Leonid B Krivdin

List of Publications by Year
in descending order

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206	3,588	159585	223800
papers	citations	30 h-index	46 g-index

210	210	210	1231
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Recent Advances in Theoretical Calculations of Indirect Spinâ€“Spin Coupling Constants. Annual Reports on NMR Spectroscopy, 2007, , 133-245.	1.5	152
2	Structural applications of one-bond carbonî—¸carbon spinâ€”spin coupling constants. Progress in Nuclear Magnetic Resonance Spectroscopy, 1989, 21, 293-448.	7.5	115
3	Modern quantum chemical methods for calculating spinâ€“spin coupling constants: theoretical basis and structural applications in chemistry. Russian Chemical Reviews, 2013, 82, 99-130.	6.5	107
4	Spinâ€”spin coupling constants between carbons separated by more than one bond. Progress in Nuclear Magnetic Resonance Spectroscopy, 1991, 23, 301-610.	7.5	83
5	Structural trends of ⁷⁷Seï£¿¹H spinâ€“spin coupling constants and conformational behavior of 2â€substituted selenophenes. Magnetic Resonance in Chemistry, 2010, 48, 44-52.	1.9	77
6	Computational protocols for calculating 13C NMR chemical shifts. Progress in Nuclear Magnetic Resonance Spectroscopy, 2019, 112-113, 103-156.	7.5	71
7	Non-empirical calculations of NMR indirect carbon-carbon coupling constants: 1. Three-membered rings. Magnetic Resonance in Chemistry, 2002, 40, 187-194.	1.9	69
8	Carbon-carbon coupling constants - a new guide in the stereochemistry of oximes. Tetrahedron Letters, 1984, 25, 4817-4820.	1.4	66
9	Theoretical grounds of relativistic methods for calculation of spinâ€“spin coupling constants in nuclear magnetic resonance spectra. Russian Chemical Reviews, 2016, 85, 356-426.	6.5	63
10	Calculation of 15 N NMR chemical shifts: Recent advances and perspectives. Progress in Nuclear Magnetic Resonance Spectroscopy, 2017, 102-103, 98-119.	7.5	58
11	Carbon-carbon spin-spin coupling constants: Practical applications of theoretical calculations. Progress in Nuclear Magnetic Resonance Spectroscopy, 2018, 105, 54-99.	7.5	56
12	NaturalJ coupling (NJC) analysis of the electron lone pair effect on NMR couplings: Part 1. The lone pair orientation effect of an ?-nitrogen atom on1J(C,C) couplings. Magnetic Resonance in Chemistry, 2001, 39, 600-606.	1.9	54
13	Theoretical calculations of carbon-hydrogen spin-spin coupling constants. Progress in Nuclear Magnetic Resonance Spectroscopy, 2018, 108, 17-73.	7.5	53
14	Relativistic effects in the NMR spectra of compounds containing heavy chalcogens. Mendeleev Communications, 2018, 28, 1-13.	1.6	51
15	Non-empirical calculations of NMR indirect carbonâ€“carbon coupling constants. Part 8â€”Monocycloalkanes. Magnetic Resonance in Chemistry, 2004, 42, 671-686.	1.9	50
16	Orange to black electrochromic behaviour in poly(2-(2-thienyl)-1H-pyrrole) thin films. Electrochimica Acta, 2007, 52, 4784-4791.	5.2	46
17	Computational ¹H NMR: Part 1. Theoretical background. Magnetic Resonance in Chemistry, 2019, 57, 897-914.	1.9	44
18	Divinyl selenide: conformational study and stereochemical behavior of its ⁷⁷Seï£¿¹H spinâ€“spin coupling constants. Magnetic Resonance in Chemistry, 2008, 46, 979-985.	1.9	43

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19	Conformational analysis and diastereotopic assignments in the series of seleniumâ€containing heterocycles by means of ⁷⁷Seâ€¹H spinâ€spin coupling constants: a combined theoretical and experimental study. Magnetic Resonance in Chemistry, 2011, 49, 389-398.	1.9	42
20	On the accuracy of the GIAOâ€DFT calculation of ¹⁵N NMR chemical shifts of the nitrogenâ€containing heterocycles â€“ a gateway to better agreement with experiment at lower computational cost. Magnetic Resonance in Chemistry, 2014, 52, 222-230.	1.9	42
21	On the HALA effect in the NMR carbon shielding constants of the compounds containing heavy pâ€elements. International Journal of Quantum Chemistry, 2016, 116, 1404-1412.	2.0	39
22	Towards the versatile DFT and MP2 computational schemes for³¹P NMR chemical shifts taking into account relativistic corrections. Magnetic Resonance in Chemistry, 2014, 52, 699-710.	1.9	38
23	Solvent effects in the GIAO-DFT calculations of the¹⁵N NMR chemical shifts of azoles and azines. Magnetic Resonance in Chemistry, 2014, 52, 686-693.	1.9	38
24	Effects of protonation on acetone: nuclear magnetic resonance and ab initio studies. Journal of the Chemical Society, Faraday Transactions, 1992, 88, 2459-2463.	1.7	36
25	Computational ¹H NMR: Part 3. Biochemical studies. Magnetic Resonance in Chemistry, 2020, 58, 15-30.	1.9	36
26	Computational ¹H NMR: Part 2. Chemical applications. Magnetic Resonance in Chemistry, 2020, 58, 5-14.	1.9	35
27	DFT computational schemes for ¹H and ¹³C NMR chemical shifts of natural products, exemplified by strychnine. Magnetic Resonance in Chemistry, 2020, 58, 56-64.	1.9	35
28	Experimental and computational studies of ⁿJ(⁷⁷Se,¹H) seleniumâ€“proton couplings in selenoglycosides. Magnetic Resonance in Chemistry, 2011, 49, 190-194.	1.9	32
29	Non-empirical calculations of NMR indirect carbon-carbon coupling constants. Part 12â€”Aliphatic and alicyclic oximes. Magnetic Resonance in Chemistry, 2005, 43, 435-443.	1.9	31
30	Benchmarking SOPPA(CC2) for the calculation of indirect nuclear spinâ€“spin coupling constants: Carbocycles. Chemical Physics, 2011, 381, 35-43.	1.9	31
31	Non-empirical calculations of NMR indirect carbon-carbon coupling constants. Part 5: Bridged bicycloalkanes. Magnetic Resonance in Chemistry, 2003, 41, 885-901.	1.9	30
32	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.	2.8	30
33	Non-empirical calculations of NMR indirect carbonâ€“carbon coupling constants. Part 6: Propellanes. Magnetic Resonance in Chemistry, 2004, 42, 1-13.	1.9	29
34	Recent advances in computational ³¹P NMR: Part 1. Chemical shifts. Magnetic Resonance in Chemistry, 2020, 58, 478-499.	1.9	28
35	Synthesis, Structure, and Spectral Properties of Bis(pyrrol-2-yl)pyridines. European Journal of Organic Chemistry, 2005, 2005, 4338-4345.	2.4	27
36	Theoretical and experimental study of ¹⁵ N NMR protonation shifts. Magnetic Resonance in Chemistry, 2015, 53, 433-441.	1.9	26

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37	Non-empirical calculations of NMR indirect carbon-carbon coupling constants: 3. Polyhedranes. Magnetic Resonance in Chemistry, 2003, 41, 157-168.	1.9	25
38	Amidine derivatives of Î±-arylglycines from N-(1-aryl-2,2,2-trichloroethyl)amides of arenesulfonic acids and secondary amines. Tetrahedron Letters, 2005, 46, 8889-8893.	1.4	25
39	Non-empirical calculations of NMR indirect carbon-carbon coupling constants. Part 4: Bicycloalkanes. Magnetic Resonance in Chemistry, 2003, 41, 417-430.	1.9	24
40	Non-empirical calculations of NMR indirect carbonâ€“carbon coupling constants. Part 9â€”Bicyclobutane-containing polycycloalkanes. Magnetic Resonance in Chemistry, 2004, 42, S168-S179.	1.9	24
41	Non-empirical calculations of NMR indirect spin-spin coupling constants. Part 13: configurational assignment of aminosulfonylamidines. Magnetic Resonance in Chemistry, 2005, 43, 937-942.	1.9	24
42	Configurational assignment of carbon, silicon and germanium containing propynal oximes by means of13Cï£¿1H,13Cï£¿13C and15Nï£¿1H spinâ€“spin coupling constants. Magnetic Resonance in Chemistry, 2007, 45, 661-666.	1.9	24
43	Quantum-chemical calculations of NMR chemical shifts of organic molecules: I. Phosphines, phosphine oxides, and phosphine sulfides. Russian Journal of Organic Chemistry, 2010, 46, 785-790.	0.8	24
44	Stereochemical behavior of ⁷⁷Seâ€“¹H spinâ€“spin coupling constants in pyrazolylâ€1,3â€diselenanes and 1,2â€diselenolane. Magnetic Resonance in Chemistry, 2012, 50, 169-173.	1.9	24
45	Computational aspects of 19F NMR. Russian Chemical Reviews, 2020, 89, 1040-1073.	6.5	24
46	Non-empirical calculations of NMR indirect carbon-carbon coupling constants. Part 11?saturated carbocycles: a reference data set and a practical guide to structural elucidation. Magnetic Resonance in Chemistry, 2005, 43, 101-116.	1.9	23
47	Nonempirical calculations of NMR indirect spin-spin coupling constants. Magnetic Resonance in Chemistry, 2006, 44, 178-187.	1.9	23
48	Non-empirical calculations of NMR indirect carbon-carbon coupling constants: 2. Strained polycarbocycles. Magnetic Resonance in Chemistry, 2003, 41, 91-101.	1.9	22
49	Non-empirical calculations of NMR indirect carbonâ€“carbon coupling constants. Part 7â€”Spiroalkanes. Magnetic Resonance in Chemistry, 2004, 42, 500-511.	1.9	22
50	Resonance assignments of diastereotopic CH₂ protons in the anomeric side chain of selenoglycosides by means of ²J(Se,H) spinâ€“spin coupling constants. Magnetic Resonance in Chemistry, 2012, 50, 488-495.	1.9	22
51	Non-empirical calculations of NMR indirect carbon-carbon coupling constants. Part 10?Carbocages. Magnetic Resonance in Chemistry, 2004, 42, 919-930.	1.9	21
52	Conformational analysis and stereochemical dependences of ³¹Pâ€“¹H spinâ€“spin coupling constants of bis(2â€phenethyl)vinylphosphine and related phosphine chalcogenides. Magnetic Resonance in Chemistry, 2009, 47, 288-299.	1.9	21
53	Computational NMR of Carbohydrates: Theoretical Background, Applications, and Perspectives. Molecules, 2021, 26, 2450.	3.8	21
54	Conformational Analysis of 2-Formylselenophene by Means of 13C - 1H, 13C - 13C, and 77Se - 1H Spin - Spin Coupling Constants. Australian Journal of Chemistry, 2009, 62, 734.	0.9	20

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55	Openâ€chain unsaturated selanyl sulfides: stereochemical structure and stereochemical behavior of their ⁷⁷Seâ€“¹H spinâ€“spin coupling constants. Magnetic Resonance in Chemistry, 2012, 50, 653-658.	1.9	20
56	Recent advances in computational ³¹P NMR: Part 2. Spinâ€“spin coupling constants. Magnetic Resonance in Chemistry, 2020, 58, 500-511.	1.9	20
57	Carbon-to-carbon coupling constants - a new guide in the stereochemistry of heteroatomic compounds. Journal of Molecular Structure, 1986, 143, 569-572.	3.6	19
58	Trivinylphosphine and trivinylphosphine chalcogenides: stereochemical trends of 31Pï£¿1H spin-spin coupling constants. Magnetic Resonance in Chemistry, 2010, 48, S48-S55.	1.9	19
59	MP2 calculation of ⁷⁷Se NMR chemical shifts taking into account relativistic corrections. Magnetic Resonance in Chemistry, 2015, 53, 485-492.	1.9	19
60	Calculation of125Te NMR Chemical Shifts at the Full Four-Component Relativistic Level with Taking into Account Solvent and Vibrational Corrections: A Gateway to Better Agreement with Experiment. Journal of Physical Chemistry A, 2017, 121, 4793-4803.	2.5	19
61	Nonempirical calculations of NMR indirect spinâ€“spin coupling constants. Part 15: pyrrolylpyridines. Magnetic Resonance in Chemistry, 2006, 44, 692-697.	1.9	18
62	Conformational study of 2-arylazo-1-vinylpyrroles. Magnetic Resonance in Chemistry, 2007, 45, 142-151.	1.9	18
63	Quantum-chemical calculations of NMR chemical shifts of organic molecules: II. Influence of medium, relativistic effects, and vibrational corrections on phosphorus magnetic shielding constants in the simplest phosphines and phosphine chalcogenides. Russian Journal of Organic Chemistry, 2011, 47, 355-362.	0.8	18
64	Benchmark calculations of ²⁹Siâ€“¹H spinâ€“spin coupling constants across double bond. Magnetic Resonance in Chemistry, 2012, 50, 278-283.	1.9	18
65	Relativistic effects in the oneâ€bond spinâ€“spin coupling constants involving selenium. Magnetic Resonance in Chemistry, 2014, 52, 500-510.	1.9	18
66	Theoretical and experimental ¹⁵N NMR study of enamineâ€“imine tautomerism of 4â€trifluoromethyl[b]benzoâ€1,4â€diazepine system. Magnetic Resonance in Chemistry, 2015, 53, 1031-1034.	1.9	18
67	Normal halogen dependence of ¹³C NMR chemical shifts of halogenomethanes revisited at the fourâ€component relativistic level. Magnetic Resonance in Chemistry, 2016, 54, 787-792.	1.9	18
68	First example of the correlated calculation of the oneâ€bond telluriumâ€“carbon spinâ€“spin coupling constants: Relativistic effects, vibrational corrections, and solvent effects. Journal of Computational Chemistry, 2016, 37, 1367-1372.	3.3	18
69	Theoretical and experimental study of the orientational nitrogen lone-pair effect on couplings in acetoxime. Journal of Magnetic Resonance, 1989, 84, 1-8.	0.5	17
70	On the significant relativistic heavy atom effect on ¹³C NMR chemical shifts of Î²- and Î³-carbons in seleno- and telluroketones. Molecular Physics, 2017, 115, 3117-3127.	1.7	17
71	Computational liquid-phase and solid-state 29Si NMR. Russian Chemical Reviews, 2020, 89, 449-468.	6.5	17
72	Computational¹H and¹³C NMR in structural and stereochemical studies. Magnetic Resonance in Chemistry, 2022, 60, 733-828.	1.9	17

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73	The first example of the configurational assignment at the CN bond of allenylthioimidates. Tetrahedron Letters, 2005, 46, 7367-7371.	1.4	16
74	Configurational Assignment and Conformational Study of Methylglyoxal Bisdimethylhydrazones Derived from the 2-Ethoxypropenal Precursor. Australian Journal of Chemistry, 2006, 59, 211.	0.9	16
75	Stereochemical Study of 2-Substituted N-Vinylpyrroles. Australian Journal of Chemistry, 2007, 60, 583.	0.9	16
76	A novel regiospecific cascade synthesis of sulfonamide derivatives from N-(2-polychloroethyl)sulfonamides via chloroaziridine intermediates in the presence of mercaptoethanol. Molecular Diversity, 2010, 14, 533-541.	3.9	16
77	Relativistic heavy atom effect on the <scp>³¹P NMR</scp> parameters of phosphine chalcogenides. Part 1. Chemical shifts. Magnetic Resonance in Chemistry, 2018, 56, 1061-1073.	1.9	16
78	Synthesis and electrochemical characterization of dipyrroles separated by diphenyleneoxide and diphenylenesulfide spacers via the Trofimov reaction. Tetrahedron, 2005, 61, 7756-7762.	1.9	15
79	Stereochemical study of iminodihydrofurans based on experimental measurements and SOPPA calculations of ¹³Cï£¿¹³C spinâ€“spin coupling constants. Magnetic Resonance in Chemistry, 2007, 45, 758-765.	1.9	15
80	Structural trends of ²⁹Siâ€“¹H spinâ€“spin coupling constants across double bond. Magnetic Resonance in Chemistry, 2012, 50, 665-671.	1.9	15
81	Algebraic-diagrammatic construction polarization propagator approach to indirect nuclear spinâ€“spin coupling constants. Journal of Chemical Physics, 2012, 137, 044119.	3.0	15
82	Stereochemical behavior of ²â€‰J(Se,H) and ³â€‰J(Se,H) spinâ€spin coupling constants across sp³ carbons: a theoretical scrutiny. Magnetic Resonance in Chemistry, 2012, 50, 557-562.	1.9	15
83	Quantum-chemical calculations of chemical shifts in NMR spectra of organic molecules: V. Stereochemical structure of unsaturated phosphonic acids dichlorides from 31P NMR spectral data. Russian Journal of Organic Chemistry, 2012, 48, 676-681.	0.8	15
84	Quantum-chemical calculations of NMR chemical shifts of organic molecules: VIII. Solvation effects on 15N NMR chemical shifts of nitrogen-containing heterocycles. Russian Journal of Organic Chemistry, 2013, 49, 379-383.	0.8	15
85	Oneâ€bond ²⁹Siâ€¹H spinâ€spin coupling constants in the series of halosilanes: benchmark SOPPA and DFT calculations, relativistic effects, and vibrational corrections. Magnetic Resonance in Chemistry, 2013, 51, 557-561.	1.9	15
86	Full fourâ€component relativistic calculations of the oneâ€bond ⁷⁷Seâ€“¹³C spinâ€spin coupling constants in the series of selenium heterocycles and their parent openâ€chain selenides. Magnetic Resonance in Chemistry, 2014, 52, 214-221.	1.9	15
87	The ¹H and ¹³C NMR chemical shifts of Strychnos alkaloids revisited at the DFT level. Magnetic Resonance in Chemistry, 2020, 58, 532-539.	1.9	15
88	anti-Markovnikov addition of tellurium tetrachloride to trimethyl ethynyl silane. Journal of Organometallic Chemistry, 2008, 693, 2509-2513.	1.8	14
89	N-(2,2-Dichloro-2-phenylethylidene)arenesulfonamides in reactions with secondary amines. Russian Journal of General Chemistry, 2008, 78, 1371-1379.	0.8	14
90	13C-13C spin-spin coupling constants in structural studies: XLIV. Carbonyl-containing oximes. Russian Journal of Organic Chemistry, 2009, 45, 481-485.	0.8	14

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91	The effects of intramolecular and intermolecular coordination on ³¹P nuclear shielding: phosphorylated azoles. Magnetic Resonance in Chemistry, 2012, 50, 120-127.	1.9	14
92	Quantum-chemical calculations of NMR chemical shifts of organic molecules: XIII. Accuracy of the calculation of 15N NMR chemical shifts of azines with account taken of solvation effects. Russian Journal of Organic Chemistry, 2014, 50, 381-388.	0.8	14
93	Relativistic effect of iodine in 13C NMR chemical shifts of iodomethanes from quantum chemical calculations within the framework of the full four-component relativistic Diracâ€"Coulomb scheme. Russian Chemical Bulletin, 2015, 64, 2756-2762.	1.5	14
94	Computational Multinuclear NMR of Platinum Complexes: A Relativistic Four-Component Study. Journal of Physical Chemistry A, 2019, 123, 4908-4920.	2.5	14
95	Recent advances in computational liquid-phase 77Se NMR. Russian Chemical Reviews, 2021, 90, 265-279.	6.5	14
96	N,N-Disubstituted Î±-Amino-Î±,Î²-unsaturated Aldehydes and their Derivatives:1H and13C NMR Study. Magnetic Resonance in Chemistry, 1997, 35, 533-537.	1.9	13
97	Structural study of 2,3,4,6-tetra(O-vinyl) methyl-Î±-d-glucopyranoside. Journal of Molecular Structure, 2006, 791, 1-9.	3.6	13
98	Stereochemical study of the sterically crowded phenylselanylalkenes by means of ⁷⁷Seï£¿¹H spinâ€"spin coupling constants. Magnetic Resonance in Chemistry, 2011, 49, 570-574.	1.9	13
99	Fourâ€component relativistic <scp>DFT</scp> calculations of ⁷⁷Se <scp>NMR</scp> chemical shifts: A gateway to a reliable computational scheme for the mediumâ€sized organoselenium molecules. Journal of Computational Chemistry, 2015, 36, 1756-1762.	3.3	13
100	<scp>¹H</scp> and <scp>¹³C NMR</scp> spectra of Strychnos alkaloids: Selected <scp>NMR</scp> updates. International Journal of Quantum Chemistry, 2020, 120, e26348.	2.0	13
101	Computational NMR of heavy nuclei involving 109Ag, 113Cd, 119Sn, 125Te, 195Pt, 199Hg, 205Tl, and 207Pb. Russian Chemical Reviews, 2021, 90, 1166-1212.	6.5	12
102	13C-13C Spin-Spin Coupling Constants in Structural Studies: XXXVII. Rotational Conformations of Hydroxy Groups in Pyranose, Furanose, and Septanose Rings. Russian Journal of Organic Chemistry, 2004, 40, 1194-1199.	0.8	11
103	Spin-spin Coupling Constants 13C-13C in Structural Studies: XXXVIII. Nonempirical Calculations: Oximes. Russian Journal of Organic Chemistry, 2005, 41, 1103-1112.	0.8	11
104	Easy Î±- to Î²-migration of an enol moiety on a pyrrole ring. Tetrahedron Letters, 2006, 47, 3645-3648.	1.4	11
105	Facile coupling of 2â€(1â€ethylthioethenyl)pyrroles with amines: A route to 2â€(1â€aminoethenyl)pyrroles and 1â€aminoâ€3â€iminopyrrolizines. Journal of Heterocyclic Chemistry, 2007, 44, 505-513.	2.6	11
106	Configurational assignment of Nâ€arylsulfonylimines of Î±â€polychloroaldehydes. Magnetic Resonance in Chemistry, 2007, 45, 980-984.	1.9	11
107	Quantum-chemical calculation of NMR chemical shifts of organic molecules: III. Intramolecular coordination effects on the 31P NMR chemical shifts of phosphorylated N-vinylazoles. Russian Journal of Organic Chemistry, 2011, 47, 1859-1864.	0.8	11
108	Quantum-chemical calculations of NMR chemical shifts of organic molecules: IV. Effect of intermolecular coordination on 31P NMR shielding constants and chemical shifts of molecular complexes of phosphorus pentachloride with azoles. Russian Journal of Organic Chemistry, 2011, 47, 1865-1869.	0.8	11

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109	Quantum chemical calculations of NMR chemical shifts of organic molecules: XI. Conformational and relativistic effects on the 31P and 77Se chemical shifts of phosphine selenides. Russian Journal of Organic Chemistry, 2013, 49, 1420-1427.	0.8	11
110	Relativistic Environmental Effects in ²⁹Si NMR Chemical Shifts of Halosilanes: Light Nucleus, Heavy Environment. Journal of Physical Chemistry A, 2015, 119, 5778-5789.	2.5	11
111	Stereochemical Applications ofCarbon-Carbon Coupling Constants in Organic Chemistry. Current Organic Chemistry, 1998, 2, 173-193.	1.6	11
112	13C-13C Spin-Spin Coupling Constants in Structural Studies: XXXVI. Stereochemical Study of the Septanose Ring. Russian Journal of Organic Chemistry, 2004, 40, 57-62.	0.8	10
113	One-Pot Vinylation of Secondary Phosphine Chalcogenides with Vinyl Sulfoxides. Phosphorus, Sulfur and Silicon and the Related Elements, 2010, 185, 1838-1844.	1.6	10
114	Quantum-chemical calculations of NMR chemical shifts of organic molecules: VII. Intramolecular coordination effect in the 29Si NMR spectra of siletanes. Russian Journal of Organic Chemistry, 2013, 49, 34-41.	0.8	10
115	Nonempirical calculations of the oneâ€bond ²⁹Siâ€“¹³C spinâ€“spin coupling constants taking into account relativistic and solvent corrections. Magnetic Resonance in Chemistry, 2014, 52, 413-421.	1.9	10
116	Quantum-chemical study of organic reaction mechanisms. Part 2. Addition of selenium dichloride to acetylene. Journal of Organometallic Chemistry, 2014, 766, 49-56.	1.8	10
117	Stereochemical behavior of geminal and vicinal ⁷⁷Seâ€“¹³C spinâ€“spin coupling constants studied at the SOPPA(CC2) level taking into account relativistic corrections. Magnetic Resonance in Chemistry, 2015, 53, 93-98.	1.9	10
118	Indirect relativistic bridge and substituent effects from the â€˜heavyâ€™ environment on the oneâ€bond and twoâ€bond ¹³Cï£¿¹H spinâ€“spin coupling constants. Magnetic Resonance in Chemistry, 2016, 54, 39-45.	1.9	10
119	Calculation of ¹⁵N and ³¹P NMR Chemical Shifts of Azoles, Phospholes, and Phosphazoles: A Gateway to Higher Accuracy at Less Computational Cost. Journal of Physical Chemistry A, 2018, 122, 6746-6759.	2.5	10
120	13C-13C Coupling Constants in Structural Studies: XXXIII. Stereochemical Study of the Pyranose Ring. Russian Journal of Organic Chemistry, 2003, 39, 663-671.	0.8	9
121	13C-13C spin-spin coupling constants in structural studies: XL. Conformational analysis of N-vinylpyrroles. Russian Journal of Organic Chemistry, 2007, 43, 880-887.	0.8	9
122	Quantum-chemical calculations of NMR chemical shifts of organic molecules: VI. Accuracy of DFT calculations of 29Si chemical shifts of four-coordinate silicon compounds. Russian Journal of Organic Chemistry, 2012, 48, 1518-1525.	0.8	9
123	Quantum-chemical study of organic reaction mechanisms: I. Addition of selenium dihalides to the double bond of vinyl ethers. Russian Journal of Organic Chemistry, 2013, 49, 508-515.	0.8	9
124	Quantum-chemical calculations of NMR chemical shifts of organic molecules: X. Dynamic equilibrium effects in the 29Si NMR spectra of silacycloalkanes. Russian Journal of Organic Chemistry, 2013, 49, 832-837.	0.8	9
125	On the accuracy factors and computational cost of the GIAOâ€“DFT calculation of ¹⁵N NMR chemical shifts of amides. Magnetic Resonance in Chemistry, 2017, 55, 1015-1021.	1.9	9
126	Geometries and NMR properties of cisplatin and transplatin revisited at the four-component relativistic level. Mendeleev Communications, 2019, 29, 315-317.	1.6	9

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127	Computational 1 H and 13 C NMR of strychnobaillonine: On the way to larger molecules calculated at lower computational costs. Magnetic Resonance in Chemistry, 2021, 59, 108-116.	1.9	9
128	Computational 1 H and 13 C NMR of the trimeric monoterpenoid indole alkaloid strychnohexamine: Selected spectral updates. Magnetic Resonance in Chemistry, 2021, 59, 691-700.	1.9	9
129	Computational ¹⁹⁹Hg NMR. Magnetic Resonance in Chemistry, 2022, 60, 929-953.	1.9	9
130	13C-13C Spin-Spin Coupling Constants in Structural Studies: XXXV. Stereochemical Study of the Furanose Ring. Russian Journal of Organic Chemistry, 2003, 39, 1764-1771.	0.8	8
131	Reactions of N-(Polychloroethylidene)arene-and - trifluoromethanesulfonamides with indoles. Russian Journal of Organic Chemistry, 2008, 44, 86-94.	0.8	8
132	Quantum-chemical calculations of NMR chemical shifts of organic molecules: XII. Calculation of the 13C NMR chemical shifts of fluoromethanes at the DFT level. Russian Journal of Organic Chemistry, 2014, 50, 160-164.	0.8	8
133	Quantum chemical studies of mechanisms of organic reactions: VI. Reaction of ethane-1,2-dithiol with vinylidene chloride. Russian Journal of Organic Chemistry, 2017, 53, 986-994.	0.8	8
134	Stereochemical Dependences of ³¹Pâ€“¹³C Spinâ€“Spin Coupling Constants of Heterocyclic Phosphines. Journal of Physical Chemistry A, 2019, 123, 6298-6303.	2.5	8
135	13C-13C spin-spin coupling constants in structural studies: XLI. Stereochemical study on N-(polychloroethylidene)arenesulfonamides and Nâ€™-arylsulfonylformimidamides. Russian Journal of Organic Chemistry, 2008, 44, 76-85.	0.8	7
136	13C-13C spin-spin coupling constants in structural studies: XLIII. Stereochemical study on functionalized 3-iminopyrrolizines. Russian Journal of Organic Chemistry, 2008, 44, 1338-1344.	0.8	7
137	Synthesis of Functionalized l-Cysteine and l-Methionine by Reaction with Electron-Deficient Acetylenes. Synthesis, 2009, 2009, 3136-3142.	2.3	7
138	Nucleophilic addition to acetylenes in superbasic catalytic systems: XVII. Vinyl ethers with furyl and cycloacetal fragments: Synthesis and structure. Russian Journal of Organic Chemistry, 2010, 46, 1383-1387.	0.8	7
139	On the longâ€range relativistic effects in the ¹⁵<scp>N NMR</scp> chemical shifts of halogenated azines. Magnetic Resonance in Chemistry, 2017, 55, 990-995.	1.9	7
140	GIAOâ€ĐFT calculation of ¹⁵N NMR chemical shifts of Schiff bases: Accuracy factors and protonation effects. Magnetic Resonance in Chemistry, 2018, 56, 727-739.	1.9	7
141	Substitution effects in the <scp>¹⁵N NMR</scp> chemical shifts of heterocyclic azines evaluated at the <scp>GIAOâ€ĐFT</scp> level. Magnetic Resonance in Chemistry, 2018, 56, 767-774.	1.9	7
142	Calculation of ¹⁵N NMR Chemical Shifts in a Diversity of Nitrogen-Containing Compounds Using Composite Method Approximation at the DFT, MP2, and CCSD Levels. Journal of Physical Chemistry A, 2019, 123, 8417-8426.	2.5	7
143	DFT computational schemes for ¹⁵N NMR chemical shifts of the condensed nitrogenâ€containing heterocycles. Magnetic Resonance in Chemistry, 2019, 57, 346-358.	1.9	7
144	Computational NMR of charged systems. Magnetic Resonance in Chemistry, 2022, 60, 8-79.	1.9	7

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145	Computational Protocols for the 19F NMR Chemical Shifts. Part 1: Methodological Aspects. Journal of Fluorine Chemistry, 2020, 238, 109625.	1.7	7
146	Simple and Versatile Scheme for the Stereochemical Identification of Natural Products and Diverse Organic Compounds with Multiple Asymmetric Centers. Journal of Physical Chemistry A, 2021, 125, 10359-10372.	2.5	7
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