Boris F Minaev

List of Publications by Year
in descending order

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	Theory and Calculation of the Phosphorescence Phenomenon. Chemical Reviews, 2017, 117, 6500-6537.	23.0	420
2	Principles of phosphorescent organic light emitting devices. Physical Chemistry Chemical Physics, 2014, 16, 1719-1758.	1.3	398
3	Time-dependent density functional calculations of phosphorescence parameters for fac-tris(2-phenylpyridine) iridium. Chemical Physics, 2007, 333, 157-167.	0.9	154
4	Response Theory and Calculations of Spin-Orbit Coupling Phenomena in Molecules. Advances in Quantum Chemistry, 1996, , 71-162.	0.4	137
5	Electronic mechanisms of activation of molecular oxygen. Russian Chemical Reviews, 2007, 76, 1059-1083.	2.5	117
6	Theoretical Study of the Cyclometalated Iridium(III) Complexes Used as Chromophores for Organic Light-Emitting Diodes. Journal of Physical Chemistry A, 2009, 113, 726-735.	1.1	111
7	Singlet Oxygen Photophysics in Liquid Solvents: Converging on a Unified Picture. Accounts of Chemical Research, 2017, 50, 1920-1927.	7.6	97
8	Spin uncoupling in surface chemisorption of unsaturated hydrocarbons. Journal of Chemical Physics, 1998, 108, 1193-1205.	1.2	94
9	Theoretical DFT study of phosphorescence from porphyrins. Chemical Physics, 2005, 315, 215-239.	0.9	94
10	Ab initio calculations of electronic g-factors by means of multiconfiguration response theory. Chemical Physics Letters, 1997, 281, 186-192.	1.2	91
11	Ab initio calculations of zero-field splitting parameters. Chemical Physics, 2002, 279, 133-142.	0.9	90
12	Theoretical Study of Phosphorescence of Iridium Complexes with Fluorineâ€Substituted Phenylpyridine Ligands. European Journal of Inorganic Chemistry, 2011, 2011, 2517-2524.	1.0	82
13	Diazadioxa[8]circulenes: Planar Antiaromatic Cyclooctatetraenes. Chemistry - A European Journal, 2013, 19, 17097-17102.	1.7	80
14	Dissociative Recombination of HCNH + : Absolute Crossâ€Sections and Branching Ratios. Astrophysical Journal, Supplement Series, 2001, 135, 275-283.	3.0	78
15	Azatrioxa[8]circulenes: Planar Antiâ€Aromatic Cyclooctatetraenes. Chemistry - A European Journal, 2013, 19, 3898-3904.	1.7	78
16	Mixing of Phosphorescent and Exciplex Emission in Efficient Organic Electroluminescent Devices. ACS Applied Materials & Interfaces, 2015, 7, 1219-1225.	4.0	78
17	Collision-induced b1Î£g+â€“a1 Î”g, b1Î£g+â€“X3 Î£g- and a1Î”gâ€“X3Î£g - transition probabilities in molecular oxygen. Journal of the Chemical Society, Faraday Transactions, 1997, 93, 2231-2239.	1.7	74
18	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.	1.5	74

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19	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.	2.0	74
20	Theoretical design of phosphorescence parameters for organic electro-luminescence devices based on iridium complexes. Chemical Physics, 2009, 358, 245-257.	0.9	73
21	Efficient â€œWarm-Whiteâ€•OLEDs Based on the Phosphorescent bis-Cyclometalated iridium(III) Complex. Journal of Physical Chemistry C, 2014, 118, 11271-11278.	1.5	73
22	Activation of Triplet Dioxygen by Glucose Oxidase:â€‰ Spinâ^'Orbit Coupling in the Superoxide Ion. Journal of Physical Chemistry B, 2002, 106, 3742-3750.	1.2	71
23	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, 308-323.	2.0	70
24	Excited States and Two-Photon Absorption of Some Novel Thiophenyl Pt(II)â^'Ethynyl Derivatives. Journal of Physical Chemistry A, 2007, 111, 244-250.	1.1	70
25	Aromaticity of the planar hetero[8]circulenes and their doubly charged ions: NICS and GIMIC characterization. Physical Chemistry Chemical Physics, 2014, 16, 15367-15374.	1.3	69
26	Molecular Phosphorescence in Polymer Matrix with Reversible Sensitivity. ACS Applied Materials & Interfaces, 2020, 12, 20765-20774.	4.0	68
27	Highly Efficient Blue Organic Light-Emitting Diodes Based on Intermolecular Tripletâ€“Singlet Energy Transfer. Journal of Physical Chemistry C, 2013, 117, 22538-22544.	1.5	65
28	Hydrogen Bonding to Tyrosyl Radical Analyzed by Ab Initio g-Tensor Calculations. Journal of Physical Chemistry A, 2000, 104, 5149-5153.	1.1	64
29	Contribution of TADF and exciplex emission for efficient â€œwarm-whiteâ€•OLEDs. Journal of Materials Chemistry C, 2018, 6, 1543-1550.	2.7	64
30	Intensities of spin-forbidden transitions in molecular oxygen and selective heavy-atom effects. International Journal of Quantum Chemistry, 1980, 17, 367-374.	1.0	63
31	Solvent induced emission of molecular 1Î”g oxygen. Computational and Theoretical Chemistry, 1989, 183, 207-214.	1.5	60
32	Magnetic phosphorescence of molecular oxygen. A study of the b1Î£g+-X3Î£gâ^' transition probability using multiconfiguration response theory. Chemical Physics, 1996, 208, 299-311.	0.9	57
33	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
34	DFT characterization of a new possible graphene allotrope. Chemical Physics Letters, 2014, 612, 229-233.	1.2	54
35	Benzoannelated aza-, oxa- and azaoxa[8]circulenes as promising blue organic emitters. Physical Chemistry Chemical Physics, 2016, 18, 28040-28051.	1.3	54
36	The interpretation of the Wulf absorption band of ozone. Chemical Physics Letters, 1994, 217, 531-538.	1.2	53

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37	Electronic structure and spectral properties of the triarylamine-dithienosilole dyes for efficient organic solar cells. Dyes and Pigments, 2012, 92, 531-536.	2.0	53
38	Tetrathio and Tetraseleno[8]circulenes: Synthesis, Structures, and Properties. Chemistry - an Asian Journal, 2015, 10, 969-975.	1.7	52
39	Experimental and theoretical study of IR and Raman spectra of tetraoxa[8]circulenes. Vibrational Spectroscopy, 2012, 61, 156-166.	1.2	51
40	On the interpretation of the external heavy atom effect on singlet-triplet transitions. Chemical Physics, 1994, 181, 15-28.	0.9	50
41	Nucleus-independent chemical shift criterion for aromaticity in Ï€-extended tetraoxa[8]circulenes. Journal of Molecular Modeling, 2013, 19, 847-850.	0.8	50
42	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.	1.7	50
43	The influence of intermolecular interaction on the forbidden near-IR transitions in molecular oxygen. Computational and Theoretical Chemistry, 1993, 284, 1-9.	1.5	49
44	Ab initio calculations of zero-field splitting parameters in linear polyacenes. Chemical Physics, 2003, 286, 127-137.	0.9	48
45	Design of nanoscaled materials based on tetraoxa[8]circulene. Physical Chemistry Chemical Physics, 2014, 16, 6555.	1.3	48
46	The vibronically induced phosphorescence in benzene. Chemical Physics, 1993, 175, 245-254.	0.9	47
47	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.	0.9	47
48	MCSCF response calculations of the excited states properties of the O2 molecule and a part of its spectrum. Physical Chemistry Chemical Physics, 2001, 3, 720-729.	1.3	47
49	Fluorescence and FTIR Spectra Analysis of Trans-A2B2-Substituted Di- and Tetra-Phenyl Porphyrins. Materials, 2010, 3, 4446-4475.	1.3	47
50	Ab initio study of the ground state properties of molecular oxygen. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2004, 60, 1027-1041.	2.0	46
51	Electronic structure, aromaticity and spectra of hetero[8]circulenes. Russian Chemical Reviews, 2015, 84, 455-484.	2.5	46
52	Spin-catalysis phenomena. International Journal of Quantum Chemistry, 1996, 57, 519-532.	1.0	45
53	Electronic states and phosphorescence of dendron functionalized platinum(II) acetylides. Journal of Luminescence, 2007, 124, 302-310.	1.5	45
54	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.	1.5	45

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55	Theoretical study of triplet state properties of free-base porphin. Chemical Physics, 2005, 312, 299-309.	0.9	44
56	Kinetic and mechanism formation of silver nanoparticles coated by synthetic humic substances. Colloids and Surfaces A: Physicochemical and Engineering Aspects, 2012, 414, 234-243.	2.3	44
57	Density functional theory study of electronic structure and spectra of tetraoxa[8]circulenes. Computational and Theoretical Chemistry, 2011, 972, 68-74.	1.1	43
58	Fragmentation of the adenine and guanine molecules induced by electron collisions. Journal of Chemical Physics, 2014, 140, 175101.	1.2	42
59	Dioxygen spectra and bioactivation. International Journal of Quantum Chemistry, 2013, 113, 1847-1867.	1.0	41
60	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.	0.3	39
61	Theoretical study of phosphorescence in dye doped light emitting diodes. Journal of Chemical Physics, 2006, 125, 234704.	1.2	38
62	Evaluation of low-scaling methods for calculation of phosphorescence parameters. Journal of Chemical Physics, 2006, 124, 114106.	1.2	37
63	Spin-spin and spin-orbit interactions in nanographene fragments: A quantum chemistry approach. Journal of Chemical Physics, 2012, 136, 104702.	1.2	37
64	Vibration and Fluorescence Spectra of Porphyrin- CoredBis(methylol)-propionic Acid Dendrimers. Sensors, 2009, 9, 1937-1966.	2.1	35
65	DFT and QTAIM study of the tetra-tert-butyltetraoxa[8]circulene regioisomers structure. Journal of Molecular Structure, 2012, 1026, 127-132.	1.8	35
66	Spin uncoupling in molecular hydrogen activation by platinum clusters. Journal of Molecular Catalysis A, 1999, 149, 179-195.	4.8	34
67	Spinâ^'Orbit Coupling Effects on the Metalâ^'Hydrogen Bond Homolysis of M(H)(CO)3(H-DAB) (M = Mn, Re;) Tj ETQq1 1 0.784314 rgBT	1.1	34
68	Aromaticity of the completely annelated tetraphenylenes: NICS and GIMIC characterization. Journal of Molecular Modeling, 2015, 21, 136.	0.8	34
69	Aromaticity of the doubly charged [8]circulenes. Physical Chemistry Chemical Physics, 2016, 18, 8980-8992.	1.3	34
70	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.	1.4	34
71	The effect of molecular structure on the properties of quinoxaline-based molecules for OLED applications. Dyes and Pigments, 2020, 173, 108008.	2.0	34
72	Schiff Base Zinc(II) Complexes as Promising Emitters for Blue Organic Light-Emitting Diodes. ACS Applied Electronic Materials, 2021, 3, 3436-3444.	2.0	34

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73	Some recent developments of high-order response theory. International Journal of Quantum Chemistry, 1998, 70, 219-239.	1.0	33
74	Quantum Chemical Model of an SN2 Reaction in a Microwave Field. Journal of Physical Chemistry A, 2002, 106, 8516-8524.	1.1	33
75	A theoretical study of the dioxygen activation by glucose oxidase and copper amine oxidase. Biochimica Et Biophysica Acta - Proteins and Proteomics, 2003, 1647, 173-178.	1.1	33
76	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, 3213-3224.	2.0	33
77	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.	1.4	33
78	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.	2.7	33
79	Spin-Orbit Coupling Induced Chemical Reactivity and Spin-Catalysis Phenomena. Collection of Czechoslovak Chemical Communications, 1995, 60, 339-371.	1.0	32
80	Internuclear distance dependence of the spinâ€“orbit coupling contributions to proton NMR chemical shifts. Chemical Physics Letters, 1998, 295, 455-461.	1.2	32
81	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.	1.3	32
82	First-principles calculations of anharmonic and deuteration effects on the photophysical properties of polyacenes and porphyrinoids. Physical Chemistry Chemical Physics, 2020, 22, 22314-22323.	1.3	32
83	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.	0.8	31
84	Approximating quasi-particle density functional calculations of small active clusters: Strong electron correlation effects. International Journal of Quantum Chemistry, 1990, 38, 779-797.	1.0	30
85	Response theory calculations of the vibronically induced 1A1gâ^'1B2u two-photon spectrum of benzene. Chemical Physics Letters, 1993, 209, 513-518.	1.2	30
86	CASSCF calculations of triplet state properties: applications to benzene derivatives. Molecular Physics, 2003, 101, 2103-2114.	0.8	30
87	The size-controllable, one-step synthesis and characterization of gold nanoparticles protected by synthetic humic substances. Materials Chemistry and Physics, 2014, 144, 168-178.	2.0	30
88	BODIPY-core 1,7-diphenyl-substituted derivatives for photovoltaics and OLED applications. Dyes and Pigments, 2020, 175, 108123.	2.0	30
89	Collision-Induced intensity of theb1?g+?a1?g transition in molecular oxygen: Model calculations for the collision complex O2 + H2. International Journal of Quantum Chemistry, 1994, 50, 279-292.	1.0	29
90	Configuration interaction study of the O2â€“C2H4exciplex: collision-induced probabilities of spin-forbidden radiative and non-radiative transitions. Journal of the Chemical Society, Faraday Transactions, 1994, 90, 1479-1486.	1.7	29

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91	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, 3387-3410.	2.0	29
92	Quantumâ€chemical study of the singlet oxygen emission. International Journal of Quantum Chemistry, 2009, 109, 500-515.	1.0	29
93	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.	1.7	28
94	Recent progress in quantum chemistry of hetero[8]circulenes. Molecular Physics, 2017, 115, 2218-2230.	0.8	28
95	New WOLEDs based on Ï€-extended azatrioxa[8]circulenes. Journal of Materials Chemistry C, 2017, 5, 4123-4128.	2.7	28
96	A Fully Conjugated Planar Heterocyclic [9]Circulene. Journal of the American Chemical Society, 2020, 142, 14058-14063.	6.6	28
97	Compressing a Nonâ€Planar Aromatic Heterocyclic [7]Helicene to a Planar Hetero[8]Circulene. Chemistry - A European Journal, 2020, 26, 4935-4940.	1.7	28
98	Magnetic field effects due to spinâ€”orbit coupling in transient intermediates. Chemical Physics, 1987, 114, 359-367.	0.9	27
99	Spin Catalysis of Ortho-Para Hydrogen Conversion. The Journal of Physical Chemistry, 1995, 99, 8936-8940.	2.9	27
100	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.	1.1	27
101	Ab initio study of low-lying triplet states of the lithium dimer. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2005, 62, 790-799.	2.0	27
102	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.	1.4	27
103	The FTIR spectra of substituted tetraoxa[8]circulenes and their assignments based on DFT calculations. Vibrational Spectroscopy, 2013, 65, 147-158.	1.2	26
104	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.	0.2	26
105	Character and spectra of triplet states in short polyenes. Chemical Physics, 1995, 194, 19-31.	0.9	25
106	Collision-induced electronic transitions in complexes between benzene and molecular oxygen. Chemical Physics, 1997, 220, 79-94.	0.9	25
107	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
108	The phosphorescence of benzene obtained byab initio and semi-empirical calculations. Theoretica Chimica Acta, 1994, 87, 343-371.	0.9	24

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109	Spin effects in activation of hydrocarbons. Journal of Molecular Catalysis A, 2001, 171, 53-72.	4.8	24
110	Singletâ€“triplet transitions in three-atomic molecules studied by time-dependent MCSCF and density functional theory. Molecular Physics, 2004, 102, 1391-1406.	0.8	24
111	Spin Transition during H2O2Formation in the Oxidative Half-Reaction of Copper Amine Oxidases. Journal of Physical Chemistry B, 2004, 108, 13882-13892.	1.2	24
112	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.	0.3	24
113	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.	1.7	24
114	Response Theory Studies of Triplet-State Spectra and Radiative Lifetimes of Naphthalene, Quinoxaline, and Phthalazine. The Journal of Physical Chemistry, 1994, 98, 3943-3949.	2.9	23
115	Response theory calculations of singlet-triplet transitions in molecular nitrogen. Chemical Physics, 1995, 190, 11-29.	0.9	23
116	Computational and Experimental Investigation of the Optical Properties of the Chromene Dyes. Journal of Physical Chemistry A, 2015, 119, 1948-1956.	1.1	23
117	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
118	Application of density functional theory for studies of excited states and phosphorescence of platinum(II) acetylides. Journal of Chemical Physics, 2006, 125, 094306.	1.2	22
119	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.	0.9	22
120	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.	2.0	22
121	Excitation of O2(a1Î”g, b1Î£g+) and I(2P12) by energy transfer from I2(A, Aâ€²3Î1,2u) in solid rare gases. Chemical Physics, 1990, 142, 445-454.	0.9	21
122	Calculation of the fine structure and intensity of the singletâ€“triplet transitions in the imidogen radical. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2005, 61, 1105-1112.	2.0	21
123	N-annelated perylenes as effective green emitters for OLEDs. RSC Advances, 2015, 5, 78150-78159.	1.7	21
124	Spin-orbit coupling of charge-transfer states and the mechanism for quenching singlet oxygen by amines. Theoretical and Experimental Chemistry, 1984, 20, 199-201.	0.2	20
125	The singlet oxygen absorption to the upper state of the Schumannâ€“Runge system: the B 3Î£u-â†’ 1Î”g and B 3Î£u-â†’ 1Î£g+ transitions intensity calculation. Physical Chemistry Chemical Physics, 1999, 1, 3403-3413.	1.3	20
126	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.	0.9	20

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127	DFT study of electronic properties, structure and spectra of aryl diazonium cations. Computational and Theoretical Chemistry, 2009, 904, 14-20.	1.5	20
128	Density functional study of ortho-substituted phenyl cations in polar medium and in the gas phase. Chemical Physics, 2011, 389, 68-74.	0.9	20
129	Structure and spectral properties of truxene dye S5. Optics and Spectroscopy (English Translation of) Tj ETQq1 1 0.784314 rgBT /Ove	0.2	20
130	Synthesis and properties of synthetic analogs of natural humic acids. Russian Journal of Applied Chemistry, 2012, 85, 296-302.	0.1	20
131	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.	0.1	19
132	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.	0.2	19
133	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.	0.2	19
134	State-Dependent Global and Local Electrophilicity of the Aryl Cations. Journal of Physical Chemistry A, 2014, 118, 3201-3210.	1.1	19
135	Thermally accessible triplet state of Ї€-nucleophiles does exist. Evidence from first principles study of ethylene interaction with copper species. RSC Advances, 2015, 5, 11558-11569.	1.7	19
136	Synthesis and properties of synthetic fulvic acid derived from hematoxylin. Journal of Molecular Structure, 2015, 1086, 25-33.	1.8	19
137	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
138	Structure and tuneable luminescence in polymeric zinc compounds based on 3-(3-pyridyl)-5-(4-pyridyl)-1,2,4-triazole. Polyhedron, 2020, 191, 114768.	1.0	19
139	Benzoselenophenylpyridine platinum complexes: green versus red phosphorescence towards hybrid OLEDs. Dalton Transactions, 2020, 49, 3393-3397.	1.6	19
140	About possibility of the triplet mechanism of the Meerwein reaction. Computational and Theoretical Chemistry, 2010, 952, 1-7.	1.5	18
141	The singletâ€“triplet energy splitting of Ї€-nucleophiles as a measure of their reaction rate with electrophilic partners. Chemical Physics Letters, 2014, 607, 75-80.	1.2	18
142	Structure and excitation-dependent emission of novel zinc complexes with pyridyltriazoles. RSC Advances, 2019, 9, 22143-22152.	1.7	18
143	Spin-dependent effects in ethylene polymerization with bis(imino)pyridine iron(II) complexes. Journal of Organometallic Chemistry, 2016, 811, 48-65.	0.8	17
144	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.	7.2	17

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145	Classification of Spin-Orbit Coupling Effects in Organic Chemical Reactions*. Zeitschrift Fur Physikalische Chemie, 1993, 182, 263-284.	1.4	16
146	A computational study of aromaticity and photophysical properties of unsymmetrical azatrioxa[8]circulenes. New Journal of Chemistry, 2017, 41, 2717-2723.	1.4	16
147	Environment friendly spin-catalysis for dioxygen activation. Chemistry and Chemical Technology, 2010, 4, 1-16.	0.2	16
148	The hyperpolarizability of molecular oxygen. Computational and Theoretical Chemistry, 1995, 336, 61-67.	1.5	15
149	Ab initio study of the PtC molecule. A new assignment of the red bands to the 1Ã‚Â3ÃŽÂÃŽÂ©(ÃŽÂ©=1,0+)Ã¢â‚¬â„¢XÃ‚Â1ÃŽÂ£+ transitions. Physical Chemistry Chemical Physics, 2000, 2, 2851-2856.	1.3	15
150	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.	1.5	15
151	The Electronic Structure of Heteroannelated Cyclooctatetraenes and their UV-Vis Absorption Spectra. Chemistry of Heterocyclic Compounds, 2014, 50, 349-363.	0.6	15
152	A Configuration Interaction Study of the (O₂)₂Dimer. Spectroscopy Letters, 1996, 29, 677-695.	0.5	14
153	Spinâ€“orbit coupling in oxygen containing diradicals. Computational and Theoretical Chemistry, 1998, 434, 193-206.	1.5	14
154	Response theory calculations of the singletâ€“triplet transition probabilities in the HOCl molecule. Journal of the Chemical Society, Faraday Transactions, 1998, 94, 2061-2067.	1.7	14
155	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.	1.2	14
156	Calculation of the phosphorescence of porphyrins by the density functional method. Optics and Spectroscopy (English Translation of Optika I Spektroskopiya), 2005, 98, 214-219.	0.2	14
157	DFT-based thermodynamics of fenton reactions rejects the â€˜pureâ€™ aquacomplex models. Computational and Theoretical Chemistry, 2011, 964, 94-99.	1.1	14
158	DFT study of electronic structure and optical properties of some Ru- and Rh-based complexes for dye-sensitized solar cells. Molecular Physics, 2011, 109, 2511-2523.	0.8	14
159	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.	1.0	14
160	Electroluminescence of Halogen Complexes with Monovalent Copper: OLED Devices and DFT Modeling. Russian Physics Journal, 2016, 58, 1205-1211.	0.2	14
161	Quantum-chemical investigation of the mechanisms of the photosensitization, luminescence, and quenching of singlet1?g oxygen in solutions. Journal of Applied Spectroscopy, 1985, 42, 518-523.	0.3	13
162	Physical properties and spectra of IO, IOâ˜ and HOI studied by ab initio methods. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2002, 58, 1039-1053.	2.0	13

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