

# Ruslan M Minyaev

## List of Publications by Year in descending order

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110  
papers

1,920  
citations

279701

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116  
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times ranked

1230  
citing authors

#	ARTICLE	IF	CITATIONS
1	A DFT insight into the structure and electronic characteristics of group 14 bis-atranes and their analogues. <i>Journal of Organometallic Chemistry</i> , 2022, 960, 122235.	0.8	0
2	1-Chloroalumole. <i>Organometallics</i> , 2022, 41, 467-471.	1.1	5
3	Phosphatetrasilatricyclo[2.1.0.02,5]pentane. <i>Mendeleev Communications</i> , 2022, 32, 33-34.	0.6	2
4	Titanium Germylidenes. <i>Angewandte Chemie - International Edition</i> , 2021, 60, 3951-3955.	7.2	6
5	Titanium Germylidenes. <i>Angewandte Chemie</i> , 2021, 133, 3997-4001.	1.6	1
6	Innenr¼cktitelbild: Titanium Germylidenes (Angew. Chem. 8/2021). <i>Angewandte Chemie</i> , 2021, 133, 4427-4427.	1.6	0
7	Computationally Designed Crystal Structures of the Supertetrahedral Ga <sub>4</sub> C and Ga <sub>4</sub> Si Solids. <i>Journal of Physical Chemistry A</i> , 2021, 125, 6556-6561.	1.1	1
8	Band Gap Engineering and 14 Electron Superatoms in 2D Superoctahedral Boranes B <sub>4</sub> X <sub>2</sub> (B, N, P, As, Sb). <i>Journal of Physical Chemistry C</i> , 2021, 125, 17280-17290.	1.5	6
9	Computational Prediction of the Low-Temperature Ferromagnetic Semiconducting 2D SiN Monolayer. <i>Physica Status Solidi (B): Basic Research</i> , 2020, 257, 1900619.	0.7	15
10	o-Quinone phenalenyl derivatives as expedient ligands for the design of magnetically active metal complexes: A computational study. <i>Chemical Physics Letters</i> , 2020, 740, 137073.	1.2	6
11	Electronic structure and magnetic properties of the triangular nanographenes with radical substituents: a DFT study. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 1288-1298.	1.3	18
12	From a (Silatrigerma)cyclobutenylium Ion to a (Silatrigerma)cyclobutenyl Radical and Back. <i>Journal of the American Chemical Society</i> , 2020, 142, 16455-16460.	6.6	16
13	Novel architectures of boron. <i>Structural Chemistry</i> , 2020, 31, 2105-2128.	1.0	15
14	Stability, electronic, and optical properties of two-dimensional phosphoborane. <i>Journal of Computational Chemistry</i> , 2020, 41, 1456-1463.	1.5	19
15	Periodic F-defects on the MgO surface as potential single-defect catalysts with non-linear optical properties. <i>Chemical Physics</i> , 2020, 532, 110680.	0.9	18
16	Theoretical Prediction for Synthetic Realization: Pyramidal Systems CIE[E <sup>2+</sup> <sub>4</sub> R <sub>4</sub> ] (E = B <sup>+</sup> , Ga, E <sup>2+</sup> = C <sup>+</sup> , Ge, R = SiMe <sub>3</sub> ), Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50 13		
17	Superoctahedral two-dimensional metallic boron with peculiar magnetic properties. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 19764-19771.	1.3	36
18	[2+2] Cycloadduct of Titanium Silylidene and Benzonitrile. <i>European Journal of Inorganic Chemistry</i> , 2019, 2019, 4224-4227.	1.0	8

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19	Structure and bonding of new boron and carbon superpolyhedra. Structural Chemistry, 2019, 30, 805-814.	1.0	12
20	Molecular dynamics study of a new metastable allotropic crystalline form of gallium—supertetrahedral gallium. Journal of Computational Chemistry, 2019, 40, 1861-1865.	1.5	4
21	Stabilization of non-typical forms of boron clusters by beryllium doping. Chemical Physics, 2019, 522, 44-54.	0.9	8
22	Computationally Designed Crystal Structures of the Supertetrahedral Al <sub>4</sub> X (X = B, C, Al). <i>Tj ETQq0 0 0 rgBT /Overlock 10 Tf</i>	1.1	5
23	From Borapyramidane to Borole Dianion. Journal of the American Chemical Society, 2018, 140, 6053-6056.	6.6	27
24	Computational Assessment of an Elusive Aromatic N <sub>3</sub> P <sub>3</sub> Molecule. ACS Omega, 2018, 3, 286-291.	1.6	6
25	Quantum chemical modeling of solid-state B <sub>4</sub> X structures containing tetrahedral B <sub>4</sub> units with X = B, C, Al, Si. Mendeleev Communications, 2018, 28, 173-175.	0.6	4
26	Stabilization of boron clusters with classical fullerene structures by combined doping effect: a quantum chemical study. Structural Chemistry, 2018, 29, 327-340.	1.0	4
27	Metalcarbonyl analogues of annelated cyclooctatetraene and cyclodecapentaene derivatives with a planar core cycle: a quantum chemical study. Physical Chemistry Chemical Physics, 2018, 20, 27830-27837.	1.3	1
28	The structurally variable network of spin couplings and migrating paramagnetic centers in binuclear <i>o</i> -quinone Co <sup>II</sup> complexes with biradical acene linkers: a computational DFT study. Dalton Transactions, 2018, 47, 15948-15956.	1.6	10
29	Difluorophosphorane-Flattened Phosphorene through Difluorination. Journal of Physical Chemistry Letters, 2018, 9, 6963-6966.	2.1	7
30	From Two- to Three-Dimensional Structures of a Supertetrahedral Boron Using Density Functional Calculations. Angewandte Chemie - International Edition, 2017, 56, 10118-10122.	7.2	24
31	From Two- to Three-Dimensional Structures of a Supertetrahedral Boron Using Density Functional Calculations. Angewandte Chemie, 2017, 129, 10252-10256.	1.6	2
32	Hybrid group 15(E 15) “group 14(E 14) element cationic pyramidal structures E 15 [E 14 4 (SiR 3) 4] + : A DFT study. Tetrahedron Letters, 2017, 58, 2054-2057.	0.7	4
33	Hypercoordinated carbon in C-doped boron fullerenes: a quantum chemical study. Structural Chemistry, 2017, 28, 357-369.	1.0	5
34	Bis(stibahousene). Journal of the American Chemical Society, 2017, 139, 13897-13902.	6.6	13
35	Supertetrahedral Aluminum — A New Allotropic Ultralight Crystalline Form of Aluminum. Journal of Physical Chemistry C, 2017, 121, 22187-22190.	1.5	11
36	Nonclassical Organosilicon Compounds. , 2017, , 3-24.		0

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37	Geometric and electronic structures of silicon fluorides ( $n = 4-6$ ) and potential energy surfaces for dissociation reactions $\text{SiF}_4 + \text{F}^+$ and $\text{SiF}_4 + \text{F}^+$ . <i>International Journal of Quantum Chemistry</i> , 2016, 116, 1358-1361.		1
38	Stabilization of non-standard conformations of the annulene rings in cyclobutadiene-framed $[n]$ annulenes ( $n=8, 10, 12, 14$ ) and their beryllium sandwich-like complexes: a quantum chemical study. <i>Structural Chemistry</i> , 2016, 27, 1229-1240.	1.0	4
39	Supermolecular design: From molecules to solid states. <i>International Journal of Quantum Chemistry</i> , 2016, 116, 259-264.	1.0	5
40	Parquet compounds on the basis of eight- and twelve-membered structure blocks: Quantum-chemical study. <i>Russian Journal of Organic Chemistry</i> , 2016, 52, 268-282.	0.3	3
41	Structure and stability of the C-doped boron fullerenes $\text{B}_6\text{C}_{12}$ and $\text{B}_8\text{C}_{12}$ with quasi-planar pentacoordinated cage carbon atoms: a quantum-chemical study. <i>Mendeleev Communications</i> , 2016, 26, 485-487.	0.6	7
42	A Cationic Phosphapyramidane. <i>Chemistry - A European Journal</i> , 2016, 22, 17585-17589.	1.7	22
43	Pyramidanes: The Covalent Form of the Ionic Compounds. <i>Organometallics</i> , 2016, 35, 346-356.	1.1	24
44	Group 14 element cationic pentagonal pyramidal complexes $\text{E}_5\text{M}^+$ ( $\text{E} = \text{Si, Ge, Sn, Pb}$ ): A quantum-chemical study. <i>Phosphorus, Sulfur and Silicon and the Related Elements</i> , 2016, 191, 609-612.	0.8	3
45	Germanium, carbon-germanium, and silicon-germanium triangulenes. <i>Journal of Computational Chemistry</i> , 2015, 36, 2193-2199.	1.5	8
46	From a $\text{Si}_3\text{Cyclopropene}$ to a $\text{Si}_3\text{Bicyclo}[1.1.0]\text{butane}$ to a $\text{Si}_3\text{Cyclopropene}$ to a $\text{Si}_3\text{S}_2\text{Bicyclo}[1.1.0]\text{butane}$ : Back and Forth and In Between. <i>Angewandte Chemie - International Edition</i> , 2015, 54, 14118-14122.	7.2	12
47	Pentagermapyramidane: Crystallizing the Transition State Structure. <i>Angewandte Chemie - International Edition</i> , 2015, 54, 5654-5657.	7.2	27
48	Dependence of the structure of alkali metal trifluoride ion pairs $\text{F}_3\text{M}^+$ on the counterion $\text{M}^+$ ( $\text{M} = \text{Tl, Rb, Cs}$ ). <i>Journal of Physical Chemistry B</i> , 2015, 119, 10000-10006.	0.6	6
49	Unidirectional migration of the iodine atom over a cyclopentadiene ring in a rotating electric field. <i>Mendeleev Communications</i> , 2015, 25, 21-23.	0.6	9
50	Assessing the Viability of Extended Nonmetal Atom Chains in $\text{M}_n\text{F}_{n+2}$ ( $\text{M} = \text{S and Se}$ ). <i>Angewandte Chemie - International Edition</i> , 2015, 54, 1476-1480.	7.2	15
51	Supertetrahedral $\text{B}_8\text{O}_{10}$ , $\text{C}_8\text{O}_{10}$ , and $\text{Al}_8\text{O}_{10}$ analogs of dodecahedrane and their substituted molecules. <i>Structural Chemistry</i> , 2015, 26, 223-229.	1.0	13
52	Binuclear sandwich and multi-decker sandwich compounds of alkali and alkaline-earth metals: a quantum chemical study. <i>Russian Chemical Bulletin</i> , 2015, 64, 540-550.	0.4	3
53	Peculiar structure of the potential energy surfaces of typical electrocyclic reactions in the areas of the symmetry-forbidden reaction paths. <i>Computational and Theoretical Chemistry</i> , 2014, 1030, 44-52.	1.1	5
54	Supertetrahedral aluminum and silicon structures and their hybrid analogues. <i>Russian Journal of Inorganic Chemistry</i> , 2014, 59, 332-336.	0.3	8

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55	Unusual reaction paths of SN2 nucleophile substitution reactions $\text{CH}_4 + \text{H}^+ \rightarrow \text{CH}_4 + \text{H}^+$ and $\text{CH}_4 + \text{F}^+ \rightarrow \text{CH}_3\text{F} + \text{H}^+$ : Quantum chemical calculations. <i>Chemical Physics</i> , 2013, 425, 170-176.	0.9	13
56	Computational design of valence tautomeric adducts of $\text{Co}^{\text{II}}$ diketonates with redox-active o-benzoquinone ligands. <i>Dalton Transactions</i> , 2013, 42, 1726-1734.	1.6	40
57	Pyramidanes. <i>Journal of the American Chemical Society</i> , 2013, 135, 8794-8797.	6.6	41
58	Supertetrahedral cubane $\text{C}_{32}\text{H}_8$ and supertetrahedral dodecahedrane $\text{C}_{80}\text{H}_{20}$ with tetrahedral $\text{C}_4\text{H}$ fragments in the vertices. <i>Mendeleev Communications</i> , 2013, 23, 131-132.	0.6	5
59	DFT Computational Design of a Ligand-Driven Light-Induced Mechanism for Spin-State Switching. <i>European Journal of Inorganic Chemistry</i> , 2013, 2013, 4203-4219.	1.0	10
60	Multi-decker tricarbonyl-bridged sandwich complexes of transition metals: structure, stability and electron-counting rules. <i>Physical Chemistry Chemical Physics</i> , 2012, 14, 14803.	1.3	9
61	Supertetrahedrane and its boron analogs. <i>Russian Chemical Bulletin</i> , 2012, 61, 1673-1680.	0.4	8
62	Silicon analogues of pyramidane: a quantum-chemical study. <i>Mendeleev Communications</i> , 2012, 22, 8-10.	0.6	9
63	Intramolecular Hypervalent Interaction in the Conjugate Five-Membered Rings. <i>Journal of Physical Chemistry A</i> , 2011, 115, 12973-12982.	1.1	13
64	Quantum-chemical simulation of boron- and halogen-containing polymers. <i>Russian Journal of Organic Chemistry</i> , 2011, 47, 1675-1681.	0.3	0
65	Sandwich Compounds of Transition Metals with Cyclopolyenes and Isolobal Boron Analogues. <i>Chemistry - A European Journal</i> , 2010, 16, 2272-2281.	1.7	15
66	A Quantum Chemical Study of Bis-(iminoquinonephenolate) Zn(II) Complexes. <i>Journal of Physical Chemistry A</i> , 2010, 114, 7780-7785.	1.1	36
67	Theoretical modeling of enantiomerization mechanisms of tetrahedral bis-( $\eta^2$ -diiminato) Ni(II) complexes. <i>Computational and Theoretical Chemistry</i> , 2009, 895, 138-141.	1.5	20
68	Theoretical modeling of the molecular and crystal structures and a square-planar to tetrahedral conformational rearrangement of trans-planar bis(N-methylsalicylaldehydato)nickel(II). <i>Mendeleev Communications</i> , 2009, 19, 64-66.	0.6	4
69	Theoretical modeling of the square-planar to tetrahedral isomerization of bis-chelate nickel(II) complexes. <i>Chemical Physics Letters</i> , 2008, 459, 27-32.	1.2	27
70	Specific and non-specific influence of the environment on dihydrogen bonding and proton transfer to $[\text{RuH}_2\{\text{P}(\text{CH}_2\text{CH}_2\text{PPh}_2)_3\}]$ . <i>Journal of Molecular Structure</i> , 2007, 844-845, 115-131.	1.8	32
71	Sandwich compounds with central hypercoordinate carbon, nitrogen, and oxygen: A quantum-chemical study. <i>Heteroatom Chemistry</i> , 2006, 17, 464-474.	0.4	12
72	Planar and Pyramidal Tetracoordinate Carbon in Organoboron Compounds. <i>Journal of Organic Chemistry</i> , 2005, 70, 6693-6704.	1.7	56

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73	A hydrocarbon dication with nonplanar hexacoordinated carbon. Mendeleev Communications, 2004, 14, 47-48.	0.6	15
74	Hypercoordinate carbon in polyhedral organic structures. Mendeleev Communications, 2004, 14, 43-46.	0.6	47
75	A quantum-chemical study of carbon sandwich compounds. Mendeleev Communications, 2004, 14, 96-98.	0.6	26
76	Poly[n]prismanes: A Family of Stable Cage Structures with Half-Planar Carbon Centers.. ChemInform, 2004, 35, no.	0.1	0
77	Hypercoordinate Carbon in Polyhedral Organic Structures. ChemInform, 2004, 35, no.	0.1	0
78	Low-Temperature IR and NMR Studies of the Interaction of Group 8 Metal Dihydrides with Alcohols. Chemistry - A European Journal, 2003, 9, 2219-2228.	1.7	48
79	Poly[n]prismanes: A Family of Stable Cage Structures with Half-Planar Carbon Centers. Journal of Organic Chemistry, 2003, 68, 8588-8594.	1.7	64
80	Non-classical structures of organic compounds: unusual stereochemistry and hypercoordination. Russian Chemical Reviews, 2002, 71, 869-892.	2.5	91
81	Low-energy barrier B4 ring puckering rearrangement of 1,6-diaza-closo-hexaborane: an ab initio study. Mendeleev Communications, 2001, 11, 132-134.	0.6	5
82	Octacoordinated main-group element centres in a planar cyclic B8 environment: an ab initio study. Mendeleev Communications, 2001, 11, 213-214.	0.6	63
83	Cyclic Aromatic Systems with Hypervalent Centers. Chemical Reviews, 2001, 101, 1247-1266.	23.0	122
84	Computational modeling of the mechanisms and stereochemistry of circumambulatory rearrangements of formylcyclopropene and 4-hydroxycyclobutenyl cation. Journal of Physical Organic Chemistry, 2000, 13, 3-12.	0.9	4
85	Stabilization of the glycine zwitterionic form by complexation with Na <sup>+</sup> and Cl <sup>-</sup> : an ab initio study. Mendeleev Communications, 2000, 10, 43-44.	0.6	6
86	Aromatic stabilization of organochalcogen compounds with the intramolecular X <sup>+</sup> O <sup>-</sup> (X = S, Se, Te) coordination. Mendeleev Communications, 2000, 10, 171-172.	0.6	11
87	Intramolecular hypervalent O <sup>+</sup> Cl interaction in the chloronium cations: an ab initio study. Mendeleev Communications, 2000, 10, 173-174.	0.6	6
88	Planar Tetracoordinate Carbon in Organoboron Compounds: ab initio Computational Study. Collection of Czechoslovak Chemical Communications, 1999, 64, 1780-1789.	1.0	30
89	Theoretical study of O - > X (S, Se, Te) coordination in organic compounds. Canadian Journal of Chemistry, 1998, 76, 776-788.	0.6	141
90	Gradient Line Reaction Paths for Hindered Internal Rotation in H <sub>2</sub> BNH <sub>2</sub> and Inversion in PF <sub>3</sub> . Journal of Physical Chemistry A, 1997, 101, 1384-1392.	1.1	16

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91	Computational modeling of the mechanisms of circumambulatory rearrangements of main-group migrants in the cyclopropene ring. <i>Computational and Theoretical Chemistry</i> , 1997, 398-399, 237-253.	1.5	4
92	A theoretical study of internal rotation in H <sub>2</sub> BOBH <sub>2</sub> and H <sub>2</sub> BNBH <sub>2</sub> . <i>Mendeleev Communications</i> , 1997, 7, 80-82.	0.6	4
93	Gradient line reaction path of ammonia addition to formaldehyde. <i>Mendeleev Communications</i> , 1997, 7, 189-191.	0.6	6
94	Internal conrotation and disrotation in H <sub>2</sub> BCH <sub>2</sub> BH <sub>2</sub> and diborylmethane 1,3 H exchange. <i>Journal of Computational Chemistry</i> , 1997, 18, 1792-1803.	1.5	12
95	An Experimental and PM3 Semiempirical Quantum-chemical Investigation of Anomalous Aluminium Dissolution in Proton-donor Solvents Containing HCl. <i>Mendeleev Communications</i> , 1995, 5, 207-208.	0.6	0
96	Rapid and Reversible Migration of the Isothiocyanate Group around the Cyclopropene Ring. <i>Mendeleev Communications</i> , 1995, 5, 213-215.	0.6	13
97	Gradient lines on multidimensional potential energy surfaces and chemical reaction mechanisms. <i>Russian Chemical Reviews</i> , 1994, 63, 883-903.	2.5	64
98	Reaction path as a gradient line on a potential energy surface. <i>International Journal of Quantum Chemistry</i> , 1994, 49, 105-127.	1.0	35
99	Gradient line reaction path of HF addition to ethylene. <i>Chemical Physics Letters</i> , 1994, 218, 413-421.	1.2	35
100	Hetero-Cope Rearrangement of S-(1,2,3-Triphenylcyclopropenyl)-O-ethylthiocarbonate. <i>Mendeleev Communications</i> , 1994, 4, 9-11.	0.6	9
101	Gradient-line reaction paths for 1,2, H shift reactions in phosphinonitrene and formaldehyde, and H <sub>2</sub> elimination from formaldehyde. <i>Journal of the Chemical Society, Faraday Transactions</i> , 1994, 90, 1839.	1.7	5
102	Transition vector symmetry and the internal pseudo-rotation and inversion paths of ClF <sub>4</sub> +. <i>Journal of the Chemical Society, Faraday Transactions</i> , 1994, 90, 1831.	1.7	15
103	Multiplicity of the inversion reaction paths for PF <sub>3</sub> . <i>Computational and Theoretical Chemistry</i> , 1992, 262, 79-85.	1.5	9
104	1,5-Sigmatropic shifts of bromine over a cyclopentadiene ring. <i>Journal of Physical Organic Chemistry</i> , 1991, 4, 31-47.	0.9	26
105	Quantum Chemistry of Organic Compounds. , 1990, , .		68
106	Pericyclic Reactions. , 1990, , 238-263.		0
107	Reaction paths of circumambulatory rearrangements of sulfur-substituted cyclopentadienes. <i>Computational and Theoretical Chemistry</i> , 1989, 186, 293-303.	1.5	6
108	Pyramidane and isoelectronic pyramidal cations. <i>Computational and Theoretical Chemistry</i> , 1984, 110, 241-253.	1.5	34

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109	A symmetrical bridged hydrogen bond in organic compounds. Computational and Theoretical Chemistry, 1983, 92, 205-216.	1.5	5
110	Polyhedral Organic Molecules and Ions " Structural Analogues of Organometallic Clusters. Russian Chemical Reviews, 1982, 51, 332-355.	2.5	13