Boris F Minaev

List of Publications by Year
in descending order

Source: https://exaly.com/author-pdf/6781682/publications.pdf

Version: 2024-02-01

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	Theory and Calculation of the Phosphorescence Phenomenon. Chemical Reviews, 2017, 117, 6500-6537.	47.7	420
2	Principles of phosphorescent organic light emitting devices. Physical Chemistry Chemical Physics, 2014, 16, 1719-1758.	2.8	398
3	Time-dependent density functional calculations of phosphorescence parameters for fac-tris(2-phenylpyridine) iridium. Chemical Physics, 2007, 333, 157-167.	1.9	154
4	Response Theory and Calculations of Spin-Orbit Coupling Phenomena in Molecules. Advances in Quantum Chemistry, 1996, , 71-162.	0.8	137
5	Electronic mechanisms of activation of molecular oxygen. Russian Chemical Reviews, 2007, 76, 1059-1083.	6.5	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.	2.5	111
7	Singlet Oxygen Photophysics in Liquid Solvents: Converging on a Unified Picture. Accounts of Chemical Research, 2017, 50, 1920-1927.	15.6	97
8	Spin uncoupling in surface chemisorption of unsaturated hydrocarbons. Journal of Chemical Physics, 1998, 108, 1193-1205.	3.0	94
9	Theoretical DFT study of phosphorescence from porphyrins. Chemical Physics, 2005, 315, 215-239.	1.9	94
10	Ab initio calculations of electronic g-factors by means of multiconfiguration response theory. Chemical Physics Letters, 1997, 281, 186-192.	2.6	91
11	Ab initio calculations of zero-field splitting parameters. Chemical Physics, 2002, 279, 133-142.	1.9	90
12	Theoretical Study of Phosphorescence of Iridium Complexes with Fluorineâ€Substituted Phenylpyridine Ligands. European Journal of Inorganic Chemistry, 2011, 2011, 2517-2524.	2.0	82
13	Diazadioxa[8]circulenes: Planar Antiaromatic Cyclooctatetraenes. Chemistry - A European Journal, 2013, 19, 17097-17102.	3.3	80
14	Dissociative Recombination of HCNH + : Absolute Crossâ€Sections and Branching Ratios. Astrophysical Journal, Supplement Series, 2001, 135, 275-283.	7.7	78
15	Azatrioxa[8]circulenes: Planar Antiâ€Aromatic Cyclooctatetraenes. Chemistry - A European Journal, 2013, 19, 3898-3904.	3.3	78
16	Mixing of Phosphorescent and Exciplex Emission in Efficient Organic Electroluminescent Devices. ACS Applied Materials & Interfaces, 2015, 7, 1219-1225.	8.0	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.	3.1	74

#	Article	IF	Citations
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.	3.9	74
20	Theoretical design of phosphorescence parameters for organic electro-luminescence devices based on iridium complexes. Chemical Physics, 2009, 358, 245-257.	1.9	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.	3.1	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.	2.6	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.	3.9	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.	2.5	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.	2.8	69
26	Molecular Phosphorescence in Polymer Matrix with Reversible Sensitivity. ACS Applied Materials & Interfaces, 2020, 12, 20765-20774.	8.0	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.	3.1	65
28	Hydrogen Bonding to Tyrosyl Radical Analyzed by Ab Initio g-Tensor Calculations. Journal of Physical Chemistry A, 2000, 104, 5149-5153.	2.5	64
29	Contribution of TADF and exciplex emission for efficient â€œwarm-whiteâ€•OLEDs. Journal of Materials Chemistry C, 2018, 6, 1543-1550.	5.5	64
30	Intensities of spin-forbidden transitions in molecular oxygen and selective heavy-atom effects. International Journal of Quantum Chemistry, 1980, 17, 367-374.	2.0	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.	1.9	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.	3.1	56
34	DFT characterization of a new possible graphene allotrope. Chemical Physics Letters, 2014, 612, 229-233.	2.6	54
35	Benzoannelated aza-, oxa- and azaoxa[8]circulenes as promising blue organic emitters. Physical Chemistry Chemical Physics, 2016, 18, 28040-28051.	2.8	54
36	The interpretation of the Wulf absorption band of ozone. Chemical Physics Letters, 1994, 217, 531-538.	2.6	53

#	Article	IF	Citations
37	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
38	Tetrathio and Tetraseleno[8]circulenes: Synthesis, Structures, and Properties. Chemistry - an Asian Journal, 2015, 10, 969-975.	3.3	52
39	Experimental and theoretical study of IR and Raman spectra of tetraoxa[8]circulenes. Vibrational Spectroscopy, 2012, 61, 156-166.	2.2	51
40	On the interpretation of the external heavy atom effect on singlet-triplet transitions. Chemical Physics, 1994, 181, 15-28.	1.9	50
41	Nucleus-independent chemical shift criterion for aromaticity in Ï€-extended tetraoxa[8]circulenes. Journal of Molecular Modeling, 2013, 19, 847-850.	1.8	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.	3.6	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.	1.9	48
45	Design of nanoscaled materials based on tetraoxa[8]circulene. Physical Chemistry Chemical Physics, 2014, 16, 6555.	2.8	48
46	The vibronically induced phosphorescence in benzene. Chemical Physics, 1993, 175, 245-254.	1.9	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.	1.9	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.	2.8	47
49	Fluorescence and FTIR Spectra Analysis of Trans-A2B2-Substituted Di- and Tetra-Phenyl Porphyrins. Materials, 2010, 3, 4446-4475.	2.9	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.	3.9	46
51	Electronic structure, aromaticity and spectra of hetero[8]circulenes. Russian Chemical Reviews, 2015, 84, 455-484.	6.5	46
52	Spin-catalysis phenomena. International Journal of Quantum Chemistry, 1996, 57, 519-532.	2.0	45
53	Electronic states and phosphorescence of dendron functionalized platinum(II) acetylides. Journal of Luminescence, 2007, 124, 302-310.	3.1	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.	3.1	45

#	Article	IF	Citations
55	Theoretical study of triplet state properties of free-base porphin. Chemical Physics, 2005, 312, 299-309.	1.9	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.	4.7	44
57	Density functional theory study of electronic structure and spectra of tetraoxa[8]circulenes. Computational and Theoretical Chemistry, 2011, 972, 68-74.	2.5	43
58	Fragmentation of the adenine and guanine molecules induced by electron collisions. Journal of Chemical Physics, 2014, 140, 175101.	3.0	42
59	Dioxygen spectra and bioactivation. International Journal of Quantum Chemistry, 2013, 113, 1847-1867.	2.0	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.	0.8	39
61	Theoretical study of phosphorescence in dye doped light emitting diodes. Journal of Chemical Physics, 2006, 125, 234704.	3.0	38
62	Evaluation of low-scaling methods for calculation of phosphorescence parameters. Journal of Chemical Physics, 2006, 124, 114106.	3.0	37
63	Spin-spin and spin-orbit interactions in nanographene fragments: A quantum chemistry approach. Journal of Chemical Physics, 2012, 136, 104702.	3.0	37
64	Vibration and Fluorescence Spectra of Porphyrin- CoredBis(methylol)-propionic Acid Dendrimers. Sensors, 2009, 9, 1937-1966.	3.8	35
65	DFT and QTAIM study of the tetra-tert-butyltetraoxa[8]circulene regioisomers structure. Journal of Molecular Structure, 2012, 1026, 127-132.	3.6	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	2.5	34
68	Aromaticity of the completely annelated tetraphenylenes: NICS and GIMIC characterization. Journal of Molecular Modeling, 2015, 21, 136.	1.8	34
69	Aromaticity of the doubly charged [8]circulenes. Physical Chemistry Chemical Physics, 2016, 18, 8980-8992.	2.8	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.	2.8	34
71	The effect of molecular structure on the properties of quinoxaline-based molecules for OLED applications. Dyes and Pigments, 2020, 173, 108008.	3.7	34
72	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

#	Article	IF	Citations
73	Some recent developments of high-order response theory. International Journal of Quantum Chemistry, 1998, 70, 219-239.	2.0	33
74	Quantum Chemical Model of an SN2 Reaction in a Microwave Field. Journal of Physical Chemistry A, 2002, 106, 8516-8524.	2.5	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.	2.3	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.	3.9	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.	2.8	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.	5.5	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.	2.6	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.	2.8	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.	2.8	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.	1.8	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.	2.0	30
85	Response theory calculations of the vibronically induced 1A1gâ^'1B2u two-photon spectrum of benzene. Chemical Physics Letters, 1993, 209, 513-518.	2.6	30
86	CASSCF calculations of triplet state properties: applications to benzene derivatives. Molecular Physics, 2003, 101, 2103-2114.	1.7	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.	4.0	30
88	BODIPY-core 1,7-diphenyl-substituted derivatives for photovoltaics and OLED applications. Dyes and Pigments, 2020, 175, 108123.	3.7	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.	2.0	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

#	Article	IF	Citations
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.	3.9	29
92	Quantumâ€chemical study of the singlet oxygen emission. International Journal of Quantum Chemistry, 2009, 109, 500-515.	2.0	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.	3.6	28
94	Recent progress in quantum chemistry of hetero[8]circulenes. Molecular Physics, 2017, 115, 2218-2230.	1.7	28
95	New WOLEDs based on Ï€-extended azatrioxa[8]circulenes. Journal of Materials Chemistry C, 2017, 5, 4123-4128.	5.5	28
96	A Fully Conjugated Planar Heterocyclic [9]Circulene. Journal of the American Chemical Society, 2020, 142, 14058-14063.	13.7	28
97	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
98	Magnetic field effects due to spinâ€”orbit coupling in transient intermediates. Chemical Physics, 1987, 114, 359-367.	1.9	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.	2.5	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.	3.9	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.	3.0	27
103	The FTIR spectra of substituted tetraoxa[8]circulenes and their assignments based on DFT calculations. Vibrational Spectroscopy, 2013, 65, 147-158.	2.2	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.	0.6	26
105	Character and spectra of triplet states in short polyenes. Chemical Physics, 1995, 194, 19-31.	1.9	25
106	Collision-induced electronic transitions in complexes between benzene and molecular oxygen. Chemical Physics, 1997, 220, 79-94.	1.9	25
107	Strong Topological States and High Charge Carrier Mobility in Tetraoxa[8]circulene Nanosheets. Journal of Physical Chemistry C, 2018, 122, 22216-22222.	3.1	25
108	The phosphorescence of benzene obtained byab initio and semi-empirical calculations. Theoretica Chimica Acta, 1994, 87, 343-371.	0.8	24

#	Article	IF	Citations
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.	1.7	24
111	Spin Transition during H2O2Formation in the Oxidative Half-Reaction of Copper Amine Oxidases. Journal of Physical Chemistry B, 2004, 108, 13882-13892.	2.6	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.	1.3	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.	3.6	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.	1.9	23
116	Computational and Experimental Investigation of the Optical Properties of the Chromene Dyes. Journal of Physical Chemistry A, 2015, 119, 1948-1956.	2.5	23
117	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
118	Application of density functional theory for studies of excited states and phosphorescence of platinum(II) acetylides. Journal of Chemical Physics, 2006, 125, 094306.	3.0	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.	1.9	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.	3.9	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.	1.9	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.	3.9	21
123	N-annelated perylenes as effective green emitters for OLEDs. RSC Advances, 2015, 5, 78150-78159.	3.6	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.	0.8	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.	2.8	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.	1.9	20

#	Article	IF	Citations
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.	1.9	20
129	Structure and spectral properties of truxene dye S5. Optics and Spectroscopy (English Translation of) Tj ETQq1 1 0.784314 rgBT /Ove	0.6	20
130	Synthesis and properties of synthetic analogs of natural humic acids. Russian Journal of Applied Chemistry, 2012, 85, 296-302.	0.5	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.	0.5	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.	0.6	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.	0.6	19
134	State-Dependent Global and Local Electrophilicity of the Aryl Cations. Journal of Physical Chemistry A, 2014, 118, 3201-3210.	2.5	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.	3.6	19
136	Synthesis and properties of synthetic fulvic acid derived from hematoxylin. Journal of Molecular Structure, 2015, 1086, 25-33.	3.6	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.	2.8	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.	2.2	19
139	Benzoselenophenylpyridine platinum complexes: green versus red phosphorescence towards hybrid OLEDs. Dalton Transactions, 2020, 49, 3393-3397.	3.3	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.	2.6	18
142	Structure and excitation-dependent emission of novel zinc complexes with pyridyltriazoles. RSC Advances, 2019, 9, 22143-22152.	3.6	18
143	Spin-dependent effects in ethylene polymerization with bis(imino)pyridine iron(II) complexes. Journal of Organometallic Chemistry, 2016, 811, 48-65.	1.8	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.	13.8	17

#	Article	IF	Citations
145	Classification of Spin-Orbit Coupling Effects in Organic Chemical Reactions*. Zeitschrift Fur Physikalische Chemie, 1993, 182, 263-284.	2.8	16
146	A computational study of aromaticity and photophysical properties of unsymmetrical azatrioxa[8]circulenes. New Journal of Chemistry, 2017, 41, 2717-2723.	2.8	16
147	Environment friendly spin-catalysis for dioxygen activation. Chemistry and Chemical Technology, 2010, 4, 1-16.	1.1	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.	2.8	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.	3.1	15
151	The Electronic Structure of Heteroannelated Cyclooctatetraenes and their UV-Vis Absorption Spectra. Chemistry of Heterocyclic Compounds, 2014, 50, 349-363.	1.2	15
152	A Configuration Interaction Study of the (O₂)₂Dimer. Spectroscopy Letters, 1996, 29, 677-695.	1.0	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.	3.0	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.	0.6	14
157	DFT-based thermodynamics of fenton reactions rejects the â€˜pureâ€™ aquacomplex models. Computational and Theoretical Chemistry, 2011, 964, 94-99.	2.5	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.	1.7	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.	2.0	14
160	Electroluminescence of Halogen Complexes with Monovalent Copper: OLED Devices and DFT Modeling. Russian Physics Journal, 2016, 58, 1205-1211.	0.4	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.	0.7	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.	3.9	13

#	Article	IF	Citations
163	Study of structure and spectral characteristics of the binuclear zinc complex with (E)-2-({2-[3-(pyridin-2-yl)-1H-1,2,4-triazol-5-yl]phenylimino}methyl)phenol. Russian Journal of General Chemistry, 2011, 81, 2332-2344.	0.8	13
164	Multidimensional Structure Conformation of Persulfurated Benzene for Highly Efficient Phosphorescence. ACS Applied Materials & Interfaces, 2021, 13, 1314-1322.	8.0	13
165	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
166	Informative energetic structure and electronic multistability of condensed state. Computational and Theoretical Chemistry, 1991, 227, 125-129.	1.5	12
167	Spin-orbit coupling in the intersystem crossing of the ring-opened oxirane biradical. International Journal of Quantum Chemistry, 1995, 55, 23-34.	2.0	12
168	Paramagnetic Exchange Spin-Catalysis of theCisâ^'TransIsomerization of Substituted Ethylenes. The Journal of Physical Chemistry, 1996, 100, 8308-8315.	2.9	12
169	Role of exchange interaction in spin catalysis mechanisms. Theoretical and Experimental Chemistry, 1996, 32, 1-12.	0.8	12
170	Solvent effects on optically detected magnetic resonance in triplet spin labels. Theoretical Chemistry Accounts, 2004, 111, 168-175.	1.4	12
171	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 ETQq1 1 0.784314 rgBT /Overlock 10 Tf 5	0.8	12
172	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
173	How cofactor-free oxygenases can overcome spin prohibition in substrates oxygenation by dioxygen. Chemical Physics, 2019, 521, 61-68.	1.9	12
174	Spin uncoupling in chemical reactions. Advances in Quantum Chemistry, 2001, 40, 191-211.	0.8	11
175	Spin-orbit coupling in oxygen near the dissociation limit. Optics and Spectroscopy (English) Tj ETQq1 1 0.784314 rgBT /Overlock 10 Tf 5	0.6	11
176	One- and two-photon Absorptions in asymmetrically substituted free-base porphyrins: A density functional theory study. Journal of Chemical Physics, 2008, 128, 074302.	3.0	11
177	Role of triplet states of aryldiazonium cations in the Meerwein reaction. Russian Journal of Applied Chemistry, 2009, 82, 840-845.	0.5	11
178	Photochemical Water Decomposition in the Troposphere: DFT Study with a Symmetrized Kohnâ€“Sham Formalism. ChemPhysChem, 2010, 11, 4028-4034.	2.1	11
179	Stabilizing hydrogen-hydrogen interactions in cationic indopolycarbocyanine dyes. Journal of Structural Chemistry, 2011, 52, 1051-1056.	1.0	11
180	Quantum-chemical study of structure and spectral properties of triphenylamine-rhodanine dye 2-(5-(4-(diphenylamine)benzylidene)-4-oxo-2-thioxothiazolidine-3-yl) acetic acid. Optics and Spectroscopy (English Translation of Optika I Spektroskopiya), 2011, 110, 216-223.	0.6	11

#	Article	IF	Citations
181	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
182	Theoretical study of the dimerization of rhodanine in various tautomeric forms. Chemistry of Heterocyclic Compounds, 2012, 47, 1268-1279.	1.2	11
183	Structure and spectral properties of triphenylamine dye functionalized with 3,4-propylenedioxythiophene. Optics and Spectroscopy (English Translation of Optika I Spektroskopiya), 2012, 112, 829-835.	0.6	11
184	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 50 617	0.6	11
185	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
186	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
187	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
188	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
189	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
190	Aromaticity of Heterocirculenes. Chemistry, 2021, 3, 1411-1436.	2.2	11
191	The removal of spin-forbidden character in the reactions of triplet molecular oxygen. Journal of Structural Chemistry, 1982, 23, 170-175.	1.0	10
192	Spin uncoupling in ethylene activation by palladium and platinum atoms. International Journal of Quantum Chemistry, 1999, 72, 581-596.	2.0	10
193	Calculation of the fine structure of the triplet state $$ilde a^3 A_2 $$ of the ozone molecule by the method of multiconfiguration self-consistent field. Optics and Spectroscopy (English Translation of) Tj ETQq1 1 0.784314 rgBT /Overlock	0.6	10
194	Ab initio calculations of vibronic activity in phosphorescence microwave double resonance spectra of p-dichlorobenzene. Theoretical Chemistry Accounts, 2005, 113, 15-27.	1.4	10
195	DFT calculations of the intermediate and transition state in the oxidation of NO by oxygen in the gas phase. Theoretical and Experimental Chemistry, 2011, 47, 93-100.	0.8	10
196	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
197	Triplet State Phosphorescence in Tris(8-hydroxyquinoline) Aluminum Light Emitting Diode Materials. Journal of Physical Chemistry C, 2013, 117, 3446-3455.	3.1	10
198	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

#	Article	IF	Citations
199	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
200	The blue vibronically resolved electroluminescence of azatrioxa[8]circulene. Chemical Physics Letters, 2019, 732, 136667.	2.6	10
201	Impact of heteroatoms (S, Se, and Te) on the aromaticity of heterocirculenes. New Journal of Chemistry, 2019, 43, 12178-12190.	2.8	10
202	Multiconfiguration response calculations on the Cameron bands of the CO molecule. Journal of the Chemical Society, Faraday Transactions, 1995, 91, 1729-1733.	1.7	9
203	Classification of Raman active modes of platinum(II) acetylides: A combined experimental and theoretical study. Chemical Physics Letters, 2009, 481, 209-213.	2.6	9
204	A quantum chemical study of the structure of O=NO-ON=O peroxide and the reaction mechanism of no oxidation in the gas phase. Journal of Structural Chemistry, 2012, 53, 1-11.	1.0	9
205	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		9
206	Spin-orbit coupling and dissociation of CO2 molecules. Optics and Spectroscopy (English Translation) Tj ETQq0 0 0 rgBT /Overlock 10 Tf	0.8	9
207	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
208	Ab Initio Study of Electronic States of Astrophysically Important Molecules. Russian Physics Journal, 2016, 59, 536-543.	0.4	9
209	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
210	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
211	Substituent-sensitive fluorescence of sequentially N-alkylated tetrabenzotetraaza[8]circulenes. New Journal of Chemistry, 2017, 41, 7621-7625.	2.8	9
212	BaZrO3 perovskite nanoparticles as emissive material for organic/inorganic hybrid light-emitting diodes. Dyes and Pigments, 2017, 145, 399-403.	3.7	9
213	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
214	External heavy-atom effects on radiative singlet-triplet transitions. Journal of Applied Spectroscopy, 1985, 43, 887-890.	0.7	8
215	The Vegard-Kaplan band and the phosphorescent decay of N2. Chemical Physics Letters, 1994, 231, 387-394.	2.6	8
216	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

#	Article	IF	Citations
217	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		
218	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
219	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
220	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
221	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
222	Study of IR spectrum of the 17β-estradiol using quantum-chemical density functional theory. Biopolymers and Cell, 2006, 22, 363-374.	0.4	8
223	Theoretical model of triplet-triplet annihilation. Soviet Physics Journal (English Translation of) Tj ETQq1 1 0.784314 rgBT /Overlock 10 Tf	0.5	7
224	Effect of spin-orbit coupling on the intensity of magnetic dipole transitions in molecular oxygen. Soviet Physics Journal (English Translation of Izvestiia Vysshykh Uchebnykh Zavedenii, Fizika), 1978, 21, 1205-1209.	0.0	7
225	Ab initio calculation of transition dipole moments for transitions between valence states in oxygen molecules. Optics and Spectroscopy (English Translation of Optika I Spektroskopiya), 2001, 91, 883-890.	0.6	7
226	Fine structure and radiative lifetime of the low-lying triplet states of the helium excimer. Physical Chemistry Chemical Physics, 2003, 5, 2314.	2.8	7
227	Intensity of singlet-triplet transitions in C60 fullerene calculated on the basis of the time-dependent density functional theory and taking into account the quadratic response. Optics and Spectroscopy (English Translation of Optika I Spektroskopiya), 2005, 98, 336-340.	0.6	7
228	Structure and spectral properties of phenyldiazonium tetrachlorocuprate (II). Russian Journal of Applied Chemistry, 2010, 83, 36-43.	0.5	7
229	Theoretical study of the conformational structure and thermodynamic properties of 5-(4-oxo-1,3-thiazolidine-2-ylidene)-rhodanine and ethyl-5-(4-oxo-1,3-thiazolidine-2-ylidene)-rhodanine-3-acetic acid as acceptor groups of indoline dyes. Journal of Structural Chemistry, 2010, 51, 817-823.	1.0	7
230	Absolute effective cross sections of ionization of adenine and guanine molecules by electron impact. Technical Physics, 2015, 60, 1430-1436.	0.7	7
231	DFT design of polyguanidine â€" a unique two-dimensional material with high-energy density. Molecular Physics, 2017, 115, 2423-2430.	1.7	7
232	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
233	Dianthracenylazatrioxa[8]circulene: Synthesis, Characterization and Application in OLEDs. Chemistry - A European Journal, 2021, 27, 11609-11617.	3.3	7
234	Calculations of quartet state spectra for diatomic species by INDO CI method including spin-orbit coupling perturbation. Collection of Czechoslovak Chemical Communications, 1981, 46, 179-193.	1.0	6

#	Article	IF	Citations
235	Quantum chemical calculation of phosphorescence microwave double resonance spectra. International Journal of Quantum Chemistry, 1982, 22, 863-869.	2.0	6
236	Phosphorescence of aromatic molecules. Journal of Molecular Structure, 1994, 311, 185-197.	3.6	6
237	Phosphorescence of aromatic molecules. Computational and Theoretical Chemistry, 1994, 311, 185-197.	1.5	6
238	Ab Initio Study of the Phosphorescence of Nitrite Ions. Journal of Fluorescence, 1999, 9, 221-232.	2.5	6
239	Ab initio study of the singletâ€“triplet transitions in hypobromous acid. Computational and Theoretical Chemistry, 1999, 492, 53-66.	1.5	6
240	Fine and hyperfine structure in three low-lying3Î£+states of molecular hydrogen. Molecular Physics, 2003, 101, 2335-2346.	1.7	6
241	Spinâ€“spin coupling in 3b2 state of oxyallyl â€“ A comparative study with trimethylenemethane. Computational and Theoretical Chemistry, 2011, 963, 51-54.	2.5	6
242	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
243	Spin-Orbit Coupling in Enzymatic Reactions and the Role of Spin in Biochemistry. , 2012, , 1067-1093.		6
244	Comparative computational IR, Raman and phosphorescence study of Ru- and Rh-based complexes. Molecular Physics, 2013, 111, 1526-1538.	1.7	6
245	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
246	Spin-Orbit Coupling in Enzymatic Reactions and the Role of Spin in Biochemistry. , 2017, , 1557-1587.		6
247	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
248	Vibronic absorption spectra of the angular fused bisindolo- and biscarbazoloanthracene blue fluorophores for OLED applications. Chemical Physics, 2018, 513, 105-111.	1.9	6
249	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
250	Calculation of the singlet-triplet magnetic and electro-quadrupole transitions intensity for Ge₂ molecule. Molecular Physics, 2022, 120, .	1.7	6
251	Spin?orbit interaction in charge-transfer complexes. Soviet Physics Journal (English Translation of) Tj ETQq1 1 0.784314 rgBT /Overlock	0.0	5
252	MINDO/3 CI Study of NCO Spectrum and the Chemiluminescent Reaction N + CO â†' NCO + h. Spectroscopy Letters, 1989, 22, 901-923.	1.0	5

#	Article	IF	Citations
253	Paramagnetic spin catalysis of a radical recombination reaction. Molecular Engineering, 1996, 6, 261-279.	0.2	5
254	Study of singlet-triplet transitions in the ozone molecule using the multiconfigurational self-consistent field theory. High Energy Chemistry, 2006, 40, 230-233.	0.9	5
255	IR, Raman and UVâ€“vis spectra of the Ru(II) cyano complexes studied by DFT. Molecular Simulation, 2011, 37, 670-677.	2.0	5
256	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
257	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
258	Optical tuning of tetrabenzo[8]circulene derivatives through pseudorotational conformational isomerization. Dyes and Pigments, 2018, 151, 372-379.	3.7	5
259	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
260	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
261	Spin-orbit coupling effects in O(2) activation by cofactor-independent 2,4-dioxygenase. Ukrainian Biochemical Journal, 2019, 91, 38-46.	0.5	5
262	Theoretical investigation of Wulf and Chappuis bands in the spectrum of ozone. Journal of Structural Chemistry, 1997, 38, 895-900.	1.0	4
263	MCSCF linear response study of the three-body dissociative recombination CH2++eâ†'C+2H. Chemical Physics, 2002, 280, 15-30.	1.9	4
264	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
265	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
266	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
267	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
268	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 13	0.6	4
269	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
270	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

#	Article	IF	Citations
271	Molecular Terms of Dioxygen and Nitric Oxide. Physchem, 2021, 1, 121-132.	1.1	4
272	CNDO/S CI calculation of spin-orbit coupling and intersystem crossing in photochemical biradical formation reaction. Collection of Czechoslovak Chemical Communications, 1981, 46, 1318-1323.	1.0	3
273	Quantum-Chemical Study of the Diatomic Hydrides Electronic Structure. Spectroscopy Letters, 1989, 22, 211-236.	1.0	3
274	Ab InitioCalculations of the Three-body C2+ H + H Dissociative Recombination Channel for the C2H2++ e Reaction. Physica Scripta, 2003, 67, 407-413.	2.5	3
275	Electronicâ€“Rotational Coupling and c1Ââ€“uâ€“b1Â+gTransition Probability in the Oxygen Molecule. High Energy Chemistry, 2004, 38, 209-214.	0.9	3
276	Vibrational spectra of corticosteroid hormones in the terahertz range. Proceedings of SPIE, 2010, , .	0.8	3
277	Theoretical study of the models of Ca2+ and Mg2+ ions binding by the methylidene rhodanine neutral and anionic forms. Russian Journal of General Chemistry, 2011, 81, 576-585.	0.8	3
278	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
279	Synthesis and spectroscopic characterization of a new (aryl-SCN)n polymer: Polythiocyanatohydroquinone. Journal of Molecular Structure, 2015, 1096, 15-20.	3.6	3
280	Computational study of IR, Raman, and NMR spectra of 4-methylmethcathinone drug. Journal of Molecular Modeling, 2021, 27, 3.	1.8	3
281	Some recent developments of highâ€order response theory. International Journal of Quantum Chemistry, 1998, 70, 219-239.	2.0	3
282	Investigation of infrared spectrum of Fe(II) porphin in different spin states by quantum chemical density functional theory. Biopolymers and Cell, 2007, 23, 519-528.	0.4	3
283	Interaction of Myoglobin Model with Ligands of Gas Exchange. Cherkasy University Bulletin Biological Sciences Series, 2019, , 13-23.	0.2	3
284	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
285	Calculation of the spectra of unsaturated hydrocarbons by the method of complete neglect of differential overlap of configurational excitation with an account of the spin-orbit interaction. Soviet Physics Journal (English Translation of Izvestiia Vysshykh Uchebnykh Zavedenii, Fizika), 1971, 14, 644-649.	0.0	2
286	Calculation of the benzene molecule with configuration interaction, spin-orbit interaction, and complete neglect of differential overlap. Soviet Physics Journal (English Translation of Izvestiia) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50 137	0.0	2
287	Effect of a magnetic field on delayed fluorescence of anthracene exciplexes. Journal of Applied Spectroscopy, 1981, 34, 287-291.	0.7	2
288	Mechanism of the cooperative vibronic emission of1?g singlet oxygen in solutions. Theoretical and Experimental Chemistry, 1986, 21, 567-569.	0.8	2

#	Article	IF	Citations
289	Non-Equilibrium Spin Polarization of the Si-S1 Centre in Silicon Induced by Spinâ€“Orbit Coupling. Physica Status Solidi (B): Basic Research, 1988, 148, 689-698.	1.5	2
290	External heavy atom effect on the intersystem crossing from the lower and higher excited states of rhodamine dyes on a silica surface. Journal of Applied Spectroscopy, 1992, 56, 146-150.	0.7	2
291	Role of spin-orbit coupling in processes of synthesis and photodegradation of ozone. Theoretical and Experimental Chemistry, 1997, 33, 188-191.	0.8	2
292	High-Resolution Spectroscopy of the A4Îrâ† ' X4Î£-Band System of MoN. Physica Scripta, 2000, 62, 417-424.	2.5	2
293	Modeling the structure and spectral properties of sensitizing black dye for nanocrystalline TiO2 solar cells. Journal of Applied Spectroscopy, 2009, 76, 772-776.	0.7	2
294	Organometallic Materials for Electroluminescent and Photovoltaic Devices. , 0, , .		2
295	Synthesis of nanostructured polymetallic composites based on palladium and quantum-chemical simulation of initial stages of the process. Russian Journal of Applied Chemistry, 2012, 85, 564-574.	0.5	2
296	Electron density distribution in the ethylene complexes with Pd-containing bimetallic clusters. Molecular Simulation, 2013, 39, 660-669.	2.0	2
297	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
298	Influence of Molecular Oxygen on Ortho-Para Conversion of Water Molecules. Russian Physics Journal, 2017, 60, 485-493.	0.4	2
299	Possible electronic mechanisms of generation and quenching of luminescence of singlet oxygen in the course of photodynamic therapy: ab initio study. Biopolymers and Cell, 2006, 22, 231-235.	0.4	2
300	Enzymatic spin-catalysis in flavin-containing oxidases and magnetic orientation of birds. Cherkasy University Bulletin Biological Sciences Series, 2018, , 114-120.	0.2	2
301	The spin-lattice relaxation mechanism in the phosphorescent triplet state. Soviet Physics Journal (English Translation of Izvestiia Vysshykh Uchebnykh Zavedenii, Fizika), 1978, 21, 571-574.	0.0	1
302	Calculation of the intensities of the infrared spectra of acetonitrile complexes with Na+, Li+, and Mg+3 cations by the CNDO/2 method. Journal of Applied Spectroscopy, 1979, 30, 249-252.	0.7	1
303	Microwave energy transfer between triplet states of molecules under optical spin orientation conditions. Soviet Physics Journal (English Translation of Izvestiia Vysshykh Uchebnykh Zavedenii,) Tj ETQq1 1 0.784314 rgBT /Overlo	0.0	1
304	Calculation of the probability for the singlet ? triplet transition in the ethylene molecule by the CNDO CI method. Journal of Applied Spectroscopy, 1980, 32, 43-47.	0.7	1
305	Calculating chemical electron-polarization in triplet-molecule reactions. Theoretical and Experimental Chemistry, 1986, 22, 189-192.	0.8	1
306	Quantum chemical calculation of the probabilities of spin allowed and forbidden transitions in CN, CO+, and BH+ molecules. Journal of Applied Spectroscopy, 1988, 48, 322-325.	0.7	1

#	Article	IF	Citations
307	Classification of Spin-Orbit Coupling Effects in Organic Chemical Reactions*. Zeitschrift Fur Physikalische Chemie, 1992, 1, 263-284.	2.8	1
308	Intermolecular interaction in radical recombination in the system O2 + H2. Theoretical and Experimental Chemistry, 1996, 32, 200-204.	0.8	1
309	The Other Chekhov. Russian Studies in Literature, 2010, 47, 74-79.	0.1	1
310	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
311	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
312	Spin-Orbit Coupling in Enzymatic Reactions and the Role of Spin in Biochemistry. , 2016, , 1-31.		1
313	Quantum-chemical modelling radiation damage of DNA components during inelastic interaction with slow electrons. Desoxyribose irradiation. Biopolymers and Cell, 2005, 21, 351-357.	0.4	1
314	Study on models of O2 binding to heme using density functional theory. Biopolymers and Cell, 2009, 25, 298-306.	0.4	1
315	Study of IR spectrum of the testosterone and ethyniltestosterone by quantum-chemical density functional theory. Biopolymers and Cell, 2010, 26, 62-71.	0.4	1
316	Furans and Their Benzo Derivatives: Structure. , 2020, , 190-190.		1
317	Crystal structure and Hirshfeld surfaces analysis of Heterocyclic-and circulenes. MATEC Web of Conferences, 2022, 355, 01020.	0.2	1
318	Calculation of trans-butadiene by the pople-santry-segal method with configurational interaction: Role of the ?? ? States in the spectra of hydrocarbons. Soviet Physics Journal (English Translation of) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 5		
319	Calculation of complexes with charge transfer and their spectra by the pariser-parr-pople method considering configurational interaction. Bulletin of the Academy of Sciences of the USSR Division of Chemical Science, 1974, 23, 2611-2615.	0.0	0
320	Calculation of the ?? and ?? states of planar unsaturated molecules by the CNDO CI method. Theoretical and Experimental Chemistry, 1974, 8, 311-315.	0.8	0
321	Comparison of one-electron energies obtained by the CNDO/2 and ab initio methods for triatomic molecules. Theoretical and Experimental Chemistry, 1975, 10, 175-177.	0.8	0
322	Study of the mechanism of the photodecomposition of aldehydes of ?type II? according to norrish, by the CNDO/3 method. Journal of Structural Chemistry, 1978, 19, 209-213.	1.0	0
323	Model of a triplet trap in the reaction of p-fluoronitrobenzene with the hydroxide anion. Theoretical and Experimental Chemistry, 1982, 17, 513-517.	0.8	0
324	A quantum-chemical study of the o-carboranyl-substituted allyl anion. Journal of Structural Chemistry, 1982, 22, 778-780.	1.0	0

#	Article	IF	Citations
325	Quantum-chemical investigation of complexes of the nitrite ion with metal cations. Theoretical and Experimental Chemistry, 1984, 20, 287-292.	0.8	0
326	Calculation of the magnetophotoselective effect in reactions of triplet molecules. Theoretical and Experimental Chemistry, 1988, 24, 88-92.	0.8	0
327	Nonequilibrium polarization of triplet centers in silicon. Soviet Physics Journal (English Translation) Tj ETQq1 1 0.784314 rgBT /Overlo	0.0	0
328	Structures and mechanism of formation of the HCO2 radical and its HCO2 + Ion. Journal of Structural Chemistry, 1989, 29, 533-537.	1.0	0
329	Interaction mechanism of molecular oxygen with excited states of luminophores in solution, in polymers, and at a surface. Journal of Applied Spectroscopy, 1989, 50, 216-221.	0.7	0
330	Mechanism of phototransfer of hydrogen atom in the model H2CO + H2O system. Theoretical and Experimental Chemistry, 1990, 25, 441-445.	0.8	0
331	Orbital-shell density functional in calculations on the intramolecular and intermolecular potentials for chromium atoms and benzene molecules. Theoretical and Experimental Chemistry, 1990, 26, 201-203.	0.8	0
332	Metastable high-spin states in chemical ionization in hydrocarbon combustion. Theoretical and Experimental Chemistry, 1991, 27, 582-586.	0.8	0
333	Mechanism of reactions of photocatalytic synthesis of chlorohydrins. Theoretical and Experimental Chemistry, 1997, 33, 16-20.	0.8	0
334	Cooperative influence of H2 and C2H4 molecules on theb-a anda-X transitions in the O2 molecule in a ternary complex. Journal of Applied Spectroscopy, 2000, 67, 617-622.	0.7	0
335	Ab Initio Calculation of the Ground and Excited States of BrOâ€“. Journal of Structural Chemistry, 2001, 42, 490-493.	1.0	0
336	Calculation of properties of the ozone molecule by the multiconfigurational self-consistent field method. Journal of Applied Spectroscopy, 2005, 72, 781-785.	0.7	0
337	Theory of singlet oxygen emission photosensitized by porphyrins. , 2006, 6401, 114.		0
338	Investigation of spectral features of progesterone, 17a-hydroxyprogesterone and cortisone in THz range. , 2010, , .		0
339	Analysis of intermolecular interactions in progesterone and 17α-hydroxyprogesterone crystals. , 2013, , .		0
340	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
341	Electronic structure models of flavoproteides and mechanism of oxidases action. Biopolymers and Cell, 2004, 20, 224-232.	0.4	0
342	DFT study on the Raman spectra of Fe(II)-porphin. Biopolymers and Cell, 2009, 25, 62-72.	0.4	0

#	Article	IF	Citations
343	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