Yuriy Rusakov

List of Publications by Year in Descending Order

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	Quantum chemical calculations of Se and Te nuclear magnetic resonance spectral parameters and their structural applications. *Magnetic Resonance in Chemistry*, **2021**, 59, 359-407	2.1	10
78	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. *Physical Chemistry Chemical Physics*, **2021**, 23, 14925-14939	3.6	2
77	Efficient J-oriented tin basis sets for the correlated calculations of indirect nuclear spin-spin coupling constants. *Magnetic Resonance in Chemistry*, **2021**, 59, 713-722	2.1	4
76	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). *Magnetic Resonance in Chemistry*, **2020**, 58, 929-940	2.1	2
75	What Most Affects the Accuracy of Te NMR Chemical Shift Calculations. *Journal of Physical Chemistry A*, **2020**, 124, 6714-6725	2.8	5
74	A New Basis Set for the Calculation of C NMR Chemical Shifts within a Non-empirical Correlated Framework. *Journal of Physical Chemistry A*, **2020**, 124, 7322-7330	2.8	2
73	Geometries and NMR properties of cisplatin and transplatin revisited at the four-component relativistic level. *Mendeleev Communications*, **2019**, 29, 315-317	1.9	5
72	On the heavy atom on light atom relativistic effect in the NMR shielding constants of phosphine tellurides. *Magnetic Resonance in Chemistry*, **2019**, 57, 1071-1083	2.1	3
71	Hierarchical Basis Sets for the Calculation of Nuclear Magnetic Resonance Spin-Spin Coupling Constants Involving Either Selenium or Tellurium Nuclei. *Journal of Physical Chemistry A*, **2019**, 123, 6564-6571	2.8	10
70	Stereochemical Dependences of P-C Spin-Spin Coupling Constants of Heterocyclic Phosphines. *Journal of Physical Chemistry A*, **2019**, 123, 6298-6303	2.8	6
69	Long-range relativistic heavy atom effect on 1H NMR chemical shifts of selenium- and tellurium-containing compounds. *International Journal of Quantum Chemistry*, **2019**, 119, e25809	2.1	11
68	Stereoselective synthesis of E-2-halovinyl tellanes, ditellanes and selenides based on tellurium tetrahalides, selenium dihalides and internal alkynes. *Journal of Organometallic Chemistry*, **2018**, 867, 300-305	2.3	10
67	Calculation of N and 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	2.8	8
66	Relativistic heavy atom effect on C NMR chemical shifts initiated by adjacent multiple chalcogens. *Magnetic Resonance in Chemistry*, **2018**, 56, 716-726	2.1	9
65	Relativistic heavy atom effect on the P NMR parameters of phosphine chalcogenides. Part 1. Chemical shifts. *Magnetic Resonance in Chemistry*, **2018**, 56, 1061-1073	2.1	9
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. *Journal of Physical Chemistry A*, **2017**, 121, 4793-4803	2.8	18
63	On the long-range relativistic effects in the N NMR chemical shifts of halogenated azines. *Magnetic Resonance in Chemistry*, **2017**, 55, 990-995	2.1	5

62	On the significant relativistic heavy atom effect on 13C NMR chemical shifts of □and □-carbons in seleno- and telluroketones. *Molecular Physics*, **2017**, 115, 3117-3127	1.7	11
61	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	0.7	5
60	Relativistic effects of chlorine in 15N NMR chemical shifts of chlorine-containing amines. *Russian Journal of Organic Chemistry*, **2017**, 53, 1738-1739	0.7	0
59	Dipropadienyl telluride. *Russian Chemical Bulletin*, **2017**, 66, 2343-2344	1.7	
58	On the HALA effect in the NMR carbon shielding constants of the compounds containing heavy p-elements. *International Journal of Quantum Chemistry*, **2016**, 116, 1404-1412	2.1	31
57	First example of the correlated calculation of the one-bond tellurium-carbon spin-spin coupling constants: Relativistic effects, vibrational corrections, and solvent effects. *Journal of Computational Chemistry*, **2016**, 37, 1367-72	3.5	14
56	Normal halogen dependence of C NMR chemical shifts of halogenomethanes revisited at the four-component relativistic level. *Magnetic Resonance in Chemistry*, **2016**, 54, 787-792	2.1	13
55	Theoretical grounds of relativistic methods for calculation of spin□spin coupling constants in nuclear magnetic resonance spectra. *Russian Chemical Reviews*, **2016**, 85, 356-426	6.8	45
54	New relativistic computational schemes for 13C NMR chemical shifts. *Russian Journal of Organic Chemistry*, **2016**, 52, 1203-1204	0.7	2
53	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. *Magnetic Resonance in Chemistry*, **2016**, 54, 39-45	2.1	9
52	Four-component relativistic DFT calculations of (77) Se NMR chemical shifts: A gateway to a reliable computational scheme for the medium-sized organoselenium molecules. *Journal of Computational Chemistry*, **2015**, 36, 1756-62	3.5	12
51	Calculations of 29Si NMR shifts of organylsilanes by DFT taking into account solvent effects and relativistic corrections. *Russian Chemical Bulletin*, **2015**, 64, 551-557	1.7	6
50	Stereochemical behavior of geminal and vicinal 77Se-13C spin-spin coupling constants studied at the SOPPA(CC2) level taking into account relativistic corrections. *Magnetic Resonance in Chemistry*, **2015**, 53, 93-8	2.1	8
49	Reaction of tellurium tetrachloride with hex-3-yne. *Russian Chemical Bulletin*, **2015**, 64, 2747-2748	1.7	5
48	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	1.7	12
47	MP2 calculation of (77) Se NMR chemical shifts taking into account relativistic corrections. *Magnetic Resonance in Chemistry*, **2015**, 53, 485-92	2.1	15
46	Relativistic environmental effects in (29)Si NMR chemical shifts of halosilanes: light nucleus, heavy environment. *Journal of Physical Chemistry A*, **2015**, 119, 5778-89	2.8	9
45	An Effective Method for the Synthesis of 3,5-bis(halomethyl)-1,4-Oxaselenanes and their Derivatives. *Chemistry of Heterocyclic Compounds*, **2014**, 49, 1821-1826	1.4	8

44	Full four-component relativistic calculations of the one-bond 77Se-13C spin-spin coupling constants in the series of selenium heterocycles and their parent open-chain selenides. *Magnetic Resonance in Chemistry*, **2014**, 52, 214-21	2.1	13
43	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	0.7	7
42	Relativistic effects in the one-bond spin-spin coupling constants involving selenium. *Magnetic Resonance in Chemistry*, **2014**, 52, 500-10	2.1	15
41	Structural and Stereochemical Applications of Computational NMR Using 29Si–1H and 77Se–1H Indirect Spin–Spin Coupling Constants **2014**, 87-110		8
40	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	0.7	4
39	Towards the versatile DFT and MP2 computational schemes for 31P NMR chemical shifts taking into account relativistic corrections. *Magnetic Resonance in Chemistry*, **2014**, 52, 699-710	2.1	30
38	Nonempirical calculations of the one-bond (29)Si-(13)C spin-spin coupling constants taking into account relativistic and solvent corrections. *Magnetic Resonance in Chemistry*, **2014**, 52, 413-21	2.1	7
37	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	3.6	26
36	Modern quantum chemical methods for calculating spin–spin coupling constants: theoretical basis and structural applications in chemistry. *Russian Chemical Reviews*, **2013**, 82, 99-130	6.8	94
35	One-bond 29Si-1H spin-spin coupling constants in the series of halosilanes: benchmark SOPPA and DFT calculations, relativistic effects, and vibrational corrections. *Magnetic Resonance in Chemistry*, **2013**, 51, 557-61	2.1	10
34	Reaction of 2-pyridylselenenyl bromide with divinyl selenide. *Chemistry of Heterocyclic Compounds*, **2012**, 48, 1129-1131	1.4	16
33	Open-chain unsaturated selanyl sulfides: stereochemical structure and stereochemical behavior of their 77Se-1H spin-spin coupling constants. *Magnetic Resonance in Chemistry*, **2012**, 50, 653-8	2.1	16
32	Structural trends of 29Si-1H spin-spin coupling constants across double bond. *Magnetic Resonance in Chemistry*, **2012**, 50, 665-71	2.1	14
31	Algebraic-diagrammatic construction polarization propagator approach to indirect nuclear spin-spin coupling constants. *Journal of Chemical Physics*, **2012**, 137, 044119	3.9	12
30	Stereochemical behavior of (77)Se-(1)H spin-spin coupling constants in pyrazolyl-1,3-diselenanes and 1,2-diselenolane. *Magnetic Resonance in Chemistry*, **2012**, 50, 169-73	2.1	20
29	Benchmark calculations of (29) Si-(1) H spin-spin coupling constants across double bond. *Magnetic Resonance in Chemistry*, **2012**, 50, 278-83	2.1	16
28	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. *Magnetic Resonance in Chemistry*, **2012**, 50, 488-95	2.1	19
27	Stereochemical behavior of (2) J(Se,H) and (3)J(Se,H) spin-spin coupling constants across sp(3) carbons: a theoretical scrutiny. *Magnetic Resonance in Chemistry*, **2012**, 50, 557-62	2.1	13

26	Regioselective dehydrobromination reaction of 5-bromo-2-bromomethyl-1,3-thiaselenolane 1,1-dioxide. *Russian Chemical Bulletin*, **2011**, 60, 196-197	1.7	2
25	Experimental and computational studies of nJ(77Se, 1H) selenium-proton couplings in selenoglycosides. *Magnetic Resonance in Chemistry*, **2011**, 49, 190-4	2.1	28
24	Conformational analysis and diastereotopic assignments in the series of selenium-containing heterocycles by means of 77Se-1H spin-spin coupling constants: a combined theoretical and experimental study. *Magnetic Resonance in Chemistry*, **2011**, 49, 389-98	2.1	36
23	Stereochemical study of the sterically crowded phenylselanylalkenes by means of (77)Se-(1)H spin-spin coupling constants. *Magnetic Resonance in Chemistry*, **2011**, 49, 570-4	2.1	10
22	Benchmarking SOPPA(CC2) for the calculation of indirect nuclear spin□spin coupling constants: Carbocycles. *Chemical Physics*, **2011**, 381, 35-43	2.3	28
21	Structural trends of 77Se-1H spin-spin coupling constants and conformational behavior of 2-substituted selenophenes. *Magnetic Resonance in Chemistry*, **2010**, 48, 44-52	2.1	69
20	Trivinylphosphine and trivinylphosphine chalcogenides: stereochemical trends of □P-□H spin-spin coupling constants. *Magnetic Resonance in Chemistry*, **2010**, 48 Suppl 1, S48-55	2.1	14
19	Incomparably easy migration of functionalized enol substituent in pyrrole ring **2010**, 44, 237		
18	Conformational analysis and stereochemical dependences of (31)P-(1)H spin-spin coupling constants of bis(2-phenethyl)vinylphosphine and related phosphine chalcogenides. *Magnetic Resonance in Chemistry*, **2009**, 47, 288-99	2.1	20
17	Conformational analysis of N-vinyl-2-phenylpyrrole. *Chemistry of Heterocyclic Compounds*, **2009**, 45, 28-34	0.4	
16	Theoretical conformational analysis of unsaturated phospines and phosphinechalcogenides. *Russian Journal of Organic Chemistry*, **2009**, 45, 667-673	0.7	5
15	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	1.2	19
14	Influence of the Introduction of Short Alkyl Chains in Poly(2-(2-Thienyl)-1H-pyrrole) on Its Electrochromic Behavior. *Macromolecules*, **2008**, 41, 6886-6894	5.5	38
13	Synthesis and conformational analysis of furfuryl vinyl ethers. *Russian Chemical Bulletin*, **2008**, 57, 2132-2138	0.7	3
12	Divinyl selenide: conformational study and stereochemical behavior of its 77Se-1H spin-spin coupling constants. *Magnetic Resonance in Chemistry*, **2008**, 46, 979-85	2.1	39
11	Incomparably easy migration of functionalized enol substituent in pyrrole ring. *Russian Journal of Organic Chemistry*, **2008**, 44, 237-246	0.7	2
10	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	0.7	6
9	Theoretical conformational analysis of divinyl selenide. *Russian Journal of Organic Chemistry*, **2008**, 44, 1418-1421	0.7	3

8	4-Dimethylaminoacetophenone O-vinyloxime: Synthesis and steric structure. *Russian Journal of Organic Chemistry*, **2008**, 44, 1497-1503	0.7	2
7	Stereochemical Study of 2-Substituted N-Vinylpyrroles. *Australian Journal of Chemistry*, **2007**, 60, 583	1.2	15
6	Facile coupling of 2-(1-ethylthioethenyl)pyrroles with amines: A route to 2-(1-aminoethenyl)pyrroles and 1-amino-3-iminopyrrolizines. *Journal of Heterocyclic Chemistry*, **2007**, 44, 505-513	1.9	10
5	Conformational study of 2-arylazo-1-vinylpyrroles. *Magnetic Resonance in Chemistry*, **2007**, 45, 142-51	2.1	16
4	Fluorescence quenching and laser photolysis of dipyrrolylbenzenes in the presence of chloromethanes. *Russian Journal of General Chemistry*, **2007**, 77, 1386-1394	0.7	9
3	13C-13C spin-spin coupling constants in structural studies: XL. Conformational analysis of N-vinylpyrroles. *Russian Journal of Organic Chemistry*, **2007**, 43, 880-887	0.7	8
2	Nonempirical calculations of NMR indirect spin-spin coupling constants. Part 15: pyrrolylpyridines. *Magnetic Resonance in Chemistry*, **2006**, 44, 692-7	2.1	17
1	Easy □to □migration of an enol moiety on a pyrrole ring. *Tetrahedron Letters*, **2006**, 47, 3645-3648	2	10