List of Publications by Year in descending order

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SEDCEL KATSVURA

#	Article	IF	CITATIONS
1	Computerâ€eided simulation of infrared spectra of ethanol conformations in gas, liquid and in <scp>CCl₄</scp> solution. Journal of Computational Chemistry, 2022, 43, 279-288.	1.5	12
2	Synthesis and optical properties of chromophores with a methoxyphenylindolizine moiety. AIP Conference Proceedings, 2022, , .	0.3	1
3	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
4	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. Polymer, 2022, 245, 124728.	1.8	4
5	Stimuli-responsive emission of quinoxalinone-based compounds. From experimental findings to theoretical insight by means of multiscale computational spectroscopy approaches. Dyes and Pigments, 2021, 184, 108797.	2.0	5
6	Towards the intercalation of Li cations to the Co(II) and Mn(II) ferrocenyl-phosphinic MOFs. Journal of Organometallic Chemistry, 2021, 932, 121641.	0.8	2
7	D-ï€-A'-ï€-A chromophores with quinoxaline core in the ï€-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
8	Mechanistic Insights for Acidâ€catalyzed Rearrangement of Quinoxalinâ€2â€one with Diamine and Enamine. ChemCatChem, 2021, 13, 1503-1508.	1.8	5
9	Switching Ion Binding Selectivity of Thiacalix[4]arene Monocrowns at Liquid–Liquid and 2D-Confined Interfaces. International Journal of Molecular Sciences, 2021, 22, 3535.	1.8	4
10	Revisiting conformations of methyl lactate in water and methanol. Journal of Chemical Physics, 2021, 155, 024507.	1.2	16
11	A rational synthetic approach to 2,3,4,5-tetraphenyl-1-monophosphole and its derivatives. Inorganic Chemistry Communication, 2021, 134, 108949.	1.8	3
12	Temperature-sensitive emission of dialkylaminostyrylhetarene dyes and their incorporation into phospholipid aggregates: Applicability for thermal sensing and cellular uptake behavior. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2021, 268, 120647.	2.0	5
13	Indolizine-based chromophores with octatetraene π-bridge and tricyanofurane acceptor: Synthesis, photophysical, electrochemical and electro-optic properties. Journal of Photochemistry and Photobiology A: Chemistry, 2020, 386, 112125.	2.0	9
14	Thermally Stable Nitrothiacalixarene Chromophores: Conformational Study and Aggregation Behavior. International Journal of Molecular Sciences, 2020, 21, 6916.	1.8	6
15	Synthesis, structure, and electrochemical properties of 4,5-diaryl-1,2,3-triphosphaferrocenes and the first example of multi(phosphaferrocene). Dalton Transactions, 2020, 49, 17252-17262.	1.6	11
16	Triple-bridged helical binuclear copper(<scp>i</scp>) complexes: Head-to-head and head-to-tail isomerism and the solid-state luminescence. Dalton Transactions, 2020, 49, 11997-12008.	1.6	11
17	Rearrangement of two 8-membered 1,5-diaza-3,7-diphosphacyclooctane rings into 16-membered P4N4 ligand on the gold(i) template. Mendeleev Communications, 2020, 30, 40-42.	0.6	5
18	Water dispersible supramolecular assemblies built from luminescent hexarhenium clusters and silver(I) complex with pyridine-2-ylphospholane for sensorics. Journal of Molecular Liquids, 2020, 305, 112853.	2.3	3

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19	Acidâ€Catalyzed Rearrangements of 3â€Aryloxiraneâ€2â€Carboxamides: Novel DFT Mechanistic Insights. ChemistryOpen, 2020, 9, 743-747.	0.9	10
20	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
21	Study of the structures and photophysical properties of 1,3-diaza-5-phosphacyclohexanes using density functional theory and optical spectroscopy. Russian Chemical Bulletin, 2020, 69, 449-457.	0.4	3
22	Principal Descriptors of Ionic Liquid Co-catalysts for the Electrochemical Reduction of CO ₂ . ACS Applied Energy Materials, 2020, 3, 4690-4698.	2.5	10
23	Characterization of Conjugation Effects in the Series of Quinoxaline-2-ones by Means of Vibrational Raman Spectroscopy. Journal of Physical Chemistry A, 2020, 124, 3865-3875.	1.1	2
24	Oneâ€Electron Reduction of Acenaphtheneâ€1,2â€Diimine Nickel(II) Complexes. Chemistry - an Asian Journal, 2019, 14, 2979-2987.	1.7	7
25	IR and Raman markers of Fe(II) spin state in the spin-crossover complex of iron(II) nitrate with tris(3,5-dimethylpyrazol-1-yl)methane. Journal of Physics: Conference Series, 2019, 1310, 012006.	0.3	0
26	Reversible temperature-responsible emission in solutions within 293–333â€ K produced by dissociative behavior of multinuclear Cu(I) complexes with aminomethylphosphines. Inorganica Chimica Acta, 2019, 498, 119125.	1.2	3
27	Fresh Look on the Nature of Dual-Band Emission of Octahedral Copper-Iodide Clusters—Promising Ratiometric Luminescent Thermometers. Journal of Physical Chemistry C, 2019, 123, 25863-25870.	1.5	26
28	Theoretical study of the excited state properties of luminescent phospholes. Dyes and Pigments, 2019, 164, 363-371.	2.0	9
29	Zn and Co redox active coordination polymers as efficient electrocatalysts. Dalton Transactions, 2019, 48, 3601-3609.	1.6	41
30	To what extent are the photophysical properties of quinoxaline- and quinoxalinone-based chromophores predictable?. Dyes and Pigments, 2019, 170, 107580.	2.0	13
31	Intriguing Near-Infrared Solid-State Luminescence of Binuclear Silver(I) Complexes Based on Pyridylphospholane Scaffolds. Inorganic Chemistry, 2019, 58, 7698-7704.	1.9	20
32	2,3-(Dibenzimidazol-2-yl)quinoxalines: Unexpected Dynamical Effect on Steady-State Electronic Absorption Spectra. Journal of Physical Chemistry B, 2019, 123, 5514-5523.	1.2	2
33	Delineation of the Critical Parameters of Salt Catalysts in the N <i>â€</i> Formylation of Amines with CO ₂ . Chemistry - A European Journal, 2019, 25, 11074-11079.	1.7	24
34	Application of density functional theory and optical spectroscopy for the prediction of the photophysical properties of Đ-pyridylphospholanes. Russian Chemical Bulletin, 2019, 68, 254-261.	0.4	3
35	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
36	Silica nanoparticles with dual visible–NIR luminescence affected by silica confinement of Tb(III) and Yb(III) complexes for cellular imaging application. Journal of Materials Science, 2019, 54, 9140-9154.	1.7	11

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37	Fast Quantum Chemical Simulations of Infrared Spectra of Organic Compounds with the B97-3c Composite Method. Journal of Physical Chemistry A, 2019, 123, 3802-3808.	1.1	26
38	Synthesis and characterization of poly([Eu or Dy] 1,1'-ferrocenediyl-bis(<i>H</i> -phosphinates)). Phosphorus, Sulfur and Silicon and the Related Elements, 2019, 194, 459-462.	0.8	6
39	Phosphorylation of pyridoxal azomethines. Synthesis of phosphorus containing azomethines and furopyridines. Phosphorus, Sulfur and Silicon and the Related Elements, 2019, 194, 120-126.	0.8	1
40	The Assembly of Unique Hexanuclear Copper(I) Complexes with Effective White Luminescence. Inorganic Chemistry, 2019, 58, 1048-1057.	1.9	34
41	Large nonlinear optical activity of chromophores with divinylquinoxaline conjugated π-bridge. Journal of Photochemistry and Photobiology A: Chemistry, 2019, 370, 58-66.	2.0	22
42	High thermally stable D–π–A chromophores with quinoxaline moieties in the conjugated bridge: Synthesis, DFT calculations and physical properties. Dyes and Pigments, 2018, 156, 175-184.	2.0	27
43	IR and UV study of reversible water-induced structural transformations of poly(manganese) Tj ETQq1 1 0.784314 of Molecular Structure, 2018, 1166, 237-242.	rgBT /Ov 1.8	erlock 10 Tf 3 14
44	Intricacies of Cation–Anion Combinations in Imidazolium Salt-Catalyzed Cycloaddition of CO ₂ Into Epoxides. ACS Catalysis, 2018, 8, 2589-2594.	5.5	129
45	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
46	Supramolecular Organization of Solid Azobenzene Chromophore Disperse Orange 3, Its Chloroform Solutions, and PMMA-Based Films. Journal of Physical Chemistry C, 2018, 122, 1779-1785.	1.5	13
47	Towards a frustrated Lewis pair-ionic liquid system. Inorganica Chimica Acta, 2018, 470, 270-274.	1.2	3
48	Synthesis, spatial and electronic structure of 1-(+)-neomenthyl-1,2-diphosphole and 1-(+)-neomenthyl-1,2,4-triphosphole tungstenpentacarbonyl complexes. Journal of Organometallic Chemistry, 2018, 867, 125-132.	0.8	11
49	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
50	Isomeric indolizine-based π-expanded push–pull NLO-chromophores: Synthesis and comparative study. Journal of Molecular Structure, 2018, 1156, 74-82.	1.8	16
51	Ferrocene-Containing Sterically Hindered Phosphonium Salts. Molecules, 2018, 23, 2773.	1.7	6
52	Composite materials containing chromophores with 3,7-(di)vinylquinoxalinone π-electron bridge doped into PMMA: Atomistic modeling and measurements of quadratic nonlinear optical activity. Dyes and Pigments, 2018, 158, 131-141.	2.0	29
53	Novel enantiopure monophospholes: synthesis, spatial and electronic structure, photophysical characteristics and conjugation effects. Dalton Transactions, 2018, 47, 11521-11529.	1.6	11
54	Nonlinear optical activity of push–pull indolizine-based chromophores with various acceptor moieties. Journal of Photochemistry and Photobiology A: Chemistry, 2018, 364, 764-772.	2.0	13

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55	Chromophores Supramolecular Organization in Polymer Materials with Quadratic Nonlinear-Optical Activity: Symmetry Aspects. Proceedings (mdpi), 2018, 2, 70.	0.2	0
56	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
57	The first representatives of tetranuclear gold(<scp>i</scp>) complexes of P,N-containing cyclophanes. Dalton Transactions, 2018, 47, 7715-7720.	1.6	7
58	The role of London dispersion interactions in strong and moderate intermolecular hydrogen bonds in the crystal and in the gas phase. Chemical Physics Letters, 2017, 672, 124-127.	1.2	11
59	Benzimidazolylquinoxalines: novel fluorophores with tuneable sensitivity to solvent effects. Physical Chemistry Chemical Physics, 2017, 19, 6095-6104.	1.3	11
60	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
61	One-pot synthesis of aryl-substituted 1,2,3-triphospholide anions. Journal of Organometallic Chemistry, 2017, 844, 1-7.	0.8	14
62	Leaching from Palladium Nanoparticles in an Ionic Liquid Leads to the Formation of Ionic Monometallic Species. Journal of Physical Chemistry Letters, 2017, 8, 3452-3456.	2.1	5
63	Push–pull isomeric chromophores with vinyl- and divinylquinoxaline-2-one units as ï€-electron bridge: Synthesis, photophysical, thermal and electro-chemical properties. Dyes and Pigments, 2017, 146, 82-91.	2.0	23
64	A Rhodium Nanoparticle–Lewis Acidic Ionic Liquid Catalyst for the Chemoselective Reduction of Heteroarenes. Angewandte Chemie - International Edition, 2016, 55, 292-296.	7.2	112
65	The influence of different substituents on the geometrical changes in the heterocyclic moiety of 1,2-diphospholes. Phosphorus, Sulfur and Silicon and the Related Elements, 2016, 191, 1646-1649.	0.8	10
66	"Host–guest―binding of a luminescent dinuclear Au(<scp>i</scp>) 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
67	Reversible Water-Induced Structural and Magnetic Transformations and Selective Water Adsorption Properties of Poly(manganese 1,1′-ferrocenediyl-bis(H-phosphinate)). Crystal Growth and Design, 2016, 16, 5084-5090.	1.4	34
68	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
69	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
70	Calorimetric and spectroscopic studies on solvation energetics for H ₂ storage in the CO ₂ /HCOOH system. Physical Chemistry Chemical Physics, 2016, 18, 10764-10773.	1.3	25
71	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
72	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

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73	Synthesis of novel pyridyl containing phospholanes and their polynuclear luminescent copper(<scp>i</scp>) complexes. Dalton Transactions, 2016, 45, 2250-2260.	1.6	63
74	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
75	Synthesis and structure of the iron(iii) tris-chelate complex based on 1,1´-ferrocenediylbis(phenylphosphinic acid). Russian Chemical Bulletin, 2015, 64, 1819-1822.	0.4	10
76	Conjugation effects and optical spectra of 1,2-diphosphole cycloadducts. Russian Chemical Bulletin, 2015, 64, 1896-1900.	0.4	10
77	First neutral dinuclear cobalt complex formed by bridging [î¼-O2P(H)R]– ligands: synthesis, X-ray crystal structure and quantum-chemical study. Mendeleev Communications, 2015, 25, 27-28.	0.6	7
78	Comparative Study of Conjugational Effects in 3,4,5-Triaryl-1- <i>R</i> -1,2-Diphospholes and 3,4,5-Triaryl-1,2-Diphosphacyclopentadienide-Anions. Phosphorus, Sulfur and Silicon and the Related Elements, 2015, 190, 858-862.	0.8	12
79	Synthesis and magnetic properties of manganese carbonyl complexes with different coordination modes of 3,4,5-triaryl-1,2-diphospholide ligands. Dalton Transactions, 2015, 44, 10259-10266.	1.6	8
80	Unexpected ligand effect on the catalytic reaction rate acceleration for hydrogen production using biomimetic nickel electrocatalysts with 1,5-diaza-3,7-diphosphacyclooctanes. Journal of Organometallic Chemistry, 2015, 789-790, 14-21.	0.8	31
81	Quantification of Conventional and Nonconventional Charge-Assisted Hydrogen Bonds in the Condensed and Gas Phases. Journal of Physical Chemistry Letters, 2015, 6, 4431-4436.	2.1	39
82	Correlations between metal spin states and vibrational spectra ofÂaÂtrinuclear Fe(II) complex exhibiting spin crossover. Journal of Molecular Structure, 2015, 1101, 8-13.	1.8	2
83	Infrared and Raman bands of cyclopentadienyl ligands as indicators of electronic configuration of metal centers in metallocenes. Journal of Organometallic Chemistry, 2015, 776, 30-34.	0.8	15
84	Conjugation in and Optical Properties of 1- <i>R</i> -1,2-Diphospholes and 1- <i>R</i> -Phospholes. Journal of Physical Chemistry A, 2014, 118, 12168-12177.	1.1	30
85	Synthesis and structure of ferrocenylphosphinic acids. Journal of Organometallic Chemistry, 2014, 766, 40-48.	0.8	36
86	Enhanced Conversion of Carbohydrates to the Platform Chemical 5â€Hydroxymethylfurfural Using Designer Ionic Liquids. ChemSusChem, 2014, 7, 1647-1654.	3.6	65
87	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
88	Is There a Simple Way to Reliable Simulations of Infrared Spectra of Organic Compounds?. Journal of Physical Chemistry A, 2013, 117, 6664-6670.	1.1	33
89	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. Journal of Physical Chemistry A, 2013, 117, 6827-6834.	1.1	24
90	Efficient synthesis and structure peculiarity of macrocycles with bi-indolizinylquinoxalinone moieties. Tetrahedron, 2013, 69, 10675-10687.	1.0	15

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91	How Strong Is Hydrogen Bonding in Ionic Liquids? Combined X-ray Crystallographic, Infrared/Raman Spectroscopic, and Density Functional Theory Study. Journal of Physical Chemistry B, 2013, 117, 9094-9105.	1.2	130
92	Bipyridine and phenanthroline IR-spectral bands as indicators of metal spin state in hexacoordinated complexes of Fe(<scp>ii</scp>), Ni(<scp>ii</scp>) and Co(<scp>ii</scp>). Dalton Transactions, 2013, 42, 1787-1797.	1.6	82
93	Synthesis, X-ray crystal structure and quantum-chemical study of new dinuclear cobalt complex {Co2[mmm-O2P(H)Mes]2(bpy)4}Br2. Mendeleev Communications, 2013, 23, 135-136.	0.6	6
94	A remarkable anion effect on palladium nanoparticle formation and stabilization in hydroxyl-functionalized ionic liquids. Physical Chemistry Chemical Physics, 2012, 14, 6026.	1.3	59
95	A cobalt(ii) acetate complex with 1-(3,5-di-tert-butyl-4-hydroxybenzyl)-1H-indole-2,3-dione 3-thiosemicarbazone: synthesis and structure. Russian Chemical Bulletin, 2012, 61, 1909-1916.	0.4	0
96	IR and Raman spectra, hydrogen bonds, and conformations of N-(2-hydroxyethyl)-4,6-dimethyl-2-oxo-1,2-dihydropyrimidine (drug Xymedone). Russian Chemical Bulletin, 2012, 61, 1199-1206.	0.4	9
97	Synthesis and Stereoselective Interconversion of Chiral 1â€Azaâ€3,6â€diphosphacycloheptanes. European Journal of Inorganic Chemistry, 2012, 2012, 1857-1866.	1.0	21
98	Rationalization of Solvation and Stabilization of Palladium Nanoparticles in Imidazoliumâ€Based Ionic Liquids by DFT and Vibrational Spectroscopy. ChemPhysChem, 2012, 13, 1781-1790.	1.0	27
99	Complex Formation of dâ€Metal Ions at the Interface of Tb ^{III} â€Doped Silica Nanoparticles as a Basis of Substrateâ€Responsive Tb ^{III} â€Centered Luminescence. ChemPhysChem, 2012, 13, 3357-3364.	1.0	35
100	Ab Initio and DFT Predictions of Infrared Intensities and Raman Activities. Journal of Physical Chemistry A, 2011, 115, 63-69.	1.1	132
101	Mass Spectrometric and Theoretical Study of Polyiodides: The Connection between Solid State, Solution, and Gas Phases. Inorganic Chemistry, 2011, 50, 9728-9733.	1.9	33
102	The Molecular Design of "Carcass―Type Phosphoranes, Based on the Reaction of P(III)-Cyclic Derivatives and Unsaturated Activated Compounds. Phosphorus, Sulfur and Silicon and the Related Elements, 2011, 186, 652-656.	0.8	15
103	Spectral study of the molecular structure of some 2-methylthio-6-methyl-4-alkyl- and alkylaminopyrimidines. Russian Journal of General Chemistry, 2011, 81, 2164-2171.	0.3	1
104	Synthesis, IR/Raman, and quantum-chemical structural analysis of new octathiotetraphosphetane ammonium salts. Heteroatom Chemistry, 2011, 22, 24-30.	0.4	10
105	IR and NMR spectra, intramolecular hydrogen bonding and conformations of para-tert-butyl-aminothiacalix[4]arene in solid state and chloroform solution. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2010, 75, 872-879.	2.0	2
106	DFT study of substitution effect on the geometry, IR spectra, spin state and energetic stability of the ferrocenes and their pentaphospholyl analogues. Journal of Organometallic Chemistry, 2010, 695, 2586-2595.	0.8	49
107	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
108	Variable temperature IR spectroscopy and quantum chemistry as the tool for diagnostics of metal spin state. Chemical Physics Letters, 2010, 495, 50-54.	1.2	8

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109	Guest-induced conformation shift of <i>p</i> -sulphonatothiacalix[4]arene in the solid state and solution manipulated by [Zn(dipy) ₃] ²⁺ . Supramolecular Chemistry, 2010, 22, 203-211.	1.5	2
110	A simple physical model for the simultaneous rationalisation of melting points and heat capacities of ionic liquids. Physical Chemistry Chemical Physics, 2010, 12, 13780.	1.3	15
111	Phosphonium ionic liquids based on bulky phosphines: synthesis, structure and properties. Dalton Transactions, 2010, 39, 5564.	1.6	39
112	Structural Studies of the Ionic Liquid 1-Ethyl-3-methylimidazolium Tetrafluoroborate in Dichloromethane Using a Combined DFT-NMR Spectroscopic Approach. Journal of Physical Chemistry B, 2009, 113, 5046-5051.	1.2	55
113	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
114	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
115	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, with an unusual conical-like conformation. Journal of Inclusion Phenomena and Macrocyclic Chemistry, 2008, 60, 321-328.	8(1,4)-teti 1.6	abenzenacy 9
116	Comparative studies of geometric and quasielastic characteristics of PP and SS bonds. Dalton Transactions, 2008, , 1465.	1.6	6
117	Application of Density Functional Theory and Vibrational Spectroscopy Toward the Rational Design of Ionic Liquids. Journal of Physical Chemistry A, 2007, 111, 352-370.	1.1	238
118	Revisiting Ether-Derivatized Imidazolium-Based Ionic Liquids. Journal of Physical Chemistry B, 2007, 111, 10095-10108.	1.2	121
119	Germylene complexes of tungsten pentacarbonyls W(CO)5GeCl2 and W(CO)5GeW(CO)5: Electrochemical synthesis and quantum-chemical computations. Journal of Organometallic Chemistry, 2007, 692, 4067-4072.	0.8	4
120	An experimental and quantum-chemical study of the Raman spectra and rotational isomerism of thiophosphites (RS) n PCl3 â^' n (R = Me, Et; n = 1, 2). Optics and Spectroscopy (English Translation of) Tj ETQqQ)0 0.2 gBT	/Overlock 10
121	Conformational analysis of mono-and bis(dimethoxyphosphoryl)benzenes. Russian Journal of General Chemistry, 2006, 76, 453-460.	0.3	0
122	Synthesis, structure, and transition metal complexes of amphiphilic 1,5-diaza-3,7-diphosphacyclooctanes. Heteroatom Chemistry, 2006, 17, 499-513.	0.4	36
123	Binding energies, vibrations and structural characteristics of small polyphosphorus molecules from quantum chemical computations. Dalton Transactions, 2005, , 1701.	1.6	12
124	Vibrational spectra, co-operative intramolecular hydrogen bonding and conformations of calix[4]arene and thiacalix[4]arene molecules and their para-tert-butyl derivatives. Organic and Biomolecular Chemistry, 2005, 3, 2558.	1.5	41
125	Energetics of intramolecular hydrogen bonds and conformations of Â-diphenylphosphoryl- and Â-diphenylthiophosphoryl-substituted aliphatic alcohol molecules. Russian Chemical Bulletin, 2004, 53, 55-59.	0.4	8
126	Molecular Structure, Vibrational Spectra, and Hydrogen Bonding of the Ionic Liquid 1-Ethyl-3-methyl-1H-imidazolium Tetrafluoroborate. Helvetica Chimica Acta, 2004, 87, 2556-2565.	1.0	197

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127	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
128	Scaled quantum mechanical computations of vibrational spectra of organoelement molecules, containing the atoms P, S, and Cl. Chemical Physics Letters, 2003, 377, 658-662.	1.2	53
129	Vibrational spectra and conformational isomerism of calixarene building blocks: 2-benzylphenolPart IV. For Parts l–III see refs. 1–3 Organic and Biomolecular Chemistry, 2003, 1, 714-719.	1.5	12
130	Vibrational spectra and conformational isomerism of calixarene building blocks. II. Bis(2-hydroxyphenyl)methaneFor previous communication see ref. 1.Electronic supplementary information (ESI) available: Table 1S. Results obtained from geometry optimisation for conformer 2.I. See http://www.rsc.org/suppdata/p2/b1/b108745b/. Perkin Transactions II RSC, 2002, , 67-71.	1.1	0
131	Vibrational spectra and conformational isomerism of calixarene building blocks. III. 2,6-Dimethylanisole and n-propyl-2,6-dimethylphenyl ether. Journal of Molecular Structure, 2002, 610, 113-125.	1.8	12
132	Cooperative intramolecular hydrogen bond and conformations of thiocalix[4]arene molecules. Russian Chemical Bulletin, 2002, 51, 825-827.	0.4	35
133	Synthesis, IR Spectra, and Steric Structure of Macrocycles Derived from Pyrimidine Compounds. Russian Journal of General Chemistry, 2002, 72, 1625-1632.	0.3	5
134	Vibrational spectra and conformational isomerism of calixarene building blocks. Part I. Diphenylmethane, (C 6 H 5) 2 CH 2. Journal of Molecular Structure, 2001, 559, 315-320.	1.8	40
135	Conformations and coordination properties of trialkyltrithiophosphites in copper(I) complexes. Journal of Molecular Structure, 2000, 554, 127-140.	1.8	15
136	New Type of Molecular Propellers with Acyclic Blades Stabilised by Phosphorus Atropoisomerism. Phosphorus, Sulfur and Silicon and the Related Elements, 1999, 144, 737-740.	0.8	0
137	Vibrational spectra, conformations, and intramolecular interactions of R(CH2)2-O-PCl2 molecules (R=Et, OMe) Journal of Molecular Structure, 1999, 475, 13-25.	1.8	1
138	Vibrational spectroscopy of tri- and tetra-coordinated phosphorus compounds. Journal of Molecular Structure, 1999, 482-483, 449-452.	1.8	0
139	Vibrational spectra, conformations, and intramolecular interactions of X(CH 2) 2 –O–PCl 2 molecules. Journal of Molecular Structure, 1999, 508, 223-231.	1.8	Ο
140	Vibrational spectra, conformations, and force constants of bis(dimethylamino)chlorophosphine and 2-chloro-1,3-dimethyl-1,3,2-diazaphospholane. Russian Chemical Bulletin, 1998, 47, 375-378.	0.4	0
141	Vibrational spectra, conformations and intramolecular interactions of the Cl2P–O–(CH2)2SCN molecule. Journal of Molecular Structure, 1997, 435, 281-288.	1.8	5
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9

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