Valentina A Minaeva

List of Publications by Year
in descending order

56	1,247	304743	377865
papers	citations	22 h-index	34 g-index

56	56	56	1176
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	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
2	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
3	Benzoannelated aza-, oxa- and azaoxa[8]circulenes as promising blue organic emitters. Physical Chemistry Chemical Physics, 2016, 18, 28040-28051.	2.8	54
4	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
5	Experimental and theoretical study of IR and Raman spectra of tetraoxa[8]circulenes. Vibrational Spectroscopy, 2012, 61, 156-166.	2.2	51
6	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
7	Design of nanoscaled materials based on tetraoxa[8]circulene. Physical Chemistry Chemical Physics, 2014, 16, 6555.	2.8	48
8	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
9	Fluorescence and FTIR Spectra Analysis of Trans-A2B2-Substituted Di- and Tetra-Phenyl Porphyrins. Materials, 2010, 3, 4446-4475.	2.9	47
10	Electronic structure, aromaticity and spectra of hetero[8]circulenes. Russian Chemical Reviews, 2015, 84, 455-484.	6.5	46
11	Density functional theory study of electronic structure and spectra of tetraoxa[8]circulenes. Computational and Theoretical Chemistry, 2011, 972, 68-74.	2.5	43
12	Fragmentation of the adenine and guanine molecules induced by electron collisions. Journal of Chemical Physics, 2014, 140, 175101.	3.0	42
13	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
14	DFT and QTAIM study of the tetra-tert-butyltetraoxa[8]circulene regioisomers structure. Journal of Molecular Structure, 2012, 1026, 127-132.	3.6	35
15	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
16	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
17	Quantumâ€chemical study of the singlet oxygen emission. International Journal of Quantum Chemistry, 2009, 109, 500-515.	2.0	29
18	Recent progress in quantum chemistry of hetero[8]circulenes. Molecular Physics, 2017, 115, 2218-2230.	1.7	28

#	ARTICLE	IF	CITATIONS
19	The FTIR spectra of substituted tetraoxa[8]circulenes and their assignments based on DFT calculations. Vibrational Spectroscopy, 2013, 65, 147-158.	2.2	26
20	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
21	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
22	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
23	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
24	Structure and spectral properties of truxene dye S5. Optics and Spectroscopy (English Translation of) Tj ETQq0 0 0 rgBT /Overlock 10 Tf	0.6	20
25	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
26	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
27	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
28	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
29	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 /Ov	0.7	12
30	Stabilizing hydrogen-hydrogen interactions in cationic indopolycarbocyanine dyes. Journal of Structural Chemistry, 2011, 52, 1051-1056.	1.0	11
31	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
32	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
33	Theoretical study of the dimerization of rhodanine in various tautomeric forms. Chemistry of Heterocyclic Compounds, 2012, 47, 1268-1279.	1.2	11
34	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 50 137	0.6	11
35	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
36	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

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37	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
38	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 ETQq0 0 0 rgBT /Overlock 10	0.6	9
39	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
40	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
41	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
42	Absolute effective cross sections of ionization of adenine and guanine molecules by electron impact. Technical Physics, 2015, 60, 1430-1436.	0.7	7
43	Ab Initio Study of the Phosphorescence of Nitrite Ions. Journal of Fluorescence, 1999, 9, 221-232.	2.5	6
44	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
45	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
46	IR, Raman and UVâ€“vis spectra of the Ru(II) cyano complexes studied by DFT. Molecular Simulation, 2011, 37, 670-677.	2.0	5
47	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
48	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
49	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
50	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
51	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 ETQq1 1 0.784314 rgBT /Overlock 10	0.6	4
52	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
53	Vibrational spectra of corticosteroid hormones in the terahertz range. Proceedings of SPIE, 2010, , .	0.8	3
54	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

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55	Investigation of spectral features of progesterone, 17a-hydroxyprogesterone and cortisone in THz range. , 2010, , .		0
56	Surface-enhanced infrared spectroscopy for cortisol analysis. , 2018, , .		0