

Valentina A Minaeva

List of Publications by Year in descending order

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56
papers

1,247
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304368

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docs citations

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times ranked

1176
citing authors

#	ARTICLE	IF	CITATIONS
1	Theoretical Study of the Cyclometalated Iridium(III) Complexes Used as Chromophores for Organic Light-Emitting Diodes. <i>Journal of Physical Chemistry A</i> , 2009, 113, 726-735.	1.1	111
2	Novel Zinc Complex with an Ethylenediamine Schiff Base for High-Luminance Blue Fluorescent OLED Applications. <i>Journal of Physical Chemistry C</i> , 2019, 123, 11850-11859.	1.5	56
3	Benzoannelated aza-, oxa- and azaoxa[8]circulenes as promising blue organic emitters. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 28040-28051.	1.3	54
4	Electronic structure and spectral properties of the triarylamine-dithienosilole dyes for efficient organic solar cells. <i>Dyes and Pigments</i> , 2012, 92, 531-536.	2.0	53
5	Experimental and theoretical study of IR and Raman spectra of tetraoxa[8]circulenes. <i>Vibrational Spectroscopy</i> , 2012, 61, 156-166.	1.2	51
6	The art of the possible: computational design of the 1D and 2D materials based on the tetraoxa[8]circulene monomer. <i>RSC Advances</i> , 2014, 4, 25843-25851.	1.7	50
7	Design of nanoscaled materials based on tetraoxa[8]circulene. <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 6555.	1.3	48
8	MCSCF response calculations of the excited states properties of the O ₂ molecule and a part of its spectrum. <i>Physical Chemistry Chemical Physics</i> , 2001, 3, 720-729.	1.3	47
9	Fluorescence and FTIR Spectra Analysis of Trans-A ₂ B ₂ -Substituted Di- and Tetra-Phenyl Porphyrins. <i>Materials</i> , 2010, 3, 4446-4475.	1.3	47
10	Electronic structure, aromaticity and spectra of hetero[8]circulenes. <i>Russian Chemical Reviews</i> , 2015, 84, 455-484.	2.5	46
11	Density functional theory study of electronic structure and spectra of tetraoxa[8]circulenes. <i>Computational and Theoretical Chemistry</i> , 2011, 972, 68-74.	1.1	43
12	Fragmentation of the adenine and guanine molecules induced by electron collisions. <i>Journal of Chemical Physics</i> , 2014, 140, 175101.	1.2	42
13	Application of Bader's atoms in molecules theory to the description of coordination bonds in the complex compounds of Ca ²⁺ and Mg ²⁺ with methyldene rhodanine and its anion. <i>Russian Journal of General Chemistry</i> , 2012, 82, 1254-1262.	0.3	39
14	DFT and QTAIM study of the tetra-tert-butyltetraoxa[8]circulene regioisomers structure. <i>Journal of Molecular Structure</i> , 2012, 1026, 127-132.	1.8	35
15	A DFT and QTAIM study of the novel d-block metal complexes with tetraoxa[8]circulene-based ligands. <i>New Journal of Chemistry</i> , 2015, 39, 7815-7821.	1.4	33
16	Single crystal architecture and absorption spectra of octathio[8]circulene and sym-tetraselenatetrathio[8]circulene: QTAIM and TD-DFT approach. <i>Journal of Molecular Modeling</i> , 2013, 19, 4511-4519.	0.8	31
17	Quantum-chemical study of the singlet oxygen emission. <i>International Journal of Quantum Chemistry</i> , 2009, 109, 500-515.	1.0	29
18	Recent progress in quantum chemistry of hetero[8]circulenes. <i>Molecular Physics</i> , 2017, 115, 2218-2230.	0.8	28

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19	The FTIR spectra of substituted tetraoxa[8]circulenes and their assignments based on DFT calculations. <i>Vibrational Spectroscopy</i> , 2013, 65, 147-158.	1.2	26
20	A comparative study of the electronic structure and spectra of tetraoxa[8]circulene and octathio[8]circulene. <i>Optics and Spectroscopy (English Translation of Optika i Spektroskopiya)</i> , 2014, 116, 33-46.	0.2	26
21	Structure of zinc complexes with 3-(pyridin-2-yl)-5-(arylideneiminophenyl)-1H-1,2,4-triazoles in different tautomeric forms: DFT and QAIM study. <i>Russian Journal of Inorganic Chemistry</i> , 2013, 58, 928-934.	0.3	24
22	Computational study of the structure, UV-vis absorption spectra and conductivity of biphenylene-based polymers and their boron nitride analogues. <i>RSC Advances</i> , 2016, 6, 49505-49516.	1.7	24
23	Structure and spectroscopic characterization of tetrathia- and tetraselena[8]circulenes as a new class of polyaromatic heterocycles. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2015, 151, 247-261.	2.0	22
24	Structure and spectral properties of truxene dye S5. <i>Optics and Spectroscopy (English Translation of Optika i Spektroskopiya)</i> , 2010, 108, 16-22.	0.2	20
25	Theoretical study of vibration spectra of sensitizing dyes for photoelectrical converters based on ruthenium(II) and iridium(III) complexes. <i>Russian Journal of Applied Chemistry</i> , 2009, 82, 1211-1221.	0.1	19
26	Quantum-chemical study of the structure and optical properties of sensitized dyes of an indoline-thiazolidine series. <i>Optics and Spectroscopy (English Translation of Optika i Spektroskopiya)</i> , 2010, 108, 16-22.	0.2	19
27	Quantum-chemical study of effect of conjugation on structure and spectral properties of C105 sensitizing dye. <i>Optics and Spectroscopy (English Translation of Optika i Spektroskopiya)</i> , 2011, 110, 393-400.	0.2	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. <i>Russian Journal of General Chemistry</i> , 2011, 81, 2332-2344.	0.3	13
29	Theoretical investigation of the structure and electronic absorption spectrum of a complex zinc bis-[8-(3,5-difluorophenylsulfanyl)amino]quinolate. <i>Optics and Spectroscopy (English Translation of Optika i Spektroskopiya)</i> , 2010, 108, 16-22.	0.2	13
30	Stabilizing hydrogen-hydrogen interactions in cationic indopolycarbocyanine dyes. <i>Journal of Structural Chemistry</i> , 2011, 52, 1051-1056.	0.3	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. <i>Optics and Spectroscopy (English Translation of Optika i Spektroskopiya)</i> , 2011, 110, 216-223.	0.2	11
32	Raman spectra of tetraoxa[8]circulenes. p-dinaphthalenodiphenylenetetrafurane and its tetraalkyl derivatives (DFT study and experiment). <i>Journal of Applied Spectroscopy</i> , 2012, 79, 695-707.	0.3	11
33	Theoretical study of the dimerization of rhodanine in various tautomeric forms. <i>Chemistry of Heterocyclic Compounds</i> , 2012, 47, 1268-1279.	0.6	11
34	Quantum-chemical investigation of the structure and electronic absorption spectra of electroluminescent zinc complexes. <i>Optics and Spectroscopy (English Translation of Optika i Spektroskopiya)</i> , 2010, 108, 16-22.	0.2	13
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. <i>Journal of Molecular Modeling</i> , 2017, 23, 55.	0.8	11
36	Raman spectra of alkyl-substituted azaoxa[8]circulenes: DFT calculation and experiment. <i>Optics and Spectroscopy (English Translation of Optika i Spektroskopiya)</i> , 2013, 114, 509-521.	0.2	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.	0.2	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 00rgBT /Overlock 10	0.2	10
39	A complete characterization of vibrational IR and Raman spectra of the highly-symmetrical octathia[8]circulene. Vibrational Spectroscopy, 2019, 100, 107-116.	1.2	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.	1.1	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.	0.3	7
42	Absolute effective cross sections of ionization of adenine and guanine molecules by electron impact. Technical Physics, 2015, 60, 1430-1436.	0.2	7
43	Ab Initio Study of the Phosphorescence of Nitrite Ions. Journal of Fluorescence, 1999, 9, 221-232.	1.3	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.	0.3	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.	0.2	6
46	IR, Raman and UV-vis spectra of the Ru(II) cyano complexes studied by DFT. Molecular Simulation, 2011, 37, 670-677.	0.9	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.	0.3	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.	0.2	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.	0.2	4
50	Analysis of the electronic, IR, and ¹ H NMR spectra of conjugated oligomers based on 4,4'-triphenylamine vinylene. Optics and Spectroscopy (English Translation of Optika I Spektroskopiya), 2016, 121, 348-356.	0.2	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 /@verlock 10	1.4	4
52	Identification of tautomeric intermediates of a novel thiazolylazonaphthol dye – A density functional theory study. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2018, 203, 324-332.	2.0	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 Ca ²⁺ and Mg ²⁺ ions binding by the methyldiene rhodanine neutral and anionic forms. Russian Journal of General Chemistry, 2011, 81, 576-585.	0.3	3

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