

Boris F Minaev

List of Publications by Year in descending order

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343
papers

8,067
citations

50170

46
h-index

88477

70
g-index

348
all docs

348
docs citations

348
times ranked

6168
citing authors

#	ARTICLE	IF	CITATIONS
1	TADF quenching properties of phenothiazine or phenoxazine-substituted benzantrones emitting in deep-red/near-infrared region towards oxygen sensing. <i>Dyes and Pigments</i> , 2022, 197, 109952.	2.0	13
2	Crystal structure and Hirshfeld surfaces analysis of Heterocyclic-and circulenes. <i>MATEC Web of Conferences</i> , 2022, 355, 01020.	0.1	1
3	Calculation of the singlet-triplet magnetic and electro-quadrupole transitions intensity for Ge ₂ molecule. <i>Molecular Physics</i> , 2022, 120, .	0.8	6
4	Impact of molecular and packing structure on the charge-transport properties of hetero[8]circulenes. <i>Journal of Materials Chemistry C</i> , 2021, 9, 1451-1466.	2.7	11
5	Computational study of IR, Raman, and NMR spectra of 4-methylmethcathinone drug. <i>Journal of Molecular Modeling</i> , 2021, 27, 3.	0.8	3
6	Dianthracenylazatrioxa[8]circulene: Synthesis, Characterization and Application in OLEDs. <i>Chemistry - A European Journal</i> , 2021, 27, 11609-11617.	1.7	7
7	Molecular Terms of Dioxygen and Nitric Oxide. <i>Physchem</i> , 2021, 1, 121-132.	0.5	4
8	Schiff Base Zinc(II) Complexes as Promising Emitters for Blue Organic Light-Emitting Diodes. <i>ACS Applied Electronic Materials</i> , 2021, 3, 3436-3444.	2.0	34
9	Hirshfeld surfaces analysis and DFT study of the structure and IR spectrum of N-ethyl-2-amino-1-(4-chlorophenyl)propan-1-one (4-CEC) hydrochloride. <i>Computational and Theoretical Chemistry</i> , 2021, 1205, 113455.	1.1	8
10	Multidimensional Structure Conformation of Persulfurated Benzene for Highly Efficient Phosphorescence. <i>ACS Applied Materials & Interfaces</i> , 2021, 13, 1314-1322.	4.0	13
11	Aromaticity of Heterocirculenes. <i>Chemistry</i> , 2021, 3, 1411-1436.	0.9	11
12	The effect of molecular structure on the properties of quinoxaline-based molecules for OLED applications. <i>Dyes and Pigments</i> , 2020, 173, 108008.	2.0	34
13	BODIPY-core 1,7-diphenyl-substituted derivatives for photovoltaics and OLED applications. <i>Dyes and Pigments</i> , 2020, 175, 108123.	2.0	30
14	Structure and tuneable luminescence in polymeric zinc compounds based on 3-(3-pyridyl)-5-(4-pyridyl)-1,2,4-triazole. <i>Polyhedron</i> , 2020, 191, 114768.	1.0	19
15	New Aspects of the Airglow Problem and Reactivity of the Dioxygen Quintet O ₂ (⁵ Δ _g) State in the MLT Region as Predicted by DFT Calculations. <i>Journal of Physical Chemistry A</i> , 2020, 124, 9638-9655.	1.1	7
16	Can attachment of tert-butyl substituents to methoxycarbazole moiety induce efficient TADF in diphenylsulfone-based blue OLED emitters?. <i>Organic Electronics</i> , 2020, 86, 105894.	1.4	6
17	A Fully Conjugated Planar Heterocyclic [9]Circulene. <i>Journal of the American Chemical Society</i> , 2020, 142, 14058-14063.	6.6	28
18	First-principles calculations of anharmonic and deuteration effects on the photophysical properties of polyacenes and porphyrinoids. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 22314-22323.	1.3	32

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19	Benzoselenophenylpyridine platinum complexes: green <i>versus</i> red phosphorescence towards hybrid OLEDs. Dalton Transactions, 2020, 49, 3393-3397.	1.6	19
20	Compressing a Non-Planar Aromatic Heterocyclic [7]Helicene to a Planar Hetero[8]Circulene. Chemistry - A European Journal, 2020, 26, 4935-4940.	1.7	28
21	Anti-Aromatic versus Induced Paratropicity: Synthesis and Interrogation of a Dihydro-diazatrioxa[9]circulene with a Proton Placed Directly above the Central Ring. Angewandte Chemie - International Edition, 2020, 59, 5144-5150.	7.2	17
22	Anti-Aromatic versus Induced Paratropicity: Synthesis and Interrogation of a Dihydro-diazatrioxa[9]circulene with a Proton Placed Directly above the Central Ring. Angewandte Chemie, 2020, 132, 5182-5188.	1.6	8
23	Flexible diphenylsulfone versus rigid dibenzothiophene-dioxide as acceptor moieties in donor-acceptor-donor TADF emitters for highly efficient OLEDs. Organic Electronics, 2020, 83, 105733.	1.4	11
24	Molecular Phosphorescence in Polymer Matrix with Reversible Sensitivity. ACS Applied Materials & Interfaces, 2020, 12, 20765-20774.	4.0	68
25	Structure, stability and electronic properties of one-dimensional tetrathia- and tetraselena[8]circulene-based materials: a comparative DFT study. New Journal of Chemistry, 2020, 44, 6872-6882.	1.4	5
26	Furans and Their Benzo Derivatives: Structure. , 2020, , 190-190.		1
27	The blue vibronically resolved electroluminescence of azatrioxa[8]circulene. Chemical Physics Letters, 2019, 732, 136667.	1.2	10
28	Structure and excitation-dependent emission of novel zinc complexes with pyridyltriazoles. RSC Advances, 2019, 9, 22143-22152.	1.7	18
29	Impact of heteroatoms (S, Se, and Te) on the aromaticity of heterocirculenes. New Journal of Chemistry, 2019, 43, 12178-12190.	1.4	10
30	How cofactor-free oxygenases can overcome spin prohibition in substrates oxygenation by dioxygen. Chemical Physics, 2019, 521, 61-68.	0.9	12
31	Aromaticity and photophysics of tetrasila- and tetragerma-annelated tetrathienylenes as new representatives of the hetero[8]circulene family. Physical Chemistry Chemical Physics, 2019, 21, 9246-9254.	1.3	19
32	Novel Zinc Complex with an Ethylenediamine Schiff Base for High-Luminance Blue Fluorescent OLED Applications. Journal of Physical Chemistry C, 2019, 123, 11850-11859.	1.5	56
33	Experimental and theoretical study of the mechanism formation of silver nanoclusters in the reduction reaction of Ag ⁺ ions by alizarin solution. Colloids and Interface Science Communications, 2019, 29, 47-54.	2.0	4
34	A complete characterization of vibrational IR and Raman spectra of the highly-symmetrical octathia[8]circulene. Vibrational Spectroscopy, 2019, 100, 107-116.	1.2	9
35	Multi-channel electroluminescence of CdTe/CdS core-shell quantum dots implemented into a QLED device. Dyes and Pigments, 2019, 162, 647-653.	2.0	23
36	Computational study of the structure and magnetic properties of the weakly-coupled tetranuclear square-planar complex of Cu(II) with a tetraporphyrin sheet. Inorganica Chimica Acta, 2019, 485, 73-79.	1.2	5

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37	Spin-orbit coupling effects in O(2) activation by cofactor-independent 2,4-dioxygenase. Ukrainian Biochemical Journal, 2019, 91, 38-46.	0.1	5
38	Interaction of Myoglobin Model with Ligands of Gas Exchange. Cherkasy University Bulletin Biological Sciences Series, 2019, , 13-23.	0.2	3
39	Wave structure of hemodynamic parameters in people with the different baseline level of cardiac output and the blood supply of the thoracic organs. Cherkasy University Bulletin Biological Sciences Series, 2019, , 37-45.	0.2	0
40	Spin-catalysis of Unsaturated Substrates Oxidation by Cofactor-free Mono- and Di-oxygenases. How Triplet Oxygen Can Overcome Spin Prohibition. Ukraïnskij Zhurnal Medicini Bãologã Ta Sportu, 2019, 4, 329-343.	0.0	3
41	The Electronic Structure and Spectra of Triphenylamines Functionalized by Phenylethynyl Groups. Optics and Spectroscopy (English Translation of Optika I Spektroskopiya), 2018, 124, 57-64.	0.2	1
42	Optical tuning of tetrabenzo[8]circulene derivatives through pseudorotational conformational isomerization. Dyes and Pigments, 2018, 151, 372-379.	2.0	5
43	Contribution of TADF and exciplex emission for efficient warm-white OLEDs. Journal of Materials Chemistry C, 2018, 6, 1543-1550.	2.7	64
44	Dynamics of Thermoluminescence under Dual-Wavelength Vis-IR Laser Excitation of Eosin Molecules in a Polyvinyl Butyral Film Containing Oxygen and Silver Nanoparticles. Optics and Spectroscopy (English Translation of Optika I Spektroskopiya), 2018, 125, 874-881.	0.2	1
45	Strong Topological States and High Charge Carrier Mobility in Tetraoxa[8]circulene Nanosheets. Journal of Physical Chemistry C, 2018, 122, 22216-22222.	1.5	25
46	Identification of tautomeric intermediates of a novel thiazolylazonaphthol dye - A density functional theory study. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2018, 203, 324-332.	2.0	4
47	Vibronic absorption spectra of the angular fused bisindolo- and biscarbazoloanthracene blue fluorophores for OLED applications. Chemical Physics, 2018, 513, 105-111.	0.9	6
48	A theoretical study of new representatives of closed- and open-circle benzofuran and benzocyclopentadienone oligomers. New Journal of Chemistry, 2018, 42, 11493-11505.	1.4	11
49	Enzymatic spin-catalysis in flavin-containing oxidases and magnetic orientation of birds. Cherkasy University Bulletin Biological Sciences Series, 2018, , 114-120.	0.2	2
50	Spin-Orbit Coupling in Enzymatic Reactions and the Role of Spin in Biochemistry. , 2017, , 1557-1587.		6
51	Super high-energy density single-bonded trigonal nitrogen allotrope - a chemical twin of the cubic gauche form of nitrogen. Physical Chemistry Chemical Physics, 2017, 19, 6698-6706.	1.3	32
52	Recent progress in quantum chemistry of hetero[8]circulenes. Molecular Physics, 2017, 115, 2218-2230.	0.8	28
53	A computational study of aromaticity and photophysical properties of unsymmetrical azatrioxa[8]circulenes. New Journal of Chemistry, 2017, 41, 2717-2723.	1.4	16
54	Calculation of the optical spectra of the copper(I) complex with triphenylphosphine, iodine, and 3-pyridine-2-yl-5-phenyl-1H-1,2,4-triazole by the DFT method. Optics and Spectroscopy (English) Tj ETQq0 0 0 rgBT (Overlock 40 Tf 50 5		

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55	DFT design of polyguanidine – a unique two-dimensional material with high-energy density. <i>Molecular Physics</i> , 2017, 115, 2423-2430.	0.8	7
56	A computational study of structural and magnetic properties of bi- and trinuclear Cu(II) complexes with extremely long Cu–Cu distances. <i>Chemical Physics</i> , 2017, 491, 48-55.	0.9	12
57	Synthesis and luminescent properties of copper(I) complexes with 3-pyridin-2-yl-5-(4-R-phenyl)-1H-1,2,4-triazoles. <i>Russian Journal of Inorganic Chemistry</i> , 2017, 62, 423-430.	0.3	5
58	Synthesis and characterisation of a carbazole-based bipolar exciplex-forming compound for efficient and color-tunable OLEDs. <i>New Journal of Chemistry</i> , 2017, 41, 559-568.	1.4	34
59	Substituent-sensitive fluorescence of sequentially N-alkylated tetrabenzotetraaza[8]circulenes. <i>New Journal of Chemistry</i> , 2017, 41, 7621-7625.	1.4	9
60	BaZrO ₃ perovskite nanoparticles as emissive material for organic/inorganic hybrid light-emitting diodes. <i>Dyes and Pigments</i> , 2017, 145, 399-403.	2.0	9
61	Comparative study of the structural and spectral properties of tetraaza- and tetraoxaannulated tetracirculenes. <i>Optics and Spectroscopy (English Translation of Optika i Spektroskopiya)</i> , 2017, 122, 523-540.	0.2	6
62	New WOLEDs based on π -extended azatrioxa[8]circulenes. <i>Journal of Materials Chemistry C</i> , 2017, 5, 4123-4128.	2.7	28
63	Theory and Calculation of the Phosphorescence Phenomenon. <i>Chemical Reviews</i> , 2017, 117, 6500-6537.	23.0	420
64	Solvatochromic effect in absorption and emission spectra of star-shaped bipolar derivatives of 1,3,5-triazine and carbazole. A time-dependent density functional study. <i>Journal of Molecular Modeling</i> , 2017, 23, 55.	0.8	11
65	Two-dimensional honeycomb (A7) and zigzag sheet (ZS) type nitrogen monolayers. A first principles study of structural, electronic, spectral, and mechanical properties. <i>Computational Materials Science</i> , 2017, 133, 122-129.	1.4	27
66	Two isomeric solid carbon nitrides with 1:1 stoichiometry which exhibit strong mechanical anisotropy. <i>New Journal of Chemistry</i> , 2017, 41, 13140-13148.	1.4	8
67	Singlet Oxygen Photophysics in Liquid Solvents: Converging on a Unified Picture. <i>Accounts of Chemical Research</i> , 2017, 50, 1920-1927.	7.6	97
68	Influence of Molecular Oxygen on Ortho-Para Conversion of Water Molecules. <i>Russian Physics Journal</i> , 2017, 60, 485-493.	0.2	2
69	Analysis of Dissociation-Recombination Processes for the CO ₂ Molecule with the Spin-Orbit Coupling Taken into Account. <i>Optics and Spectroscopy (English Translation of Optika i Spektroskopiya)</i> , 2017, 122, 523-540.	0.2	6
70	Nine-ring angular fused bis-carbazoloanthracene displaying a solid state based excimer emission suitable for OLED application. <i>Journal of Materials Chemistry C</i> , 2016, 4, 5795-5805.	2.7	33
71	Highly Luminous Sky-Blue Organic Light-Emitting Diodes Based on the Bis[(1,2)(5,6)]indoloanthracene Emissive Layer. <i>Journal of Physical Chemistry C</i> , 2016, 120, 6206-6217.	1.5	45
72	Computational study of the structure, UV-vis absorption spectra and conductivity of biphenylene-based polymers and their boron nitride analogues. <i>RSC Advances</i> , 2016, 6, 49505-49516.	1.7	24

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73	Ab initio investigation of electric and magnetic dipole electronic transitions in the complex of oxygen with benzene. <i>Journal of Molecular Modeling</i> , 2016, 22, 214.	0.8	5
74	Ab Initio Study of Electronic States of Astrophysically Important Molecules. <i>Russian Physics Journal</i> , 2016, 59, 536-543.	0.2	9
75	Benzoannelated aza-, oxa- and azaoxa[8]circulenes as promising blue organic emitters. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 28040-28051.	1.3	54
76	Anion-induced exchange interactions in binuclear complexes of Cu(II) with flexible hexadentate bispicolylamidrazone ligands. <i>Chemical Physics Letters</i> , 2016, 661, 48-52.	1.2	9
77	Analysis of the electronic, IR, and ¹ H NMR spectra of conjugated oligomers based on 4,4'-triphenylamine vinylene. <i>Optics and Spectroscopy (English Translation of Optika i Spektroskopiya)</i> , 2016, 121, 348-356.	0.2	4
78	Quantum-chemical study of the structure and magnetic properties of mono- and binuclear Cu(II) complexes with 1,3-bis(3-(pyrimidin-2-yl)-1H-1,2,4-triazol-5-yl)propane. <i>Russian Journal of Inorganic Chemistry</i> , 2016, 61, 588-593.	0.3	9
79	Electroluminescence of Halogen Complexes with Monovalent Copper: OLED Devices and DFT Modeling. <i>Russian Physics Journal</i> , 2016, 58, 1205-1211.	0.2	14
80	Spin-dependent effects in ethylene polymerization with bis(imino)pyridine iron(II) complexes. <i>Journal of Organometallic Chemistry</i> , 2016, 811, 48-65.	0.8	17
81	Aromaticity of the doubly charged [8]circulenes. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 8980-8992.	1.3	34
82	Spin-Orbit Coupling in Enzymatic Reactions and the Role of Spin in Biochemistry. , 2016, , 1-31.		1
83	Photochemistry and Spectroscopy of Singlet Oxygen in Solvents. <i>Recent Advances which Support the Old Theory. Chemistry and Chemical Technology</i> , 2016, 10, 519-530.	0.2	8
84	The effect of a heteroatom on the structure and vibrational spectra of Heteroannulated tetraphenylenes. <i>Optics and Spectroscopy (English Translation of Optika i Spektroskopiya)</i> , 2015, 119, 620-632.	0.2	4
85	Electronic structure, aromaticity and spectra of hetero[8]circulenes. <i>Russian Chemical Reviews</i> , 2015, 84, 455-484.	2.5	46
86	Temperature effects in low-frequency Raman spectra of corticosteroid hormones. <i>Optics and Spectroscopy (English Translation of Optika i Spektroskopiya)</i> , 2015, 118, 214-223.	0.2	10
87	Quantum-chemical investigation of the structure and electronic absorption spectra of symmetric triphenylamine oligomers conjugated to vinylene, imine, azine, and ethynylene groups. <i>Optics and Spectroscopy (English Translation of Optika i Spektroskopiya)</i> , 2015, 118, 703-710.	0.2	2
88	Structure and spectral and luminescence properties of the trinuclear zinc complex with (E)-5-((2,6-diethylphenylimino)methyl)-2-methylquinolin-8-ol: Experimental and DFT study. <i>Russian Journal of Inorganic Chemistry</i> , 2015, 60, 1560-1567.	0.3	6
89	Thermally accessible triplet state of $\dot{\text{I}}\text{C}\text{-nucleophiles}$ does exist. Evidence from first principles study of ethylene interaction with copper species. <i>RSC Advances</i> , 2015, 5, 11558-11569.	1.7	19
90	Alkali and alkaline-earth metal complexes with tetraoxa[8]circulene sheet: a computational study by DFT and QTAIM methods. <i>RSC Advances</i> , 2015, 5, 24299-24305.	1.7	28

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91	Synthesis and properties of synthetic fulvic acid derived from hematoxylin. <i>Journal of Molecular Structure</i> , 2015, 1086, 25-33.	1.8	19
92	DFT simulation of the heteroannulated octatetraenes vibronic spectra with the Franck-Condon and Herzberg-Teller approaches including Duschinsky effect. <i>Chemical Physics</i> , 2015, 459, 65-71.	0.9	22
93	A DFT and QTAIM study of the novel d-block metal complexes with tetraoxa[8]circulene-based ligands. <i>New Journal of Chemistry</i> , 2015, 39, 7815-7821.	1.4	33
94	Structure and spectroscopic characterization of tetrathia- and tetraselena[8]circulenes as a new class of polyaromatic heterocycles. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2015, 151, 247-261.	2.0	22
95	A combined experimental and density functional study of 1-(arylsulfonyl)-2-chloro-2-butenes reactivity towards the allylic chlorine. <i>Journal of Physical Organic Chemistry</i> , 2015, 28, 403-413.	0.9	0
96	Computational and Experimental Investigation of the Optical Properties of the Chromene Dyes. <i>Journal of Physical Chemistry A</i> , 2015, 119, 1948-1956.	1.1	23
97	Aromaticity of the completely annulated tetraphenylenes: NICS and GIMIC characterization. <i>Journal of Molecular Modeling</i> , 2015, 21, 136.	0.8	34
98	Synthesis and spectroscopic characterization of a new (aryl-SCN) _n polymer: Polythiocyanatohydroquinone. <i>Journal of Molecular Structure</i> , 2015, 1096, 15-20.	1.8	3
99	Features of terahertz adsorption and Raman scattering of mineralocorticoid hormones. <i>Bulletin of the Russian Academy of Sciences: Physics</i> , 2015, 79, 1196-1201.	0.1	4
100	Absolute effective cross sections of ionization of adenine and guanine molecules by electron impact. <i>Technical Physics</i> , 2015, 60, 1430-1436.	0.2	7
101	N-annulated perylenes as effective green emitters for OLEDs. <i>RSC Advances</i> , 2015, 5, 78150-78159.	1.7	21
102	Mixing of Phosphorescent and Exciplex Emission in Efficient Organic Electroluminescent Devices. <i>ACS Applied Materials & Interfaces</i> , 2015, 7, 1219-1225.	4.0	78
103	Tetrathio and Tetraselena[8]circulenes: Synthesis, Structures, and Properties. <i>Chemistry - an Asian Journal</i> , 2015, 10, 969-975.	1.7	52
104	Tuning optical and electronic properties of poly(4,4'-triphenylamine vinylene)s by post-modification reactions. <i>Dyes and Pigments</i> , 2015, 113, 227-238.	2.0	10
105	Spin-orbit coupling and dissociation of CO ₂ molecules. <i>Optics and Spectroscopy (English Translation)</i> Tj ETQq1 1 0,784314 rgBT /Overl	0.2	8
106	Plasmon amplification and quenching of the fluorescence and phosphorescence of anionic and cationic dyes in various media. <i>Journal of Optical Technology (A Translation of Opticheskii Zhurnal)</i> , 2014, 81, 625.	0.2	8
107	The size-controllable, one-step synthesis and characterization of gold nanoparticles protected by synthetic humic substances. <i>Materials Chemistry and Physics</i> , 2014, 144, 168-178.	2.0	30
108	State-Dependent Global and Local Electrophilicity of the Aryl Cations. <i>Journal of Physical Chemistry A</i> , 2014, 118, 3201-3210.	1.1	19

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109	Efficient "Warm-White" OLEDs Based on the Phosphorescent bis-Cyclometalated iridium(III) Complex. <i>Journal of Physical Chemistry C</i> , 2014, 118, 11271-11278.	1.5	73
110	The Electronic Structure of Heteroannulated Cyclooctatetraenes and their UV-Vis Absorption Spectra. <i>Chemistry of Heterocyclic Compounds</i> , 2014, 50, 349-363.	0.6	15
111	Principles of phosphorescent organic light emitting devices. <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 1719-1758.	1.3	398
112	Design of nanoscaled materials based on tetraoxa[8]circulene. <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 6555.	1.3	48
113	A comparative study of the electronic structure and spectra of tetraoxa[8]circulene and octathio[8]circulene. <i>Optics and Spectroscopy (English Translation of Optika i Spektroskopiya)</i> , 2014, 116, 33-46.	0.2	26
114	The art of the possible: computational design of the 1D and 2D materials based on the tetraoxa[8]circulene monomer. <i>RSC Advances</i> , 2014, 4, 25843-25851.	1.7	50
115	Electronic descriptors for analytical use of the benzidine-based compounds and the mechanism of oxidative coupling of anilines. <i>Journal of Physical Organic Chemistry</i> , 2014, 27, 640-651.	0.9	11
116	DFT characterization of a new possible graphene allotrope. <i>Chemical Physics Letters</i> , 2014, 612, 229-233.	1.2	54
117	Fragmentation of the adenine and guanine molecules induced by electron collisions. <i>Journal of Chemical Physics</i> , 2014, 140, 175101.	1.2	42
118	A study of the role played by the Hartree-Fock orbital exchange in the formation of the energy of the first singlet charge-transfer excited state by the example of JK-62 and JK-201 sensitizing dye molecules. <i>Optics and Spectroscopy (English Translation of Optika i Spektroskopiya)</i> , 2014, 116, 431-437.	0.2	4
119	Aromaticity of the planar hetero[8]circulenes and their doubly charged ions: NICS and GIMIC characterization. <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 15367-15374.	1.3	69
120	Theoretical Study of Relationships between Structural, Optical, Energetic, and Magnetic Properties and Reactivity Parameters of Benzidine and Its Oxidized Forms. <i>Journal of Physical Chemistry A</i> , 2014, 118, 8872-8882.	1.1	9
121	Quantum-chemical simulation of the synthesis of structural fragments of humic substances analogs. <i>Russian Journal of General Chemistry</i> , 2014, 84, 848-852.	0.3	3
122	The singlet-triplet energy splitting of π -nucleophiles as a measure of their reaction rate with electrophilic partners. <i>Chemical Physics Letters</i> , 2014, 607, 75-80.	1.2	18
123	Raman spectra of alkyl-substituted azaoxa[8]circulenes: DFT calculation and experiment. <i>Optics and Spectroscopy (English Translation of Optika i Spektroskopiya)</i> , 2013, 114, 509-521.	0.2	10
124	Triplet State Phosphorescence in Tris(8-hydroxyquinoline) Aluminum Light Emitting Diode Materials. <i>Journal of Physical Chemistry C</i> , 2013, 117, 3446-3455.	1.5	10
125	Comparative computational IR, Raman and phosphorescence study of Ru- and Rh-based complexes. <i>Molecular Physics</i> , 2013, 111, 1526-1538.	0.8	6
126	Highly Efficient Blue Organic Light-Emitting Diodes Based on Intermolecular Triplet-Singlet Energy Transfer. <i>Journal of Physical Chemistry C</i> , 2013, 117, 22538-22544.	1.5	65

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127	Structural and Electronic Properties of Poly(9,9-dialkylfluorene)-Based Alternating Copolymers in Solution: An NMR Spectroscopy and Density Functional Theory Study. <i>Journal of Physical Chemistry C</i> , 2013, 117, 17969-17982.	1.5	15
128	Structure of zinc complexes with 3-(pyridin-2-yl)-5-(arylideneiminophenyl)-1H-1,2,4-triazoles in different tautomeric forms: DFT and QTAIM study. <i>Russian Journal of Inorganic Chemistry</i> , 2013, 58, 928-934.	0.3	24
129	Structure and electronic absorption spectra of isotruxene dyes for dye-sensitized solar cells: Investigation by the DFT, TDDFT, and QTAIM methods. <i>Optics and Spectroscopy (English Translation of Optika i Laser)</i> , 2013, 38, 1027-1034.	1.0	14
130	Dioxygen spectra and bioactivation. <i>International Journal of Quantum Chemistry</i> , 2013, 113, 1847-1867.	1.0	41
131	Nucleus-independent chemical shift criterion for aromaticity in π -extended tetraoxa[8]circulenes. <i>Journal of Molecular Modeling</i> , 2013, 19, 847-850.	0.8	50
132	Diazadioxo[8]circulenes: Planar Antiaromatic Cyclooctatetraenes. <i>Chemistry - A European Journal</i> , 2013, 19, 17097-17102.	1.7	80
133	Azatrioxa[8]circulenes: Planar Antiaromatic Cyclooctatetraenes. <i>Chemistry - A European Journal</i> , 2013, 19, 3898-3904.	1.7	78
134	Spectroscopy study of silver nanoparticles fabrication using synthetic humic substances and their antimicrobial activity. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2013, 108, 115-122.	2.0	74
135	The FTIR spectra of substituted tetraoxa[8]circulenes and their assignments based on DFT calculations. <i>Vibrational Spectroscopy</i> , 2013, 65, 147-158.	1.2	26
136	Quantum-chemical investigation of the structure and electronic absorption spectra of electroluminescent zinc complexes. <i>Optics and Spectroscopy (English Translation of Optika i Laser)</i> , 2013, 38, 1027-1034.	1.0	14
137	Theoretical study of the triplet state aryl cations recombination: A possible route to unusually stable doubly charged biphenyl cations. <i>International Journal of Quantum Chemistry</i> , 2013, 113, 2580-2588.	1.0	14
138	Analysis of intermolecular interactions in progesterone and 17 β -hydroxyprogesterone crystals. , 2013, , .		0
139	Single crystal architecture and absorption spectra of octathio[8]circulene and sym-tetraselenatetrathio[8]circulene: QTAIM and TD-DFT approach. <i>Journal of Molecular Modeling</i> , 2013, 19, 4511-4519.	0.8	31
140	Electron density distribution in the ethylene complexes with Pd-containing bimetallic clusters. <i>Molecular Simulation</i> , 2013, 39, 660-669.	0.9	2
141	Spin-spin and spin-orbit interactions in nanographene fragments: A quantum chemistry approach. <i>Journal of Chemical Physics</i> , 2012, 136, 104702.	1.2	37
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