemical Physics Letters</i> , 2003, 372, 750-757.	1.2	22
67	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
68	Electron spin resonance parameters of bulk oxygen vacancy in semiconducting tin dioxide. <i>Physical Review B</i> , 2010, 81, .	1.1	21
69	Nuclear spin optical rotation and Faraday effect in gaseous and liquid water. <i>Journal of Chemical Physics</i> , 2012, 136, 184502.	1.2	21
70	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
71	Nuclear spin circular dichroism. <i>Journal of Chemical Physics</i> , 2014, 140, 134103.	1.2	20
72	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

#	ARTICLE	IF	CITATIONS
73	Magnetic-field dependence of ^{59}Co nuclear magnetic shielding in Co(III) complexes. <i>Physical Review A</i> , 2004, 69, .	1.0	19
74	Magnetic Properties of $\text{Ni}^{2+}(\text{aq})$ from First Principles. <i>Journal of Chemical Theory and Computation</i> , 2011, 7, 3248-3260.	2.3	19
75	Nuclear spin-induced Cotton-Mouton effect in molecules. <i>Journal of Chemical Physics</i> , 2013, 138, 204110.	1.2	19
76	Magnetic-Field-Induced Quadrupole Splitting in Gaseous and Liquid ^{13}C NMR: Quadratic and Quartic Field Dependence. <i>Physical Review Letters</i> , 2001, 86, 3268-3271.	2.9	18
77	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
78	^{13}C NMR spectroscopy of methane adsorbed in SAPO-11 molecular sieve. <i>Chemical Physics Letters</i> , 1996, 261, 425-430.	1.2	17
79	Perturbational relativistic theory of electron spin resonance g-tensor. <i>Journal of Chemical Physics</i> , 2004, 121, 1258-1265.	1.2	17
80	Charge localization in alcohol isomers studied by Compton scattering. <i>Journal of Chemical Physics</i> , 2009, 130, 034506.	1.2	17
81	Nuclear spin relaxation due to chemical shift anisotropy of gas-phase ^{129}Xe . <i>Physical Chemistry Chemical Physics</i> , 2011, 13, 13704.	1.3	17
82	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
83	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
84	Calculation of isotropic Compton profiles with Gaussian basis sets. <i>Physical Chemistry Chemical Physics</i> , 2011, 13, 5630.	1.3	16
85	Anisotropy of the ^1H and ^{13}C shielding tensors in chloroform. <i>Chemical Physics Letters</i> , 1996, 253, 340-348.	1.2	15
86	Laser-induced splittings in the nuclear magnetic resonance spectra of the rare gas atoms. <i>Chemical Physics Letters</i> , 2004, 400, 226-230.	1.2	15
87	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
88	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
89	Surface relaxation of the (100) face of wurtzite CdS. <i>Surface Science</i> , 1996, 352-354, 77-82.	0.8	14
90	Constant-pressure simulations of Gay-Berne liquid-crystalline phases in cylindrical nanocavities. <i>Physical Chemistry Chemical Physics</i> , 2013, 15, 14047.	1.3	14

#	ARTICLE	IF	CITATIONS
91	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
92	Pseudo-Contact NMR Shifts over the Paramagnetic Metalloprotein CoMMP-12 from First Principles. <i>Angewandte Chemie</i> , 2016, 128, 14933-14937.	1.6	14
93	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
94	Experimental and quantum-chemical determination of the ^2H quadrupole coupling tensor in deuterated benzenes. <i>Physical Chemistry Chemical Physics</i> , 2007, 9, 481-490.	1.3	13
95	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
96	Communication: Nuclear quadrupole moment-induced Cotton-Mouton effect in noble gas atoms. <i>Journal of Chemical Physics</i> , 2013, 139, 181102.	1.2	13
97	Curie-type paramagnetic NMR relaxation in the aqueous solution of Ni(II). <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 6916-6924.	1.3	13
98	Spin dynamics simulation of electron spin relaxation in Ni ²⁺ (aq). <i>Journal of Chemical Physics</i> , 2014, 141, 014109.	1.2	12
99	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
100	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
101	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
102	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
103	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
104	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
105	Solvation Structure and Dynamics of Ni ²⁺ (aq) from First Principles. <i>Journal of Chemical Theory and Computation</i> , 2011, 7, 2937-2946.	2.3	11
106	Nuclear quadrupole moment-induced Cotton-Mouton effect in molecules. <i>Journal of Chemical Physics</i> , 2014, 140, 024103.	1.2	11
107	Characteristic Spectral Patterns in the ^{13}C Nuclear Magnetic Resonance Spectra of Hexagonal and Crenellated Graphene Fragments. <i>ChemPhysChem</i> , 2014, 15, 1799-1808.	1.0	11
108	Nuclear-Spin-Induced Cotton-Mouton Effect in a Strong External Magnetic Field. <i>ChemPhysChem</i> , 2014, 15, 2337-2350.	1.0	10

#	ARTICLE	IF	CITATIONS
109	Paramagnetic Pyrazolylborate Complexes $Tp^{2+}M$ and $Tp^{2+}M: ^1H$, ^{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
110	^{13}C NMR of methane in an $AlPO_4$ molecular sieve: Exchange effects and shielding anisotropy. <i>Physical Review B</i> , 1998, 58, 14833-14836.	1.1	9
111	Nuclear spin circular dichroism in fullerenes: a computational study. <i>Chemical Communications</i> , 2014, 50, 15228-15231.	2.2	9
112	Chemical shift extremum of $^{129}Xe(aq)$ reveals details of hydrophobic solvation. <i>Scientific Reports</i> , 2018, 8, 7023.	1.6	9
113	Influence of Hydrogen Bonding in the Paramagnetic NMR Shieldings of Nitronyl Nitroxide Derivative Molecules. <i>Journal of Physical Chemistry B</i> , 2004, 108, 1197-1206.	1.2	8
114	^{19}F spin-spin coupling in peri-difluoronaphthalene. <i>Physical Chemistry Chemical Physics</i> , 2009, 11, 4136.	1.3	8
115	Rovibrational effects on NMR shieldings in a heavy-element system: XeF_2 . <i>Journal of Chemical Physics</i> , 2012, 137, 214309.	1.2	8
116	Experimental and First-Principles NMR Analysis of Pt(II) Complexes With $<i>O</i>$, $<i>O</i>$ -Dialkyldithiophosphate Ligands. <i>Journal of Physical Chemistry A</i> , 2016, 120, 8326-8338.	1.1	8
117	Liquid-state paramagnetic relaxation from first principles. <i>Physical Review A</i> , 2016, 94, .	1.0	8
118	Paramagnetic Enhancement of Nuclear Spin-Spin Coupling. <i>Journal of Chemical Theory and Computation</i> , 2017, 13, 1275-1283.	2.3	8
119	Calculation of scalar nuclear spin-spin coupling in a noble-gas mixture. <i>Physical Review A</i> , 2019, 99, .	1.0	8
120	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
121	Inequivalence of single CH_a and 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
122	Chemical Shift in Paramagnetic Systems. <i>Science and Technology of Atomic, Molecular, Condensed Matter and Biological Systems</i> , 2013, , 41-67.	0.6	7
123	Magnetic field-induced nuclear quadrupole coupling in atomic ^{131}Xe . <i>Molecular Physics</i> , 2013, 111, 1390-1400.	0.8	7
124	Solvation chemical shifts of perylenic antenna molecules from molecular dynamics simulations. <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 22309-22320.	1.3	7
125	Nuclear magnetic resonance parameters in water dimer. <i>Theoretical Chemistry Accounts</i> , 2011, 129, 313-324.	0.5	6
126	Electron correlation and relativistic effects in the secondary NMR isotope shifts of CSe_2 . <i>Physical Chemistry Chemical Physics</i> , 2013, 15, 17468.	1.3	6

#	ARTICLE	IF	CITATIONS
127	Nuclear spin-spin coupling anisotropy in the van der Waals-bonded ^{129}Xe dimer. <i>Physical Chemistry Chemical Physics</i> , 2013, 15, 11427.	1.3	6
128	Electron and nuclear spin polarization in Rb-Xe spin-exchange optical hyperpolarization. <i>Physical Review A</i> , 2017, 95, .	1.0	6
129	Ratcheting rotation or speedy spinning: EPR and dynamics of $\text{Sc}^{3+}\text{C}_2@C_{80}$. <i>Chemical Communications</i> , 2017, 53, 8992-8995.	2.2	6
130	Relation between molecular electronic structure and nuclear spin-induced circular dichroism. <i>Scientific Reports</i> , 2017, 7, 46617.	1.6	6
131	Magnetic-field-induced quadrupole coupling in the nuclear magnetic resonance of noble-gas atoms and molecules. <i>Physical Review A</i> , 2004, 70, .	1.0	5
132	Effect of molecular size on the parity-non-conserving contributions to the nuclear magnetic resonance shielding constant. <i>Theoretical Chemistry Accounts</i> , 2008, 121, 53-57.	0.5	5
133	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
134	Direct magnetic-field dependence of NMR chemical shift. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 8485-8490.	1.3	4
135	Brownian Translational Dynamics on a Flexible Surface: Nuclear Spin Relaxation of Fluid Membrane Phases. <i>Langmuir</i> , 2018, 34, 3755-3766.	1.6	2
136	Solvation structure and dynamics of $\text{Ni}^{2+}(\text{aq})$ from a polarizable force field. <i>Chemical Physics</i> , 2014, 443, 112-122.	0.9	1
137	Polarization transfer in a spin-exchange optical-pumping experiment. <i>Physical Review A</i> , 2020, 102, .	1.0	1
138	Au ₃₂ : A 24-Carat Golden Fullerene.. <i>ChemInform</i> , 2004, 35, no.	0.1	0
139	Direct enantiomeric discrimination through antisymmetric hyperfine coupling. <i>Chemical Communications</i> , 2021, 57, 8264-8267.	2.2	0