Boris F Minaev

List of Publications by Citations

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	Principles of phosphorescent organic light emitting devices. *Physical Chemistry Chemical Physics*, **2014**, 16, 1719-58	3.6	327
333	Theory and Calculation of the Phosphorescence Phenomenon. *Chemical Reviews*, **2017**, 117, 6500-6537	68.1	289
332	Time-dependent density functional calculations of phosphorescence parameters for fac-tris(2-phenylpyridine) iridium. *Chemical Physics*, **2007**, 333, 157-167	2.3	134
331	Response Theory and Calculations of Spin-Orbit Coupling Phenomena in Molecules. *Advances in Quantum Chemistry*, **1996**, 71-162	1.4	124
330	Theoretical study of the cyclometalated iridium(III) complexes used as chromophores for organic light-emitting diodes. *Journal of Physical Chemistry A*, **2009**, 113, 726-35	2.8	104
329	Electronic mechanisms of activation of molecular oxygen. *Russian Chemical Reviews*, **2007**, 76, 1059-1083	3.8	100
328	Spin uncoupling in surface chemisorption of unsaturated hydrocarbons. *Journal of Chemical Physics*, **1998**, 108, 1193-1205	3.9	92
327	Ab initio calculations of electronic g-factors by means of multiconfiguration response theory. *Chemical Physics Letters*, **1997**, 281, 186-192	2.5	84
326	Theoretical DFT study of phosphorescence from porphyrins. *Chemical Physics*, **2005**, 315, 215-239	2.3	84
325	Ab initio calculations of zero-field splitting parameters. *Chemical Physics*, **2002**, 279, 133-142	2.3	77
324	Theoretical Study of Phosphorescence of Iridium Complexes with Fluorine-Substituted Phenylpyridine Ligands. *European Journal of Inorganic Chemistry*, **2011**, 2011, 2517-2524	2.3	76
323	Mixing of phosphorescent and exciplex emission in efficient organic electroluminescent devices. *ACS Applied Materials & Interfaces*, **2015**, 7, 1219-25	9.5	74
322	Diazadioxa[8]circulenes: planar antiaromatic cyclooctatetraenes. *Chemistry - A European Journal*, **2013**, 19, 17097-102	4.8	74
321	Theoretical design of phosphorescence parameters for organic electro-luminescence devices based on iridium complexes. *Chemical Physics*, **2009**, 358, 245-257	2.3	72
320	Dissociative Recombination of HCNH + : Absolute Cross-Sections and Branching Ratios. *Astrophysical Journal, Supplement Series*, **2001**, 135, 275-283	8	70
319	Density Functional Theory Study of Photophysical Properties of Iridium(III) Complexes with Phenylisoquinoline and Phenylpyridine Ligands. *Journal of Physical Chemistry C*, **2011**, 115, 20724-20731	3.8	69
318	Excited states and two-photon absorption of some novel thiophenyl Pt(II)-ethynyl derivatives. *Journal of Physical Chemistry A*, **2007**, 111, 244-50	2.8	69

317	Azatrioxa[8]circulenes: planar anti-aromatic cyclooctatetraenes. *Chemistry - A European Journal*, **2013**, 19, 3898-904	4.8	68
316	Singlet Oxygen Photophysics in Liquid Solvents: Converging on a Unified Picture. *Accounts of Chemical Research*, **2017**, 50, 1920-1927	24.3	67
315	Collision-inducedb1g+âa1g,b1g+âX3g- anda1gâX3g- transition probabilities in molecularoxygen. *Journal of the Chemical Society, Faraday Transactions*, **1997**, 93, 2231-2239		67
314	Efficient âWarm-WhiteâOLEDs Based on the Phosphorescent bis-Cyclometalated iridium(III) Complex. *Journal of Physical Chemistry C*, **2014**, 118, 11271-11278	3.8	66
313	Density functional theory study of vibronic structure of the first absorption Qx band in free-base porphin. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2006**, 65, 308-23	4.4	64
312	Activation of Triplet Dioxygen by Glucose Oxidase: SpinâOrbit Coupling in the Superoxide Ion. *Journal of Physical Chemistry B*, **2002**, 106, 3742-3750	3.4	64
311	Hydrogen Bonding to Tyrosyl Radical Analyzed by Ab Initio g-Tensor Calculations. *Journal of Physical Chemistry A*, **2000**, 104, 5149-5153	2.8	63
310	Contribution of TADF and exciplex emission for efficient âWarm-whiteâOLEDs. *Journal of Materials Chemistry C*, **2018**, 6, 1543-1550	7.1	59
309	Aromaticity of the planar hetero[8]circulenes and their doubly charged ions: NICS and GIMIC characterization. *Physical Chemistry Chemical Physics*, **2014**, 16, 15367-74	3.6	59
308	Highly Efficient Blue Organic Light-Emitting Diodes Based on Intermolecular Tripletâ Singlet Energy Transfer. *Journal of Physical Chemistry C*, **2013**, 117, 22538-22544	3.8	58
307	Solvent induced emission of molecular 1g oxygen. *Computational and Theoretical Chemistry*, **1989**, 183, 207-214		57
306	Intensities of spin-forbidden transitions in molecular oxygen and selective heavy-atom effects. *International Journal of Quantum Chemistry*, **1980**, 17, 367-374	2.1	55
305	Magnetic phosphorescence of molecular oxygen. A study of the b1g+-X3gâtransition probability using multiconfiguration response theory. *Chemical Physics*, **1996**, 208, 299-311	2.3	52
304	Spectroscopy study of silver nanoparticles fabrication using synthetic humic substances and their antimicrobial activity. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2013**, 108, 115-22	4.4	50
303	Electronic structure and spectral properties of the triarylamine-dithienosilole dyes for efficient organic solar cells. *Dyes and Pigments*, **2012**, 92, 531-536	4.6	49
302	The interpretation of the Wulf absorption band of ozone. *Chemical Physics Letters*, **1994**, 217, 531-538	2.5	49
301	Experimental and theoretical study of IR and Raman spectra of tetraoxa[8]circulenes. *Vibrational Spectroscopy*, **2012**, 61, 156-166	2.1	48
300	The influence of intermolecular interaction on the forbidden near-IR transitions in molecular oxygen. *Computational and Theoretical Chemistry*, **1993**, 284, 1-9		48

299	Benzoannelated aza-, oxa- and azaoxa[8]circulenes as promising blue organic emitters. *Physical Chemistry Chemical Physics*, **2016**, 18, 28040-28051	3.6	45
298	The vibronically induced phosphorescence in benzene. *Chemical Physics*, **1993**, 175, 245-254	2.3	45
297	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	3.7	44
296	Linear response calculations of electronic g-factors and spin-rotational coupling constants for diatomic molecules with a triplet ground state. *Chemical Physics*, **1998**, 237, 149-158	2.3	44
295	On the interpretation of the external heavy atom effect on singlet-triplet transitions. *Chemical Physics*, **1994**, 181, 15-28	2.3	44
294	Tetrathio and tetraseleno[8]circulenes: synthesis, structures, and properties. *Chemistry - an Asian Journal*, **2015**, 10, 969-75	4.5	43
293	Nucleus-independent chemical shift criterion for aromaticity in extended tetraoxa[8]circulenes. *Journal of Molecular Modeling*, **2013**, 19, 847-50	2	43
292	Electronic states and phosphorescence of dendron functionalized platinum(II) acetylides. *Journal of Luminescence*, **2007**, 124, 302-310	3.8	43
291	Design of nanoscaled materials based on tetraoxa[8]circulene. *Physical Chemistry Chemical Physics*, **2014**, 16, 6555-9	3.6	42
290	Theoretical study of triplet state properties of free-base porphin. *Chemical Physics*, **2005**, 312, 299-309	2.3	42
289	Density functional theory study of electronic structure and spectra of tetraoxa[8]circulenes. *Computational and Theoretical Chemistry*, **2011**, 972, 68-74	2	41
288	Ab initio calculations of zero-field splitting parameters in linear polyacenes. *Chemical Physics*, **2003**, 286, 127-137	2.3	41
287	MCSCF response calculations of the excited states properties of theO2 molecule and a part of its spectrum. *Physical Chemistry Chemical Physics*, **2001**, 3, 720-729	3.6	41
286	Ab initio study of the ground state properties of molecular oxygen. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2004**, 60, 1027-41	4.4	40
285	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	3.8	40
284	Fluorescence and FTIR Spectra Analysis of Trans-AâBâSubstituted Di- and Tetra-Phenyl Porphyrins. *Materials*, **2010**, 3, 4446-4475	3.5	39
283	Novel Zinc Complex with an Ethylenediamine Schiff Base for High-Luminance Blue Fluorescent OLED Applications. *Journal of Physical Chemistry C*, **2019**, 123, 11850-11859	3.8	37
282	DFT characterization of a new possible graphene allotrope. *Chemical Physics Letters*, **2014**, 612, 229-233	2.5	36

281	Electronic structure, aromaticity and spectra of hetero[8]circulenes. *Russian Chemical Reviews*, **2015**, 84, 455-484	6.8	34
280	Spin-catalysis phenomena. *International Journal of Quantum Chemistry*, **1996**, 57, 519-532	2.1	34
279	Fragmentation of the adenine and guanine molecules induced by electron collisions. *Journal of Chemical Physics*, **2014**, 140, 175101	3.9	33
278	Dioxygen spectra and bioactivation. *International Journal of Quantum Chemistry*, **2013**, 113, 1847-1867	2.1	33
277	DFT and QTAIM study of the tetra-tert-butyltetraoxa[8]circulene regioisomers structure. *Journal of Molecular Structure*, **2012**, 1026, 127-132	3.4	33
276	Kinetic and mechanism formation of silver nanoparticles coated by synthetic humic substances. *Colloids and Surfaces A: Physicochemical and Engineering Aspects*, **2012**, 414, 234-243	5.1	33
275	Spin uncoupling in molecular hydrogen activation by platinum clusters. *Journal of Molecular Catalysis A*, **1999**, 149, 179-195		33
274	Spin-spin and spin-orbit interactions in nanographene fragments: a quantum chemistry approach. *Journal of Chemical Physics*, **2012**, 136, 104702	3.9	31
273	Theoretical study of phosphorescence in dye doped light emitting diodes. *Journal of Chemical Physics*, **2006**, 125, 234704	3.9	31
272	A theoretical study of the dioxygen activation by glucose oxidase and copper amine oxidase. *Biochimica Et Biophysica Acta - Proteins and Proteomics*, **2003**, 1647, 173-8	4	31
271	Spinâ□Orbit Coupling Effects on the Metalâ□Hydrogen Bond Homolysis of M(H)(CO)3(H-DAB) (M = Mn, Re; H-DAB = 1,4-Diaza-1,3-butadiene). *Journal of Physical Chemistry A*, **1999**, 103, 5766-5772	2.8	31
270	Application of Baderâ□ 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	0.7	30
269	Some recent developments of high-order response theory. *International Journal of Quantum Chemistry*, **1998**, 70, 219-239	2.1	30
268	Theoretical study of the external heavy atom effect on phosphorescence of free-base porphin molecule. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2004**, 60, 3213-24	4.4	30
267	Quantum Chemical Model of an SN2 Reaction in a Microwave Field. *Journal of Physical Chemistry A*, **2002**, 106, 8516-8524	2.8	30
266	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	7.1	30
265	Aromaticity of the completely annelated tetraphenylenes: NICS and GIMIC characterization. *Journal of Molecular Modeling*, **2015**, 21, 136	2	29
264	Vibration and Fluorescence Spectra of Porphyrin-Cored 2,2-Bis(methylol)-propionic Acid Dendrimers. *Sensors*, **2009**, 9, 1937-66	3.8	29

263	Evaluation of low-scaling methods for calculation of phosphorescence parameters. *Journal of Chemical Physics*, **2006**, 124, 114106	3.9	29
262	Response theory calculations of the vibronically induced 1A1gâ1B2u two-photon spectrum of benzene. *Chemical Physics Letters*, **1993**, 209, 513-518	2.5	29
261	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, 4511-9	2	28
260	Internuclear distance dependence of the spinâorbit coupling contributions to proton NMR chemical shifts. *Chemical Physics Letters*, **1998**, 295, 455-461	2.5	28
259	CASSCF calculations of triplet state properties: applications to benzene derivatives. *Molecular Physics*, **2003**, 101, 2103-2114	1.7	28
258	Spin-Orbit Coupling Induced Chemical Reactivity and Spin-Catalysis Phenomena. *Collection of Czechoslovak Chemical Communications*, **1995**, 60, 339-371		28
257	Aromaticity of the doubly charged [8]circulenes. *Physical Chemistry Chemical Physics*, **2016**, 18, 8980-92	3.6	27
256	Configuration interaction study of the O2â2H4 exciplex: collision-induced probabilities of spin-forbidden radiative and non-radiative transitions. *Journal of the Chemical Society, Faraday Transactions*, **1994**, 90, 1479-1486		27
255	Approximating quasi-particle density functional calculations of small active clusters: Strong electron correlation effects. *International Journal of Quantum Chemistry*, **1990**, 38, 779-797	2.1	27
254	Molecular Phosphorescence in Polymer Matrix with Reversible Sensitivity. *ACS Applied Materials & Interfaces*, **2020**, 12, 20765-20774	9.5	26
253	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	0.7	26
252	Quantum-chemical study of the singlet oxygen emission. *International Journal of Quantum Chemistry*, **2009**, 109, 500-515	2.1	26
251	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	3.6	25
250	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	3.6	25
249	The size-controllable, one-step synthesis and characterization of gold nanoparticles protected by synthetic humic substances. *Materials Chemistry and Physics*, **2014**, 144, 168-178	4.4	25
248	The FTIR spectra of substituted tetraoxa[8]circulenes and their assignments based on DFT calculations. *Vibrational Spectroscopy*, **2013**, 65, 147-158	2.1	25
247	Response calculations of electronic and vibrational transitions in molecular oxygen induced by interaction with noble gases. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2003**, 59, 3387-410	4.4	25
246	Ab initio study of low-lying triplet states of the lithium dimer. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2005**, 62, 790-9	4.4	25

245	The Singletâ□Triplet Absorption and Photodissociation of the HOCl, HOBr, and HOI Molecules Calculated by the MCSCF Quadratic Response Method. *Journal of Physical Chemistry A*, **1999**, 103, 7294-7309	2.8	25
244	Character and spectra of triplet states in short polyenes. *Chemical Physics*, **1995**, 194, 19-31	2.3	25
243	Magnetic field effects due to spinâ□orbit coupling in transient intermediates. *Chemical Physics*, **1987**, 114, 359-367	2.3	25
242	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	3.7	24
241	Collision-induced electronic transitions in complexes between benzene and molecular oxygen. *Chemical Physics*, **1997**, 220, 79-94	2.3	24
240	Spin Transition during H2O2Formation in the Oxidative Half-Reaction of Copper Amine Oxidases. *Journal of Physical Chemistry B*, **2004**, 108, 13882-13892	3.4	24
239	Collision-Induced intensity of the b1□g+â□1□g transition in molecular oxygen: Model calculations for the collision complex O2 + H2. *International Journal of Quantum Chemistry*, **1994**, 50, 279-292	2.1	24
238	The phosphorescence of benzene obtained byab initio and semi-empirical calculations. *Theoretica Chimica Acta*, **1994**, 87, 343-371		24
237	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	3.6	23
236	Recent progress in quantum chemistry of hetero[8]circulenes. *Molecular Physics*, **2017**, 115, 2218-2230	1.7	22
235	Singletâ□riplet transitions in three-atomic molecules studied by time-dependent MCSCF and density functional theory. *Molecular Physics*, **2004**, 102, 1391-1406	1.7	22
234	New WOLEDs based on □extended azatrioxa[8]circulenes. *Journal of Materials Chemistry C*, **2017**, 5, 4123-4128	7.1	21
233	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	2.3	21
232	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, 247-61	4.4	21
231	N-annelated perylenes as effective green emitters for OLEDs. *RSC Advances*, **2015**, 5, 78150-78159	3.7	21
230	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	1.5	21
229	Application of density functional theory for studies of excited states and phosphorescence of platinum(II) acetylides. *Journal of Chemical Physics*, **2006**, 125, 094306	3.9	21
228	Spin effects in activation of hydrocarbons. *Journal of Molecular Catalysis A*, **2001**, 171, 53-72		21

227	Computational and experimental investigation of the optical properties of the chromene dyes. *Journal of Physical Chemistry A*, **2015**, 119, 1948-56	2.8	20
226	Structure and spectral properties of truxene dye S5. *Optics and Spectroscopy (English Translation of Optika I Spektroskopiya)*, **2012**, 112, 168-174	0.7	20
225	Spin Catalysis of Ortho-Para Hydrogen Conversion. *The Journal of Physical Chemistry*, **1995**, 99, 8936-8940		20
224	Response Theory Studies of Triplet-State Spectra and Radiative Lifetimes of Naphthalene, Quinoxaline, and Phthalazine. *The Journal of Physical Chemistry*, **1994**, 98, 3943-3949		20
223	Density functional study of ortho-substituted phenyl cations in polar medium and in the gas phase. *Chemical Physics*, **2011**, 389, 68-74	2.3	19
222	Quantum-chemical study of the structure and optical properties of sensitized dyes of an indoline-thiazolidine series. *Optics and Spectroscopy (English Translation of Optika I Spektroskopiya)*, **2010**, 108, 16-22	0.7	19
221	Synthesis and properties of synthetic analogs of natural humic acids. *Russian Journal of Applied Chemistry*, **2012**, 85, 296-302	0.8	18
220	Thermally accessible triplet state of ⊟nucleophiles does exist. Evidence from first principles study of ethylene interaction with copper species. *RSC Advances*, **2015**, 5, 11558-11569	3.7	18
219	Quantum-chemical study of effect of conjugation on structure and spectral properties of C105 sensitizing dye. *Optics and Spectroscopy (English Translation of Optika I Spektroskopiya)*, **2011**, 110, 393-400	0.7	18
218	Theoretical study of vibration spectra of sensitizing dyes for photoelectrical converters based on ruthenium(II) and iridium(III) complexes. *Russian Journal of Applied Chemistry*, **2009**, 82, 1211-1221	0.8	18
217	About possibility of the triplet mechanism of the Meerwein reaction. *Computational and Theoretical Chemistry*, **2010**, 952, 1-7		18
216	Calculation of the fine structure and intensity of the singlet-triplet transitions in the imidogen radical. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2005**, 61, 1105-12	4.4	18
215	Oxygen absorption below and near the Herzberg I continuum. Ab initio calculation of the transitions probability from metastable states.. *Chemical Physics*, **2000**, 252, 25-46	2.3	18
214	Response theory calculations of singlet-triplet transitions in molecular nitrogen. *Chemical Physics*, **1995**, 190, 11-29	2.3	18
213	The singletâ⊟riplet energy splitting of ⊟nucleophiles as a measure of their reaction rate with electrophilic partners. *Chemical Physics Letters*, **2014**, 607, 75-80	2.5	17
212	DFT study of electronic properties, structure and spectra of aryl diazonium cations. *Computational and Theoretical Chemistry*, **2009**, 904, 14-20		17
211	The singlet oxygen absorption to the upper state of the Schumannâ⊟unge system: the B 3⊟-⊟⊡a 1⊟g and B 3⊟-⊟⊡b 1⊟g+ transitions intensity calculation. *Physical Chemistry Chemical Physics*, **1999**, 1, 3403-3413	3.6	17
210	Excitation of O2(a1⊟g, b1⊟g+) and I(2P12) by energy transfer from I2(A, A?3⊟1,2u) in solid rare gases. *Chemical Physics*, **1990**, 142, 445-454	2.3	17

209	Multi-channel electroluminescence of CdTe/CdS core-shell quantum dots implemented into a QLED device. *Dyes and Pigments*, **2019**, 162, 647-653	4.6	17
208	Strong Topological States and High Charge Carrier Mobility in Tetraoxa[8]circulene Nanosheets. *Journal of Physical Chemistry C*, **2018**, 122, 22216-22222	3.8	17
207	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	3.2	16
206	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	3.6	16
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204	Spin-orbit coupling of charge-transfer states and the mechanism for quenching singlet oxygen by amines. *Theoretical and Experimental Chemistry*, **1984**, 20, 199-201	1.3	16
203	A computational study of aromaticity and photophysical properties of unsymmetrical azatrioxa[8]circulenes. *New Journal of Chemistry*, **2017**, 41, 2717-2723	3.6	15
202	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	3.8	15
201	Classification of Spin-Orbit Coupling Effects in Organic Chemical Reactions*. *Zeitschrift Fur Physikalische Chemie*, **1993**, 182, 263-284	3.1	15
200	The effect of molecular structure on the properties of quinoxaline-based molecules for OLED applications. *Dyes and Pigments*, **2020**, 173, 108008	4.6	15
199	A Fully Conjugated Planar Heterocyclic [9]Circulene. *Journal of the American Chemical Society*, **2020**, 142, 14058-14063	16.4	15
198	First-principles calculations of anharmonic and deuteration effects on the photophysical properties of polyacenes and porphyrinoids. *Physical Chemistry Chemical Physics*, **2020**, 22, 22314-22323	3.6	15
197	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	3.7	15
196	Compressing a Non-Planar Aromatic Heterocyclic [7]Helicene to a Planar Hetero[8]Circulene. *Chemistry - A European Journal*, **2020**, 26, 4935-4940	4.8	14
195	Spin-dependent effects in ethylene polymerization with bis(imino)pyridine iron(II) complexes. *Journal of Organometallic Chemistry*, **2016**, 811, 48-65	2.3	14
194	The Electronic Structure of Heteroannelated Cyclooctatetraenes and their UV-Vis Absorption Spectra. *Chemistry of Heterocyclic Compounds*, **2014**, 50, 349-363	1.4	14
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190	BODIPY-core 1,7-diphenyl-substituted derivatives for photovoltaics and OLED applications. *Dyes and Pigments*, **2020**, 175, 108123	4.6	14
189	Benzoselenophenylpyridine platinum complexes: green versus red phosphorescence towards hybrid OLEDs. *Dalton Transactions*, **2020**, 49, 3393-3397	4.3	13
188	Synthesis and properties of synthetic fulvic acid derived from hematoxylin. *Journal of Molecular Structure*, **2015**, 1086, 25-33	3.4	13
187	Response theory calculations of the singletâ□triplet transition probabilities in the HOCl molecule. *Journal of the Chemical Society, Faraday Transactions*, **1998**, 94, 2061-2067		13
186	Ab initio study of nonhomogeneous broadening of the zero-field splitting of triplet guest molecules in diluted glasses. *Journal of Chemical Physics*, **2003**, 119, 3120-3129	3.9	13
185	Calculation of the phosphorescence of porphyrins by the density functional method. *Optics and Spectroscopy (English Translation of Optika I Spektroskopiya)*, **2005**, 98, 214-219	0.7	13
184	The hyperpolarizability of molecular oxygen. *Computational and Theoretical Chemistry*, **1995**, 336, 61-67		13
183	Environment friendly spin-catalysis for dioxygen activation. *Chemistry and Chemical Technology*, **2010**, 4, 1-16	0.9	13
182	Spinâ□rbit coupling in oxygen containing diradicals. *Computational and Theoretical Chemistry*, **1998**, 434, 193-206		12
181	Solvent effects on optically detected magnetic resonance in triplet spin labels. *Theoretical Chemistry Accounts*, **2004**, 111, 168-175	1.9	12
180	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	16.4	11
179	Electronic descriptors for analytical use of the benzidine-based compounds and the mechanism of oxidative coupling of anilines. *Journal of Physical Organic Chemistry*, **2014**, 27, 640-651	2.1	11
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177	Quantum-chemical investigation of the structure and electronic absorption spectra of electroluminescent zinc complexes. *Optics and Spectroscopy (English Translation of Optika I Spektroskopiya)*, **2013**, 114, 30-40	0.7	11
176	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
175	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 Optika I Spektroskopiya)*, **2012**, 113, 298-304	0.7	11
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