## Leonid B Krivdin

List of Publications by Year in descending order

Source: https://exaly.com/author-pdf/8589441/publications.pdf

Version: 2024-02-01



#	Article	IF	CITATIONS
1	Computational NMR of charged systems. Magnetic Resonance in Chemistry, 2022, 60, 8-79.	1.9	7
2	Four omponent relativistic calculations of NMR shielding constants of the transition metal complexes. Part 1: Pentaammines of cobalt, rhodium, and iridium. Magnetic Resonance in Chemistry, 2022, 60, 463-468.	1.9	4
3	Computational NMR of natural products: on the way to super large molecules exemplified with alasmontamine A. Magnetic Resonance in Chemistry, 2022, , .	1.9	3
4	Computational <sup>1</sup> H and <sup>13</sup> C NMR in structural and stereochemical studies. Magnetic Resonance in Chemistry, 2022, 60, 733-828.	1.9	17
5	Combined Computational NMR and Molecular Docking Scrutiny of Potential Natural SARS-CoV-2 M <sup>pro</sup> Inhibitors. Journal of Physical Chemistry B, 2022, 126, 2173-2187.	2.6	7
6	Stereochemical dependence of substituent <i>γ</i> â€effects in the <sup>19</sup> F NMR shielding constants. Magnetic Resonance in Chemistry, 2022, 60, 869-876.	1.9	1
7	Fluorine spin–spin coupling constants of pentafluorobenzene revisited at the ab initio correlated levels. Magnetic Resonance in Chemistry, 2022, , .	1.9	3
8	Computational <sup>199</sup> Hg NMR. Magnetic Resonance in Chemistry, 2022, 60, 929-953.	1.9	9
9	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
10	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
11	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
12	Benchmark density functional theory calculations of 13 C NMR chemical shifts of the natural antimalarial compounds with a new basis set $3z\hat{a}\in \mathbf{S}$ . International Journal of Quantum Chemistry, 2021, 121, e26639.	2.0	4
13	Recent advances in computational liquid-phase 77Se NMR. Russian Chemical Reviews, 2021, 90, 265-279.	6.5	14
14	Computational NMR of Carbohydrates: Theoretical Background, Applications, and Perspectives. Molecules, 2021, 26, 2450.	3.8	21
15	COMPUTATIONAL NMR OF CARBOHYDRATES: THEORETICAL BACKGROUND, APPLICATIONS, AND PERSPECTIVES. Modern Technologies and Scientific and Technological Progress, 2021, 1, 36-37.	0.1	0
16	HIGH-PRECISION CALCULATION OF 1H AND 13C NMR CHEMICAL SHIFTS OF STRICHNINA ALKALOIDS. Modern Technologies and Scientific and Technological Progress, 2021, 1, 40-42.	0.1	0
17	MECHANISMS OF TRANSMISSION OF THE SPIN-SPIN INTERACTION OF CARBON-CARBON IN A SERIES OF BICYCLOBUTANE DERIVATIVES. Scientific Papers Collection of the Angarsk State Technical University, 2021, 2021, 77-87.	0.1	0
18	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

#	Article	IF	CITATIONS
19	Computational <sup>1</sup> H NMR: Part 2. Chemical applications. Magnetic Resonance in Chemistry, 2020, 58, 5-14.	1.9	35
20	Computational <sup>1</sup> H NMR: Part 3. Biochemical studies. Magnetic Resonance in Chemistry, 2020, 58, 15-30.	1.9	36
21	DFT computational schemes for <sup>1</sup> H and <sup>13</sup> C NMR chemical shifts of natural products, exemplified by strychnine. Magnetic Resonance in Chemistry, 2020, 58, 56-64.	1.9	35
22	The <sup>1</sup> H and <sup>13</sup> C NMR chemical shifts of <i>Strychnos</i> alkaloids revisited at the DFT level. Magnetic Resonance in Chemistry, 2020, 58, 532-539.	1.9	15
23	Recent advances in computational <sup>31</sup> P NMR: Part 1. Chemical shifts. Magnetic Resonance in Chemistry, 2020, 58, 478-499.	1.9	28
24	Recent advances in computational <sup>31</sup> P NMR: Part 2. Spin–spin coupling constants. Magnetic Resonance in Chemistry, 2020, 58, 500-511.	1.9	20
25	Four-component relativistic computational NMR study of ferrous, cobalt and nickel bisglycinates. Mendeleev Communications, 2020, 30, 476-478.	1.6	3
26	Computational aspects of 19F NMR. Russian Chemical Reviews, 2020, 89, 1040-1073.	6.5	24
27	A New Basis Set for the Calculation of <sup>13</sup> C NMR Chemical Shifts within a Non-empirical Correlated Framework. Journal of Physical Chemistry A, 2020, 124, 7322-7330.	2.5	4
28	Computational liquid-phase and solid-state 29Si NMR. Russian Chemical Reviews, 2020, 89, 449-468.	6.5	17
29	<scp><sup>1</sup>H</scp> and <scp><sup>13</sup>C NMR</scp> spectra of <i>Strychnos</i> alkaloids: Selected <scp>NMR</scp> updates. International Journal of Quantum Chemistry, 2020, 120, e26348.	2.0	13
30	Computational Protocols for the 19F NMR Chemical Shifts. Part 1: Methodological Aspects. Journal of Fluorine Chemistry, 2020, 238, 109625.	1.7	7
31	Quantum-chemical Study of the Mechanisms of Organic Reactions: VIII. On the Reaction of Ethane-1,2-dithiol with 1,3-Dichlorobut-2-ene in the Hydrazine Hydrate–KOH System. Russian Journal of Organic Chemistry, 2019, 55, 662-669.	0.8	2
32	Stereochemical Dependences of <sup>31</sup> P– <sup>13</sup> C Spin–Spin Coupling Constants of Heterocyclic Phosphines. Journal of Physical Chemistry A, 2019, 123, 6298-6303.	2.5	8
33	Calculation of <sup>15</sup> N 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
34	Geometries and NMR properties of cisplatin and transplatin revisited at the four-component relativistic level. Mendeleev Communications, 2019, 29, 315-317.	1.6	9
35	Computational protocols for calculating 13C NMR chemical shifts. Progress in Nuclear Magnetic Resonance Spectroscopy, 2019, 112-113, 103-156.	7.5	71
36	Computational Multinuclear NMR of Platinum Complexes: A Relativistic Four-Component Study. Journal of Physical Chemistry A, 2019, 123, 4908-4920.	2.5	14

#	Article	IF	CITATIONS
37	Computational <sup>1</sup> H NMR: Part 1. Theoretical background. Magnetic Resonance in Chemistry, 2019, 57, 897-914.	1.9	44
38	DFT computational schemes for <sup>15</sup> N NMR chemical shifts of the condensed nitrogenâ€containing heterocycles. Magnetic Resonance in Chemistry, 2019, 57, 346-358.	1.9	7
39	GIAOâ€DFT calculation of <sup>15</sup> N NMR chemical shifts of Schiff bases: Accuracy factors and protonation effects. Magnetic Resonance in Chemistry, 2018, 56, 727-739.	1.9	7
40	Carbon-carbon spin-spin coupling constants: Practical applications of theoretical calculations. Progress in Nuclear Magnetic Resonance Spectroscopy, 2018, 105, 54-99.	7.5	56
41	Relativistic effects in the NMR spectra of compounds containing heavy chalcogens. Mendeleev Communications, 2018, 28, 1-13.	1.6	51
42	Substitution effects in the <scp><sup>15</sup>N NMR</scp> chemical shifts of heterocyclic azines evaluated at the <scp>GIAOâ€DFT</scp> level. Magnetic Resonance in Chemistry, 2018, 56, 767-774.	1.9	7
43	Quantum Chemical Study of Mechanisms of Organic Reactions: VII. Reaction of Ethane-1,2-dithiol with 1,3-Dichloropropene in the System Hydrazine Hydrate–KOH. Russian Journal of Organic Chemistry, 2018, 54, 1446-1452.	0.8	5
44	Theoretical calculations of carbon-hydrogen spin-spin coupling constants. Progress in Nuclear Magnetic Resonance Spectroscopy, 2018, 108, 17-73.	7.5	53
45	Relativistic heavy atom effect on the <scp><sup>31</sup>P NMR</scp> parameters of phosphine chalcogenides. Part 1. Chemical shifts. Magnetic Resonance in Chemistry, 2018, 56, 1061-1073.	1.9	16
46	Calculation of <sup>15</sup> N and <sup>31</sup> P 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
47	On the accuracy factors and computational cost of the GIAO–DFT calculation of <sup>15</sup> N NMR chemical shifts of amides. Magnetic Resonance in Chemistry, 2017, 55, 1015-1021.	1.9	9
48	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
49	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
50	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
51	On the longâ€range relativistic effects in the <sup>15</sup> <scp>N NMR</scp> chemical shifts of halogenated azines. Magnetic Resonance in Chemistry, 2017, 55, 990-995.	1.9	7
52	On the significant relativistic heavy atom effect on <sup>13</sup> C NMR chemical shifts of β- and γ-carbons in seleno- and telluroketones. Molecular Physics, 2017, 115, 3117-3127.	1.7	17
53	Quantum-chemical calculations of NMR chemical shifts of organic molecules: XV. Relativistic calculations of 29Si NMR chemical shifts of silanes. Russian Journal of Organic Chemistry, 2017, 53, 643-651.	0.8	6
54	Relativistic effects of chlorine in 15N NMR chemical shifts of chlorine-containing amines. Russian Journal of Organic Chemistry, 2017, 53, 1738-1739.	0.8	2

#	Article	IF	CITATIONS
55	Calculation of 15N NMR chemical shifts of amines in the framework of the density functional theory. Russian Chemical Bulletin, 2017, 66, 2248-2252.	1.5	1
56	Normal halogen dependence of <sup>13</sup> C NMR chemical shifts of halogenomethanes revisited at the fourâ€component relativistic level. Magnetic Resonance in Chemistry, 2016, 54, 787-792.	1.9	18
57	Theoretical grounds of relativistic methods for calculation of spin–spin coupling constants in nuclear magnetic resonance spectra. Russian Chemical Reviews, 2016, 85, 356-426.	6.5	63
58	Accounting for intermolecular effects in the calculation of 15N NMR chemical shifts of protonated nitrogen-containing compounds. Russian Journal of Organic Chemistry, 2016, 52, 1695-1696.	0.8	0
59	New relativistic computational schemes for 13C NMR chemical shifts. Russian Journal of Organic Chemistry, 2016, 52, 1203-1204.	0.8	2
60	Indirect relativistic bridge and substituent effects from the â€~heavy' environment on the oneâ€bond and twoâ€bond <sup>13</sup> Cï£; <sup>1</sup> H spin–spin coupling constants. Magnetic Resonance in Chemistry, 2016, 54, 39-45.	1.9	10
61	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
62	Quantum chemical study of mechanisms of organic reactions: V. Addition of ethane-1,2-dithiol to 4-hydroxy-4-methylpent-2-ynenitrile. Russian Journal of Organic Chemistry, 2016, 52, 1267-1276.	0.8	2
63	First example of the correlated calculation of the oneâ€bond tellurium–carbon spin–spin coupling constants: Relativistic effects, vibrational corrections, and solvent effects. Journal of Computational Chemistry, 2016, 37, 1367-1372.	3.3	18
64	Relativistic effect of iodine in 13C NMR chemical shifts of iodomethanes from quantum chemical calculations within the framework of the full four-component relativistic Dirac—Coulomb scheme. Russian Chemical Bulletin, 2015, 64, 2756-2762.	1.5	14
65	Theoretical and experimental <sup>15</sup> N NMR study of enamine–imine tautomerism of 4â€trifluoromethyl[b]benzoâ€1,4â€diazepine system. Magnetic Resonance in Chemistry, 2015, 53, 1031-1034.	1.9	18
66	MP2 calculation of <sup>77</sup> Se NMR chemical shifts taking into account relativistic corrections. Magnetic Resonance in Chemistry, 2015, 53, 485-492.	1.9	19
67	Relativistic Environmental Effects in <sup>29</sup> Si NMR Chemical Shifts of Halosilanes: Light Nucleus, Heavy Environment. Journal of Physical Chemistry A, 2015, 119, 5778-5789.	2.5	11
68	Quantum chemical study of mechanisms of organic reactions. Russian Chemical Bulletin, 2015, 64, 511-517.	1.5	4
69	Theoretical and experimental study of <sup>15</sup> N NMR protonation shifts. Magnetic Resonance in Chemistry, 2015, 53, 433-441.	1.9	26
70	Quantum chemical study of mechanisms of organic reactions: IV. Nucleophilic addition of ethylene glycol to 4-hydroxybut-2-ynenitrile. Russian Journal of Organic Chemistry, 2015, 51, 313-318.	0.8	5
71	Fourâ€component relativistic <scp>DFT</scp> calculations of <sup>77</sup> Se <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
72	Calculations of 29Si NMR shifts of organylsilanes by DFT taking into account solvent effects and relativistic corrections. Russian Chemical Bulletin, 2015, 64, 551-557.	1.5	6

#	Article	IF	CITATIONS
73	Stereochemical behavior of geminal and vicinal <sup>77</sup> Se– <sup>13</sup> C spin–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
74	Quantum-chemical calculations of NMR chemical shifts of organic molecules: XIV. Solvation effects in calculations of chemical shifts in 13C NMR spectra of chlorine-containing compounds. Russian Journal of Organic Chemistry, 2014, 50, 1082-1086.	0.8	4
75	Towards the versatile DFT and MP2 computational schemes for <sup>31</sup> P NMR chemical shifts taking into account relativistic corrections. Magnetic Resonance in Chemistry, 2014, 52, 699-710.	1.9	38
76	Nonempirical calculations of the oneâ€bond <sup>29</sup> Si– <sup>13</sup> C spin–spin coupling constants taking into account relativistic and solvent corrections. Magnetic Resonance in Chemistry, 2014, 52, 413-421.	1.9	10
77	On the accuracy of the GIAOâ€DFT calculation of <sup>15</sup> N NMR chemical shifts of the nitrogenâ€containing heterocycles – a gateway to better agreement with experiment at lower computational cost. Magnetic Resonance in Chemistry, 2014, 52, 222-230.	1.9	42
78	Full fourâ€component relativistic calculations of the oneâ€bond <sup>77</sup> Se– <sup>13</sup> C 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
79	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
80	Relativistic effects in the oneâ€bond spin–spin coupling constants involving selenium. Magnetic Resonance in Chemistry, 2014, 52, 500-510.	1.9	18
81	Solvent effects in the GIAO-DFT calculations of the <sup>15</sup> N NMR chemical shifts of azoles and azines. Magnetic Resonance in Chemistry, 2014, 52, 686-693.	1.9	38
82	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
83	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
84	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
85	First example of a high-level correlated calculation of the indirect spin–spin coupling constants involving tellurium: tellurophene and divinyl telluride. Physical Chemistry Chemical Physics, 2013, 15, 13101-13107.	2.8	30
86	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
87	Quantum-chemical calculations of NMR chemical shifts of organic molecules: IX. Electronic structure of [dimethylamino(chloro)methylideneamino]trichlorophosphonium hexachlorophosphate: Azomethine or azophosphine?. Russian Journal of Organic Chemistry, 2013, 49, 195-197.	0.8	6
88	Modern quantum chemical methods for calculating spin–spin coupling constants: theoretical basis and structural applications in chemistry. Russian Chemical Reviews, 2013, 82, 99-130.	6.5	107
89	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
90	Karplus dependence of spin–spin coupling constants revisited theoretically. Part 1: second-order double perturbation theory. Physical Chemistry Chemical Physics, 2013, 15, 18195.	2.8	5

#	Article	IF	CITATIONS
91	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
92	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
93	Oneâ€bond <sup>29</sup> Siâ€ <sup>1</sup> H 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
94	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
95	Openâ€chain unsaturated selanyl sulfides: stereochemical structure and stereochemical behavior of their <sup>77</sup> Se– <sup>1</sup> H spin–spin coupling constants. Magnetic Resonance in Chemistry, 2012, 50, 653-658.	1.9	20
96	Structural trends of <sup>29</sup> Si– <sup>1</sup> H spin–spin coupling constants across double bond. Magnetic Resonance in Chemistry, 2012, 50, 665-671.	1.9	15
97	Algebraic-diagrammatic construction polarization propagator approach to indirect nuclear spin–spin coupling constants. Journal of Chemical Physics, 2012, 137, 044119.	3.0	15
98	The effects of intramolecular and intermolecular coordination on <sup>31</sup> P nuclear shielding: phosphorylated azoles. Magnetic Resonance in Chemistry, 2012, 50, 120-127.	1.9	14
99	Stereochemical behavior of <sup>77</sup> Seâ€ <sup>1</sup> H spinâ€spin coupling constants in pyrazolylâ€1,3â€diselenanes and 1,2â€diselenolane. Magnetic Resonance in Chemistry, 2012, 50, 169-173.	1.9	24
100	Benchmark calculations of <sup>29</sup> Si– <sup>1</sup> H spin–spin coupling constants across double bond. Magnetic Resonance in Chemistry, 2012, 50, 278-283.	1.9	18
101	Resonance assignments of diastereotopic CH <sub>2</sub> protons in the anomeric side chain of selenoglycosides by means of <sup>2</sup> <i>J</i> (Se,H) spinâ€spin coupling constants. Magnetic Resonance in Chemistry, 2012, 50, 488-495.	1.9	22
102	Stereochemical behavior of <sup>2</sup> <i>J</i> (Se,H) and <sup>3</sup> <i>J</i> (Se,H) spinâ€spin coupling constants across sp <sup>3</sup> carbons: a theoretical scrutiny. Magnetic Resonance in Chemistry, 2012, 50, 557-562.	1.9	15
103	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
104	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
105	Cascade synthesis of 2-amino-5-(4-methoxyphenyl)-4-phenyl-1,3-thiazole by reaction of 4-chloro-N-[2,2-dichloro-1-(4-methoxyphenyl)-2-phenylethyl]benzenesulfonamide with thiourea. Russian Journal of Organic Chemistry, 2011, 47, 572-576.	0.8	2
106	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
107	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
108	Experimental and computational studies of <sup><i>n</i></sup> <i>J</i> ( <sup>77</sup> Se, <sup>1</sup> H) selenium–proton couplings in selenoglycosides. Magnetic Resonance in Chemistry, 2011, 49, 190-194.	1.9	32

#	Article	IF	CITATIONS
109	Conformational analysis and diastereotopic assignments in the series of seleniumâ€containing heterocycles by means of <sup>77</sup> Seâ€ <sup>1</sup> H spinâ€spin coupling constants: a combined theoretical and experimental study. Magnetic Resonance in Chemistry, 2011, 49, 389-398.	1.9	42
110	Stereochemical study of the sterically crowded phenylselanylalkenes by means of <sup>77</sup> Se <sup>1</sup> H spin–spin coupling constants. Magnetic Resonance in Chemistry, 2011, 49, 570-574.	1.9	13
111	Benchmarking SOPPA(CC2) for the calculation of indirect nuclear spin–spin coupling constants: Carbocycles. Chemical Physics, 2011, 381, 35-43.	1.9	31
112	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
113	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
114	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
115	Structural trends of <sup>77</sup> Se <sup>1</sup> H spin–spin coupling constants and conformational behavior of 2â€substituted selenophenes. Magnetic Resonance in Chemistry, 2010, 48, 44-52.	1.9	77
116	Trivinylphosphine and trivinylphosphine chalcogenides: stereochemical trends of 31P1H spin-spin coupling constants. Magnetic Resonance in Chemistry, 2010, 48, S48-S55.	1.9	19
117	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
118	Synthesis of Functionalized l-Cysteine and l-Methionine by Reaction with Electron-Deficient Acetylenes. Synthesis, 2009, 2009, 3136-3142.	2.3	7
119	Conformational analysis and stereochemical dependences of <sup>31</sup> P– <sup>1</sup> H spin–spin coupling constants of bis(2â€phenethyl)vinylphosphine and related phosphine chalcogenides. Magnetic Resonance in Chemistry, 2009, 47, 288-299.	1.9	21
120	Conformational analysis of N-vinyl-2-phenylpyrrole. Chemistry of Heterocyclic Compounds, 2009, 45, 28-34.	1.2	1
121	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
122	Theoretical conformational analysis of unsaturated phospines and phosphinechalcogenides. Russian Journal of Organic Chemistry, 2009, 45, 667-673.	0.8	5
123	C-amidoalkylation of pyrroles with N-trifluoromethylsulfonyl and N-arylsulfonyl polychloroaldehyde imines. Russian Journal of Organic Chemistry, 2009, 45, 1365-1374.	0.8	1
124	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
125	Synthesis and conformational analysis of furfuryl vinyl ethers. Russian Chemical Bulletin, 2008, 57, 2132-2138.	1.5	3
126	Divinyl selenide: conformational study and stereochemical behavior of its <sup>77</sup> Se <sup>1</sup> H spin–spin coupling constants. Magnetic Resonance in Chemistry, 2008, 46, 979-985.	1.9	43

#	Article	IF	CITATIONS
127	anti-Markovnikov addition of tellurium tetrachloride to trimethyl ethynyl silane. Journal of Organometallic Chemistry, 2008, 693, 2509-2513.	1.8	14
128	N-(2,2-Dichloro-2-phenylethylidene)arenesulfonamides in reactions with secondary amines. Russian Journal of General Chemistry, 2008, 78, 1371-1379.	0.8	14
129	13C-13C spin-spin coupling constants in structural studies: XLI. Stereochemical study on N-(polychloroethylidene)arenesulfonamides and N'-arylsulfonylformimidamides. Russian Journal of Organic Chemistry, 2008, 44, 76-85.	0.8	7
130	Reactions of N-(Polychloroethylidene)arene-and - trifluoromethanesulfonamides with indoles. Russian Journal of Organic Chemistry, 2008, 44, 86-94.	0.8	8
131	Incomparably easy migration of functionalized enol substituent in pyrrole ring. Russian Journal of Organic Chemistry, 2008, 44, 237-246.	0.8	3
132	13C-13C spin-spin coupling constants in structural studies: XLII. Stereochemical study on functionalized 2,5-dihydrofuran-2-imines. Russian Journal of Organic Chemistry, 2008, 44, 388-396.	0.8	6
133	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
134	Theoretical conformational analysis of divinyl selenide. Russian Journal of Organic Chemistry, 2008, 44, 1418-1421.	0.8	3
135	4-Dimethylaminoacetophenone O-vinyloxime: Synthesis and steric structure. Russian Journal of Organic Chemistry, 2008, 44, 1497-1503.	0.8	2
136	Small spiroalkanes: ring strain effects and carbon-carbon spin-spin coupling constants. Arkivoc, 2008, 2008, 68-73.	0.5	3
137	Recent Advances in Theoretical Calculations of Indirect Spin–Spin Coupling Constants. Annual Reports on NMR Spectroscopy, 2007, , 133-245.	1.5	152
138	Stereochemical Study of 2-Substituted N-Vinylpyrroles. Australian Journal of Chemistry, 2007, 60, 583.	0.9	16
139	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
140	Conformational study of 2-arylazo-1-vinylpyrroles. Magnetic Resonance in Chemistry, 2007, 45, 142-151.	1.9	18
141	Configurational assignment of carbon, silicon and germanium containing propynal oximes by means of13Cï£į1H,13Cï£į13C and15Nï£į1H spin–spin coupling constants. Magnetic Resonance in Chemistry, 2007, 45, 661-666.	1.9	24
142	Stereochemical study of iminodihydrofurans based on experimental measurements and SOPPA calculations of <sup>13</sup> C <sup>13</sup> C spin–spin coupling constants. Magnetic Resonance in Chemistry, 2007, 45, 758-765.	1.9	15
143	Configurational assignment of <i>N</i> â€arylsulfonylimines of αâ€polychloroaldehydes. Magnetic Resonance in Chemistry, 2007, 45, 980-984.	1.9	11
144	Orange to black electrochromic behaviour in poly(2-(2-thienyl)-1H-pyrrole) thin films. Electrochimica Acta, 2007, 52, 4784-4791.	5.2	46

#	Article	IF	CITATIONS
145	2,5-dihalothiophenes in the reaction with chlorosulfonic acid. Russian Journal of General Chemistry, 2007, 77, 926-931.	0.8	2
146	13C-13C spin-spin coupling constants in structural studies: XXXIX. Nonempirical calculations of heteroaromatic oximes. Russian Journal of Organic Chemistry, 2007, 43, 872-879.	0.8	5
147	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
148	Configurational Assignment and Conformational Study of Methylglyoxal Bisdimethylhydrazones Derived from the 2-Ethoxypropenal Precursor. Australian Journal of Chemistry, 2006, 59, 211.	0.9	16
149	Structural study of 2,3,4,6-tetra(O-vinyl) methyl-α-d-glucopyranoside. Journal of Molecular Structure, 2006, 791, 1-9.	3.6	13
150	Easy α- to Î <sup>2</sup> -migration of an enol moiety on a pyrrole ring. Tetrahedron Letters, 2006, 47, 3645-3648.	1.4	11
151	Nonempirical calculations of NMR indirect spin-spin coupling constants. Magnetic Resonance in Chemistry, 2006, 44, 178-187.	1.9	23
152	Nonempirical calculations of NMR indirect spin–spin coupling constants. Part 15: pyrrolylpyridines. Magnetic Resonance in Chemistry, 2006, 44, 692-697.	1.9	18
153	The first example of the configurational assignment at the CN bond of allenylthioimidates. Tetrahedron Letters, 2005, 46, 7367-7371.	1.4	16
154	Amidine derivatives of α-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
155	Synthesis and electrochemical characterization of dipyrroles separated by diphenyleneoxide and diphenylenesulfide spacers via the Trofimov reaction. Tetrahedron, 2005, 61, 7756-7762.	1.9	15
156	Synthesis, Structure, and Spectral Properties of Bis(pyrrol-2-yl)pyridines. European Journal of Organic Chemistry, 2005, 2005, 4338-4345.	2.4	27
157	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
158	Non-empirical calculations of NMR indirect carbon-carbon coupling constants. Part 12—Aliphatic and alicyclic oximes. Magnetic Resonance in Chemistry, 2005, 43, 435-443.	1.9	31
159	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
160	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
161	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
162	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

#	Article	IF	CITATIONS
163	Non-empirical calculations of NMR indirect carbon–carbon coupling constants. Part 6: Propellanes. Magnetic Resonance in Chemistry, 2004, 42, 1-13.	1.9	29
164	Non-empirical calculations of NMR indirect carbon–carbon coupling constants. Part 7—Spiroalkanes. Magnetic Resonance in Chemistry, 2004, 42, 500-511.	1.9	22
165	Non-empirical calculations of NMR indirect carbon–carbon coupling constants. Part 8—Monocycloalkanes. Magnetic Resonance in Chemistry, 2004, 42, 671-686.	1.9	50
166	Non-empirical calculations of NMR indirect carbon–carbon coupling constants. Part 9—Bicyclobutane-containing polycycloalkanes. Magnetic Resonance in Chemistry, 2004, 42, S168-S179.	1.9	24
167	Non-empirical calculations of NMR indirect carbon-carbon coupling constants. Part 10?Carbocages. Magnetic Resonance in Chemistry, 2004, 42, 919-930.	1.9	21
168	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
169	Title is missing!. Russian Journal of Organic Chemistry, 2003, 39, 698-704.	0.8	6
170	13C-13C Spin-Spin Coupling Constants in Structural Studies: XXXIV. Nonempirical Calculations: Small Heterocycles. Russian Journal of Organic Chemistry, 2003, 39, 1618-1628.	0.8	4
171	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
172	Non-empirical calculations of NMR indirect carbon-carbon coupling constants: 2. Strained polycarbocycles. Magnetic Resonance in Chemistry, 2003, 41, 91-101.	1.9	22
173	Non-empirical calculations of NMR indirect carbon-carbon coupling constants: 3. Polyhedranes. Magnetic Resonance in Chemistry, 2003, 41, 157-168.	1.9	25
174	Non-empirical calculations of NMR indirect carbon-carbon coupling constants. Part 4: Bicycloalkanes. Magnetic Resonance in Chemistry, 2003, 41, 417-430.	1.9	24
175	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
176	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
177	Title is missing!. Russian Journal of Organic Chemistry, 2002, 38, 394-398.	0.8	5
178	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
179	Stereochemical Applications ofCarbon-Carbon Coupling Constants in Organic Chemistry. Current Organic Chemistry, 1998, 2, 173-193.	1.6	11
180	N,N-Disubstituted α-Amino-α,β-unsaturated Aldehydes and their Derivatives:1H and13C NMR Study. Magnetic Resonance in Chemistry, 1997, 35, 533-537.	1.9	13

#	Article	IF	CITATIONS
181	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
182	Spin—spin coupling constants between carbons separated by more than one bond. Progress in Nuclear Magnetic Resonance Spectroscopy, 1991, 23, 301-610.	7.5	83
183	Question of the reverse polarization of triple bonds. Journal of Structural Chemistry, 1991, 32, 59-64.	1.0	1
184	Effects of conjugation and the conformational structure of aromatic selenides. Bulletin of the Academy of Sciences of the USSR Division of Chemical Science, 1989, 38, 54-58.	0.0	2
185	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
186	Structural applications of one-bond carbonî—,carbon spin—spin coupling constants. Progress in Nuclear Magnetic Resonance Spectroscopy, 1989, 21, 293-448.	7.5	115
187	Direct13C-13C spin-spin coupling constants for the triple bond in activated acetylenes. Bulletin of the Academy of Sciences of the USSR Division of Chemical Science, 1988, 37, 1132-1136.	0.0	0
188	2,6-Di-tert-butylphenylvinyl ether: Effect of the unshared oxygen electron pair on the13C-13C spin-spin interaction constant. Bulletin of the Academy of Sciences of the USSR Division of Chemical Science, 1987, 36, 69-72.	0.0	0
189	Establishing the configuration of imine nitrogen compounds: Influence of alkyl groups on13C-13C spin-spin coupling constant in alkyl phenyl ketoximes. Bulletin of the Academy of Sciences of the USSR Division of Chemical Science, 1987, 36, 694-697.	0.0	2
190	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
191	An example of nonadditivity of the substituent effect on direct13C-13C spin-spin coupling constants in the benzene ring. Bulletin of the Academy of Sciences of the USSR Division of Chemical Science, 1986, 35, 455-455.	0.0	0
192	Synthesis of monosubstituted divinyl sulfides. Bulletin of the Academy of Sciences of the USSR Division of Chemical Science, 1986, 35, 639-641.	0.0	1
193	Effect of the nitrogen unshared electron pair on the direct13C-13C spin-spin coupling constant of a neighboring bond in oximes. Bulletin of the Academy of Sciences of the USSR Division of Chemical Science, 1986, 35, 1103-1103.	0.0	2
194	Effect of the unshared electron pair of the oxygen atom on the direct13C-13C spin-spin coupling constants in dibenzofuran. Bulletin of the Academy of Sciences of the USSR Division of Chemical Science, 1986, 35, 2190-2190.	0.0	0
195	Use of13C-13C spin-spin coupling constants for establishing the configuration of 1-alkoxy-1-aminoxyethanes. Bulletin of the Academy of Sciences of the USSR Division of Chemical Science, 1985, 34, 1975-1977.	0.0	0
196	Study of conjugation effects by NMR spectroscopy. XXIV. Determination of the conformational composition of alkyl phenyl ethers with branched alkyl radicals from the13C-1H and13C-13C spin-spin coupling constants. Bulletin of the Academy of Sciences of the USSR Division of Chemical Science, 1985, 34, 2278-2281.	0.0	0
197	Use of 13C-13C spin-spin coupling constants for the establishment of the configuration of aromatic oximes. Bulletin of the Academy of Sciences of the USSR Division of Chemical Science, 1984, 33, 2596-2596.	0.0	3
198	Carbon-carbon coupling constants - a new guide in the stereochemistry of oximes. Tetrahedron Letters, 1984, 25, 4817-4820.	1.4	66

#	Article	IF	CITATIONS
199	Study of conjugation effects by means of NMR spectroscopy 21. Factor analysis of NMR parameters of alkyl phenyl ethers and sulfides. Bulletin of the Academy of Sciences of the USSR Division of Chemical Science, 1983, 32, 953-958.	0.0	1
200	Study of the effects of coupling by NMR spectroscopy 16.1H-1H spin-spin coupling constants in phenyl alkyl ethers. Bulletin of the Academy of Sciences of the USSR Division of Chemical Science, 1982, 31, 251-255.	0.0	0
201	An NMR spectroscopic study of the effects of conjugation. Bulletin of the Academy of Sciences of the USSR Division of Chemical Science, 1982, 31, 502-506.	0.0	1
202	An NMR spectroscopic study of the effects of conjugation. Bulletin of the Academy of Sciences of the USSR Division of Chemical Science, 1982, 31, 506-512.	0.0	0
203	Direct13C-13C spin-spin coupling constants of olefinic carbons in vinyl ethers. Bulletin of the Academy of Sciences of the USSR Division of Chemical Science, 1982, 31, 1981-1983.	0.0	0
204	NMR spectroscopic study of conjugation effects Communication 19. Electronic effects in trialkyl phenoxy derivatives of silicon, germanium, and tin. Bulletin of the Academy of Sciences of the USSR Division of Chemical Science, 1982, 31, 1799-1802.	0.0	1
205	NMR study of conjugation effects 15.13C-13C spin-spin coupling constants in phenyl alkyl ether. Bulletin of the Academy of Sciences of the USSR Division of Chemical Science, 1982, 31, 105-110.	0.0	1
206	Substitution effects and parameters of PMR spectra of the benzene ring in trialkylphenoxysilanes, trialkylphenoxygermanes, and trialkylphenoxystannanes. Bulletin of the Academy of Sciences of the USSR Division of Chemical Science, 1982, 31, 2501-2503.	0.0	0