

Yuriy Rusakov

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79
papers

1,076
citations

17
h-index

26
g-index

87
ext. papers

1,236
ext. citations

2.1
avg, IF

4.79
L-index

#	Paper	IF	Citations
79	Modern quantum chemical methods for calculating spin-spin coupling constants: theoretical basis and structural applications in chemistry. <i>Russian Chemical Reviews</i> , 2013 , 82, 99-130	6.8	94
78	Structural trends of ⁷⁷ Se- ¹ H spin-spin coupling constants and conformational behavior of 2-substituted selenophenes. <i>Magnetic Resonance in Chemistry</i> , 2010 , 48, 44-52	2.1	69
77	Theoretical grounds of relativistic methods for calculation of spin-spin coupling constants in nuclear magnetic resonance spectra. <i>Russian Chemical Reviews</i> , 2016 , 85, 356-426	6.8	45
76	Divinyl selenide: conformational study and stereochemical behavior of its ⁷⁷ Se- ¹ H spin-spin coupling constants. <i>Magnetic Resonance in Chemistry</i> , 2008 , 46, 979-85	2.1	39
75	Influence of the Introduction of Short Alkyl Chains in Poly(2-(2-Thienyl)-1H-pyrrole) on Its Electrochromic Behavior. <i>Macromolecules</i> , 2008 , 41, 6886-6894	5.5	38
74	Conformational analysis and diastereotopic assignments in the series of selenium-containing heterocycles by means of ⁷⁷ Se- ¹ H spin-spin coupling constants: a combined theoretical and experimental study. <i>Magnetic Resonance in Chemistry</i> , 2011 , 49, 389-98	2.1	36
73	On the HALA effect in the NMR carbon shielding constants of the compounds containing heavy p-elements. <i>International Journal of Quantum Chemistry</i> , 2016 , 116, 1404-1412	2.1	31
72	Towards the versatile DFT and MP2 computational schemes for ³¹ P NMR chemical shifts taking into account relativistic corrections. <i>Magnetic Resonance in Chemistry</i> , 2014 , 52, 699-710	2.1	30
71	Experimental and computational studies of nJ(⁷⁷ Se, ¹ H) selenium-proton couplings in selenoglycosides. <i>Magnetic Resonance in Chemistry</i> , 2011 , 49, 190-4	2.1	28
70	Benchmarking SOPPA(CC2) for the calculation of indirect nuclear spin-spin coupling constants: Carbocycles. <i>Chemical Physics</i> , 2011 , 381, 35-43	2.3	28
69	First example of a high-level correlated calculation of the indirect spin-spin coupling constants involving tellurium: tellurophene and divinyl telluride. <i>Physical Chemistry Chemical Physics</i> , 2013 , 15, 13101-13107	2.6	26
68	Stereochemical behavior of (⁷⁷ Se)-(¹ H) spin-spin coupling constants in pyrazolyl-1,3-diselenanes and 1,2-diselenolane. <i>Magnetic Resonance in Chemistry</i> , 2012 , 50, 169-73	2.1	20
67	Conformational analysis and stereochemical dependences of (³¹ P)-(¹ H) spin-spin coupling constants of bis(2-phenethyl)vinylphosphine and related phosphine chalcogenides. <i>Magnetic Resonance in Chemistry</i> , 2009 , 47, 288-99	2.1	20
66	Resonance assignments of diastereotopic CH(2) protons in the anomeric side chain of selenoglycosides by means of (2) J(Se,H) spin-spin coupling constants. <i>Magnetic Resonance in Chemistry</i> , 2012 , 50, 488-95	2.1	19
65	Conformational Analysis of 2-Formylselenophene by Means of ¹³ C - ¹ H, ¹³ C - ¹³ C, and ⁷⁷ Se - ¹ H Spin - Spin Coupling Constants. <i>Australian Journal of Chemistry</i> , 2009 , 62, 734	1.2	19
64	Calculation of Te 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. <i>Journal of Physical Chemistry A</i> , 2017 , 121, 4793-4803	2.8	18
63	Nonempirical calculations of NMR indirect spin-spin coupling constants. Part 15: pyrrolylpyridines. <i>Magnetic Resonance in Chemistry</i> , 2006 , 44, 692-7	2.1	17

62	Reaction of 2-pyridylselenenyl bromide with divinyl selenide. <i>Chemistry of Heterocyclic Compounds</i> , 2012 , 48, 1129-1131	1.4	16
61	Open-chain unsaturated selanyl sulfides: stereochemical structure and stereochemical behavior of their ^{77}Se - ^1H spin-spin coupling constants. <i>Magnetic Resonance in Chemistry</i> , 2012 , 50, 653-8	2.1	16
60	Benchmark calculations of (^{29}Si) - (^1H) spin-spin coupling constants across double bond. <i>Magnetic Resonance in Chemistry</i> , 2012 , 50, 278-83	2.1	16
59	Conformational study of 2-aryloxy-1-vinylpyrroles. <i>Magnetic Resonance in Chemistry</i> , 2007 , 45, 142-51	2.1	16
58	Relativistic effects in the one-bond spin-spin coupling constants involving selenium. <i>Magnetic Resonance in Chemistry</i> , 2014 , 52, 500-10	2.1	15
57	MP2 calculation of (^{77}Se) NMR chemical shifts taking into account relativistic corrections. <i>Magnetic Resonance in Chemistry</i> , 2015 , 53, 485-92	2.1	15
56	Stereochemical Study of 2-Substituted N-Vinylpyrroles. <i>Australian Journal of Chemistry</i> , 2007 , 60, 583	1.2	15
55	First example of the correlated calculation of the one-bond tellurium-carbon spin-spin coupling constants: Relativistic effects, vibrational corrections, and solvent effects. <i>Journal of Computational Chemistry</i> , 2016 , 37, 1367-72	3.5	14
54	Structural trends of ^{29}Si - ^1H spin-spin coupling constants across double bond. <i>Magnetic Resonance in Chemistry</i> , 2012 , 50, 665-71	2.1	14
53	Trivinylphosphine and trivinylphosphine chalcogenides: stereochemical trends of P-H spin-spin coupling constants. <i>Magnetic Resonance in Chemistry</i> , 2010 , 48 Suppl 1, S48-55	2.1	14
52	Full four-component relativistic calculations of the one-bond ^{77}Se - ^{13}C spin-spin coupling constants in the series of selenium heterocycles and their parent open-chain selenides. <i>Magnetic Resonance in Chemistry</i> , 2014 , 52, 214-21	2.1	13
51	Stereochemical behavior of $(^2)J(\text{Se,H})$ and $(^3)J(\text{Se,H})$ spin-spin coupling constants across $\text{sp}(3)$ carbons: a theoretical scrutiny. <i>Magnetic Resonance in Chemistry</i> , 2012 , 50, 557-62	2.1	13
50	Normal halogen dependence of C NMR chemical shifts of halogenomethanes revisited at the four-component relativistic level. <i>Magnetic Resonance in Chemistry</i> , 2016 , 54, 787-792	2.1	13
49	Four-component relativistic DFT calculations of (^{77}Se) NMR chemical shifts: A gateway to a reliable computational scheme for the medium-sized organoselenium molecules. <i>Journal of Computational Chemistry</i> , 2015 , 36, 1756-62	3.5	12
48	Relativistic effect of iodine in ^{13}C NMR chemical shifts of iodomethanes from quantum chemical calculations within the framework of the full four-component relativistic Dirac-Coulomb scheme. <i>Russian Chemical Bulletin</i> , 2015 , 64, 2756-2762	1.7	12
47	Algebraic-diagrammatic construction polarization propagator approach to indirect nuclear spin-spin coupling constants. <i>Journal of Chemical Physics</i> , 2012 , 137, 044119	3.9	12
46	On the significant relativistic heavy atom effect on ^{13}C NMR chemical shifts of α and β -carbons in seleno- and telluroketones. <i>Molecular Physics</i> , 2017 , 115, 3117-3127	1.7	11
45	Long-range relativistic heavy atom effect on ^1H NMR chemical shifts of selenium- and tellurium-containing compounds. <i>International Journal of Quantum Chemistry</i> , 2019 , 119, e25809	2.1	11

44	Stereoselective synthesis of E-2-halovinyl tellanes, ditellanes and selenides based on tellurium tetrahalides, selenium dihalides and internal alkynes. <i>Journal of Organometallic Chemistry</i> , 2018 , 867, 300-305	2.3	10
43	Hierarchical Basis Sets for the Calculation of Nuclear Magnetic Resonance Spin-Spin Coupling Constants Involving Either Selenium or Tellurium Nuclei. <i>Journal of Physical Chemistry A</i> , 2019 , 123, 6564-6571	2.8	10
42	One-bond ²⁹ Si- ¹ H spin-spin coupling constants in the series of halosilanes: benchmark SOPPA and DFT calculations, relativistic effects, and vibrational corrections. <i>Magnetic Resonance in Chemistry</i> , 2013 , 51, 557-61	2.1	10
41	Stereochemical study of the sterically crowded phenylselanylalkenes by means of (⁷⁷ Se)-(¹ H) spin-spin coupling constants. <i>Magnetic Resonance in Chemistry</i> , 2011 , 49, 570-4	2.1	10
40	Facile coupling of 2-(1-ethylthioethyl)pyrroles with amines: A route to 2-(1-aminoethyl)pyrroles and 1-amino-3-iminopyrrolizines. <i>Journal of Heterocyclic Chemistry</i> , 2007 , 44, 505-513	1.9	10
39	Easy β -to α Migration of an enol moiety on a pyrrole ring. <i>Tetrahedron Letters</i> , 2006 , 47, 3645-3648	2	10
38	Quantum chemical calculations of Se and Te nuclear magnetic resonance spectral parameters and their structural applications. <i>Magnetic Resonance in Chemistry</i> , 2021 , 59, 359-407	2.1	10
37	Relativistic heavy atom effect on C NMR chemical shifts initiated by adjacent multiple chalcogens. <i>Magnetic Resonance in Chemistry</i> , 2018 , 56, 716-726	2.1	9
36	Relativistic environmental effects in (²⁹ Si) NMR chemical shifts of halosilanes: light nucleus, heavy environment. <i>Journal of Physical Chemistry A</i> , 2015 , 119, 5778-89	2.8	9
35	Fluorescence quenching and laser photolysis of dipyrrolylbenzenes in the presence of chloromethanes. <i>Russian Journal of General Chemistry</i> , 2007 , 77, 1386-1394	0.7	9
34	Indirect relativistic bridge and substituent effects from the heavy environment on the one-bond and two-bond (¹³ C)-(¹ H) spin-spin coupling constants. <i>Magnetic Resonance in Chemistry</i> , 2016 , 54, 39-45	2.1	9
33	Relativistic heavy atom effect on the P NMR parameters of phosphine chalcogenides. Part 1. Chemical shifts. <i>Magnetic Resonance in Chemistry</i> , 2018 , 56, 1061-1073	2.1	9
32	Stereochemical behavior of geminal and vicinal ⁷⁷ Se- ¹³ C spin-spin coupling constants studied at the SOPPA(CC2) level taking into account relativistic corrections. <i>Magnetic Resonance in Chemistry</i> , 2015 , 53, 93-8	2.1	8
31	Calculation of N and P NMR Chemical Shifts of Azoles, Phospholes, and Phosphazoles: A Gateway to Higher Accuracy at Less Computational Cost. <i>Journal of Physical Chemistry A</i> , 2018 , 122, 6746-6759	2.8	8
30	An Effective Method for the Synthesis of 3,5-bis(halomethyl)-1,4-Oxaselenanes and their Derivatives. <i>Chemistry of Heterocyclic Compounds</i> , 2014 , 49, 1821-1826	1.4	8
29	Structural and Stereochemical Applications of Computational NMR Using ²⁹ Si- ¹ H and ⁷⁷ Se- ¹ H Indirect Spin-Spin Coupling Constants 2014 , 87-110		8
28	¹³ C- ¹³ C spin-spin coupling constants in structural studies: XL. Conformational analysis of N-vinylpyrroles. <i>Russian Journal of Organic Chemistry</i> , 2007 , 43, 880-887	0.7	8
27	Quantum-chemical calculations of NMR chemical shifts of organic molecules: XII. Calculation of the ¹³ C NMR chemical shifts of fluoromethanes at the DFT level. <i>Russian Journal of Organic Chemistry</i> , 2014 , 50, 160-164	0.7	7

26	Nonempirical calculations of the one-bond (29)Si-(13)C spin-spin coupling constants taking into account relativistic and solvent corrections. <i>Magnetic Resonance in Chemistry</i> , 2014 , 52, 413-21	2.1	7
25	Calculations of 29Si NMR shifts of organylsilanes by DFT taking into account solvent effects and relativistic corrections. <i>Russian Chemical Bulletin</i> , 2015 , 64, 551-557	1.7	6
24	Stereochemical Dependences of P-C Spin-Spin Coupling Constants of Heterocyclic Phosphines. <i>Journal of Physical Chemistry A</i> , 2019 , 123, 6298-6303	2.8	6
23	13C-13C spin-spin coupling constants in structural studies: XLIII. Stereochemical study on functionalized 3-iminopyrrolizines. <i>Russian Journal of Organic Chemistry</i> , 2008 , 44, 1338-1344	0.7	6
22	Geometries and NMR properties of cisplatin and transplatin revisited at the four-component relativistic level. <i>Mendeleev Communications</i> , 2019 , 29, 315-317	1.9	5
21	On the long-range relativistic effects in the N NMR chemical shifts of halogenated azines. <i>Magnetic Resonance in Chemistry</i> , 2017 , 55, 990-995	2.1	5
20	Quantum-chemical calculations of NMR chemical shifts of organic molecules: XV. Relativistic calculations of 29Si NMR chemical shifts of silanes. <i>Russian Journal of Organic Chemistry</i> , 2017 , 53, 643-651	0.7	5
19	Reaction of tellurium tetrachloride with hex-3-yne. <i>Russian Chemical Bulletin</i> , 2015 , 64, 2747-2748	1.7	5
18	Theoretical conformational analysis of unsaturated phosphines and phosphinechalcogenides. <i>Russian Journal of Organic Chemistry</i> , 2009 , 45, 667-673	0.7	5
17	What Most Affects the Accuracy of Te NMR Chemical Shift Calculations. <i>Journal of Physical Chemistry A</i> , 2020 , 124, 6714-6725	2.8	5
16	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. <i>Russian Journal of Organic Chemistry</i> , 2014 , 50, 1082-1086	0.7	4
15	Efficient J-oriented tin basis sets for the correlated calculations of indirect nuclear spin-spin coupling constants. <i>Magnetic Resonance in Chemistry</i> , 2021 , 59, 713-722	2.1	4
14	On the heavy atom on light atom relativistic effect in the NMR shielding constants of phosphine tellurides. <i>Magnetic Resonance in Chemistry</i> , 2019 , 57, 1071-1083	2.1	3
13	Synthesis and conformational analysis of furfuryl vinyl ethers. <i>Russian Chemical Bulletin</i> , 2008 , 57, 2132-2138		3
12	Theoretical conformational analysis of divinyl selenide. <i>Russian Journal of Organic Chemistry</i> , 2008 , 44, 1418-1421	0.7	3
11	Correlated ab initio calculations of one-bond P-Se and P-Te spin-spin coupling constants in a series of P-Se and P-Te systems accounting for relativistic effects (part 2). <i>Magnetic Resonance in Chemistry</i> , 2020 , 58, 929-940	2.1	2
10	Regioselective dehydrobromination reaction of 5-bromo-2-bromomethyl-1,3-thiaselenolane 1,1-dioxide. <i>Russian Chemical Bulletin</i> , 2011 , 60, 196-197	1.7	2
9	Incomparably easy migration of functionalized enol substituent in pyrrole ring. <i>Russian Journal of Organic Chemistry</i> , 2008 , 44, 237-246	0.7	2

8	4-Dimethylaminoacetophenone O-vinyloxime: Synthesis and steric structure. <i>Russian Journal of Organic Chemistry</i> , 2008 , 44, 1497-1503	0.7	2
7	A New Basis Set for the Calculation of C NMR Chemical Shifts within a Non-empirical Correlated Framework. <i>Journal of Physical Chemistry A</i> , 2020 , 124, 7322-7330	2.8	2
6	New relativistic computational schemes for ¹³ C NMR chemical shifts. <i>Russian Journal of Organic Chemistry</i> , 2016 , 52, 1203-1204	0.7	2
5	An efficient method for generating property-energy consistent basis sets. New pecJ- (= 1, 2) basis sets for high-quality calculations of indirect nuclear spin-spin coupling constants involving H, C, N, and F nuclei. <i>Physical Chemistry Chemical Physics</i> , 2021 , 23, 14925-14939	3.6	2
4	Relativistic effects of chlorine in ¹⁵ N NMR chemical shifts of chlorine-containing amines. <i>Russian Journal of Organic Chemistry</i> , 2017 , 53, 1738-1739	0.7	0
3	Dipropadienyl telluride. <i>Russian Chemical Bulletin</i> , 2017 , 66, 2343-2344	1.7	
2	Conformational analysis of N-vinyl-2-phenylpyrrole. <i>Chemistry of Heterocyclic Compounds</i> , 2009 , 45, 28-34.4		
1	Incomparably easy migration of functionalized enol substituent in pyrrole ring 2010 , 44, 237		