# Juha Vaara

## List of Publications by Year in descending order

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| 139 | 4,953 | 94433 | 114465 |
|---|---|---|---|
| papers | citations | 37 h-index | 63 g-index |

| 144 | 144 | 144 | 2715 |
|---|---|---|---|
| all docs | docs citations | times ranked | citing authors |

| # | Article | IF | Citations |
|---|---|---|---|
| 1 | Au32: A 24-Carat Golden Fullerene. Angewandte Chemie - International Edition, 2004, 43, 2678-2681. | 13.8 | 285 |
| 2 | Theory and computation of nuclear magnetic resonance parameters. Physical Chemistry Chemical Physics, 2007, 9, 5399. | 2.8 | 226 |
| 3 | Density Functional Calculations of Electronicg-Tensors Using Spinâˆ’Orbit Pseudopotentials and Mean-Field All-Electron Spinâˆ’Orbit Operators. Journal of the American Chemical Society, 2000, 122, 9206-9218. | 13.7 | 222 |
| 4 | Spinâ€“spin coupling tensors as determined by experiment and computational chemistry. Progress in Nuclear Magnetic Resonance Spectroscopy, 2002, 41, 233-304. | 7.5 | 169 |
| 5 | Perturbationalab initiocalculations of relativistic contributions to nuclear magnetic resonance shielding tensors. Journal of Chemical Physics, 2003, 119, 2623-2637. | 3.0 | 124 |
| 6 | Rovibrational effects, temperature dependence, and isotope effects on the nuclear shielding tensors of water: A new 17O absolute shielding scale. Journal of Chemical Physics, 1998, 109, 8388-8397. | 3.0 | 115 |
| 7 | Leading-order relativistic effects on nuclear magnetic resonance shielding tensors. Journal of Chemical Physics, 2005, 122, 114107. | 3.0 | 113 |
| 8 | Nuclear Magnetic Resonance Chemical Shift in an Arbitrary Electronic Spin State. Physical Review Letters, 2008, 100, 133002. | 7.8 | 111 |
| 9 | Relativistic, nearly basis-set-limit nuclear magnetic shielding constants of the rare gases Heâ€“Rn: A way to absolute nuclear magnetic resonance shielding scales. Journal of Chemical Physics, 2003, 118, 2973-2976. | 3.0 | 109 |
| 10 | Study of relativistic effects on nuclear shieldings using density-functional theory and spinâ€“orbit pseudopotentials. Journal of Chemical Physics, 2001, 114, 61. | 3.0 | 101 |
| 11 | Quadratic response calculations of the electronic spin-orbit contribution to nuclear shielding tensors. Journal of Chemical Physics, 1998, 109, 1212-1222. | 3.0 | 97 |
| 12 | 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. | 13.7 | 94 |
| 13 | Relativistic spin-orbit effects on hyperfine coupling tensors by density-functional theory. Journal of Chemical Physics, 2004, 120, 2127-2139. | 3.0 | 89 |
| 14 | Experimental and TheoreticalabInitioStudy of the13Câˆ’13C Spinâˆ’Spin Coupling and1H and13C Shielding Tensors in Ethane, Ethene, and Ethyne. Journal of the American Chemical Society, 1998, 120, 3993-4005. | 13.7 | 86 |
| 15 | Systematic Gaussian basis-set limit using completeness-optimized primitive sets. A case for magnetic properties. Journal of Computational Chemistry, 2006, 27, 434-445. | 3.3 | 75 |
| 16 | Second- and third-order spin-orbit contributions to nuclear shielding tensors. Journal of Chemical Physics, 1999, 111, 2900-2909. | 3.0 | 74 |
| 17 | Calculations of nuclear magnetic shielding in paramagnetic molecules. Journal of Chemical Physics, 2003, 118, 2550. | 3.0 | 71 |
| 18 | Spinâ€“spin coupling tensors by density-functional linear response theory. Journal of Chemical Physics, 2002, 117, 5998-6009. | 3.0 | 70 |

| # | Article | IF | Citations |
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| 19 | Magnetic Couplings in the Chemical Shift of Paramagnetic NMR. Journal of Chemical Theory and Computation, 2015, 11, 4840-4849. | 5.3 | 69 |
| 20 | Spinâ^'Orbit Effects on Hyperfine Coupling Tensors in Transition Metal Complexes Using Hybrid Density Functionals and Accurate Spinâ^'Orbit Operators. Journal of Physical Chemistry A, 2004, 108, 5026-5033. | 2.5 | 62 |
| 21 | Nuclear Magnetic Shielding and Quadrupole Coupling Tensors in Liquid Water:Â A Combined Molecular Dynamics Simulation and Quantum Chemical Study. Journal of the American Chemical Society, 2004, 126, 11093-11102. | 13.7 | 60 |
| 22 | Toward Calculations of the <sup>129</sup>Xe Chemical Shift in Xe@C<sub>60</sub> at Experimental Conditions:â€‰ Relativity, Correlation, and Dynamics. Journal of Physical Chemistry A, 2008, 112, 2658-2668. | 2.5 | 60 |
| 23 | 13Câ^'13C Spinâ^'Spin Coupling Tensors in Benzene As Determined Experimentally by Liquid Crystal NMR and Theoretically byab InitioCalculations. Journal of the American Chemical Society, 1996, 118, 8879-8886. | 13.7 | 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. | 2.8 | 52 |
| 26 | <sup>1</sup>H Chemical Shifts in Paramagnetic Co(II) Pyrazolylborate Complexes: A First-Principles Study. Journal of Chemical Theory and Computation, 2015, 11, 1683-1691. | 5.3 | 52 |
| 27 | Pseudoâ€Contact NMR Shifts over the Paramagnetic Metalloprotein CoMMPâ€12 from First Principles. Angewandte Chemie - International Edition, 2016, 55, 14713-14717. | 13.8 | 51 |
| 28 | Density-functional calculations of relativistic spin-orbit effects on nuclear magnetic shielding in paramagnetic molecules. Journal of Chemical Physics, 2005, 123, 174102. | 3.0 | 50 |
| 29 | NMR Properties of Formamide:â€‰ A First Principles and Experimental Study. Journal of Physical Chemistry A, 1997, 101, 5069-5081. | 2.5 | 48 |
| 30 | Correlated response calculations of the spin-orbit interaction contribution to nuclear spin-spin couplings. Journal of Computational Chemistry, 1999, 20, 1314-1327. | 3.3 | 48 |
| 31 | Relativistic heavy-atom effects on heavy-atom nuclear shieldings. Journal of Chemical Physics, 2006, 125, 184113. | 3.0 | 48 |
| 32 | A London-type formula for the dispersion interactions of endohedral A@B systems. Physical Chemistry Chemical Physics, 2007, 9, 2954. | 2.8 | 48 |
| 33 | Understanding the NMR chemical shifts for 6-halopurines: role of structure, solvent and relativistic effects. Physical Chemistry Chemical Physics, 2010, 12, 5126. | 2.8 | 44 |
| 34 | Calculation of binary magnetic properties and potential energy curve in xenon dimer: Second virial coefficient of 129Xe nuclear shielding. Journal of Chemical Physics, 2004, 121, 5908-5919. | 3.0 | 40 |
| 35 | Chemical Distinction by Nuclear Spin Optical Rotation. Physical Review Letters, 2010, 105, 153001. | 7.8 | 39 |
| 36 | Exploring the Stability of Golden Fullerenes. Journal of Physical Chemistry C, 2008, 112, 19311-19315. | 3.1 | 37 |

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| 37 | Relativistic effects in the intermolecular interaction-induced nuclear magnetic resonance parameters of xenon dimer. Journal of Chemical Physics, 2007, 127, 164313. | 3.0 | 36 |
| 38 | Theoretical predictions of nuclear magnetic resonance parameters in a novel organo-xenon species: Chemical shifts and nuclear quadrupole couplings in HXeCCH. Journal of Chemical Physics, 2007, 127, 234314. | 3.0 | 36 |
| 39 | Perturbational calculations of parity-violating effects in nuclear-magnetic-resonance parameters. Journal of Chemical Physics, 2005, 123, 054501. | 3.0 | 35 |
| 40 | Relativistic effects on group-12 metal nuclear shieldings. Physical Chemistry Chemical Physics, 2011, 13, 21016. | 2.8 | 35 |
| 41 | Application of Self-Organizing Maps in Conformational Analysis of Lipids. Journal of the American Chemical Society, 2001, 123, 810-816. | 13.7 | 33 |
| 42 | Xe129 chemical shift by the perturbational relativistic method: Xenon fluorides. Journal of Chemical Physics, 2007, 127, 084312. | 3.0 | 33 |
| 43 | Internuclear distance dependence of the spinâ€“orbit coupling contributions to proton NMR chemical shifts. Chemical Physics Letters, 1998, 295, 455-461. | 2.6 | 32 |
| 44 | Exploring new 129Xe chemical shift ranges in HXeY compounds: hydrogen more relativistic than xenon. Physical Chemistry Chemical Physics, 2012, 14, 10944. | 2.8 | 32 |
| 45 | Dynamics and magnetic resonance properties of Sc3C2@C80 and its monoanion. Physical Chemistry Chemical Physics, 2008, 10, 7158. | 2.8 | 31 |
| 46 | Observation of Optical Chemical Shift by Precision Nuclear Spin Optical Rotation Measurements and Calculations. Journal of Physical Chemistry Letters, 2013, 4, 437-441. | 4.6 | 30 |
| 47 | Isotope and temperature effects on the 13C and 77Se nuclear shielding in carbon diselenide. Journal of Chemical Physics, 1997, 107, 1350-1361. | 3.0 | 29 |
| 48 | Density Functional Calculations of 3He Chemical Shift in Endohedral Helium Fullerenes:â€‰ Neutral, Anionic, and Di-Helium Species. Journal of Physical Chemistry A, 2006, 110, 12338-12341. | 2.5 | 29 |
| 49 | Indirect Fluorine Coupling Anisotropies inp-Difluorobenzene:Â Implications to Orientation and Structure Determination of Fluorinated Liquid Crystals. Journal of Physical Chemistry A, 1999, 103, 5675-5684. | 2.5 | 28 |
| 50 | 14N and 2H NMR Study of the Mesophases of Cetyltrimethylammonium Bromide in Formamide. Journal of Physical Chemistry B, 1997, 101, 32-38. | 2.6 | 27 |
| 51 | NMR tensors in planar hydrocarbons of increasing size. Physical Chemistry Chemical Physics, 2009, 11, 11404. | 2.8 | 27 |
| 52 | Nuclear Magnetic Resonance Chemical Shifts and Quadrupole Couplings for Different Hydrogen-Bonding Cases Occurring in Liquid Water:Â A Computational Study. Journal of Physical Chemistry A, 2007, 111, 182-192. | 2.5 | 26 |
| 53 | Laser-induced nuclear magnetic resonance splitting in hydrocarbons. Journal of Chemical Physics, 2008, 129, 124102. | 3.0 | 26 |
| 54 | Toward Reproducing Sequence Trends in Phosphorus Chemical Shifts for Nucleic Acids by MD/DFT Calculations. Journal of Chemical Theory and Computation, 2013, 9, 1641-1656. | 5.3 | 26 |

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| 55 | Nuclear magnetic resonance predictions for graphenes: concentric finite models and extrapolation to large systems. Physical Chemistry Chemical Physics, 2013, 15, 4634. | 2.8 | 26 |
| 56 | Relativistic Approximations to Paramagnetic NMR Chemical Shift and Shielding Anisotropy in Transition Metal Systems. Journal of Chemical Theory and Computation, 2017, 13, 3731-3745. | 5.3 | 26 |
| 57 | Vibrationally averaged magnetizabilities and rotational g tensors of the water molecule. Chemical Physics Letters, 1998, 297, 467-474. | 2.6 | 25 |
| 58 | Spin-Spin Coupling Tensors in Fluoromethanes. Chemistry - A European Journal, 2000, 6, 1395-1406. | 3.3 | 25 |
| 59 | Relativistic Spinâ^'Orbit Coupling Effects on Secondary Isotope Shifts of13C Nuclear Shielding in CX2(X) Tj ETQq1 1 0.784314 rgBT /Ov | 13.7 | 25 |
| 60 | Characteristic Spinâ^'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. | 13.7 | 25 |
| 61 | Ferrocene-like iron bis(dicarbollide), [3-FeIII-(1,2-C2B9H11)2]â^'. The first experimental and theoretical refinement of a paramagnetic 11B NMR spectrum. Physical Chemistry Chemical Physics, 2010, 12, 7018. | 2.8 | 25 |
| 62 | Rovibrationally Averaged Nuclear Shielding Constants in OCS. Journal of Magnetic Resonance, 1998, 135, 444-453. | 2.1 | 24 |
| 63 | Xe129 adsorbed in AlPO4-11 molecular sieve: Molecular dynamics simulation of adsorbate dynamics and NMR chemical shift. Journal of Chemical Physics, 1997, 107, 6470-6478. | 3.0 | 23 |
| 64 | Pairwise additivity in the nuclear magnetic resonance interactions of atomic xenon. Physical Chemistry Chemical Physics, 2009, 11, 2485. | 2.8 | 23 |
| 65 | Fully Relativistic Calculations of Faraday and Nuclear Spin-Induced Optical Rotation in Xenon. Journal of Chemical Theory and Computation, 2012, 8, 91-98. | 5.3 | 23 |
| 66 | Magnetic field dependence of nuclear magnetic shielding in closed-shell atomic systems. Chemical Physics Letters, 2003, 372, 750-757. | 2.6 | 22 |
| 67 | Calculations of nuclear quadrupole coupling in noble gasâ€“noble metal fluorides: Interplay of relativistic and electron correlation effects. Journal of Chemical Physics, 2006, 125, 174315. | 3.0 | 22 |
| 68 | Electron spin resonance parameters of bulk oxygen vacancy in semiconducting tin dioxide. Physical Review B, 2010, 81, . | 3.2 | 21 |
| 69 | Nuclear spin optical rotation and Faraday effect in gaseous and liquid water. Journal of Chemical Physics, 2012, 136, 184502. | 3.0 | 21 |
| 70 | Effect of correlating core orbitals in calculations of nuclear spinâ€“spin couplings. Journal of Chemical Physics, 2001, 114, 5482-5490. | 3.0 | 20 |
| 71 | Nuclear spin circular dichroism. Journal of Chemical Physics, 2014, 140, 134103. | 3.0 | 20 |
| 72 | Density Functional Theory Calculations of Electron Paramagnetic Resonance Parameters of a Nitroxide Spin Label in Tissue Factor and Factor VIIa Protein Complex. Journal of Physical Chemistry B, 2002, 106, 12354-12360. | 2.6 | 19 |

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| 73 | Magnetic-field dependence of59Conuclear magnetic shielding in Co(III) complexes. Physical Review A, 2004, 69, . | 2.5 | 19 |
| 74 | Magnetic Properties of Ni<sup>2+</sup>(aq) from First Principles. Journal of Chemical Theory and Computation, 2011, 7, 3248-3260. | 5.3 | 19 |
| 75 | Nuclear spin-induced Cotton-Mouton effect in molecules. Journal of Chemical Physics, 2013, 138, 204110. | 3.0 | 19 |
| 76 | Magnetic-Field-Induced Quadrupole Splitting in Gaseous and LiquidX131eNMR: Quadratic and Quartic Field Dependence. Physical Review Letters, 2001, 86, 3268-3271. | 7.8 | 18 |
| 77 | Methodological aspects in the calculation of parity-violating effects in nuclear magnetic resonance parameters. Journal of Chemical Physics, 2007, 126, 074107. | 3.0 | 18 |
| 78 | 13C NMR spectroscopy of methane adsorbed in SAPO-11 molecular sieve. Chemical Physics Letters, 1996, 261, 425-430. | 2.6 | 17 |
| 79 | Perturbational relativistic theory of electron spin resonance g-tensor. Journal of Chemical Physics, 2004, 121, 1258-1265. | 3.0 | 17 |
| 80 | Charge localization in alcohol isomers studied by Compton scattering. Journal of Chemical Physics, 2009, 130, 034506. | 3.0 | 17 |
| 81 | Nuclear spin relaxation due to chemical shift anisotropy of gas-phase 129Xe. Physical Chemistry Chemical Physics, 2011, 13, 13704. | 2.8 | 17 |
| 82 | Faraday Rotation in Graphene Quantum Dots: Interplay of Size, Perimeter Type, and Functionalization. Journal of Physical Chemistry C, 2014, 118, 23996-24005. | 3.1 | 17 |
| 83 | Assignment of solid-state 13 C and 1 H NMR spectra of paramagnetic Ni(II) acetylacetonate complexes aided by first-principles computations. Solid State Nuclear Magnetic Resonance, 2017, 87, 29-37. | 2.3 | 17 |
| 84 | Calculation of isotropic Compton profiles with Gaussian basis sets. Physical Chemistry Chemical Physics, 2011, 13, 5630. | 2.8 | 16 |
| 85 | Anisotropy of the 1H and 13C shielding tensors in chloroform. Chemical Physics Letters, 1996, 253, 340-348. | 2.6 | 15 |
| 86 | Laser-induced splittings in the nuclear magnetic resonance spectra of the rare gas atoms. Chemical Physics Letters, 2004, 400, 226-230. | 2.6 | 15 |
| 87 | Comment on â€œCalculation of nuclear magnetic shieldings using an analytically differentiated relativistic shielding formulaâ€•[J. Chem. Phys. 123, 114102 (2005)]. Journal of Chemical Physics, 2006, 124, 137101. | 3.0 | 15 |
| 88 | Characterization of pore structures of hydrated cements and natural shales by 129 Xe NMR spectroscopy. Microporous and Mesoporous Materials, 2017, 253, 49-54. | 4.4 | 15 |
| 89 | Surface relaxation of the (100) face of wurtzite CdS. Surface Science, 1996, 352-354, 77-82. | 1.9 | 14 |
| 90 | Constant-pressure simulations of Gayâ€“Berne liquid-crystalline phases in cylindrical nanocavities. Physical Chemistry Chemical Physics, 2013, 15, 14047. | 2.8 | 14 |

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| 91 | Xenon NMR of liquid crystals confined to cylindrical nanocavities: a simulation study. Physical Chemistry Chemical Physics, 2015, 17, 7158-7171. | 2.8 | 14 |
| 92 | Pseudoâ€Contact NMR Shifts over the Paramagnetic Metalloprotein CoMMPâ€12 from First Principles. Angewandte Chemie, 2016, 128, 14933-14937. | 2.0 | 14 |
| 93 | Ab initio paramagnetic NMR shifts via point-dipole approximation in a large magnetic-anisotropy Co(ii) complex. Physical Chemistry Chemical Physics, 2018, 20, 22547-22555. | 2.8 | 14 |
| 94 | Experimental and quantum-chemical determination of the2H quadrupole coupling tensor in deuterated benzenes. Physical Chemistry Chemical Physics, 2007, 9, 481-490. | 2.8 | 13 |
| 95 | Nuclear spin-spin coupling in a van der Waals-bonded system: Xenon dimer. Journal of Chemical Physics, 2013, 138, 104313. | 3.0 | 13 |
| 96 | Communication: Nuclear quadrupole moment-induced Cotton-Mouton effect in noble gas atoms. Journal of Chemical Physics, 2013, 139, 181102. | 3.0 | 13 |
| 97 | Curie-type paramagnetic NMR relaxation in the aqueous solution of Ni(<scp>ii</scp>). Physical Chemistry Chemical Physics, 2014, 16, 6916-6924. | 2.8 | 13 |
| 98 | Spin dynamics simulation of electron spin relaxation in Ni2 +(aq). Journal of Chemical Physics, 2014, 141, 014109. | 3.0 | 12 |
| 99 | Spin Doublet Point Defects in Graphenes: Predictions for ESR and NMR Spectral Parameters. Journal of Chemical Theory and Computation, 2015, 11, 3746-3754. | 5.3 | 12 |
| 100 | Remarkable reversal of <sup>13</sup>C-NMR assignment in d<sup>1</sup>, d<sup>2</sup> compared to d<sup>8</sup>, d<sup>9</sup> acetylacetonate complexes: analysis and explanation based on solid-state MAS NMR and computations. Physical Chemistry Chemical Physics, 2020, 22, 8048-8059. | 2.8 | 12 |
| 101 | Computational and experimental study of NMR relaxation of quadrupolar noble gas nuclei in organic solvents. Molecular Physics, 1994, 82, 13-27. | 1.7 | 11 |
| 102 | Deuterium quadrupole coupling tensors in methyl halides:Ab initioeffective core potential and liquid crystal nuclear magnetic resonance study. Journal of Chemical Physics, 1997, 107, 1744-1752. | 3.0 | 11 |
| 103 | Experimental and Theoretical Study of the Spinâ^'Spin Coupling Tensors in Methylsilane. Journal of Physical Chemistry A, 1999, 103, 9669-9677. | 2.5 | 11 |
| 104 | Nuclear magnetic resonance parameters of atomic xenon dissolved in Gay-Berne model liquid crystal. Physical Review E, 2007, 75, 031707. | 2.1 | 11 |
| 105 | Solvation Structure and Dynamics of Ni<sup>2+</sup>(aq) from First Principles. Journal of Chemical Theory and Computation, 2011, 7, 2937-2946. | 5.3 | 11 |
| 106 | Nuclear quadrupole moment-induced Cotton-Mouton effect in molecules. Journal of Chemical Physics, 2014, 140, 024103. | 3.0 | 11 |
| 107 | Characteristic Spectral Patterns in the Carbonâ€13 Nuclear Magnetic Resonance Spectra of Hexagonal and Crenellated Graphene Fragments. ChemPhysChem, 2014, 15, 1799-1808. | 2.1 | 11 |
| 108 | Nuclearâ€Spinâ€Induced Cottonâ€“Mouton Effect in a Strong External Magnetic Field. ChemPhysChem, 2014, 15, 2337-2350. | 2.1 | 10 |

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| 109 | Paramagnetic Pyrazolylborate Complexes Tp<sub>2</sub>M and Tp*<sub>2</sub>M: <sup>1</sup>H, <sup>13</sup>C, <sup>11</sup>B, and <sup>14</sup>N NMR Spectra and First-Principles Studies of Chemical Shifts. Inorganic Chemistry, 2020, 59, 9294-9307. | 4.0 | 10 |
| 110 | 13CNMR of methane in anAlPO4â"11molecular sieve: Exchange effects and shielding anisotropy. Physical Review B, 1998, 58, 14833-14836. | 3.2 | 9 |
| 111 | Nuclear spin circular dichroism in fullerenes: a computational study. Chemical Communications, 2014, 50, 15228-15231. | 4.1 | 9 |
| 112 | Chemical shift extremum of 129Xe(aq) reveals details of hydrophobic solvation. Scientific Reports, 2018, 8, 7023. | 3.3 | 9 |
| 113 | Influence of Hydrogen Bonding in the Paramagnetic NMR Shieldings of Nitronylnitroxide Derivative Molecules. Journal of Physical Chemistry B, 2004, 108, 1197-1206. | 2.6 | 8 |
| 114 | 19F spinâ€"spin coupling in peri-difluoronaphthalene. Physical Chemistry Chemical Physics, 2009, 11, 4136. | 2.8 | 8 |
| 115 | Rovibrational effects on NMR shieldings in a heavy-element system: XeF2. Journal of Chemical Physics, 2012, 137, 214309. | 3.0 | 8 |
| 116 | Experimental and First-Principles NMR Analysis of Pt(II) Complexes With O,Oâ€²-Dialkyldithiophosphate Ligands. Journal of Physical Chemistry A, 2016, 120, 8326-8338. | 2.5 | 8 |
| 117 | Liquid-state paramagnetic relaxation from first principles. Physical Review A, 2016, 94, . | 2.5 | 8 |
| 118 | Paramagnetic Enhancement of Nuclear Spinâ€"Spin Coupling. Journal of Chemical Theory and Computation, 2017, 13, 1275-1283. | 5.3 | 8 |
| 119 | Calculation of scalar nuclear spin-spin coupling in a noble-gas mixture. Physical Review A, 2019, 99, . | 2.5 | 8 |
| 120 | Effects of two double bonds on the hydrocarbon interior of a phospholipid bilayer. Chemical Physics Letters, 1995, 246, 300-306. | 2.6 | 7 |
| 121 | Inequivalence of single CHa and CHb methylene bonds in the interior of a diunsaturated lipid bilayer from a molecular dynamics simulation. Chemical Physics Letters, 1997, 268, 55-60. | 2.6 | 7 |
| 122 | Chemical Shift in Paramagnetic Systems. Science and Technology of Atomic, Molecular, Condensed Matter and Biological Systems, 2013, , 41-67. | 0.6 | 7 |
| 123 | Magnetic field-induced nuclear quadrupole coupling in atomic<sup>131</sup>Xe. Molecular Physics, 2013, 111, 1390-1400. | 1.7 | 7 |
| 124 | Solvation chemical shifts of perylenic antenna molecules from molecular dynamics simulations. Physical Chemistry Chemical Physics, 2014, 16, 22309-22320. | 2.8 | 7 |
| 125 | Nuclear magnetic resonance parameters in water dimer. Theoretical Chemistry Accounts, 2011, 129, 313-324. | 1.4 | 6 |
| 126 | Electron correlation and relativistic effects in the secondary NMR isotope shifts of CSe2. Physical Chemistry Chemical Physics, 2013, 15, 17468. | 2.8 | 6 |

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| 127 | Nuclear spinâ€“spin coupling anisotropy in the van der Waals-bonded 129Xe dimer. Physical Chemistry Chemical Physics, 2013, 15, 11427. | 2.8 | 6 |
| 128 | Electron and nuclear spin polarization in Rb-Xe spin-exchange optical hyperpolarization. Physical Review A, 2017, 95, . | 2.5 | 6 |
| 129 | Ratcheting rotation or speedy spinning: EPR and dynamics of Sc<sub>3</sub>C<sub>2</sub>@C<sub>80</sub>. Chemical Communications, 2017, 53, 8992-8995. | 4.1 | 6 |
| 130 | Relation between molecular electronic structure and nuclear spin-induced circular dichroism. Scientific Reports, 2017, 7, 46617. | 3.3 | 6 |
| 131 | Magnetic-field-induced quadrupole coupling in the nuclear magnetic resonance of noble-gas atoms and molecules. Physical Review A, 2004, 70, . | 2.5 | 5 |
| 132 | Effect of molecular size on the parity-non-conserving contributions to the nuclear magnetic resonance shielding constant. Theoretical Chemistry Accounts, 2008, 121, 53-57. | 1.4 | 5 |
| 133 | Energetics and exchange of xenon and water in a prototypic cryptophane-A biosensor structure. Physical Chemistry Chemical Physics, 2022, 24, 17946-17950. | 2.8 | 5 |
| 134 | Direct magnetic-field dependence of NMR chemical shift. Physical Chemistry Chemical Physics, 2020, 22, 8485-8490. | 2.8 | 4 |
| 135 | Brownian Translational Dynamics on a Flexible Surface: Nuclear Spin Relaxation of Fluid Membrane Phases. Langmuir, 2018, 34, 3755-3766. | 3.5 | 2 |
| 136 | Solvation structure and dynamics of Ni2+(aq) from a polarizable force field. Chemical Physics, 2014, 443, 112-122. | 1.9 | 1 |
| 137 | Polarization transfer in a spin-exchange optical-pumping experiment. Physical Review A, 2020, 102, . | 2.5 | 1 |
| 138 | Au32: A 24-Carat Golden Fullerene.. ChemInform, 2004, 35, no. | 0.0 | 0 |
| 139 | Direct enantiomeric discrimination through antisymmetric hyperfine coupling. Chemical Communications, 2021, 57, 8264-8267. | 4.1 | 0 |