

# Sergei Katsyuba

## List of Publications by Year in descending order

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167  
papers

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171  
docs citations

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times ranked

3721  
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#	ARTICLE	IF	CITATIONS
1	Application of Density Functional Theory and Vibrational Spectroscopy Toward the Rational Design of Ionic Liquids. <i>Journal of Physical Chemistry A</i> , 2007, 111, 352-370.	1.1	238
2	Molecular Structure, Vibrational Spectra, and Hydrogen Bonding of the Ionic Liquid 1-Ethyl-3-methyl-1H-imidazolium Tetrafluoroborate. <i>Helvetica Chimica Acta</i> , 2004, 87, 2556-2565.	1.0	197
3	Ab Initio and DFT Predictions of Infrared Intensities and Raman Activities. <i>Journal of Physical Chemistry A</i> , 2011, 115, 63-69.	1.1	132
4	How Strong Is Hydrogen Bonding in Ionic Liquids? Combined X-ray Crystallographic, Infrared/Raman Spectroscopic, and Density Functional Theory Study. <i>Journal of Physical Chemistry B</i> , 2013, 117, 9094-9105.	1.2	130
5	Intricacies of Cation-Anion Combinations in Imidazolium Salt-Catalyzed Cycloaddition of CO <sub>2</sub> Into Epoxides. <i>ACS Catalysis</i> , 2018, 8, 2589-2594.	5.5	129
6	Revisiting Ether-Derivatized Imidazolium-Based Ionic Liquids. <i>Journal of Physical Chemistry B</i> , 2007, 111, 10095-10108.	1.2	121
7	A Rhodium Nanoparticle-Lewis Acidic Ionic Liquid Catalyst for the Chemoselective Reduction of Heteroarenes. <i>Angewandte Chemie - International Edition</i> , 2016, 55, 292-296.	7.2	112
8	Bipyridine and phenanthroline IR-spectral bands as indicators of metal spin state in hexacoordinated complexes of Fe(II), Ni(II) and Co(II). <i>Dalton Transactions</i> , 2013, 42, 1787-1797.	1.6	82
9	Enhanced Conversion of Carbohydrates to the Platform Chemical 5-Hydroxymethylfurfural Using Designer Ionic Liquids. <i>ChemSusChem</i> , 2014, 7, 1647-1654.	3.6	65
10	Synthesis of novel pyridyl containing phospholanes and their polynuclear luminescent copper(I) complexes. <i>Dalton Transactions</i> , 2016, 45, 2250-2260.	1.6	63
11	A remarkable anion effect on palladium nanoparticle formation and stabilization in hydroxyl-functionalized ionic liquids. <i>Physical Chemistry Chemical Physics</i> , 2012, 14, 6026.	1.3	59
12	Structural Studies of the Ionic Liquid 1-Ethyl-3-methylimidazolium Tetrafluoroborate in Dichloromethane Using a Combined DFT-NMR Spectroscopic Approach. <i>Journal of Physical Chemistry B</i> , 2009, 113, 5046-5051.	1.2	55
13	Scaled quantum mechanical computations of vibrational spectra of organoelement molecules, containing the atoms P, S, and Cl. <i>Chemical Physics Letters</i> , 2003, 377, 658-662.	1.2	53
14	DFT study of substitution effect on the geometry, IR spectra, spin state and energetic stability of the ferrocenes and their pentaphospholyl analogues. <i>Journal of Organometallic Chemistry</i> , 2010, 695, 2586-2595.	0.8	49
15	Vibrational spectra, co-operative intramolecular hydrogen bonding and conformations of calix[4]arene and thiacalix[4]arene molecules and their para-tert-butyl derivatives. <i>Organic and Biomolecular Chemistry</i> , 2005, 3, 2558.	1.5	41
16	Zn and Co redox active coordination polymers as efficient electrocatalysts. <i>Dalton Transactions</i> , 2019, 48, 3601-3609.	1.6	41
17	Vibrational spectra and conformational isomerism of calixarene building blocks. Part I. Diphenylmethane, (C <sub>6</sub> H <sub>5</sub> ) <sub>2</sub> CH <sub>2</sub> . <i>Journal of Molecular Structure</i> , 2001, 559, 315-320.	1.8	40
18	Phosphonium ionic liquids based on bulky phosphines: synthesis, structure and properties. <i>Dalton Transactions</i> , 2010, 39, 5564.	1.6	39

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19	Quantification of Conventional and Nonconventional Charge-Assisted Hydrogen Bonds in the Condensed and Gas Phases. <i>Journal of Physical Chemistry Letters</i> , 2015, 6, 4431-4436.	2.1	39
20	Synthesis, structure, and transition metal complexes of amphiphilic 1,5-diaza-3,7-diphosphacyclooctanes. <i>Heteroatom Chemistry</i> , 2006, 17, 499-513.	0.4	36
21	Synthesis and structure of ferrocenylphosphinic acids. <i>Journal of Organometallic Chemistry</i> , 2014, 766, 40-48.	0.8	36
22	Cooperative intramolecular hydrogen bond and conformations of thioalix[4]arene molecules. <i>Russian Chemical Bulletin</i> , 2002, 51, 825-827.	0.4	35
23	Complex Formation of $\text{Tb}^{\text{III}}$ -Doped Silica Nanoparticles as a Basis of Substrate-Responsive $\text{Tb}^{\text{III}}$ -Centered Luminescence. <i>ChemPhysChem</i> , 2012, 13, 3357-3364.	1.0	35
24	Reversible Water-Induced Structural and Magnetic Transformations and Selective Water Adsorption Properties of Poly(manganese 1,1'-ferrocenediyl-bis(H-phosphinate)). <i>Crystal Growth and Design</i> , 2016, 16, 5084-5090.	1.4	34
25	The Assembly of Unique Hexanuclear Copper(I) Complexes with Effective White Luminescence. <i>Inorganic Chemistry</i> , 2019, 58, 1048-1057.	1.9	34
26	Mass Spectrometric and Theoretical Study of Polyiodides: The Connection between Solid State, Solution, and Gas Phases. <i>Inorganic Chemistry</i> , 2011, 50, 9728-9733.	1.9	33
27	Is There a Simple Way to Reliable Simulations of Infrared Spectra of Organic Compounds?. <i>Journal of Physical Chemistry A</i> , 2013, 117, 6664-6670.	1.1	33
28	Unexpected ligand effect on the catalytic reaction rate acceleration for hydrogen production using biomimetic nickel electrocatalysts with 1,5-diaza-3,7-diphosphacyclooctanes. <i>Journal of Organometallic Chemistry</i> , 2015, 789-790, 14-21.	0.8	31
29	Conjugation in and Optical Properties of 1,1'-2-Diphospholes and 1,1'-Phospholes. <i>Journal of Physical Chemistry A</i> , 2014, 118, 12168-12177.	1.1	30
30	Composite materials containing chromophores with 3,7-(di)vinylquinoxalinone $\pi$ -electron bridge doped into PMMA: Atomistic modeling and measurements of quadratic nonlinear optical activity. <i>Dyes and Pigments</i> , 2018, 158, 131-141.	2.0	29
31	Rationalization of Solvation and Stabilization of Palladium Nanoparticles in Imidazolium-Based Ionic Liquids by DFT and Vibrational Spectroscopy. <i>ChemPhysChem</i> , 2012, 13, 1781-1790.	1.0	27
32	High thermally stable $\pi$ -A chromophores with quinoxaline moieties in the conjugated bridge: Synthesis, DFT calculations and physical properties. <i>Dyes and Pigments</i> , 2018, 156, 175-184.	2.0	27
33	Fresh Look on the Nature of Dual-Band Emission of Octahedral Copper-Iodide Clusters—Promising Ratiometric Luminescent Thermometers. <i>Journal of Physical Chemistry C</i> , 2019, 123, 25863-25870.	1.5	26
34	Fast Quantum Chemical Simulations of Infrared Spectra of Organic Compounds with the B97-3c Composite Method. <i>Journal of Physical Chemistry A</i> , 2019, 123, 3802-3808.	1.1	26
35	Calorimetric and spectroscopic studies on solvation energetics for $\text{H}_2$ storage in the $\text{CO}_2/\text{HCOOH}$ system. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 10764-10773.	1.3	25
36	Application of Time-Dependent Density Functional Theory and Optical Spectroscopy toward the Rational Design of Novel 3,4,5-Triaryl-1-R-1,2-diphospholes. <i>Journal of Physical Chemistry A</i> , 2013, 117, 6827-6834.	1.1	24

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37	Delineation of the Critical Parameters of Salt Catalysts in the N-Formylation of Amines with CO <sub>2</sub> . Chemistry - A European Journal, 2019, 25, 11074-11079.	1.7	24
38	Solvation of Palladium Clusters in an Ionic Liquid: A QM/MM Molecular Dynamics Study. Journal of Physical Chemistry C, 2016, 120, 4596-4604.	1.5	23
39	Push-pull isomeric chromophores with vinyl- and divinylquinoxaline-2-one units as $\pi$ -electron bridge: Synthesis, photophysical, thermal and electro-chemical properties. Dyes and Pigments, 2017, 146, 82-91.	2.0	23
40	High-temperature spin-crossover in coordination compounds of iron(II) with tris(pyrazol-1-yl)methane. Inorganica Chimica Acta, 2010, 363, 4059-4064.	1.2	22
41	Solvation and stabilization of palladium nanoparticles in phosphonium-based ionic liquids: a combined infrared spectroscopic and density functional theory study. Physical Chemistry Chemical Physics, 2014, 16, 20672-20680.	1.3	22
42	Novel amphiphilic conjugates of p-tert-butylthiacalix[4]arene with 10,12-pentacosadiynoic acid in 1,3-alternate stereoisomeric form. Synthesis and chromatic properties in the presence of metal ions. New Journal of Chemistry, 2018, 42, 2942-2951.	1.4	22
43	Large nonlinear optical activity of chromophores with divinylquinoxaline conjugated $\pi$ -bridge. Journal of Photochemistry and Photobiology A: Chemistry, 2019, 370, 58-66.	2.0	22
44	Synthesis and Stereoselective Interconversion of Chiral 1,3,6,8-tetraphosphacycloheptanes. European Journal of Inorganic Chemistry, 2012, 2012, 1857-1866.	1.0	21
45	Novel quinoxalinone-based push-pull chromophores with highly sensitive emission and absorption properties towards small structural modifications. Physical Chemistry Chemical Physics, 2018, 20, 21515-21527.	1.3	21
46	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.	1.7	20
47	Intriguing Near-Infrared Solid-State Luminescence of Binuclear Silver(I) Complexes Based on Pyridylphospholane Scaffolds. Inorganic Chemistry, 2019, 58, 7698-7704.	1.9	20
48	Vibrational spectra, conformations and force constants of dialkylphosphites (RO) <sub>2</sub> P(O)H. Journal of Molecular Structure, 1992, 269, 1-21.	1.8	19
49	$\pi$ -host-guest-binding of a luminescent dinuclear Au( <sup>sc</sup> ) complex based on cyclic diphosphine with organic substrates as a reason for luminescence tuneability. New Journal of Chemistry, 2016, 40, 9853-9861.	1.4	19
50	Fast and Accurate Quantum Chemical Modeling of Infrared Spectra of Condensed-Phase Systems. Journal of Physical Chemistry B, 2020, 124, 6664-6670.	1.2	18
51	The hydrogen bonding and tautomerism of pyrimidine containing macrocycles. IR, UV and quantum chemical studies. Journal of Molecular Structure, 2004, 707, 1-9.	1.8	16
52	Pyridyl Containing 1,5-Diaza-3,7-diphosphacyclooctanes as Bridging Ligands for Dinuclear Copper(I) Complexes. Zeitschrift Fur Anorganische Und Allgemeine Chemie, 2017, 643, 895-902.	0.6	16
53	Novel water soluble cationic Au(I) complexes with cyclic PNNP ligand as building blocks for heterometallic supramolecular assemblies with anionic hexarhenium cluster units. Journal of Luminescence, 2018, 196, 485-491.	1.5	16
54	Isomeric indolizine-based $\pi$ -expanded push-pull NLO-chromophores: Synthesis and comparative study. Journal of Molecular Structure, 2018, 1156, 74-82.	1.8	16

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55	Revisiting conformations of methyl lactate in water and methanol. <i>Journal of Chemical Physics</i> , 2021, 155, 024507.	1.2	16
56	Conformations and coordination properties of trialkyltrithiophosphites in copper(I) complexes. <i>Journal of Molecular Structure</i> , 2000, 554, 127-140.	1.8	15
57	A simple physical model for the simultaneous rationalisation of melting points and heat capacities of ionic liquids. <i>Physical Chemistry Chemical Physics</i> , 2010, 12, 13780.	1.3	15
58	The Molecular Design of "Carcass"-Type Phosphoranes, Based on the Reaction of P(III)-Cyclic Derivatives and Unsaturated Activated Compounds. <i>Phosphorus, Sulfur and Silicon and the Related Elements</i> , 2011, 186, 652-656.	0.8	15
59	Efficient synthesis and structure peculiarity of macrocycles with bi-indolizinyloquinoline moieties. <i>Tetrahedron</i> , 2013, 69, 10675-10687.	1.0	15
60	Infrared and Raman bands of cyclopentadienyl ligands as indicators of electronic configuration of metal centers in metallocenes. <i>Journal of Organometallic Chemistry</i> , 2015, 776, 30-34.	0.8	15
61	One-pot synthesis of aryl-substituted 1,2,3-triphospholide anions. <i>Journal of Organometallic Chemistry</i> , 2017, 844, 1-7.	0.8	14
62	IR and UV study of reversible water-induced structural transformations of poly(manganese) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50 467 To of <i>Journal of Molecular Structure</i> , 2018, 1166, 237-242.	1.8	14
63	Supramolecular Organization of Solid Azobenzene Chromophore Disperse Orange 3, Its Chloroform Solutions, and PMMA-Based Films. <i>Journal of Physical Chemistry C</i> , 2018, 122, 1779-1785.	1.5	13
64	Nonlinear optical activity of push-pull indolizine-based chromophores with various acceptor moieties. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2018, 364, 764-772.	2.0	13
65	To what extent are the photophysical properties of quinoxaline- and quinoxalinone-based chromophores predictable?. <i>Dyes and Pigments</i> , 2019, 170, 107580.	2.0	13
66	Vibrational spectra and conformational isomerism of calixarene building blocks. III. 2,6-Dimethylanisole and n-propyl-2,6-dimethylphenyl ether. <i>Journal of Molecular Structure</i> , 2002, 610, 113-125.	1.8	12
67	Vibrational spectra and conformational isomerism of calixarene building blocks: 2-benzylphenol Part IV. For Parts I-III see refs. 1-3. <i>Organic and Biomolecular Chemistry</i> , 2003, 1, 714-719.	1.5	12
68	Binding energies, vibrations and structural characteristics of small polyphosphorus molecules from quantum chemical computations. <i>Dalton Transactions</i> , 2005, , 1701.	1.6	12
69	Comparative Study of Conjugational Effects in 3,4,5-Triaryl-1,2-Diphospholes and 3,4,5-Triaryl-1,2-Diphosphacyclopentadienide-Anions. <i>Phosphorus, Sulfur and Silicon and the Related Elements</i> , 2015, 190, 858-862.	0.8	12
70	Computer-aided simulation of infrared spectra of ethanol conformations in gas, liquid and in CCl <sub>4</sub> solution. <i>Journal of Computational Chemistry</i> , 2022, 43, 279-288.	1.5	12
71	The role of London dispersion interactions in strong and moderate intermolecular hydrogen bonds in the crystal and in the gas phase. <i>Chemical Physics Letters</i> , 2017, 672, 124-127.	1.2	11
72	Benzimidazolylquinoxalines: novel fluorophores with tuneable sensitivity to solvent effects. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 6095-6104.	1.3	11

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73	Synthesis, spatial and electronic structure of 1-(+)-neomenthyl-1,2-diphosphole and 1-(+)-neomenthyl-1,2,4-triphosphole tungstenpentacarbonyl complexes. <i>Journal of Organometallic Chemistry</i> , 2018, 867, 125-132.	0.8	11
74	Novel enantiopure monophospholes: synthesis, spatial and electronic structure, photophysical characteristics and conjugation effects. <i>Dalton Transactions</i> , 2018, 47, 11521-11529.	1.6	11
75	Silica nanoparticles with dual visible-NIR luminescence affected by silica confinement of Tb(III) and Yb(III) complexes for cellular imaging application. <i>Journal of Materials Science</i> , 2019, 54, 9140-9154.	1.7	11
76	Synthesis, structure, and electrochemical properties of 4,5-diaryl-1,2,3-triphosphaferrocenes and the first example of multi(phosphaferrocene). <i>Dalton Transactions</i> , 2020, 49, 17252-17262.	1.6	11
77	Triple-bridged helical binuclear copper( $\mu_3$ ) complexes: Head-to-head and head-to-tail isomerism and the solid-state luminescence. <i>Dalton Transactions</i> , 2020, 49, 11997-12008.	1.6	11
78	Synthesis, IR/Raman, and quantum-chemical structural analysis of new octathiotetraphosphetane ammonium salts. <i>Heteroatom Chemistry</i> , 2011, 22, 24-30.	0.4	10
79	Synthesis and structure of the iron(III) tris-chelate complex based on 1,1'-ferrocenediylbis(phenylphosphinic acid). <i>Russian Chemical Bulletin</i> , 2015, 64, 1819-1822.	0.4	10
80	Conjugation effects and optical spectra of 1,2-diphosphole cycloadducts. <i>Russian Chemical Bulletin</i> , 2015, 64, 1896-1900.	0.4	10
81	The influence of different substituents on the geometrical changes in the heterocyclic moiety of 1,2-diphospholes. <i>Phosphorus, Sulfur and Silicon and the Related Elements</i> , 2016, 191, 1646-1649.	0.8	10
82	Acid-Catalyzed Rearrangements of 3-Aryloxirane-2-Carboxamides: Novel DFT Mechanistic Insights. <i>ChemistryOpen</i> , 2020, 9, 743-747.	0.9	10
83	Principal Descriptors of Ionic Liquid Co-catalysts for the Electrochemical Reduction of CO <sub>2</sub> . <i>ACS Applied Energy Materials</i> , 2020, 3, 4690-4698.	2.5	10
84	13,17,53,57-Tetraphenyl-13,17,53,57-tetrathio-3,7-dithia-1,5(1,5)-di(1,5-diaza-3,7-diphosphacyclooctana)-2,4,6,8(1,4)-tetrabenzenacyclooctane with an unusual conical-like conformation. <i>Journal of Inclusion Phenomena and Macrocyclic Chemistry</i> , 2008, 60, 321-328.	1.6	9
85	IR and Raman spectra, hydrogen bonds, and conformations of N-(2-hydroxyethyl)-4,6-dimethyl-2-oxo-1,2-dihydropyrimidine (drug Xymedone). <i>Russian Chemical Bulletin</i> , 2012, 61, 1199-1206.	0.4	9
86	Theoretical study of the excited state properties of luminescent phospholes. <i>Dyes and Pigments</i> , 2019, 164, 363-371.	2.0	9
87	Indolizine-based chromophores with octatetraene $\pi$ -bridge and tricyanofurane acceptor: Synthesis, photophysical, electrochemical and electro-optic properties. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2020, 386, 112125.	2.0	9
88	Energetics of intramolecular hydrogen bonds and conformations of $\hat{A}$ -diphenylphosphoryl- and $\hat{A}$ -diphenylthiophosphoryl-substituted aliphatic alcohol molecules. <i>Russian Chemical Bulletin</i> , 2004, 53, 55-59.	0.4	8
89	Variable temperature IR spectroscopy and quantum chemistry as the tool for diagnostics of metal spin state. <i>Chemical Physics Letters</i> , 2010, 495, 50-54.	1.2	8
90	Synthesis and magnetic properties of manganese carbonyl complexes with different coordination modes of 3,4,5-triaryl-1,2-diphospholide ligands. <i>Dalton Transactions</i> , 2015, 44, 10259-10266.	1.6	8

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91	Synthesis and photophysical properties of 2,3,4,5-tetraphenyl-1-n-octyl-1-monophosphole. Russian Chemical Bulletin, 2019, 68, 445-448.	0.4	8
92	D- $\pi$ -A' $\pi$ -A chromophores with quinoxaline core in the $\pi$ -electron bridge and charged heterocyclic acceptor moiety: Synthesis, DFT calculations, photophysical and electro-chemical properties. Journal of Photochemistry and Photobiology A: Chemistry, 2021, 407, 113042.	2.0	8
93	IR and NMR spectra, intramolecular hydrogen bonding and conformations of mercaptothiacalix[4]arene molecules and their para-tert-butyl-derivative. Journal of Inclusion Phenomena and Macrocyclic Chemistry, 2008, 60, 281-291.	1.6	7
94	Quantum chemical investigation of the structures of ionic liquids based on 1-ethyl-3-methylimidazolium halides: IR spectra and hydrogen bonds. Russian Chemical Bulletin, 2009, 58, 1812-1816.	0.4	7
95	First neutral dinuclear cobalt complex formed by bridging $[\frac{1}{4}\text{-O}_2\text{P(H)R}]^{\ominus}$ ligands: synthesis, X-ray crystal structure and quantum-chemical study. Mendeleev Communications, 2015, 25, 27-28.	0.6	7
96	The first representatives of tetranuclear gold( $\text{I}$ ) complexes of P,N-containing cyclophanes. Dalton Transactions, 2018, 47, 7715-7720.	1.6	7
97	One-electron Reduction of Acenaphthene-1,2-dithiimine Nickel(II) Complexes. Chemistry - an Asian Journal, 2019, 14, 2979-2987.	1.7	7
98	Comparative studies of geometric and quasielastic characteristics of PP and SS bonds. Dalton Transactions, 2008, , 1465.	1.6	6
99	Synthesis, X-ray crystal structure and quantum-chemical study of new dinuclear cobalt complex $\{\text{Co}_2[\text{mmm-O}_2\text{P(H)Mes}]_2(\text{bpy})_4\}\text{Br}_2$ . Mendeleev Communications, 2013, 23, 135-136.	0.6	6
100	Thermal stability of primary and secondary phosphine oxides formed as a reaction of phosphine oxide with ketones. Phosphorus, Sulfur and Silicon and the Related Elements, 2016, 191, 1480-1481.	0.8	6
101	A fresh look at participation of phosphorus atom in conjugation. Phosphorus, Sulfur and Silicon and the Related Elements, 2016, 191, 417-422.	0.8	6
102	Ferrocene-Containing Sterically Hindered Phosphonium Salts. Molecules, 2018, 23, 2773.	1.7	6
103	Synthesis and characterization of poly([Eu or Dy] 1,1'-ferrocenediyl-bis( $\text{H}$ -phosphinates)). Phosphorus, Sulfur and Silicon and the Related Elements, 2019, 194, 459-462.	0.8	6
104	Thermally Stable Nitrothiacalixarene Chromophores: Conformational Study and Aggregation Behavior. International Journal of Molecular Sciences, 2020, 21, 6916.	1.8	6
105	What quantum chemical simulations tell us about the infrared spectra, structure and interionic interactions of a bulk ionic liquid. Physical Chemistry Chemical Physics, 2022, 24, 7349-7355.	1.3	6
106	Vibrational spectra, conformations and intramolecular interactions of the $\text{Cl}_2\text{P}(\text{O})(\text{CH}_2)_2\text{SCN}$ molecule. Journal of Molecular Structure, 1997, 435, 281-288.	1.8	5
107	Synthesis, IR Spectra, and Steric Structure of Macrocycles Derived from Pyrimidine Compounds. Russian Journal of General Chemistry, 2002, 72, 1625-1632.	0.3	5
108	The effect of stacking arrangement on the conjugation in azochromophores revealed by combination of Raman spectroscopy and DFT calculations. Chemical Physics Letters, 2016, 659, 242-246.	1.2	5



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109	Leaching from Palladium Nanoparticles in an Ionic Liquid Leads to the Formation of Ionic Monometallic Species. <i>Journal of Physical Chemistry Letters</i> , 2017, 8, 3452-3456.	2.1	5
110	Rearrangement of two 8-membered 1,5-diaza-3,7-diphosphacyclooctane rings into 16-membered P4N4 ligand on the gold(i) template. <i>Mendeleev Communications</i> , 2020, 30, 40-42.	0.6	5
111	Stimuli-responsive emission of quinoxalinone-based compounds. From experimental findings to theoretical insight by means of multiscale computational spectroscopy approaches. <i>Dyes and Pigments</i> , 2021, 184, 108797.	2.0	5
112	Mechanistic Insights for Acid-catalyzed Rearrangement of Quinoxalinone with Diamine and Enamine. <i>ChemCatChem</i> , 2021, 13, 1503-1508.	1.8	5
113	Temperature-sensitive emission of dialkylaminostyrylhetarene dyes and their incorporation into phospholipid aggregates: Applicability for thermal sensing and cellular uptake behavior. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2021, 268, 120647.	2.0	5
114	Germylene complexes of tungsten pentacarbonyls W(CO) <sub>5</sub> GeCl <sub>2</sub> and W(CO) <sub>5</sub> GeW(CO) <sub>5</sub> : Electrochemical synthesis and quantum-chemical computations. <i>Journal of Organometallic Chemistry</i> , 2007, 692, 4067-4072.	0.8	4
115	Switching Ion Binding Selectivity of Thiacalix[4]arene Monocrowns at Liquid-Liquid and 2D-Confined Interfaces. <i>International Journal of Molecular Sciences</i> , 2021, 22, 3535.	1.8	4
116	The incorporation of upper vs lower rim substituted thia- and calix[4]arene ligands into polydiacethylene polymeric bilayers for rational design of sensors to heavy metal ions. <i>Polymer</i> , 2022, 245, 124728.	1.8	4
117	Force constants and vibrational spectra of molecules RP(X)F <sub>2</sub> . <i>Journal of Applied Spectroscopy</i> , 1985, 42, 173-177.	0.3	3
118	Towards a frustrated Lewis pair-ionic liquid system. <i>Inorganica Chimica Acta</i> , 2018, 470, 270-274.	1.2	3
119	Reversible temperature-responsive emission in solutions within 293-333 K produced by dissociative behavior of multinuclear Cu(I) complexes with aminomethylphosphines. <i>Inorganica Chimica Acta</i> , 2019, 498, 119125.	1.2	3
120	Application of density functional theory and optical spectroscopy for the prediction of the photophysical properties of $\delta$ -pyridylphospholanes. <i>Russian Chemical Bulletin</i> , 2019, 68, 254-261.	0.4	3
121	Water dispersible supramolecular assemblies built from luminescent hexarhenium clusters and silver(I) complex with pyridine-2-ylphospholane for sensorics. <i>Journal of Molecular Liquids</i> , 2020, 305, 112853.	2.3	3
122	Study of the structures and photophysical properties of 1,3-diaza-5-phosphacyclohexanes using density functional theory and optical spectroscopy. <i>Russian Chemical Bulletin</i> , 2020, 69, 449-457.	0.4	3
123	A rational synthetic approach to 2,3,4,5-tetraphenyl-1-monophosphole and its derivatives. <i>Inorganic Chemistry Communication</i> , 2021, 134, 108949.	1.8	3
124	Structural information content of the stretching vibration frequencies of PN and PO bonds in five-membered heterocyclic compounds. <i>Bulletin of the Academy of Sciences of the USSR Division of Chemical Science</i> , 1985, 34, 2064-2067.	0.0	2
125	Spectroscopic study of compounds with P-H bonds: Vibrational spectra and rotational isomers of ethyl ethylphosphite. <i>Journal of Applied Spectroscopy</i> , 1991, 54, 540-544.	0.3	2
126	IR and NMR spectra, intramolecular hydrogen bonding and conformations of para-tert-butyl-aminothiacalix[4]arene in solid state and chloroform solution. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2010, 75, 872-879.	2.0	2



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127	Guest-induced conformation shift of <i>p</i> -sulphonatocalix[4]arene in the solid state and solution manipulated by [Zn(dipy) <sub>3</sub> ] <sup>2+</sup> . <i>Supramolecular Chemistry</i> , 2010, 22, 203-211.	1.5	2
128	Correlations between metal spin states and vibrational spectra of a trinuclear Fe(II) complex exhibiting spin crossover. <i>Journal of Molecular Structure</i> , 2015, 1101, 8-13.	1.8	2
129	2,3-(Dibenzimidazol-2-yl)quinoxalines: Unexpected Dynamical Effect on Steady-State Electronic Absorption Spectra. <i>Journal of Physical Chemistry B</i> , 2019, 123, 5514-5523.	1.2	2
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