Denis Chachkov

List of Publications by Year in Descending Order

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The third column is the impact factor (IF) of the journal, and the fourth column is the number of citations of the article.

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	Amendment to: Structural changes at complexing of 3d (4d) elements with "template" tetradentate ligand 1,8-diimino-1,8-dimercapto-3,6-diazaoctadien-3,5-dithione-2,7: DFT analysis. *Journal of Chemical Sciences*, **2022**, 134, 1	1.8	
200	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
199	Structural changes at complexing of 3d (4d) elements with template tetradentate ligand 1,8-diimino-1,8-dimercapto- 3,6-diazaoctadien-3,5-dithione-2,7: DFT analysis. *Journal of Chemical Sciences*, **2021**, 133, 1	1.8	
198	A new chemical compound with an unusual ratio of number of carbon and nitrogen atoms - C(N): quantum-chemical modelling.. *RSC Advances*, **2021**, 11, 35974-35981	3.7	1
197	Experimental and DFT investigation of structure and IR spectra of H-bonded associates of p-(3-carboxy-1-adamantyl)thiacalix[4]arene. *Journal of Molecular Modeling*, **2021**, 27, 135	2	
196	(H,H)-Isomerism of cis- and trans-di[benzo]porphyrazines: Quantum chemical modeling within the framework of the DFT method. *Journal of Porphyrins and Phthalocyanines*, **2021**, 25, 858-865	1.8	1
195	Models of Molecular Structures of Hexa-Nuclear AlFe Metal Clusters (n + m = 6): DFT Quantum-Chemical Design. *Materials*, **2021**, 14,	3.5	1
194	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
193	Molecular Structures of Heteroligand Macrotetracyclic Complexes of 3d Ions with Phthalocyanine and Fluoride Anion Studied by Density Functional Theory. *Russian Journal of Physical Chemistry A*, **2021**, 95, 310-316	0.7	
192	Radical character of non-IPR isomer 17418 (C1) of fullerene C76. *Fullerenes Nanotubes and Carbon Nanostructures*, **2021**, 29, 678-684	1.8	1
191	Heteroligand macrotetracyclic complexes of 3d elements with phthalocyanine and two fluoride anions: molecular structures and thermodynamic parameters, as determined from DFT calculations. *Russian Chemical Bulletin*, **2021**, 70, 1438-1445	1.7	1
190	Conformational Analysis of -Alkyl--[2-(diphenylphosphoryl)ethyl]amides of Diphenylphosphorylacetic Acid: Dipole Moments, IR Spectroscopy, DFT Study. *Molecules*, **2021**, 26,	4.8	2
189	Polarity and Conformational Analysis of Tri(1-naphthyl)phosphine, Tri(2-naphthyl)phosphine, and Their Chalcogenides. *Russian Journal of Organic Chemistry*, **2021**, 57, 1245-1255	0.7	
188	Study of p-(3-carboxymethyl-1-adamantyl)calix[4]arene and tetrapropoxy-p-(3-carboxymethyl-1-adamantyl)calix[4]arene by vibrational spectroscopy and DFT. *Journal of Molecular Structure*, **2021**, 1239, 130508	3.4	
187	Conformational Analysis of Dibutylphosphorylacetic Acid N,N-Dibutylamide in Solution. *Russian Journal of General Chemistry*, **2021**, 91, 2581-2587	0.7	
186	The decay mechanism of 1,1,2,2-tetranitroxyethane according to theoretical calculations. *Journal of Physics: Conference Series*, **2020**, 1658, 012007	0.3	
185	The effect of molecular structure on the O NO2 bond dissociation energy and the activation energy of the radical decay of cellotriose nitrates. *Journal of Physics: Conference Series*, **2020**, 1658, 012026	0.3	

184	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
183	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
182	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
181	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
180	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
179	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
178	About of Possibility of Existence of Zn(IV) Oxidation State in Heteroligand Complexes with Porphyrazine, trans-Di[benzo]porphyrazine, Phthalocyanine, and Oxo Ligands: Quantum-Chemical Review. *Comments on Inorganic Chemistry*, **2020**, 40, 107-115	3.9	1
177	Quantum-Chemical Design of Molecular Structures of Tetra-, Penta- and Hexanuclear Metal Clusters Containing Aluminum and 3-Element Atoms. *Materials*, **2020**, 13,	3.5	1
176	Experimental and Theoretical Conformational Analysis of Tris(4-methylphenyl)phosphine and Its Chalcogenides. *Russian Journal of Organic Chemistry*, **2020**, 56, 2098-2103	0.7	1
175	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
174	MOLECULAR STRUCTURE MODELS OF Al2Ti3 AND Al2V3 CLUSTERS ACCORDING TO DFT QUANTUM-CHEMICAL CALCULATION. *European Chemical Bulletin*, **2020**, 9, 62	0.5	13
173	Novel modifications of elemental nitrogen and their molecular structures – a quantumchemical calculation. *European Chemical Bulletin*, **2020**, 9, 78	0.5	11
172	NOVEL OXIDATION DEGREE – 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
171	DFT study on the relative stability of isomeric macrocyclic metal chelates of divalent 4D-element ions with tetradentate (NSSN)- and (NNNN)- “template” ligands. *European Chemical Bulletin*, **2020**, 9, 329	0.5	4
170	Quantum Chemical Study of the Addition of Secondary Phosphine Chalcogenides to Vinyl Selenides. *Russian Journal of Organic Chemistry*, **2020**, 56, 1696-1701	0.7	
169	Tetra-, hexa-, and octanitrogen molecules: a quantum chemical design and thermodynamic properties. *Russian Chemical Bulletin*, **2020**, 69, 2067-2072	1.7	1
168	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
167	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

166	Density Functional Theory Modeling of Molecular Structures of Heteroligand 3d M(IV) Complexes with Porphyrazine and Oxo Anion. *Russian Journal of Inorganic Chemistry*, **2020**, 65, 1019-1024	1.5	2
165	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
164	3d-Unusual Macrotetracyclic Chelates of 3d Elements with a 17-Membered Macrocyclic Ligand and Their Molecular Structures in Terms of DFT Quantum-Chemical Simulation. *Russian Journal of Inorganic Chemistry*, **2020**, 65, 81-87	1.5	0
163	Combination of phthalocyanine and fluoride ligand for Zn(III) stabilization: Quantum-chemical consideration. *Inorganic Chemistry Communication*, **2019**, 108, 107526	3.1	2
162	Quantum-chemical calculation of molecular structures of Al2Mn3 and Al2Zn3 clusters by using DFT method. *Structural Chemistry*, **2019**, 30, 1289-1299	1.8	4
161	Quantum-Chemical DFT Calculation of the Molecular Structures of Template Heteroligand (6666)Macrotetracyclic 3d M(II) Chelates with a 16-Membered Macrocyclic Ligand and Cl Ions. *Russian Journal of Inorganic Chemistry*, **2019**, 64, 628-636	1.5	
160	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
159	Mechanism of Hydrolysis of 1,1,1-Trisubstituted Hyposilatranes and Hypogermatranes. *Russian Journal of Organic Chemistry*, **2019**, 55, 227-233	0.7	3
158	Transition state structure of the reaction of homolytic dissociation of the C-N bond and competition between dif erent mechanisms of the primary act of gas-phase monomolecular decomposition of nitrobenzene. *Russian Chemical Bulletin*, **2019**, 68, 1510-1519	1.7	2
157	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
156	Polarity and Structure of Se-Esters of Diselenophosphinic Acids: Experimental and Theoretical Conformational Analysis in Solution. *Russian Journal of General Chemistry*, **2019**, 89, 929-938	0.7	
155	DFT Quantum-Chemical Calculation of the Molecular Structures of (5665)Macrotetracyclic Chelates in the M(II) 4,5-Diaminoacridone 2-[(2-Formylphenyl)amino]benzenecarbaldehyde Systems (M = Mn, Fe, Co, Ni, Cu, Zn). *Russian Journal of Inorganic Chemistry*, **2019**, 64, 230-236	1.5	
154	Structural Changes in Macrocycles of Tetrathio-Substituted 1,8-Dioxa-, 1,8-Dithia-3,6,10,13-Tetraazacyclotetradecane and 1,3,5,8,10,12-Hexaazacyclotetradecane upon the Complexation with 3d M(II) Ions according to Density Functional Theory Calculations. *Russian Journal of Inorganic Chemistry*, **2019**, 64, 496-502	1.5	1
153	Novel oxidation state 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
152	Alternative mechanisms of thermal decomposition of o-nitrotoluene in the gas phase. *Russian Chemical Bulletin*, **2018**, 67, 274-281	1.7	3
151	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
150	DFT calculation of molecular structures of Al2Fe3 and Al2Cu3 heterobinuclear clusters. *Structural Chemistry*, **2018**, 29, 1543-1549	1.8	7
149	Experimental Study of a Borehole Acoustic Radiator with a Ring in a Long Cylindrical Chamber. *Acoustical Physics*, **2018**, 64, 237-244	1.1	4

148	Structural Changes in the Macrocycles of Tetrathioand Dithiodioxo-Substituted 1,8-Dioxa-3,6,10,13-tetraazacyclotetradecane Caused by Complexation with 3d M(II) Ions according to Quantum-Chemical DFT Calculation. *Russian Journal of Inorganic Chemistry*, **2018**, 63, 911-916	1.5	
147	Molecular Structures of (5454)Macrotetracyclic 3d M(II) Chelates Forming in Ternary Systems M(II)–1,2-Ethandiamine–Trioxosulfidosulfate(VI) Anion According to DFT Data. *Russian Journal of Inorganic Chemistry*, **2018**, 63, 1199-1203	1.5	
146	Molecular Structures of Tetranuclear (Al, Fe) Metal Clusters. *Glass Physics and Chemistry*, **2018**, 44, 339-345	0.7	2
145	Conformational Analysis of Tris(3-methylphenyl)phosphine and Its Chalcogenides. *Russian Journal of General Chemistry*, **2018**, 88, 2251-2256	0.7	2
144	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
143	Effect of Nozzle Shape on Amplitude of Well Acoustic Emitter Generation. *Acoustical Physics*, **2018**, 64, 492-502	1.1	5
142	Models of Molecular Structures of Template (5676)Macrotetracyclic 3d M(II) Chelates with a 16-Membered Macrocyclic Ligand according to Density Functional Theory Data. *Russian Journal of Inorganic Chemistry*, **2018**, 63, 1056-1061	1.5	
141	Polarity and structure of derivatives of bis(2-phenylethyl)selenophosphinic acid. *Pure and Applied Chemistry*, **2017**, 89, 393-401	2.1	3
140	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
139	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
138	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
137	Quantum Chemical Calculation of Molecular Structures of Al2Fe2 and Al2FeCo Tetranuclear Metalloclusters. *Glass Physics and Chemistry*, **2017**, 43, 597-604	0.7	3
136	On the possibility of the existence of molecular nitrogen allotropes. *Russian Journal of Inorganic Chemistry*, **2017**, 62, 955-959	1.5	1
135	Energy barriers to gas-phase unimolecular decomposition of trinitrotoluenes. *Russian Journal of Organic Chemistry*, **2017**, 53, 999-1011	0.7	2
134	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
133	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
132	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
131	Molecular structures of (454)macrotricyclic chelates in the M(II) ion–thiosulfate anion–ethylenediamine systems according to quantum-chemical DFT calculations. *Russian Journal of Inorganic Chemistry*, **2017**, 62, 1614-1618	1.5	2

130	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
129	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
128	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
127	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
126	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
125	DFT OPBE/TZVP ~~al~~culation 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
124	Polarity and structure of P(X)-modified (X = O, S) arylcarbamoylmethylphosphine oxides and sulfides. *Russian Journal of Organic Chemistry*, **2016**, 52, 1413-1418	0.7	2
123	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
122	Synthesis and conformational analysis of phosphine selenides. *Russian Journal of General Chemistry*, **2016**, 86, 590-601	0.7	4
121	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
120	Energy barriers to gas-phase unimolecular decomposition of mono- and dinitrotoluenes. *Russian Journal of Organic Chemistry*, **2016**, 52, 791-805	0.7	6
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	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
117	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
116	Mechanism of the Reactions of (2,2-Dimethyl-1-((Trimethylsilyl)Oxy)Propylidene)-(Trimethylsilyl)Phosphine with Nucleophilic and Electrophilic Reagents. *Phosphorus, Sulfur and Silicon and the Related Elements*, **2015**, 190, 918-921	1	0
115	Effect of molecular structure of nitroalkanes on the C-NO2 bond strength and activation energy of the gas-phase radical decomposition according to the quantum-chemical simulation. *Russian Journal of General Chemistry*, **2015**, 85, 1801-1807	0.7	0
114	Phosphoryl- and thiophosphoryl-functionalized enamino ketones. Polarity and conformational analysis. *Russian Journal of Organic Chemistry*, **2015**, 51, 1264-1267	0.7	
113	Dipole moments and quantum chemical study of the structure of furan-containing gem-bromonitroethenes. *Russian Journal of Organic Chemistry*, **2015**, 51, 1282-1285	0.7	

112	Synthesis, polarity, and structure of 2-chloro-N-[2-(methylsulfanyl)phenyl]- and 2-(diphenylthiophosphoryl)-N-[2-(methylsulfanyl)phenyl]acetamides. *Russian Journal of Organic Chemistry*, **2015**, 51, 943-946	0.7	1
111	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
110	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
109	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
108	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
107	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
106	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
105	Conformational Analysis of 2-Chloro-N-[2-((Diphenylphosphoryl)Methyl)Phenyl]-Acetamide and 2-Chloro-N-[2-((Diphenylthiophosphoryl)Methyl)Phenyl]Acetamide. *Phosphorus, Sulfur and Silicon and the Related Elements*, **2015**, 190, 803-805	1	1
104	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
103	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
102	Conformational analysis of 2-aminophenyl-, 2-aminobenzyl-, and 2-nitrobenzyl(diphenyl)phosphine oxides. *Russian Journal of Organic Chemistry*, **2014**, 50, 796-799	0.7	1
101	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*	1.5	23
100	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
99	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
98	Quantum-chemical study of the reaction of 2-methylbenzo[d][1,3,2]dioxaphosphinin-4(4H)-one with hexafluoroacetonimine. *Russian Journal of General Chemistry*, **2014**, 84, 969-970	0.7	1
97	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
96	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
95	(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

94	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
93	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
92	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
91	Study of the structure of 1-nitro-3,3,3-trifluoro- and 1-nitro-3,3,3-tribromopropenes by the methods of dipole moments and quantum chemistry. *Russian Journal of Organic Chemistry*, **2014**, 50, 1562-1564	0.7	1
90	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
89	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
88	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
87	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
86	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
85	Calix[4]resorcinols bearing □-aminoacetal groups on the upper rim. Synthesis and properties. *Russian Journal of General Chemistry*, **2013**, 83, 319-324	0.7	2
84	Molecular structures of metalmacrocyclic chelates of 3d-elements formed at template synthesis in the ion M(II)- thiooxamide-guanidine-formaldehyde quaternary systems. *Open Chemistry*, **2013**, 11, 1822-1829	1.6	1
83	Theoretical study of the structure of N-arylmaleimides and bis-maleimides. *Russian Journal of Organic Chemistry*, **2013**, 49, 1482-1485	0.7	
82	Polarity and structure of □-nitrocinnamic acid esters. *Russian Journal of General Chemistry*, **2013**, 83, 1771-1774	0.7	
81	Polarity and structure of diphosphorus-substituted isoxazole and 1,2,3-triazole. *Russian Journal of Organic Chemistry*, **2013**, 49, 1369-1372	0.7	2
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