Denis Chachkov

List of Publications by Citations

201 papers	1,154 citations	15 h-index	23 g-index
217 ext. papers	1,267 ext. citations	1.4 avg, IF	5.21 L-index

#	Paper	IF	Citations
201	DFT B3LYP calculation of the spatial structure of Co(II), Ni(II), and Cu(II) template complexes formed in ternary systems metal(II) ion-dithiooxamide-formaldehyde. *Russian Journal of Inorganic Chemistry*, **2009**, 54, 1952-1956	1.5	46
200	Mechanisms of gas phase decomposition of C-nitro compounds from quantum chemical data. *Russian Chemical Reviews*, **2009**, 78, 903-943	6.8	41
199	Geometric parameters and energies of molecular structures of macrocyclic metal chelates in the ternary 3d M(II) ion-ethanedithioamide-ethanedial systems according to quantum-chemical DFT B3LYP calculations. *Russian Journal of Inorganic Chemistry*, **2012**, 57, 205-210	1.5	27
198	Molecular structure and thermodynamic parameters of (5656)macrotetracyclic chelates in the 3d-element(ii) ion-hydrazinomethanethiohydrazide-2,3-butanedione ternary system according to density functional quantum-chemical calculations. *Russian Journal of Inorganic Chemistry*, **2013**, 58, 174-179	1.5	27
197	Calculation of geometric parameters and energies of macrocyclic metal chelates in the ternary M(II) ion-thiocarbamoylmethanamide-formaldehyde systems. *Russian Journal of Inorganic Chemistry*, **2011**, 56, 1935-1942	1.5	27
196	Molecular structures of (5456)metalmacrocyclic chelates with 7-imino-1-oxa-3,6,8,11-tetraazacyclododecanetetrathione-4,5,9,10 formed at template synthesis according to DFT OPBE/TZVP method data. *Inorganica Chimica Acta*, **2013**, 408, 246-250	2.7	26
195	Calculation of geometric parameters of macrocyclic metal chelates formed by template synthesis in tertiary systems M(II) ion-ethanedithioamide-formaldehyde-ammonia. *Russian Journal of Inorganic Chemistry*, **2011**, 56, 223-231	1.5	26
194	DFT Calculations of Space Structures of MII Complexes with (N,N,N,N)-Coordinating Macroheterocyclic Ligand 1,8-Dioxa-3,6,10,13-tetraazacyclotetradecanetetrathione-4,5,11,12. *Macroheterocycles*, **2009**, 2, 271-274	2.2	26
193	Structure of (5656)macrotetracyclic chelates in the ternary systems M(II)-ethanedithioamide-acetone (M = Mn, Fe, Co, Ni, Cu, Zn) according to DFT calculations. *Russian Journal of Inorganic Chemistry*, **2013**, 58, 1073-1078	1.5	25
192	Quantum-chemical calculation of molecular structures of (5656)macrotetracyclic 3d-metal complexes self-assembled in quaternary systems M(II) ion-ethanedithioamide-formaldehyde-ammonia by the density functional theory method. *Russian Journal of Inorganic Chemistry*, **2014**, 59, 218-223	1.5	23
191	Density functional theory calculation of molecular structures of (5656)macrotetracyclic 3d metal complexes with 4,12-Dithiooxo-1,8-dioxa-3,6,10,13-tetraazacyclotetradecanedione-5,11. *Russian Journal of Inorganic Chemistry*, **2012**, 57, 981-986	1.5	23
190	Self-assembly of supramolecular Ni(II) and Cu(II) metalmacrocyclic compounds with tetraazamacrocyclic ligand into a gelatin-immobilized matrix. *Journal of Coordination Chemistry*, **2010**, 63, 4309-4318	1.6	21
189	Structure of the template complex formed in the Co(III)-dithiooxamide-acetone ternary system during complex formation in the KCoFe(CN)6-gelatin immobilized matrices. *Russian Journal of Inorganic Chemistry*, **2010**, 55, 1243-1247	1.5	20
188	Theoretical Study of the Mechanism of the Nitro-Nitrite Rearrangement and Its Role in Gas-Phase Monomolecular Decomposition of C-Nitro Compounds. *Russian Journal of General Chemistry*, **2004**, 74, 908-920	0.7	19
187	Molecular structures of (5656)macrotetracyclic 3d metal chelates formed in the M(II) ion-ethanedithioamide-formaldehyde systems according to the density functional theory method. *Russian Journal of Inorganic Chemistry*, **2015**, 60, 1117-1122	1.5	18
186	A novel acid-catalyzed rearrangement of 2-substituted-3-(2-nitrophenyl)oxiranes for the synthesis of di- and mono-oxalamides. *RSC Advances*, **2016**, 6, 27885-27895	3.7	15
185	Formation enthalpies and bond dissociation enthalpies for C1–C4 mononitroalkanes by composite and DFT/B3LYP methods. *Computational and Theoretical Chemistry*, **2010**, 958, 1-6		14

184	Structures of metalmacrocyclic compounds arising from self-assembly in ion 3d-element dithiooxamide-2-hydroxysubstituted acetaldehyde ternary systems. *Inorganica Chimica Acta*, **2013**, 408, 199-203	2.7	13
183	Molecular structures of (5656)macrotetracyclic chelates formed in the M(II) ion ethanedithioamide-2-thiapropanediol-1,3 systems according to density functional theory calculations. *Russian Journal of Inorganic Chemistry*, **2015**, 60, 1354-1359	1.5	13
182	On the possibility of template synthesis in the ternary system of vanadium(IV)-dithiooxamide-formaldehyde. *Russian Journal of General Chemistry*, **2009**, 79, 1122-1128	0.7	13
181	Energy of the O NO2 bond dissociation and the mechanism of the gas-phase monomolecular decomposition of aliphatic alcohol nitroesters. *Computational and Theoretical Chemistry*, **2004**, 686, 185-192		13
180	MOLECULAR STRUCTURE MODELS OF Al2Ti3 AND Al2V3 CLUSTERS ACCORDING TO DFT QUANTUM-CHEMICAL CALCULATION. *European Chemical Bulletin*, **2020**, 9, 62	0.5	13
179	Molecular structures of template (5555)macrotetracyclic chelates of 3d M(II) ions with 1,4,7,10-tetraaza-1,3,8-dodecatriene-5,6,11,12-tetrathione according to DFT quantum-chemical calculations. *Russian Journal of Inorganic Chemistry*, **2013**, 58, 1315-1320	1.5	12
178	The influence of molecular structure on the change of the arrhenius factor of gas-phase elimination of nitric acid from nitroalkanes. *International Journal of Quantum Chemistry*, **2007**, 107, 2343-2352	2.1	12
177	Quantum-chemical calculation of steric structure of the complexes formed at template synthesis in three-component systems of Co(II) [Ni(II), Cu(II)] ion-bithiooxamide-acetone. *Russian Journal of General Chemistry*, **2008**, 78, 1849-1861	0.7	12
176	DFT OPBE/TZVP alculation of Molecular Structures of (5656) Macroheterocyclic Chelates of Double Charged 3d-Element Ions with 1,5,8,11-Tetraazacyclotetradecanetetrathione-2,3,9,10 and Its Dioxa- and Dithia Analogs. *Macroheterocycles*, **2016**, 9, 268-276	2.2	12
175	Template Synthesis into Gelatin-Immobilized Matrix as Perspective Method of Obtaining Supramolecular Macroheterocyclic Compounds. *Macroheterocycles*, **2008**, 1, 90-97	2.2	12
174	About possibility of stabilization of unusual copper(IV) oxidation state in complexes with porphyrazine and two fluorine ligands: Quantum-chemical design. *Inorganic Chemistry Communication*, **2019**, 106, 224-227	3.1	11
173	Specifics of molecular structures of (565)macrotricyclic 3d-Metal chelates in the ternary systems M(II)-hydrazinecarbothioamide-2,4-Pentanedione according to DFT calculations. *Russian Journal of Inorganic Chemistry*, **2013**, 58, 548-553	1.5	11
172	Enthalpies of formation of mono substituted nitrobenzenes: A quantum chemistry study. *Computational and Theoretical Chemistry*, **2013**, 1011, 37-43	2	11
171	Effect of the molecular structure on the strength of the C-NO2 bond in a series of monofunctional nitrobenzene derivatives. *Russian Journal of General Chemistry*, **2011**, 81, 2273-2287	0.7	11
170	Estimations of activation and enthalpies of reaction for HONO elimination from C2 4 mononitroalkanes: A theoretical study. *Computational and Theoretical Chemistry*, **2011**, 966, 265-271	2	11
169	Novel modifications of elemental nitrogen and their molecular structures a quantumchemical calculation. *European Chemical Bulletin*, **2020**, 9, 78	0.5	11
168	Molecular structures of (5454) macrotetracyclic chelates of 3d M(II) ions with 4,5,9,10-tetramethyl-1,3,6,8-tetraaza-5,8-cyclodecadiene-2,7-diimine according to DFT quantum-chemical calculations. *Russian Journal of Inorganic Chemistry*, **2014**, 59, 349-354	1.5	10
167	(5656)Macrotetracyclic chelates of doubly charged 3d-element ions with 1,4,8,11-tetraazacyclotetradecane-2,3,9,10-tetrathione and their molecular structures according to density functional theory data. *Russian Journal of Inorganic Chemistry*, **2014**, 59, 1276-1282	1.5	10

166	Molecular structures of (555)macrotricyclic chelates appearing in 3d-element(ii) ion-hydrazinomethanethioamide-ethanedial systems according to density functional theory calculations. *Russian Journal of Inorganic Chemistry*, **2012**, 57, 1570-1575	1.5	10
165	Theoretical study of substituents effect on C–NO2 bond strength in mono substituted nitrobenzenes. *Computational and Theoretical Chemistry*, **2013**, 1017, 7-13	2	10
164	The relative stability of macrotricyclic metal complexes in M(II)-thiocarbohydrazide-acetone (M = Mn, Fe, Co, Ni, Cu, Zn) ternary systems according to the data of quantum-chemical calculations. *Russian Journal of Physical Chemistry A*, **2011**, 85, 152-155	0.7	10
163	Mild template synthesis in the iron(III)-ethanedithioamide-1,2-formaldehyde triple system on a K[Fe2(CN)6] gelatin-immobilized matrix. *Journal of Coordination Chemistry*, **2009**, 62, 1058-1066	1.6	10
162	Ab Initio quantum chemical calculation of the structures of coordination compounds arising at template synthesis in ion M(II)-hydrozinomethane thiohydrazide-acetone (M = Co, Ni, Cu) systems. *Journal of Structural Chemistry*, **2009**, 50, 613-617	0.9	10
161	Quantum-chemical calculations of molecular structure of trans-isomeric chelate of Ni(II) with hydrazinomethanethioamide using different versions of DFT method. *Russian Journal of General Chemistry*, **2013**, 83, 911-914	0.7	9
160	Specifics of the molecular structures of "template" (5456)macrotetracyclic chelates of 3d M(II) Ions with 5,7,9-triimino-1-oxa-3,6,8,11-tetraazacyclododecane-4,10-dithione according to DFT calculations. *Russian Journal of Inorganic Chemistry*, **2013**, 58, 1203-1209	1.5	9
159	DFT B3LYP Quantum-Chemical Calculation of Molecular Structures of (6.6.6)-Macrotricyclic MII Comp-lexes with (N,N,N,N)-Coordinating Ligand Formed in the MII– Hydrazinomethanethiohydrazide–Propanone Triple Systems. *Macroheterocycles*, **2010**, 3, 171-175	2.2	9
158	DFT Quantum-Chemical Modeling Molecular Structures of Cobalt Macrocyclic Complexes with Porphyrazine or Its Benzo-Derivatives and Two Oxygen Acido Ligands. *International Journal of Molecular Sciences*, **2020**, 21,	6.3	9
157	On the molecular structures of (545)macrotricyclic chelates in the M(II) ion-2,3-butanedione-aminomethanamidine ternary systems. *Russian Journal of Inorganic Chemistry*, **2014**, 59, 101-106	1.5	8
156	Quantum-chemical calculation of the molecular structures of 3d metal chelates with ligands self-assembled in the M(II)-hydrazinomethane thiohydrazide-acetone systems. *Russian Journal of Inorganic Chemistry*, **2012**, 57, 1100-1106	1.5	8
155	Geometry and vibrational frequencies of the helical polypeptide complexes with ligand molecules. *International Journal of Quantum Chemistry*, **2011**, 111, 2525-2539	2.1	8
154	Molecular structures of asymmetric (555)macrotricyclic chelates formed in 3d metal ion-ethanedithioamide-hydrazinomethanethioamide-2,3-butanedione quaternary systems. *Russian Journal of Inorganic Chemistry*, **2015**, 60, 187-193	1.5	7
153	Study of p-(3-carboxy-1-adamantyl)-calix[4]arene with hydrogen bonds along the upper and lower rim by IR spectroscopy and DFT. *Journal of Molecular Modeling*, **2020**, 26, 179	2	7
152	DFT calculation of molecular structures of Al2Fe3 and Al2Cu3 heterobinuclear clusters. *Structural Chemistry*, **2018**, 29, 1543-1549	1.8	7
151	Structural peculiarities of macrocyclic chelates, products of self-assembly in the M(II) ion-2-amino-2-thioheptanoic acid-guanidine-formaldehyde system, as shown by quantum-chemical simulation. *Russian Journal of General Chemistry*, **2014**, 84, 315-319	0.7	7
150	On the possibility of template synthesis through "cross-linkage" of chelate rings with trans-arranged donor atoms in M(II)–ethandithioamide–formaldehyde systems. *Russian Journal of Inorganic Chemistry*, **2015**, 60, 1253-1257	1.5	7
149	Quantum-chemical simulation of structure of isomeric asymmetric (555)macrotricyclic chelates of 3d elements arising via self-assembly in quaternary systems metal(II)-ethanedithioamide-hydrazinomethanethioamide-ethanedial. *Russian Journal of General Chemistry*, **2014**, 84, 1962-1969	0.7	7

148	Stability of isomerous chelates in M(II)-thiocarbamoylmethanamide-ethandial systems according to the DFT B3LYP method (M = Mn, Fe, Co, Ni, Cu, Zn). *Russian Journal of Physical Chemistry A*, **2011**, 85, 1475-1477	0.7	7
147	Theoretical Study of the Tautomeric Reactions of Dinitromethane and Its Radical Cation. *Journal of Energetic Materials*, **2009**, 27, 263-295	1.6	7
146	Dipole moments, structure, and transannular interactions in silatranes containing planar fragments. *Russian Journal of General Chemistry*, **2008**, 78, 1350-1353	0.7	7
145	Possibility of template synthesis with junction of metallacycles containing trans-located nitrogen atoms in the 3d metal(II) ion-dithiooxamide-acetone systems as predicted by DFT simulation data. *Russian Journal of General Chemistry*, **2015**, 85, 628-633	0.7	6
144	Stabilization of unusual metal oxidation state +4 in the iron, cobalt, nickel, and copper complexes with trans-di[benzo]porphyrazine and two fluoride anions: a DFT quantum chemical analysis. *Russian Chemical Bulletin*, **2020**, 69, 893-898	1.7	6
143	Molecular structures of (5656)macrotetracyclic chelates in M(II) ion–ethanedithioamide–methanimine–hydrogen cyanide quaternary systems by DFT calculations. *Russian Journal of Inorganic Chemistry*, **2016**, 61, 616-622	1.5	6
142	Novel oxidation state of zinc(III) in chelate with 3,7,11,15-tetraazaporphine and one fluorine ligand: Quantum-chemical modeling. *Journal of Porphyrins and Phthalocyanines*, **2019**, 23, 685-689	1.8	6
141	Mutual stability and molecular structures of asymmetric (555)macrotricyclic 3d-metal chelates formed by self-assembly in M(II) ion-ethanedithioamide-hydrazinomethanethioamide-2-oxopropanal quaternary systems according to density functional theory calculations. *Russian Journal of Inorganic Chemistry*, **2014**, 59, 489-495	1.5	6
140	On template synthesis in the ternary system Ni(II)-thiosemicarbazide-diacetyl. *Russian Journal of Inorganic Chemistry*, **2013**, 58, 1518-1522	1.5	6
139	Molecular structures and stability of isomeric asymmetric (565)macrotricyclic chelates of 3d metals in the M(II)-dithiooxamide-thiosemicarbazide-formaldehyde systems according to DFT calculations. *Russian Journal of Inorganic Chemistry*, **2014**, 59, 1472-1479	1.5	6
138	Conformational analysis of secondary arylalkylphosphine selenides. *Russian Journal of Organic Chemistry*, **2012**, 48, 1320-1322	0.7	6
137	Conformational analysis of 2-substituted 1-nitro-and 1-bromo-1-nitroethenes. *Russian Journal of General Chemistry*, **2007**, 77, 894-898	0.7	6
136	Quantum-chemical calculations of (5.6.5)Macrotricyclic Complexes in Some MII (N,S)-Ambidentate Ligson (O)-Ligson Triple Systems. *Macroheterocycles*, **2010**, 3, 161-166	2.2	6
135	NOVEL OXIDATION DEGREE OF Zn+3 IN THE MACROCYCLIC COMPOUND WITH TRANS-DI[BENZO]PORPHYRAZINE AND FLUORIDE LIGAND: QUANTUM-CHEMICAL CONSIDERATION. *European Chemical Bulletin*, **2020**, 9, 160	0.5	6
134	Energy barriers to gas-phase unimolecular decomposition of mono- and dinitrotoluenes. *Russian Journal of Organic Chemistry*, **2016**, 52, 791-805	0.7	6
133	Models of molecular structures of aluminum–iron clusters AlFe3, Al2Fe3, and Al2Fe4 according to quantum-chemical DFT calculations. *Russian Journal of Inorganic Chemistry*, **2017**, 62, 336-343	1.5	5
132	Quantum-chemical modeling of template synthesis in the ternary system metal(II) ion-thiosemicarbazide-diacetyl. *Russian Journal of Inorganic Chemistry*, **2015**, 60, 964-969	1.5	5
131	Thermodynamics of Al2M3 (M = 3d Element) Metal Clusters in the Frame of DFT Quantum-Chemical Modeling. *Russian Journal of Inorganic Chemistry*, **2020**, 65, 646-649	1.5	5

130	Mechanism of the hydrolysis reactions of 1-hydroxysilatrane and 1-hydroxygermatrane, 2,2-dihydroxysilocane and 2,2-dihydroxygermocane. *Phosphorus, Sulfur and Silicon and the Related Elements*, **2016**, 191, 496-501	1	5
129	Polarity and structure of 2-(1-methylbenzimidazol-2-yl)-1-phenyl- and -1,2-diphenyl-1-nitroethenes. *Russian Journal of General Chemistry*, **2012**, 82, 911-920	0.7	5
128	Self-assembly and quantum chemical design of macrotricyclic and macrotetracyclic 3d-element metal chelates formed in the gelatin-immobilized matrix. *Russian Chemical Bulletin*, **2015**, 64, 1757-1771	1.7	5
127	Molecular structures of asymmetric (565)macrotricyclic chelates formed in 3d metal ion-ethanedithioamide-hydrazinomethanethioamide-propanone quaternary systems. *Russian Journal of Inorganic Chemistry*, **2015**, 60, 889-895	1.5	5
126	Polarity and structure of 1,3,5,11-tetraoxa-8-aza-4-germaspiro [3,7]undecan-2-one. *Russian Journal of Organic Chemistry*, **2014**, 50, 1225-1226	0.7	5
125	Quantum chemical calculation of the molecular structures of (666)macrotricyclic chelates of 3D elements in the M(II)-propanedithioamide-formaldehyde systems by the density functional theory method. *Russian Journal of Inorganic Chemistry*, **2014**, 59, 1283-1289	1.5	5
124	Geometric parameters of molecular structures of macrotricyclic chelates in MII ion–hydrazinomethane thioamide–butane-2,3-dione ternary systems (M = Co, Ni, Cu) according to the DFT B3LYP quantum chemical calculation. *Russian Chemical Bulletin*, **2012**, 61, 1531-1535	1.7	5
123	CuIV Oxidation State Stabilization in the Macrocyclic Compound With Phthalocyanine and Two Fluoro Ligands: DFT Quantum-Chemical Research. *European Chemical Bulletin*, **2020**, 9, 313	0.5	5
122	Quantum-chemical modeling of the molecular structures of (555)macrotricyclic chelates in M(II) ion–thiooxamide–glyoxal ternary systems (M = Mn, Fe, Co, Ni, Cu, Zn). *Russian Journal of Inorganic Chemistry*, **2016**, 61, 208-216	1.5	5
121	Effect of Nozzle Shape on Amplitude of Well Acoustic Emitter Generation. *Acoustical Physics*, **2018**, 64, 492-502	1.1	5
120	Quantum-chemical calculation of molecular structures of Al2Mn3 and Al2Zn3 clusters by using DFT method. *Structural Chemistry*, **2019**, 30, 1289-1299	1.8	4
119	Polarity and structure of 1,1-dihalo-2,8-dioxa-5-azagermocanes. *Russian Journal of Organic Chemistry*, **2015**, 51, 750-752	0.7	4
118	M(VI) Oxidation State Stabilization in Iron, Cobalt and Nickel Heteroligand Metal Chelates Containing 3,7,11,15-Tetraazaporphine and Two Axial Oxo Ligands: Quantum-Chemical Simulation. *International Journal of Molecular Sciences*, **2020**, 21,	6.3	4
117	DFT analysis of molecular structure of 14-membered tetraaza-, dioxotetraaza-, and hexaazamacroheterocyclic ligands and their metal complexes. *Russian Journal of General Chemistry*, **2016**, 86, 1102-1107	0.7	4
116	Experimental Study of a Borehole Acoustic Radiator with a Ring in a Long Cylindrical Chamber. *Acoustical Physics*, **2018**, 64, 237-244	1.1	4
115	Comparative stability of isomeric (565)macrotricyclic chelates of 3d-elements formed in the systems M(II)-thiosemicarbazide-formaldehyde according to DFT B3LYP data. *Russian Journal of General Chemistry*, **2013**, 83, 1123-1130	0.7	4
114	Mechanism of the reaction of 3,3-dimethyl-2-trimethylsiloxy-1-trimethylsilyl-1-phosphabut-1-ene with diethyl phosphite. *Russian Journal of General Chemistry*, **2012**, 82, 1951-1953	0.7	4
113	Conformational analysis of 4-methyl-2-trimethylsiloxy-1,3,2-dioxaphosphinane. *Russian Journal of Organic Chemistry*, **2012**, 48, 1326-1328	0.7	4

112	Computational Study of Main Mechanisms for Gas-Phase Decomposition of 1,1- and 1,2-Dinitroethane. *Journal of Energetic Materials*, **2010**, 28, 318-337	1.6	4
111	Empirical and ab initio calculations of thermochemical parameters of aminoacids: II. Diaminomonocarboxylic acids, hydroxyamino acids, thioamino acids, and heterocyclic amino(imino) acids. *Russian Journal of General Chemistry*, **2009**, 79, 1490-1493	0.7	4
110	Mechanism of Depolymerization of Polymeric p-Dinitrosobenzene in Vulcanization of Unsaturated Rubbers: A Quantum-Chemical Study. *Russian Journal of Applied Chemistry*, **2005**, 78, 315-318	0.8	4
109	Effect of Molecular Structure on the C-N Bond Strength in a Nitroalkane Series: I. Nitromethane, Fluoronitromethanes, Chloronitromethanes, and Fluorochloronitromethanes. *Russian Journal of General Chemistry*, **2001**, 71, 1449-1456	0.7	4
108	DFT study on the relative stability of isomeric macrocyclic metal chelates of divalent 4D-element ions with tetradentate (NSSN)- and (NNNN)- □emplate□ligands. *European Chemical Bulletin*, **2020**, 9, 329	0.5	4
107	Copper (IV) Stabilization in Macrocyclic Complexes with 3,7,11,15-Tetraazaporphine, Its Di[benzo]- or Tetra[benzo] Derivatives and Oxide Anion: Quantum-Chemical Research. *Materials*, **2020**, 13,	3.5	4
106	DFT Quantum-Chemical Calculations of Molecular Structures for Heteroligand M(III) Complexes of 3d Elements with Porphyrazine and Fluoride Ion. *Russian Journal of Inorganic Chemistry*, **2020**, 65, 887-892	1.5	4
105	Synthesis and conformational analysis of phosphine selenides. *Russian Journal of General Chemistry*, **2016**, 86, 590-601	0.7	4
104	Models of molecular structures of macrocyclic metal chelates in the ternary 4d M(II) ion□ethanedithioamide□ethanedial systems according to quantum-chemical DFT calculations. *Russian Journal of Inorganic Chemistry*, **2016**, 61, 1104-1110	1.5	4
103	Molecular structures of heteroligand ScIII complexes with porphyrazine, its dibenzo and tetrabenzo derivatives, and fluoride anion, as determined from DFT calculations. *Russian Chemical Bulletin*, **2021**, 70, 276-282	1.7	4
102	Polarity and structure of derivatives of bis(2-phenylethyl)selenophosphinic acid. *Pure and Applied Chemistry*, **2017**, 89, 393-401	2.1	3
101	Molecular structure of hexatomic heteronuclear (AlFe) metal clusters as determined by the DFT quantum-chemical calculation. *Russian Journal of General Chemistry*, **2017**, 87, 670-678	0.7	3
100	DFT quantum-chemical calculations of molecular structures for template heteroligand (5757)macrocyclic M(II) chelates of 3d elements with a 16-membered macrocyclic ligand and Br□ ions. *Russian Journal of Inorganic Chemistry*, **2017**, 62, 1191-1196	1.5	3
99	DFT Quantum Chemical Calculation of the Molecular Structures of the Metal Clusters Al2Cu3 and Al2Ag3. *Russian Journal of Inorganic Chemistry*, **2019**, 64, 79-87	1.5	3
98	Mechanism of Hydrolysis of 1,1,1-Trisubstituted Hyposilatranes and Hypogermatranes. *Russian Journal of Organic Chemistry*, **2019**, 55, 227-233	0.7	3
97	Molecular structures and thermodynamics of stable N4, N6 and N8 neutral poly-nitrogens according to data of QCISD(T)/TZVP method. *Chemical Physics Letters*, **2020**, 753, 137594	2.5	3
96	Mechanism of Reactions of 1-Substituted Silatranes and Germatranes, 2,2-Disubstituted Silocanes and Germocanes, 1,1,1-Trisubstituted Hyposilatranes and Hypogermatranes with Alcohols (Methanol, Ethanol): DFT Study. *Molecules*, **2020**, 25,	4.8	3
95	Quantum Chemical Calculation of Molecular Structures of Al2Fe2 and Al2FeCo Tetranuclear Metalloclusters. *Glass Physics and Chemistry*, **2017**, 43, 597-604	0.7	3

94	Alternative mechanisms of thermal decomposition of o-nitrotoluene in the gas phase. *Russian Chemical Bulletin*, **2018**, 67, 274-281	1.7	3
93	Models of molecular structure of heteronuclear clusters Al2Fe3, Al2Co3, and Al2Ni3 according to the data of quantum-chemical density functional simulation. *Russian Journal of General Chemistry*, **2016**, 86, 1991-1999	0.7	3
92	Dipole moments and conformational analysis of tris(2-pyridyl)phosphine and tris(2-pyridyl)phosphine chalcogenides. Experimental and theoretical study. *Journal of Molecular Structure*, **2014**, 1076, 285-290	3.4	3
91	Mechanism of the reaction of 3,3-dimethyl-1-trimethylsilyl-2-trimethylsiloxy-1-phosphabut-1-ene with chlorobis(o-phenylenedioxy)phosphorane. *Russian Journal of Organic Chemistry*, **2014**, 50, 608-610	0.7	3
90	Conformational analysis of arylphosphine selenides. *Russian Journal of Organic Chemistry*, **2013**, 49, 1709-1711	0.7	3
89	Molecular structure of the macrocyclic copper(II) chelate with 6,7,13,14-tetramethyl-3,10-dithio-1,2,4,5,8,9,11,12-octaazatetradecatetraene-1,5,7,11 according to quantum-chemical DFT calculations. *Russian Journal of General Chemistry*, **2013**, 83, 1937-1940	0.7	3
88	Modeling of molecular structures of (464)macrotricyclic chelates in ternary systems M(II) ion–mercaptomethanethioamide–formaldehyde. *Russian Journal of Inorganic Chemistry*, **2017**, 62, 948-954	1.5	3
87	Molecular structures of (575)macrotricyclic 3d-metal chelates in M(II)–N-methylthiocarbohydrazide–hexanedione-2,5 according to density functional theory calculations. *Russian Journal of Inorganic Chemistry*, **2017**, 62, 1366-1370	1.5	3
86	Molecular structures of macrotricyclic 4d M(II) chelates with the (NNNN)-donor ligand 2,7-dithio-3,6-diazaoctadiene-3,5-dithioamide-1,8 according to quantum-chemical density functional theory calculations. *Russian Journal of Inorganic Chemistry*, **2017**, 62, 450-456	1.5	3
85	Vibrational spectra and structure of isopropylbenzene. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2008**, 71, 1128-33	4.4	3
84	Mechanism of Hydrolysis of 2,2-Disubstituted Silocanes and Germocanes and 1-Substituted Silatranes and Germatranes. *Russian Journal of Organic Chemistry*, **2018**, 54, 490-499	0.7	3
83	Heteroligand complexes of chromium, manganese, and iron with trans-dibenzoporphyrazine and two oxo ligands: DFT calculations. *Russian Chemical Bulletin*, **2022**, 71, 656-664	1.7	3
82	Combination of phthalocyanine and fluoride ligand for Zn(III) stabilization: Quantum-chemical consideration. *Inorganic Chemistry Communication*, **2019**, 108, 107526	3.1	2
81	Models of Molecular Structures of Al2Cr3 and Al2Mo3 Metal Clusters according to Density Functional Theory Calculations. *Russian Journal of Inorganic Chemistry*, **2018**, 63, 786-799	1.5	2
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