Yuriy Rusakov

List of Publications by Year
in descending order

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82 papers	1,359 citations	448610 19 h-index	511568 30 g-index
87 all docs	87 docs citations	87 times ranked	509 citing authors

#	Article	IF	Citations
1	Fluorine spinâ€“spin coupling constants of pentafluorobenzene revisited at the ab initio correlated levels. Magnetic Resonance in Chemistry, 2022, , .	1.1	3
2	New pecS-n (n = 1, 2) basis sets for quantum chemical calculations of the NMR chemical shifts of H, C, N, and O nuclei. Journal of Chemical Physics, 2022, 156, .	1.2	6
3	Computational ¹⁹⁹Hg NMR. Magnetic Resonance in Chemistry, 2022, 60, 929-953.	1.1	9
4	Quantum chemical calculations of ⁷⁷Se and ¹²⁵Te nuclear magnetic resonance spectral parameters and their structural applications. Magnetic Resonance in Chemistry, 2021, 59, 359-407.	1.1	21
5	An efficient method for generating property-energy consistent basis sets. New pecJ-n (n =) Tj ETQq1 1 0.784314 rgBT /Ov involving ¹H, ¹³C, ¹⁵N, and ¹⁹F nuclei. Physical Chemistry Chemical Physics, 2021, 23, 14925-14939.	1.3	11
6	Efficient Jâ€oriented tin basis sets for the correlated calculations of indirect nuclear spinâ€“spin coupling constants. Magnetic Resonance in Chemistry, 2021, 59, 713-722.	1.1	8
7	What Most Affects the Accuracy of ¹²⁵Te NMR Chemical Shift Calculations. Journal of Physical Chemistry A, 2020, 124, 6714-6725.	1.1	11
8	A New Basis Set for the Calculation of ¹³C NMR Chemical Shifts within a Non-empirical Correlated Framework. Journal of Physical Chemistry A, 2020, 124, 7322-7330.	1.1	4
9	Correlated ab initio calculations of oneâ€bond ³¹Pï£¿⁷⁷Se and ³¹Pï£¿¹²⁵Te spinâ€“spin coupling constants in a series of Pï£¾Se and Pï£¾Te systems accounting for relativistic effects (part 2). Magnetic Resonance in Chemistry, 2020, 58, 929-940.	1.1	9
10	Hierarchical Basis Sets for the Calculation of Nuclear Magnetic Resonance Spinâ€“Spin Coupling Constants Involving Either Selenium or Tellurium Nuclei. Journal of Physical Chemistry A, 2019, 123, 6564-6571.	1.1	18
11	Stereochemical Dependences of ³¹Pâ€“¹³C Spinâ€“Spin Coupling Constants of Heterocyclic Phosphines. Journal of Physical Chemistry A, 2019, 123, 6298-6303.	1.1	8
12	Geometries and NMR properties of cisplatin and transplatin revisited at the four-component relativistic level. Mendeleev Communications, 2019, 29, 315-317.	0.6	9
13	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.	1.1	8
14	Longâ€range relativistic heavy atom effect on ¹H NMR chemical shifts of seleniumâ€and telluriumâ€containing compounds. International Journal of Quantum Chemistry, 2019, 119, e25809.	1.0	17
15	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.	0.8	16
16	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.	1.1	16
17	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.	1.1	10
18	Relativistic heavy atom effect on ¹³<scp>C NMR</scp> chemical shifts initiated by adjacent multiple chalcogens. Magnetic Resonance in Chemistry, 2018, 56, 716-726.	1.1	15

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19	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.	1.1	19
20	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.	1.1	7
21	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.	0.8	17
22	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.	0.3	6
23	Relativistic effects of chlorine in 15N NMR chemical shifts of chlorine-containing amines. Russian Journal of Organic Chemistry, 2017, 53, 1738-1739.	0.3	2
24	Dipropadienyl telluride. Russian Chemical Bulletin, 2017, 66, 2343-2344.	0.4	1
25	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.	1.1	18
26	Theoretical grounds of relativistic methods for calculation of spinâ€“spin coupling constants in nuclear magnetic resonance spectra. Russian Chemical Reviews, 2016, 85, 356-426.	2.5	63
27	New relativistic computational schemes for 13C NMR chemical shifts. Russian Journal of Organic Chemistry, 2016, 52, 1203-1204.	0.3	2
28	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.	1.1	10
29	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.	1.0	39
30	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.	1.5	18
31	Reaction of tellurium tetrachloride with hex-3-yne. Russian Chemical Bulletin, 2015, 64, 2747-2748.	0.4	6
32	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.	0.4	14
33	MP2 calculation of ⁷⁷Se NMR chemical shifts taking into account relativistic corrections. Magnetic Resonance in Chemistry, 2015, 53, 485-492.	1.1	19
34	Relativistic Environmental Effects in ²⁹Si NMR Chemical Shifts of Halosilanes: Light Nucleus, Heavy Environment. Journal of Physical Chemistry A, 2015, 119, 5778-5789.	1.1	11
35	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.	1.5	13
36	Calculations of 29Si NMR shifts of organylsilanes by DFT taking into account solvent effects and relativistic corrections. Russian Chemical Bulletin, 2015, 64, 551-557.	0.4	6

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37	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.	1.1	10
38	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.	0.3	4
39	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.	1.1	38
40	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.	1.1	10
41	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.	0.6	9
42	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.	1.1	15
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.	0.3	8
44	Relativistic effects in the oneâ€bond spinâ€“spin coupling constants involving selenium. Magnetic Resonance in Chemistry, 2014, 52, 500-510.	1.1	18
45	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.	1.3	30
46	Modern quantum chemical methods for calculating spinâ€“spin coupling constants: theoretical basis and structural applications in chemistry. Russian Chemical Reviews, 2013, 82, 99-130.	2.5	107
47	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.	1.1	15
48	Reaction of 2-pyridylselenenyl bromide with divinyl selenide. Chemistry of Heterocyclic Compounds, 2012, 48, 1129-1131.	0.6	21
49	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.	1.1	20
50	Structural trends of ²⁹Siâ€“¹H spinâ€“spin coupling constants across double bond. Magnetic Resonance in Chemistry, 2012, 50, 665-671.	1.1	15
51	Algebraic-diagrammatic construction polarization propagator approach to indirect nuclear spinâ€“spin coupling constants. Journal of Chemical Physics, 2012, 137, 044119.	1.2	15
52	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.	1.1	24
53	Benchmark calculations of ²⁹Siâ€“¹H spinâ€“spin coupling constants across double bond. Magnetic Resonance in Chemistry, 2012, 50, 278-283.	1.1	18
54	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.	1.1	22

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55	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.	1.1	15
56	Regioselective dehydrobromination reaction of 5-bromo-2-bromomethyl-1,3-thiaselenolane 1,1-dioxide. Russian Chemical Bulletin, 2011, 60, 196-197.	0.4	3
57	Experimental and computational studies of ⁿJ(⁷⁷Se,¹H) seleniumâ€“proton couplings in selenoglycosides. Magnetic Resonance in Chemistry, 2011, 49, 190-194.	1.1	32
58	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.	1.1	42
59	Stereochemical study of the sterically crowded phenylselanylalkenes by means of ⁷⁷Seï£¿¹H spinâ€“spin coupling constants. Magnetic Resonance in Chemistry, 2011, 49, 570-574.	1.1	13
60	Benchmarking SOPPA(CC2) for the calculation of indirect nuclear spinâ€“spin coupling constants: Carbocycles. Chemical Physics, 2011, 381, 35-43.	0.9	31
61	Structural trends of ⁷⁷Seï£¿¹H spinâ€“spin coupling constants and conformational behavior of 2â€substituted selenophenes. Magnetic Resonance in Chemistry, 2010, 48, 44-52.	1.1	77
62	Trivinylphosphine and trivinylphosphine chalcogenides: stereochemical trends of 31Pï£¿1H spin-spin coupling constants. Magnetic Resonance in Chemistry, 2010, 48, S48-S55.	1.1	19
63	10.1007/s11178-008-2009-4. , 2010, 44, 237.		0
64	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.	1.1	21
65	Conformational analysis of N-vinyl-2-phenylpyrrole. Chemistry of Heterocyclic Compounds, 2009, 45, 28-34.	0.6	1
66	Theoretical conformational analysis of unsaturated phospines and phosphinechalcogenides. Russian Journal of Organic Chemistry, 2009, 45, 667-673.	0.3	5
67	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.	0.5	20
68	Synthesis and conformational analysis of furfuryl vinyl ethers. Russian Chemical Bulletin, 2008, 57, 2132-2138.	0.4	3
69	Divinyl selenide: conformational study and stereochemical behavior of its ⁷⁷Seï£¿¹H spinâ€“spin coupling constants. Magnetic Resonance in Chemistry, 2008, 46, 979-985.	1.1	43
70	Incomparably easy migration of functionalized enol substituent in pyrrole ring. Russian Journal of Organic Chemistry, 2008, 44, 237-246.	0.3	3
71	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.	0.3	7
72	Theoretical conformational analysis of divinyl selenide. Russian Journal of Organic Chemistry, 2008, 44, 1418-1421.	0.3	3

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73	4-Dimethylaminoacetophenone O-vinyloxime: Synthesis and steric structure. Russian Journal of Organic Chemistry, 2008, 44, 1497-1503.	0.3	2
74	Influence of the Introduction of Short Alkyl Chains in Poly(2-(2-Thienyl)-1H-pyrrole) on Its Electrochromic Behavior. Macromolecules, 2008, 41, 6886-6894.	2.2	42
75	Stereochemical Study of 2-Substituted N-Vinylpyrroles. Australian Journal of Chemistry, 2007, 60, 583.	0.5	16
76	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.	1.4	11
77	Conformational study of 2-arylazo-1-vinylpyrroles. Magnetic Resonance in Chemistry, 2007, 45, 142-151.	1.1	18
78	Fluorescence quenching and laser photolysis of dipyrrolylbenzenes in the presence of chloromethanes. Russian Journal of General Chemistry, 2007, 77, 1386-1394.	0.3	9
79	13C-13C spin-spin coupling constants in structural studies: XL. Conformational analysis of N-vinylpyrroles. Russian Journal of Organic Chemistry, 2007, 43, 880-887.	0.3	9
80	Easy Î±- to Î²-migration of an enol moiety on a pyrrole ring. Tetrahedron Letters, 2006, 47, 3645-3648.	0.7	11
81	Nonempirical calculations of NMR indirect spinâ€“spin coupling constants. Part 15: pyrrolylpyridines. Magnetic Resonance in Chemistry, 2006, 44, 692-697.	1.1	18
82	Two-components ion flow in a low voltage vacuum spark. , 2004, , .		0