Valentina A Minaeva

List of Publications by Year
in descending order

56	1,247	304368	377514
papers	citations	22 h-index	34 g-index

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

#	Article	IF	Citations
1	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
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.	1.5	56
3	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
4	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.	2.0	4
5	Surface-enhanced infrared spectroscopy for cortisol analysis. , 2018, , .		0
6	Recent progress in quantum chemistry of hetero[8]circulenes. Molecular Physics, 2017, 115, 2218-2230.	0.8	28
7	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	1.1	2
8	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
9	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
10	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.	0.8	11
11	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
12	Benzoannelated aza-, oxa- and azaoxa[8]circulenes as promising blue organic emitters. Physical Chemistry Chemical Physics, 2016, 18, 28040-28051.	1.3	54
13	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.	0.2	4
14	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
15	Electronic structure, aromaticity and spectra of hetero[8]circulenes. Russian Chemical Reviews, 2015, 84, 455-484.	2.5	46
16	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
17	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
18	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

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19	Absolute effective cross sections of ionization of adenine and guanine molecules by electron impact. Technical Physics, 2015, 60, 1430-1436.	0.2	7
20	Design of nanoscaled materials based on tetraoxa[8]circulene. Physical Chemistry Chemical Physics, 2014, 16, 6555.	1.3	48
21	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
22	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
23	Fragmentation of the adenine and guanine molecules induced by electron collisions. Journal of Chemical Physics, 2014, 140, 175101.	1.2	42
24	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
25	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.	0.2	10
26	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
27	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		
28	The FTIR spectra of substituted tetraoxa[8]circulenes and their assignments based on DFT calculations. Vibrational Spectroscopy, 2013, 65, 147-158.	1.2	26
29	Quantum-chemical investigation of the structure and electronic absorption spectra of electroluminescent zinc complexes. Optics and Spectroscopy (English Translation of Optika I) Tj ETQq1 1 0.784314 rgBT /Overlock 10 T		
30	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
31	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
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.	0.3	11
33	DFT and QTAIM study of the tetra-tert-butyltetraoxa[8]circulene regioisomers structure. Journal of Molecular Structure, 2012, 1026, 127-132.	1.8	35
34	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
35	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 /Over		
36	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

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37	Theoretical study of the dimerization of rhodanine in various tautomeric forms. Chemistry of Heterocyclic Compounds, 2012, 47, 1268-1279.	0.6	11
38	Experimental and theoretical study of IR and Raman spectra of tetraoxa[8]circulenes. Vibrational Spectroscopy, 2012, 61, 156-166.	1.2	51
39	Structure and spectral properties of truxene dye S5. Optics and Spectroscopy (English Translation of) Tj ETQq1 1 0.784314 rgBT /Ove	0.2	20
40	Density functional theory study of electronic structure and spectra of tetraoxa[8]circulenes. Computational and Theoretical Chemistry, 2011, 972, 68-74.	1.1	43
41	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
42	Stabilizing hydrogen-hydrogen interactions in cationic indopolycarbocyanine dyes. Journal of Structural Chemistry, 2011, 52, 1051-1056.	0.3	11
43	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.	0.3	3
44	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.	0.3	13
45	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.	0.2	11
46	IR, Raman and UVâ€“vis spectra of the Ru(II) cyano complexes studied by DFT. Molecular Simulation, 2011, 37, 670-677.	0.9	5
47	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
48	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
49	Fluorescence and FTIR Spectra Analysis of Trans-A2B2-Substituted Di- and Tetra-Phenyl Porphyrins. Materials, 2010, 3, 4446-4475.	1.3	47
50	Investigation of spectral features of progesterone, 17a-hydroxyprogesterone and cortisone in THz range. , 2010, , .		0
51	Vibrational spectra of corticosteroid hormones in the terahertz range. Proceedings of SPIE, 2010, , .	0.8	3
52	Quantumâ€chemical study of the singlet oxygen emission. International Journal of Quantum Chemistry, 2009, 109, 500-515.	1.0	29
53	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
54	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

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55	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
56	Ab Initio Study of the Phosphorescence of Nitrite Ions. Journal of Fluorescence, 1999, 9, 221-232.	1.3	6