Boris F Minaev

List of Publications by Year
in descending order

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343 papers	8,067 citations	50276 46 h-index	88630 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 benzanthrones emitting in deep-red/near-infrared region towards oxygen sensing. Dyes and Pigments, 2022, 197, 109952.	3.7	13
2	Crystal structure and Hirshfeld surfaces analysis of Heterocyclic-and circulenes. MATEC Web of Conferences, 2022, 355, 01020.	0.2	1
3	Calculation of the singlet-triplet magnetic and electro-quadrupole transitions intensity for Ge₂ molecule. Molecular Physics, 2022, 120, .	1.7	6
4	Impact of molecular and packing structure on the charge-transport properties of hetero[8]circulenes. Journal of Materials Chemistry C, 2021, 9, 1451-1466.	5.5	11
5	Computational study of IR, Raman, and NMR spectra of 4-methylmethcathinone drug. Journal of Molecular Modeling, 2021, 27, 3.	1.8	3
6	Dianthracenylazatrioxa[8]circulene: Synthesis, Characterization and Application in OLEDs. Chemistry - A European Journal, 2021, 27, 11609-11617.	3.3	7
7	Molecular Terms of Dioxygen and Nitric Oxide. Physchem, 2021, 1, 121-132.	1.1	4
8	Schiff Base Zinc(II) Complexes as Promising Emitters for Blue Organic Light-Emitting Diodes. ACS Applied Electronic Materials, 2021, 3, 3436-3444.	4.3	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. Computational and Theoretical Chemistry, 2021, 1205, 113455.	2.5	8
10	Multidimensional Structure Conformation of Persulfurated Benzene for Highly Efficient Phosphorescence. ACS Applied Materials & Interfaces, 2021, 13, 1314-1322.	8.0	13
11	Aromaticity of Heterocirculenes. Chemistry, 2021, 3, 1411-1436.	2.2	11
12	The effect of molecular structure on the properties of quinoxaline-based molecules for OLED applications. Dyes and Pigments, 2020, 173, 108008.	3.7	34
13	BODIPY-core 1,7-diphenyl-substituted derivatives for photovoltaics and OLED applications. Dyes and Pigments, 2020, 175, 108123.	3.7	30
14	Structure and tuneable luminescence in polymeric zinc compounds based on 3-(3-pyridyl)-5-(4-pyridyl)-1,2,4-triazole. Polyhedron, 2020, 191, 114768.	2.2	19
15	New Aspects of the Airglow Problem and Reactivity of the Dioxygen Quintet O₂(⁵Î_g) State in the MLT Region as Predicted by DFT Calculations. Journal of Physical Chemistry A, 2020, 124, 9638-9655.	2.5	7
16	Can attachment of tert-butyl substituents to methoxycarbazole moiety induce efficient TADF in diphenylsulfone-based blue OLED emitters?. Organic Electronics, 2020, 86, 105894.	2.6	6
17	A Fully Conjugated Planar Heterocyclic [9]Circulene. Journal of the American Chemical Society, 2020, 142, 14058-14063.	13.7	28
18	First-principles calculations of anharmonic and deuteration effects on the photophysical properties of polyacenes and porphyrinoids. Physical Chemistry Chemical Physics, 2020, 22, 22314-22323.	2.8	32

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19	Benzoselenophenylpyridine platinum complexes: green versus red phosphorescence towards hybrid OLEDs. Dalton Transactions, 2020, 49, 3393-3397.	3.3	19
20	Compressing a Nonâ€Planar Aromatic Heterocyclic [7]Helicene to a Planar Hetero[8]Circulene. Chemistry - A European Journal, 2020, 26, 4935-4940.	3.3	28
21	Antiâ€Aromatic versus Induced Paratropicity: Synthesis and Interrogation of a Dihydroâ€diazatrioxa[9]circulene with a Proton Placed Directly above the Central Ring. Angewandte Chemie - International Edition, 2020, 59, 5144-5150.	13.8	17
22	Antiâ€Aromatic versus Induced Paratropicity: Synthesis and Interrogation of a Dihydroâ€diazatrioxa[9]circulene with a Proton Placed Directly above the Central Ring. Angewandte Chemie, 2020, 132, 5182-5188.	2.0	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.	2.6	11
24	Molecular Phosphorescence in Polymer Matrix with Reversible Sensitivity. ACS Applied Materials & Interfaces, 2020, 12, 20765-20774.	8.0	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.	2.8	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.	2.6	10
28	Structure and excitation-dependent emission of novel zinc complexes with pyridyltriazoles. RSC Advances, 2019, 9, 22143-22152.	3.6	18
29	Impact of heteroatoms (S, Se, and Te) on the aromaticity of heterocirculenes. New Journal of Chemistry, 2019, 43, 12178-12190.	2.8	10
30	How cofactor-free oxygenases can overcome spin prohibition in substrates oxygenation by dioxygen. Chemical Physics, 2019, 521, 61-68.	1.9	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.	2.8	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.	3.1	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.	4.1	4
34	A complete characterization of vibrational IR and Raman spectra of the highly-symmetrical octathia[8]circulene. Vibrational Spectroscopy, 2019, 100, 107-116.	2.2	9
35	Multi-channel electroluminescence of CdTe/CdS core-shell quantum dots implemented into a QLED device. Dyes and Pigments, 2019, 162, 647-653.	3.7	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.	2.4	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.	0.5	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	Spinâ€“catalysis of Unsaturated Substrates Oxidation by Cofactorâ€“free Monoâ€“ and Diâ€“oxygenases. How Triplet Oxygen Can Overcome Spin Prohibition. UkraÃ¯nsÊ¹kij Å¾urnal Medicini BÃ¬ologÃ¬Ã¯ Ta Sportu, 2019, 4, 329-343.	0.2	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.	0.6	1
42	Optical tuning of tetrabenzo[8]circulene derivatives through pseudorotational conformational isomerization. Dyes and Pigments, 2018, 151, 372-379.	3.7	5
43	Contribution of TADF and exciplex emission for efficient â€œwarm-whiteâ€•OLEDs. Journal of Materials Chemistry C, 2018, 6, 1543-1550.	5.5	64
44	Dynamics of Thermoluminescence under Dual-Wavelength Visâ€“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.	0.6	1
45	Strong Topological States and High Charge Carrier Mobility in Tetraoxa[8]circulene Nanosheets. Journal of Physical Chemistry C, 2018, 122, 22216-22222.	3.1	25
46	Identification of tautomeric intermediates of a novel thiazolylazonaphthol dye â€“ A density functional theory study. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2018, 203, 324-332.	3.9	4
47	Vibronic absorption spectra of the angular fused bisindolo- and biscarbazoloanthracene blue fluorophores for OLED applications. Chemical Physics, 2018, 513, 105-111.	1.9	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.	2.8	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 allotropeâ€”a chemical twin of the cubic gauche form of nitrogen. Physical Chemistry Chemical Physics, 2017, 19, 6698-6706.	2.8	32
52	Recent progress in quantum chemistry of hetero[8]circulenes. Molecular Physics, 2017, 115, 2218-2230.	1.7	28
53	A computational study of aromaticity and photophysical properties of unsymmetrical azatrioxa[8]circulenes. New Journal of Chemistry, 2017, 41, 2717-2723.	2.8	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 10 Tf 50 57	1.6	4

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55	DFT design of polyguanidine â€“ a unique two-dimensional material with high-energy density. Molecular Physics, 2017, 115, 2423-2430.	1.7	7
56	A computational study of structural and magnetic properties of bi- and trinuclear Cu(II) complexes with extremely long Cu---Cu distances. Chemical Physics, 2017, 491, 48-55.	1.9	12
57	Synthesis and luminescent properties of copper(I) complexes with 3-pyridin-2-yl-5-(4-R-phenyl)-1H-1,2,4-triazoles. Russian Journal of Inorganic Chemistry, 2017, 62, 423-430.	1.3	5
58	Synthesis and characterisation of a carbazole-based bipolar exciplex-forming compound for efficient and color-tunable OLEDs. New Journal of Chemistry, 2017, 41, 559-568.	2.8	34
59	Substituent-sensitive fluorescence of sequentially N-alkylated tetrabenzotetraaza[8]circulenes. New Journal of Chemistry, 2017, 41, 7621-7625.	2.8	9
60	BaZrO3 perovskite nanoparticles as emissive material for organic/inorganic hybrid light-emitting diodes. Dyes and Pigments, 2017, 145, 399-403.	3.7	9
61	Comparative study of the structural and spectral properties of tetraaza- and tetraoxaannelated tetracirculenes. Optics and Spectroscopy (English Translation of Optika I Spektroskopiya), 2017, 122, 523-540.	0.6	6
62	New WOLEDs based on Ï€-extended azatrioxa[8]circulenes. Journal of Materials Chemistry C, 2017, 5, 4123-4128.	5.5	28
63	Theory and Calculation of the Phosphorescence Phenomenon. Chemical Reviews, 2017, 117, 6500-6537.	47.7	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. Journal of Molecular Modeling, 2017, 23, 55.	1.8	11
65	Two-dimensional honeycomb (A7) and zigzag sheet (ZS) type nitrogen monolayers. A first principles study of structural, electronic, spectral, and mechanical properties. Computational Materials Science, 2017, 133, 122-129.	3.0	27
66	Two isomeric solid carbon nitrides with 1â€‰:â€‰1 stoichiometry which exhibit strong mechanical anisotropy. New Journal of Chemistry, 2017, 41, 13140-13148.	2.8	8
67	Singlet Oxygen Photophysics in Liquid Solvents: Converging on a Unified Picture. Accounts of Chemical Research, 2017, 50, 1920-1927.	15.6	97
68	Influence of Molecular Oxygen on Ortho-Para Conversion of Water Molecules. Russian Physics Journal, 2017, 60, 485-493.	0.4	2
69	Analysis of Dissociationâ€"Recombination Processes for the CO2 Molecule with the Spinâ€"Orbit Coupling Taken into Account. Optics and Spectroscopy (English Translation of Optika I) Tj ETQq1 1 0.784314 rgBT /Overlock 10 Tf 50 1	0.6	8
70	Nine-ring angular fused biscarbazoloanthracene displaying a solid state based excimer emission suitable for OLED application. Journal of Materials Chemistry C, 2016, 4, 5795-5805.	5.5	33
71	Highly Luminous Sky-Blue Organic Light-Emitting Diodes Based on the Bis[(1,2)(5,6)]indoloanthracene Emissive Layer. Journal of Physical Chemistry C, 2016, 120, 6206-6217.	3.1	45
72	Computational study of the structure, UV-vis absorption spectra and conductivity of biphenylene-based polymers and their boron nitride analogues. RSC Advances, 2016, 6, 49505-49516.	3.6	24

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73	Ab initio investigation of electric and magnetic dipole electronic transitions in the complex of oxygen with benzene. Journal of Molecular Modeling, 2016, 22, 214.	1.8	5
74	Ab Initio Study of Electronic States of Astrophysically Important Molecules. Russian Physics Journal, 2016, 59, 536-543.	0.4	9
75	Benzoannelated aza-, oxa- and azaoxa[8]circulenes as promising blue organic emitters. Physical Chemistry Chemical Physics, 2016, 18, 28040-28051.	2.8	54
76	Anion-induced exchange interactions in binuclear complexes of Cu(II) with flexible hexadentate bispicolylamidrazone ligands. Chemical Physics Letters, 2016, 661, 48-52.	2.6	9
77	Analysis of the electronic, IR, and 1H NMR spectra of conjugated oligomers based on 4,4'-triphenylamine vinylene. Optics and Spectroscopy (English Translation of Optika I Spektroskopiya), 2016, 121, 348-356.	0.6	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. Russian Journal of Inorganic Chemistry, 2016, 61, 588-593.	1.3	9
79	Electroluminescence of Halogen Complexes with Monovalent Copper: OLED Devices and DFT Modeling. Russian Physics Journal, 2016, 58, 1205-1211.	0.4	14
80	Spin-dependent effects in ethylene polymerization with bis(imino)pyridine iron(II) complexes. Journal of Organometallic Chemistry, 2016, 811, 48-65.	1.8	17
81	Aromaticity of the doubly charged [8]circulenes. Physical Chemistry Chemical Physics, 2016, 18, 8980-8992.	2.8	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. Recent Advances which Support the Old Theory. Chemistry and Chemical Technology, 2016, 10, 519-530.	1.1	8
84	The effect of a heteroatom on the structure and vibrational spectra of Heteroannulated tetraphenylenes. Optics and Spectroscopy (English Translation of Optika I Spektroskopiya), 2015, 119, 620-632.	0.6	4
85	Electronic structure, aromaticity and spectra of hetero[8]circulenes. Russian Chemical Reviews, 2015, 84, 455-484.	6.5	46
86	Temperature effects in low-frequency Raman spectra of corticosteroid hormones. Optics and Spectroscopy (English Translation of Optika I Spektroskopiya), 2015, 118, 214-223.	0.6	10
87	Quantum-chemical investigation of the structure and electronic absorption spectra of symmetric triphenylamine oligomers conjugated to vinylene, imine, azine, and ethynylene groups. Optics and Spectroscopy (English Translation of Optika I Spektroskopiya), 2015, 118, 703-710.	0.6	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. Russian Journal of Inorganic Chemistry, 2015, 60, 1560-1567.	1.3	6
89	Thermally accessible triplet state of Ï€-nucleophiles does exist. Evidence from first principles study of ethylene interaction with copper species. RSC Advances, 2015, 5, 11558-11569.	3.6	19
90	Alkali and alkaline-earth metal complexes with tetraoxa[8]circulene sheet: a computational study by DFT and QTAIM methods. RSC Advances, 2015, 5, 24299-24305.	3.6	28

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91	Synthesis and properties of synthetic fulvic acid derived from hematoxylin. Journal of Molecular Structure, 2015, 1086, 25-33.	3.6	19
92	DFT simulation of the heteroannelated octatetraenes vibronic spectra with the Franckâ€“Condon and Herzbergâ€“Teller approaches including Duschinsky effect. Chemical Physics, 2015, 459, 65-71.	1.9	22
93	A DFT and QTAIM study of the novel d-block metal complexes with tetraoxa[8]circulene-based ligands. New Journal of Chemistry, 2015, 39, 7815-7821.	2.8	33
94	Structure and spectroscopic characterization of tetrathia- and tetraselena[8]circulenes as a new class of polyaromatic heterocycles. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2015, 151, 247-261.	3.9	22
95	A combined experimental and density functional study of 1-(arylsulfonyl)-2-R-4-chloro-2-butenes reactivity towards the allylic chlorine. Journal of Physical Organic Chemistry, 2015, 28, 403-413.	1.9	0
96	Computational and Experimental Investigation of the Optical Properties of the Chromene Dyes. Journal of Physical Chemistry A, 2015, 119, 1948-1956.	2.5	23
97	Aromaticity of the completely annelated tetraphenylenes: NICS and GIMIC characterization. Journal of Molecular Modeling, 2015, 21, 136.	1.8	34
98	Synthesis and spectroscopic characterization of a new (aryl-SCN)n polymer: Polythiocyanatohydroquinone. Journal of Molecular Structure, 2015, 1096, 15-20.	3.6	3
99	Features of terahertz adsorption and Raman scattering of mineralocorticoid hormones. Bulletin of the Russian Academy of Sciences: Physics, 2015, 79, 1196-1201.	0.6	4
100	Absolute effective cross sections of ionization of adenine and guanine molecules by electron impact. Technical Physics, 2015, 60, 1430-1436.	0.7	7
101	N-annelated perylenes as effective green emitters for OLEDs. RSC Advances, 2015, 5, 78150-78159.	3.6	21
102	Mixing of Phosphorescent and Exciplex Emission in Efficient Organic Electroluminescent Devices. ACS Applied Materials & Interfaces, 2015, 7, 1219-1225.	8.0	78
103	Tetrathio and Tetraseleno[8]circulenes: Synthesis, Structures, and Properties. Chemistry - an Asian Journal, 2015, 10, 969-975.	3.3	52
104	Tuning optical and electronic properties of poly(4,4'-triphenylamine vinylene)s by post-modification reactions. Dyes and Pigments, 2015, 113, 227-238.	3.7	10
105	Spin-orbit coupling and dissociation of CO2 molecules. Optics and Spectroscopy (English Translation) Tj ETQq1 1 0.784314 rgBT /Ove	0.6	9
106	Plasmon amplification and quenching of the fluorescence and phosphorescence of anionic and cationic dyes in various media. Journal of Optical Technology (A Translation of Opticheskii Zhurnal), 2014, 81, 625.	0.4	8
107	The size-controllable, one-step synthesis and characterization of gold nanoparticles protected by synthetic humic substances. Materials Chemistry and Physics, 2014, 144, 168-178.	4.0	30
108	State-Dependent Global and Local Electrophilicity of the Aryl Cations. Journal of Physical Chemistry A, 2014, 118, 3201-3210.	2.5	19

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109	Efficient â€œWarm-Whiteâ€•OLEDs Based on the Phosphorescent bis-Cyclometalated iridium(III) Complex. Journal of Physical Chemistry C, 2014, 118, 11271-11278.	3.1	73
110	The Electronic Structure of Heteroannelated Cyclooctatetraenes and their UV-Vis Absorption Spectra. Chemistry of Heterocyclic Compounds, 2014, 50, 349-363.	1.2	15
111	Principles of phosphorescent organic light emitting devices. Physical Chemistry Chemical Physics, 2014, 16, 1719-1758.	2.8	398
112	Design of nanoscaled materials based on tetraoxa[8]circulene. Physical Chemistry Chemical Physics, 2014, 16, 6555.	2.8	48
113	A comparative study of the electronic structure and spectra of tetraoxa[8]circulene and octathio[8]circulene. Optics and Spectroscopy (English Translation of Optika I Spektroskopiya), 2014, 116, 33-46.	0.6	26
114	The art of the possible: computational design of the 1D and 2D materials based on the tetraoxa[8]circulene monomer. RSC Advances, 2014, 4, 25843-25851.	3.6	50
115	Electronic descriptors for analytical use of the benzidineâ€based compounds and the mechanism of oxidative coupling of anilines. Journal of Physical Organic Chemistry, 2014, 27, 640-651.	1.9	11
116	DFT characterization of a new possible graphene allotrope. Chemical Physics Letters, 2014, 612, 229-233.	2.6	54
117	Fragmentation of the adenine and guanine molecules induced by electron collisions. Journal of Chemical Physics, 2014, 140, 175101.	3.0	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. Optics and Spectroscopy (English Translation of Optika I Spektroskopiya), 2014, 116, 431-437.	0.6	4
119	Aromaticity of the planar hetero[8]circulenes and their doubly charged ions: NICS and GIMIC characterization. Physical Chemistry Chemical Physics, 2014, 16, 15367-15374.	2.8	69
120	Theoretical Study of Relationships between Structural, Optical, Energetic, and Magnetic Properties and Reactivity Parameters of Benzidine and Its Oxidized Forms. Journal of Physical Chemistry A, 2014, 118, 8872-8882.	2.5	9
121	Quantum-chemical simulation of the synthesis of structural fragments of humic substances analogs. Russian Journal of General Chemistry, 2014, 84, 848-852.	0.8	3
122	The singletâ€“triplet energy splitting of Ï€-nucleophiles as a measure of their reaction rate with electrophilic partners. Chemical Physics Letters, 2014, 607, 75-80.	2.6	18
123	Raman spectra of alkyl-substituted azaoxa[8]circulenes: DFT calculation and experiment. Optics and Spectroscopy (English Translation of Optika I Spektroskopiya), 2013, 114, 509-521.	0.6	10
124	Triplet State Phosphorescence in Tris(8-hydroxyquinoline) Aluminum Light Emitting Diode Materials. Journal of Physical Chemistry C, 2013, 117, 3446-3455.	3.1	10
125	Comparative computational IR, Raman and phosphorescence study of Ru- and Rh-based complexes. Molecular Physics, 2013, 111, 1526-1538.	1.7	6
126	Highly Efficient Blue Organic Light-Emitting Diodes Based on Intermolecular Tripletâ€“Singlet Energy Transfer. Journal of Physical Chemistry C, 2013, 117, 22538-22544.	3.1	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. Journal of Physical Chemistry C, 2013, 117, 17969-17982.	3.1	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. Russian Journal of Inorganic Chemistry, 2013, 58, 928-934.	1.3	24
129	Structure and electronic absorption spectra of isotruxene dyes for dye-sensitized solar cells: Investigation by the DFT, TDDFT, and QTAIM methods. Optics and Spectroscopy (English Translation of) Tj ETQq1 1 0.784314 rgBT /Ove	1.1	9
130	Dioxygen spectra and bioactivation. International Journal of Quantum Chemistry, 2013, 113, 1847-1867.	2.0	41
131	Nucleus-independent chemical shift criterion for aromaticity in Ï€-extended tetraoxa[8]circulenes. Journal of Molecular Modeling, 2013, 19, 847-850.	1.8	50
132	Diazadioxa[8]circulenes: Planar Antiaromatic Cyclooctatetraenes. Chemistry - A European Journal, 2013, 19, 17097-17102.	3.3	80
133	Azatrioxa[8]circulenes: Planar Antiâ€Aromatic Cyclooctatetraenes. Chemistry - A European Journal, 2013, 19, 3898-3904.	3.3	78
134	Spectroscopy study of silver nanoparticles fabrication using synthetic humic substances and their antimicrobial activity. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2013, 108, 115-122.	3.9	74
135	The FTIR spectra of substituted tetraoxa[8]circulenes and their assignments based on DFT calculations. Vibrational Spectroscopy, 2013, 65, 147-158.	2.2	26
136	Quantum-chemical investigation of the structure and electronic absorption spectra of electroluminescent zinc complexes. Optics and Spectroscopy (English Translation of Optika I) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50 377	0.6	11
137	Theoretical study of the triplet state aryl cations recombination: A possible route to unusually stable doubly charged biphenyl cations. International Journal of Quantum Chemistry, 2013, 113, 2580-2588.	2.0	14
138	Analysis of intermolecular interactions in progesterone and 17α-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. Journal of Molecular Modeling, 2013, 19, 4511-4519.	1.8	31
140	Electron density distribution in the ethylene complexes with Pd-containing bimetallic clusters. Molecular Simulation, 2013, 39, 660-669.	2.0	2
141	Spin-spin and spin-orbit interactions in nanographene fragments: A quantum chemistry approach. Journal of Chemical Physics, 2012, 136, 104702.	3.0	37
142	Application of Baderâ€™s atoms in molecules theory to the description of coordination bonds in the complex compounds of Ca2+ and Mg2+ with methylidene rhodanine and its anion. Russian Journal of General Chemistry, 2012, 82, 1254-1262.	0.8	39
143	Raman spectra of tetraoxa[8]circulenes. p-dinaphthalenodiphenylenotetrafuran and its tetraalkyl derivatives (DFT study and experiment). Journal of Applied Spectroscopy, 2012, 79, 695-707.	0.7	11
144	DFT and QTAIM study of the tetra-tert-butyltetraoxa[8]circulene regioisomers structure. Journal of Molecular Structure, 2012, 1026, 127-132.	3.6	35

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145	Structure and intramolecular stabilization of geometric isomers of Bi- and trithiazolidine-4-ones and their methyl derivatives: A DFT and QTAIM study. Journal of Structural Chemistry, 2012, 53, 428-435.	1.0	6
146	Theoretical investigation of the structure and electronic absorption spectrum of a complex zinc bis-[8-(3,5-difluorophenylsulfanylamino)quinolinate]. Optics and Spectroscopy (English Translation of) Tj ETQq0 0 0 rgBT /Overlock 10 T	0.6	12
147	Kinetic and mechanism formation of silver nanoparticles coated by synthetic humic substances. Colloids and Surfaces A: Physicochemical and Engineering Aspects, 2012, 414, 234-243.	4.7	44
148	Electronic structure and spectral properties of the triarylamine-dithienosilole dyes for efficient organic solar cells. Dyes and Pigments, 2012, 92, 531-536.	3.7	53
149	Spin-Orbit Coupling in Enzymatic Reactions and the Role of Spin in Biochemistry. , 2012, , 1067-1093.		6
150	Theoretical study of the dimerization of rhodanine in various tautomeric forms. Chemistry of Heterocyclic Compounds, 2012, 47, 1268-1279.	1.2	11
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