

Boris F Minaev

List of Publications by Year in Descending Order

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

334
papers

6,746
citations

43
h-index

63
g-index

348
ext. papers

7,358
ext. citations

2.8
avg, IF

6.25
L-index

#	Paper	IF	Citations
334	Crystal structure and Hirshfeld surfaces analysis of Heterocyclic-and circulenes. <i>MATEC Web of Conferences</i> , 2022 , 355, 01020	0.3	0
333	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	4.6	1
332	Aromaticity of Heterocirculenes. <i>Chemistry</i> , 2021 , 3, 1411-1436	2.1	1
331	Multidimensional Structure Conformation of Persulfurated Benzene for Highly Efficient Phosphorescence. <i>ACS Applied Materials & Interfaces</i> , 2021 , 13, 1314-1322	9.5	8
330	Dianthracenylazatrioxa[8]circulene: Synthesis, Characterization and Application in OLEDs. <i>Chemistry - A European Journal</i> , 2021 , 27, 11609-11617	4.8	4
329	Molecular Terms of Dioxygen and Nitric Oxide. <i>Physchem</i> , 2021 , 1, 121-132		1
328	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	7.1	3
327	Computational study of IR, Raman, and NMR spectra of 4-methylmethcathinone drug. <i>Journal of Molecular Modeling</i> , 2021 , 27, 3	2	2
326	Schiff Base Zinc(II) Complexes as Promising Emitters for Blue Organic Light-Emitting Diodes. <i>ACS Applied Electronic Materials</i> , 2021 , 3, 3436-3444	4	1
325	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	2	3
324	Benzoselenophenylpyridine platinum complexes: green versus red phosphorescence towards hybrid OLEDs. <i>Dalton Transactions</i> , 2020 , 49, 3393-3397	4.3	13
323	Compressing a Non-Planar Aromatic Heterocyclic [7]Helicene to a Planar Hetero[8]Circulene. <i>Chemistry - A European Journal</i> , 2020 , 26, 4935-4940	4.8	14
322	Anti-Aromatic versus Induced Paratropicity: Synthesis and Interrogation of a Dihydro-diazatrioxa[9]circulene with a Proton Placed Directly above the Central Ring. <i>Angewandte Chemie - International Edition</i> , 2020 , 59, 5144-5150	16.4	11
321	Anti-Aromatic versus Induced Paratropicity: Synthesis and Interrogation of a Dihydro-diazatrioxa[9]circulene with a Proton Placed Directly above the Central Ring. <i>Angewandte Chemie</i> , 2020 , 132, 5182-5188	3.6	7
320	Flexible diphenylsulfone versus rigid dibenzothiophene-dioxide as acceptor moieties in donor-acceptor-donor TADF emitters for highly efficient OLEDs. <i>Organic Electronics</i> , 2020 , 83, 105733	3.5	5
319	Molecular Phosphorescence in Polymer Matrix with Reversible Sensitivity. <i>ACS Applied Materials & Interfaces</i> , 2020 , 12, 20765-20774	9.5	26
318	Furans and Their Benzo Derivatives: Structure 2020 , 190-190		1

317	The effect of molecular structure on the properties of quinoxaline-based molecules for OLED applications. <i>Dyes and Pigments</i> , 2020 , 173, 108008	4.6	15
316	BODIPY-core 1,7-diphenyl-substituted derivatives for photovoltaics and OLED applications. <i>Dyes and Pigments</i> , 2020 , 175, 108123	4.6	14
315	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	2.7	10
314	New Aspects of the Airglow Problem and Reactivity of the Dioxygen Quintet O(Δ) State in the MLT Region as Predicted by DFT Calculations. <i>Journal of Physical Chemistry A</i> , 2020 , 124, 9638-9655	2.8	3
313	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	3.5	4
312	A Fully Conjugated Planar Heterocyclic [9]Circulene. <i>Journal of the American Chemical Society</i> , 2020 , 142, 14058-14063	16.4	15
311	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	3.6	15
310	Structure, stability and electronic properties of one-dimensional tetrathia- and tetraselena[8]circulene-based materials: a comparative DFT study. <i>New Journal of Chemistry</i> , 2020 , 44, 6872-6882	3.6	2
309	How cofactor-free oxygenases can overcome spin prohibition in substrates oxygenation by dioxygen. <i>Chemical Physics</i> , 2019 , 521, 61-68	2.3	7
308	Aromaticity and photophysics of tetrasila- and tetra-germa-annelated tetrathienylenes as new representatives of the hetero[8]circulene family. <i>Physical Chemistry Chemical Physics</i> , 2019 , 21, 9246-9254	3.6	16
307	Novel Zinc Complex with an Ethylenediamine Schiff Base for High-Luminance Blue Fluorescent OLED Applications. <i>Journal of Physical Chemistry C</i> , 2019 , 123, 11850-11859	3.8	37
306	The blue vibronically resolved electroluminescence of azatrioxa[8]circulene. <i>Chemical Physics Letters</i> , 2019 , 732, 136667	2.5	7
305	Structure and excitation-dependent emission of novel zinc complexes with pyridyltriazoles.. <i>RSC Advances</i> , 2019 , 9, 22143-22152	3.7	8
304	Impact of heteroatoms (S, Se, and Te) on the aromaticity of heterocirculenes. <i>New Journal of Chemistry</i> , 2019 , 43, 12178-12190	3.6	4
303	Spin-orbit coupling effects in O(2) activation by cofactor-independent 2,4-dioxygenase. <i>Ukrainian Biochemical Journal</i> , 2019 , 91, 38-46	0.7	2
302	Spin-catalysis of Unsaturated Substrates Oxidation by Cofactor-free Mono- and Dioxygenases. How Triplet Oxygen Can Overcome Spin Prohibition. <i>Ukrainian Journal of Medicine and Biology</i> , 2019 , 4, 329-343	0.1	0
301	Experimental and theoretical study of the mechanism formation of silver nanoclusters in the reduction reaction of Ag ⁺ ions by alizarin solution. <i>Colloids and Interface Science Communications</i> , 2019 , 29, 47-54	5.4	4
300	A complete characterization of vibrational IR and Raman spectra of the highly-symmetrical octathia[8]circulene. <i>Vibrational Spectroscopy</i> , 2019 , 100, 107-116	2.1	9

299	Multi-channel electroluminescence of CdTe/CdS core-shell quantum dots implemented into a QLED device. <i>Dyes and Pigments</i> , 2019 , 162, 647-653	4.6	17
298	Computational study of the structure and magnetic properties of the weakly-coupled tetranuclear square-planar complex of Cu(II) with a tetraporphyrin sheet. <i>Inorganica Chimica Acta</i> , 2019 , 485, 73-79	2.7	4
297	The Electronic Structure and Spectra of Triphenylamines Functionalized by Phenylethynyl Groups. <i>Optics and Spectroscopy (English Translation of Optika I Spektroskopiya)</i> , 2018 , 124, 57-64	0.7	1
296	Optical tuning of tetrabenz[8]circulene derivatives through pseudorotational conformational isomerization. <i>Dyes and Pigments</i> , 2018 , 151, 372-379	4.6	4
295	Contribution of TADF and exciplex emission for efficient "warm-white" OLEDs. <i>Journal of Materials Chemistry C</i> , 2018 , 6, 1543-1550	7.1	59
294	Vibronic absorption spectra of the angular fused bisindolo- and biscarbazoloanthracene blue fluorophores for OLED applications. <i>Chemical Physics</i> , 2018 , 513, 105-111	2.3	2
293	A theoretical study of new representatives of closed- and open-circle benzofuran and benzocyclopentadienone oligomers. <i>New Journal of Chemistry</i> , 2018 , 42, 11493-11505	3.6	9
292	Dynamics of Thermoluminescence under Dual-Wavelength Vis-IR Laser Excitation of Eosin Molecules in a Polyvinyl Butyral Film Containing Oxygen and Silver Nanoparticles. <i>Optics and Spectroscopy (English Translation of Optika I Spektroskopiya)</i> , 2018 , 125, 874-881	0.7	1
291	Strong Topological States and High Charge Carrier Mobility in Tetraoxa[8]circulene Nanosheets. <i>Journal of Physical Chemistry C</i> , 2018 , 122, 22216-22222	3.8	17
290	Identification of tautomeric intermediates of a novel thiazolylazonaphthol dye - A density functional theory study. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2018 , 203, 324-332	4.4	4
289	Spin-Orbit Coupling in Enzymatic Reactions and the Role of Spin in Biochemistry 2017 , 1557-1587		4
288	Super high-energy density single-bonded trigonal nitrogen allotrope-a chemical twin of the cubic gauche form of nitrogen. <i>Physical Chemistry Chemical Physics</i> , 2017 , 19, 6698-6706	3.6	23
287	Recent progress in quantum chemistry of hetero[8]circulenes. <i>Molecular Physics</i> , 2017 , 115, 2218-2230	1.7	22
286	A computational study of aromaticity and photophysical properties of unsymmetrical azatrioxa[8]circulenes. <i>New Journal of Chemistry</i> , 2017 , 41, 2717-2723	3.6	15
285	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. <i>Optics and Spectroscopy (English Translation of Optika I Spektroskopiya)</i> , 2017 , 122, 175-183	0.7	2
284	DFT design of polyguanidine - a unique two-dimensional material with high-energy density. <i>Molecular Physics</i> , 2017 , 115, 2423-2430	1.7	7
283	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	2.3	10
282	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 ^{1.5}		4

281	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	3.6	25
280	Substituent-sensitive fluorescence of sequentially N-alkylated tetrabenzotetraaza[8]circulenes. <i>New Journal of Chemistry</i> , 2017 , 41, 7621-7625	3.6	9
279	BaZrO ₃ perovskite nanoparticles as emissive material for organic/inorganic hybrid light-emitting diodes. <i>Dyes and Pigments</i> , 2017 , 145, 399-403	4.6	7
278	Comparative study of the structural and spectral properties of tetraaza- and tetraoxaannelated tetracirculenes. <i>Optics and Spectroscopy (English Translation of Optika I Spektroskopiya)</i> , 2017 , 122, 523-540	0.7	6
277	New WOLEDs based on extended azatrioxa[8]circulenes. <i>Journal of Materials Chemistry C</i> , 2017 , 5, 4123-4128	7.1	21
276	Theory and Calculation of the Phosphorescence Phenomenon. <i>Chemical Reviews</i> , 2017 , 117, 6500-6537	68.1	289
275	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	2	10
274	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	3.2	16
273	Two isomeric solid carbon nitrides with 1 : 1 stoichiometry which exhibit strong mechanical anisotropy. <i>New Journal of Chemistry</i> , 2017 , 41, 13140-13148	3.6	8
272	Singlet Oxygen Photophysics in Liquid Solvents: Converging on a Unified Picture. <i>Accounts of Chemical Research</i> , 2017 , 50, 1920-1927	24.3	67
271	Influence of Molecular Oxygen on Ortho-Para Conversion of Water Molecules. <i>Russian Physics Journal</i> , 2017 , 60, 485-493	0.7	1
270	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	2	4
269	Ab Initio Study of Electronic States of Astrophysically Important Molecules. <i>Russian Physics Journal</i> , 2016 , 59, 536-543	0.7	7
268	Benzoannelated aza-, oxa- and azaoxa[8]circulenes as promising blue organic emitters. <i>Physical Chemistry Chemical Physics</i> , 2016 , 18, 28040-28051	3.6	45
267	Anion-induced exchange interactions in binuclear complexes of Cu(II) with flexible hexadentate bispicolylamidrazone ligands. <i>Chemical Physics Letters</i> , 2016 , 661, 48-52	2.5	8
266	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	0.7	4
265	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	1.5	9
264	Electroluminescence of Halogen Complexes with Monovalent Copper: OLED Devices and DFT Modeling. <i>Russian Physics Journal</i> , 2016 , 58, 1205-1211	0.7	10

263	Spin-dependent effects in ethylene polymerization with bis(imino)pyridine iron(II) complexes. <i>Journal of Organometallic Chemistry</i> , 2016 , 811, 48-65	2.3	14
262	Aromaticity of the doubly charged [8]circulenes. <i>Physical Chemistry Chemical Physics</i> , 2016 , 18, 8980-92	3.6	27
261	Photochemistry and Spectroscopy of Singlet Oxygen in Solvents. Recent Advances which Support the Old Theory. <i>Chemistry and Chemical Technology</i> , 2016 , 10, 519-530	0.9	7
260	Spin-Orbit Coupling in Enzymatic Reactions and the Role of Spin in Biochemistry 2016 , 1-31		1
259	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> , 2016 , 120, 345-351	0.7	7
258	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	7.1	30
257	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	3.8	40
256	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	3.7	15
255	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	2.3	21
254	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	3.6	25
253	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, 247-61	4.4	21
252	A combined experimental and density functional study of 1-(arylsulfonyl)-2-R-4-chloro-2-butenes reactivity towards the allylic chlorine. <i>Journal of Physical Organic Chemistry</i> , 2015 , 28, 403-413	2.1	
251	Computational and experimental investigation of the optical properties of the chromene dyes. <i>Journal of Physical Chemistry A</i> , 2015 , 119, 1948-56	2.8	20
250	Aromaticity of the completely annulated tetraphenylenes: NICS and GIMIC characterization. <i>Journal of Molecular Modeling</i> , 2015 , 21, 136	2	29
249	Synthesis and spectroscopic characterization of a new (aryl-SCN) _n polymer: Polythiocyanatohydroquinone. <i>Journal of Molecular Structure</i> , 2015 , 1096, 15-20	3.4	2
248	Features of terahertz adsorption and Raman scattering of mineralocorticoid hormones. <i>Bulletin of the Russian Academy of Sciences: Physics</i> , 2015 , 79, 1196-1201	0.4	2
247	Absolute effective cross sections of ionization of adenine and guanine molecules by electron impact. <i>Technical Physics</i> , 2015 , 60, 1430-1436	0.5	5
246	N-annulated perylenes as effective green emitters for OLEDs. <i>RSC Advances</i> , 2015 , 5, 78150-78159	3.7	21

245	Mixing of phosphorescent and exciplex emission in efficient organic electroluminescent devices. <i>ACS Applied Materials & Interfaces</i> , 2015 , 7, 1219-25	9.5	74
244	Tetrathio and tetraseleno[8]circulenes: synthesis, structures, and properties. <i>Chemistry - an Asian Journal</i> , 2015 , 10, 969-75	4.5	43
243	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	4.6	7
242	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	0.7	3
241	Electronic structure, aromaticity and spectra of hetero[8]circulenes. <i>Russian Chemical Reviews</i> , 2015 , 84, 455-484	6.8	34
240	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	0.7	8
239	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	0.7	2
238	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	1.5	6
237	Thermally accessible triplet state of nucleophiles does exist. Evidence from first principles study of ethylene interaction with copper species. <i>RSC Advances</i> , 2015 , 5, 11558-11569	3.7	18
236	Alkali and alkaline-earth metal complexes with tetraoxa[8]circulene sheet: a computational study by DFT and QAIM methods. <i>RSC Advances</i> , 2015 , 5, 24299-24305	3.7	24
235	Synthesis and properties of synthetic fulvic acid derived from hematoxylin. <i>Journal of Molecular Structure</i> , 2015 , 1086, 25-33	3.4	13
234	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	4.4	25
233	State-dependent global and local electrophilicity of the aryl cations. <i>Journal of Physical Chemistry A</i> , 2014 , 118, 3201-10	2.8	16
232	Efficient "Warm-White" LEDs Based on the Phosphorescent bis-Cyclometalated iridium(III) Complex. <i>Journal of Physical Chemistry C</i> , 2014 , 118, 11271-11278	3.8	66
231	The Electronic Structure of Heteroannulated Cyclooctatetraenes and their UV-Vis Absorption Spectra. <i>Chemistry of Heterocyclic Compounds</i> , 2014 , 50, 349-363	1.4	14
230	Principles of phosphorescent organic light emitting devices. <i>Physical Chemistry Chemical Physics</i> , 2014 , 16, 1719-58	3.6	327
229	Design of nanoscaled materials based on tetraoxa[8]circulene. <i>Physical Chemistry Chemical Physics</i> , 2014 , 16, 6555-9	3.6	42
228	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	0.7	26

227	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	3.7	44
226	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	2.1	11
225	DFT characterization of a new possible graphene allotrope. <i>Chemical Physics Letters</i> , 2014 , 612, 229-233	2.5	36
224	Fragmentation of the adenine and guanine molecules induced by electron collisions. <i>Journal of Chemical Physics</i> , 2014 , 140, 175101	3.9	33
223	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	0.7	4
222	Aromaticity of the planar hetero[8]circulenes and their doubly charged ions: NICS and GIMIC characterization. <i>Physical Chemistry Chemical Physics</i> , 2014 , 16, 15367-74	3.6	59
221	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, 8872-82	2.8	9
220	Quantum-chemical simulation of the synthesis of structural fragments of humic substances analogs. <i>Russian Journal of General Chemistry</i> , 2014 , 84, 848-852	0.7	3
219	The singlet-triplet energy splitting of nucleophiles as a measure of their reaction rate with electrophilic partners. <i>Chemical Physics Letters</i> , 2014 , 607, 75-80	2.5	17
218	Spin-orbit coupling and dissociation of CO ₂ molecules. <i>Optics and Spectroscopy (English Translation of Optika i Spektroskopiya)</i> , 2014 , 117, 695-702	0.7	8
217	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 Opticheski Zhurnal)</i> , 2014 , 81, 625	0.9	6
216	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	0.7	10
215	Triplet State Phosphorescence in Tris(8-hydroxyquinoline) Aluminum Light Emitting Diode Materials. <i>Journal of Physical Chemistry C</i> , 2013 , 117, 3446-3455	3.8	9
214	Comparative computational IR, Raman and phosphorescence study of Ru- and Rh-based complexes. <i>Molecular Physics</i> , 2013 , 111, 1526-1538	1.7	5
213	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	3.8	58
212	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	3.8	15
211	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	1.5	21
210	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 Spektroskopiya)</i> , 2013 , 115, 484-490	0.7	8

209	Dioxygen spectra and bioactivation. <i>International Journal of Quantum Chemistry</i> , 2013 , 113, 1847-1867	2.1	33
208	Nucleus-independent chemical shift criterion for aromaticity in extended tetraoxa[8]circulenes. <i>Journal of Molecular Modeling</i> , 2013 , 19, 847-50	2	43
207	Diazadioxa[8]circulenes: planar antiaromatic cyclooctatetraenes. <i>Chemistry - A European Journal</i> , 2013 , 19, 17097-102	4.8	74
206	Azatrioxa[8]circulenes: planar anti-aromatic cyclooctatetraenes. <i>Chemistry - A European Journal</i> , 2013 , 19, 3898-904	4.8	68
205	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, 115-22	4.4	50
204	The FTIR spectra of substituted tetraoxa[8]circulenes and their assignments based on DFT calculations. <i>Vibrational Spectroscopy</i> , 2013 , 65, 147-158	2.1	25
203	Quantum-chemical investigation of the structure and electronic absorption spectra of electroluminescent zinc complexes. <i>Optics and Spectroscopy (English Translation of Optika i Spektroskopiya)</i> , 2013 , 114, 30-40	0.7	11
202	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 ^{2,1}	2.1	14
201	Single crystal architecture and absorption spectra of octathio[8]circulene and sym-tetraselenatetrathio[8]circulene: QAIM and TD-DFT approach. <i>Journal of Molecular Modeling</i> , 2013 , 19, 4511-9	2	28
200	Electron density distribution in the ethylene complexes with Pd-containing bimetallic clusters. <i>Molecular Simulation</i> , 2013 , 39, 660-669	2	2
199	Experimental and theoretical study of IR and Raman spectra of tetraoxa[8]circulenes. <i>Vibrational Spectroscopy</i> , 2012 , 61, 156-166	2.1	48
198	A quantum chemical study of the structure of O=NO-ON=O peroxide and the reaction mechanism of no oxidation in the gas phase. <i>Journal of Structural Chemistry</i> , 2012 , 53, 1-11	0.9	7
197	Structure and spectral properties of truxene dye S5. <i>Optics and Spectroscopy (English Translation of Optika i Spektroskopiya)</i> , 2012 , 112, 168-174	0.7	20
196	Structure and spectral properties of triphenylamine dye functionalized with 3,4-propylenedioxythiophene. <i>Optics and Spectroscopy (English Translation of Optika i Spektroskopiya)</i> , 2012 , 112, 829-835	0.7	11
195	Synthesis and properties of synthetic analogs of natural humic acids. <i>Russian Journal of Applied Chemistry</i> , 2012 , 85, 296-302	0.8	18
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