

Vladimir Lukeš

List of Publications by Year in descending order

Source: <https://exaly.com/author-pdf/8283185/publications.pdf>

Version: 2024-02-01

130
papers

2,571
citations

218677

26
h-index

223800

46
g-index

130
all docs

130
docs citations

130
times ranked

2796
citing authors

#	ARTICLE	IF	CITATIONS
1	Study of the solvent effect on the enthalpies of homolytic and heterolytic N-H bond cleavage in p-phenylenediamine and tetracyano-p-phenylenediamine. <i>Computational and Theoretical Chemistry</i> , 2010, 952, 25-30.	1.5	281
2	DFT/B3LYP study of tocopherols and chromans antioxidant action energetics. <i>Chemical Physics</i> , 2007, 336, 51-57.	1.9	152
3	Theoretical Study of Vibrational and Optical Spectra of Methylene-Bridged Oligofluorenes. <i>Journal of Physical Chemistry A</i> , 2005, 109, 10232-10238.	2.5	129
4	DFT/B3LYP Study of the Substituent Effect on the Reaction Enthalpies of the Individual Steps of Single Electron Transfer-Proton Transfer and Sequential Proton Loss Electron Transfer Mechanisms of Phenols Antioxidant Action. <i>Journal of Physical Chemistry A</i> , 2006, 110, 12312-12320.	2.5	114
5	System-Dependent Signatures of Electronic and Vibrational Coherences in Electronic Two-Dimensional Spectra. <i>Journal of Physical Chemistry Letters</i> , 2012, 3, 1497-1502.	4.6	80
6	Study of gas-phase O-H bond dissociation enthalpies and ionization potentials of substituted phenols - Applicability of ab initio and DFT/B3LYP methods. <i>Chemical Physics</i> , 2006, 330, 515-525.	1.9	74
7	Vibronic modulation of lineshapes in two-dimensional electronic spectra. <i>Chemical Physics Letters</i> , 2008, 459, 94-99.	2.6	69
8	DFT/B3LYP study of O-H bond dissociation enthalpies of para and meta substituted phenols: Correlation with the phenolic C-O bond length. <i>Computational and Theoretical Chemistry</i> , 2006, 767, 43-50.	1.5	66
9	Study of N-H, O-H, and S-H bond dissociation enthalpies and ionization potentials of substituted anilines, phenols, and thiophenols. <i>Computational and Theoretical Chemistry</i> , 2006, 758, 149-159.	1.5	62
10	Dependence of Optical Properties of Oligo-para-phenylenes on Torsional Modes and Chain Length. <i>Journal of Physical Chemistry B</i> , 2007, 111, 7954-7962.	2.6	62
11	On the energetics of homolytic and heterolytic OH bond cleavage in flavonoids. <i>Computational and Theoretical Chemistry</i> , 2012, 991, 192-200.	2.5	61
12	Vibrational wave packet induced oscillations in two-dimensional electronic spectra. I. Experiments. <i>Journal of Chemical Physics</i> , 2010, 132, .	3.0	55
13	Protective role of quercetin against copper(II)-induced oxidative stress: A spectroscopic, theoretical and DNA damage study. <i>Food and Chemical Toxicology</i> , 2017, 110, 340-350.	3.6	55
14	Oxidation of sterols: Energetics of C-H and O-H bond cleavage. <i>Food Chemistry</i> , 2012, 133, 1435-1440.	8.2	54
15	Vibrational wave packet induced oscillations in two-dimensional electronic spectra. II. Theory. <i>Journal of Chemical Physics</i> , 2010, 132, .	3.0	53
16	Effect of N-Substituents on Redox, Optical, and Electronic Properties of Naphthalene Bisimides Used for Field-Effect Transistors Fabrication. <i>Journal of Physical Chemistry B</i> , 2010, 114, 1803-1809.	2.6	51
17	Ultrafast photo-induced charge transfer unveiled by two-dimensional electronic spectroscopy. <i>Journal of Chemical Physics</i> , 2012, 136, 204503.	3.0	49
18	Electronic ground state conformers of Î²-carotene and their role in ultrafast spectroscopy. <i>Chemical Physics Letters</i> , 2011, 506, 122-127.	2.6	40

#	ARTICLE	IF	CITATIONS
19	Study of natural anthraquinone colorants by EPR and UV/vis spectroscopy. <i>Dyes and Pigments</i> , 2016, 132, 79-93.	3.7	39
20	Vibronic energy relaxation approach highlighting deactivation pathways in carotenoids. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 19491-19499.	2.8	34
21	From phenols to quinones: Thermodynamics of radical scavenging activity of para-substituted phenols. <i>Phytochemistry</i> , 2019, 166, 112077.	2.9	34
22	DFT/B3LYP study of the substituent effect on the reaction enthalpies of the individual steps of sequential proton loss electron transfer mechanism of phenols antioxidant action: Correlation with phenolic CO bond length. <i>Computational and Theoretical Chemistry</i> , 2007, 805, 153-160.	1.5	32
23	Effect of substituents on redox, spectroscopic and structural properties of conjugated diaryltetrazines—a combined experimental and theoretical study. <i>Physical Chemistry Chemical Physics</i> , 2011, 13, 2690-2700.	2.8	32
24	Shape memory effect of dehydrochlorinated crosslinked poly(vinyl chloride). <i>Macromolecular Chemistry and Physics</i> , 1997, 198, 3161-3172.	2.2	28
25	Highly Charged Cations from N^2 , N^3 , N^4 -Tetrakis(4-aminophenyl)benzidine and Its N^2 , N^3 , N^4 -Tetrakis(4-methoxyphenyl)-Substituted Homologue Studied by Thin-Layer in Situ Electron Spin Resonance/UV-Vis-NIR Spectroelectrochemistry. <i>Journal of Physical Chemistry B</i> , 2010, 114, 4451-4460.	2.6	28
26	On the enthalpies of homolytic and heterolytic H bond cleavage in para and meta substituted thiophenols. <i>Computational and Theoretical Chemistry</i> , 2011, 967, 273-283.	2.5	28
27	Physicochemical and biological properties of luteolin-7-O- β -D-glucoside (cynaroside) isolated from <i>Anthriscus sylvestris</i> (L.) Hoffm.. <i>Monatshefte für Chemie</i> , 2014, 145, 1307-1318.	1.8	25
28	On relativistic effects in ground state potential curves of Zn_2 , Cd_2 , and Hg_2 dimers. A CCSD(T) study. <i>Journal of Computational Chemistry</i> , 2009, 30, 65-74.	3.3	24
29	Charged States of 1,3,5-Triazine Molecules as Models for Star-shaped Molecular Architecture: A DFT and Spectroelectrochemical Study. <i>Journal of Physical Chemistry B</i> , 2011, 115, 3344-3353.	2.6	23
30	Torsional potentials and full-dimensional simulation of electronic absorption and fluorescence spectra of para-phenylene oligomers using the semiempirical self-consistent charge density-functional tight binding approach. <i>Journal of Chemical Physics</i> , 2008, 129, 164905.	3.0	21
31	The validation of quantum chemical lipophilicity prediction of alcohols. <i>Acta Chimica Slovaca</i> , 2016, 9, 89-94.	0.8	21
32	The applicability of AM1 and PM3 semi-empirical methods for the study of N-H bond dissociation enthalpies and ionisation potentials of amine type antioxidants. <i>Polymer Degradation and Stability</i> , 2006, 91, 262-270.	5.8	20
33	Thermodynamic study of vitamin B6 antioxidant potential. <i>Computational and Theoretical Chemistry</i> , 2016, 1077, 32-38.	2.5	20
34	A study of the energetics of antioxidant action of p-phenylenediamines. <i>Polymer Degradation and Stability</i> , 2005, 88, 548-554.	5.8	18
35	On the structure and physical origin of van der Waals interaction in zinc, cadmium and mercury dimers. <i>Chemical Physics Letters</i> , 2006, 424, 199-203.	2.6	18
36	Theoretical investigation of the structure and the electron-vibrational dynamics of 9,9- spiro bifluorene. <i>Chemical Physics</i> , 2008, 349, 226-233.	1.9	18

#	ARTICLE	IF	CITATIONS
37	Two-dimensional electronic spectra of an aggregating dye: simultaneous measurement of monomeric and dimeric line-shapes. <i>Physical Chemistry Chemical Physics</i> , 2009, 11, 5986.	2.8	18
38	Optical properties of furanic and thiophenic ethane-1,2-diones. <i>Synthetic Metals</i> , 2003, 138, 399-408.	3.9	17
39	On the toxicity of para-substituted phenols and their quinone metabolites: Quantum chemical study. <i>Chemical Physics Letters</i> , 2018, 709, 71-76.	2.6	17
40	Interaction energy anisotropy of the pyrrole dimer: ab initio theoretical study. <i>Theoretical Chemistry Accounts</i> , 1999, 101, 319-324.	1.4	16
41	Perturbation calculation of the interaction energy using orthogonalized orbitals. <i>Theoretical Chemistry Accounts</i> , 1998, 99, 53-59.	1.4	15
42	Non-linear optical properties of new bridged bis-thienyls. <i>Synthetic Metals</i> , 2001, 124, 279-286.	3.9	15
43	Synthesis, theoretical characterisation and spectra of thiophene-fluorene-conjugated derivatives. <i>Synthetic Metals</i> , 2005, 148, 179-186.	3.9	15
44	Stable Radical Trianions from Reversibly Formed Sigma-Dimers of Selenadiazoloquinolones Studied by In Situ EPR/UV-vis Spectroelectrochemistry and Quantum Chemical Calculations. <i>Journal of Physical Chemistry A</i> , 2012, 116, 9919-9927.	2.5	15
45	Theoretical Study of Structure, Electronic Properties, and Photophysics of Cyano-Substituted Thiophenes and Terthiophenes. <i>Journal of Physical Chemistry A</i> , 2008, 112, 10931-10938.	2.5	14
46	Homolytic N-H bond cleavage in anilines: Energetics and substituent effect. <i>Computational and Theoretical Chemistry</i> , 2013, 1014, 60-67.	2.5	14
47	Synthesis and Optical Properties of Various Thienyl Derivatives of Pyrene. <i>Journal of Fluorescence</i> , 2014, 24, 153-160.	2.5	14
48	The ab initio study of halogen and hydrogen N-bonded para-substituted pyridine(X 2 /XY/HX) complexes. <i>Chemical Physics Letters</i> , 2015, 619, 7-13.	2.6	14
49	Solvent- and concentration-induced self-assembly of an amphiphilic perylene dye. <i>New Journal of Chemistry</i> , 2020, 44, 892-899.	2.8	14
50	Theoretical study of structure and electronic properties of cyano-substituted pyrroles. <i>Chemical Physics</i> , 2008, 353, 177-184.	1.9	13
51	TORSIONAL POTENTIALS AND FULL-DIMENSIONAL SIMULATION OF ELECTRONIC ABSORPTION SPECTRA OF <i>para</i> -PHENYLENEVINYLENE OLIGOMERS USING SEMIEMPIRICAL HAMILTONIANS. <i>Journal of Theoretical and Computational Chemistry</i> , 2010, 09, 249-263.	1.8	13
52	Charged States of \pm -Dicyano β -Dibutylquaterthiophene as Studied by in Situ ESR UV-Vis NIR Spectroelectrochemistry. <i>Journal of Physical Chemistry A</i> , 2010, 114, 11545-11551.	2.5	13
53	Theoretical and spectroscopic study of ethyl 1,4-dihydro-4-oxoquinoline-3-carboxylate and its 6-fluoro and 8-nitro derivatives in neutral and radical anion forms. <i>Journal of Molecular Structure</i> , 2011, 994, 61-69.	3.6	12
54	Design of Novel Generations of Planar Sunflower Molecules: Theoretical Comparative Study of Electronic Structure and Charge Transport Characteristics. <i>Journal of Physical Chemistry C</i> , 2019, 123, 22752-22766.	3.1	12

#	ARTICLE	IF	CITATIONS
55	Perturbative calculation of the Hartree-Fock interaction energy using orthogonalized orbitals. <i>International Journal of Quantum Chemistry</i> , 1999, 75, 81-88.	2.0	11
56	Optical properties of 2,3-diaza-1,3-butadiene bridged oligothiophenes. <i>Synthetic Metals</i> , 2002, 129, 85-94.	3.9	11
57	Structure, electronic and optical characterization of oligothiophenes terminated with (9H-fluoren-9-ylidene)methyl chromophores. <i>Synthetic Metals</i> , 2007, 157, 770-778.	3.9	11
58	Theoretical study of structural and optical properties of lithium cation complexes with dimethyl sulfoxide. <i>Computational and Theoretical Chemistry</i> , 2011, 963, 503-509.	2.5	10
59	Density-functional theoretical study of fluorination effect on the electronic structure and electron drift mobilities of symmetric pentacene derivatives. <i>Synthetic Metals</i> , 2018, 240, 67-76.	3.9	10
60	On the Relation Between Conformational Changes and Optical Properties in Oligothiophenes, 2. Linear and Nonlinear Optical Properties. <i>Macromolecular Theory and Simulations</i> , 2001, 10, 592-599.	1.4	9
61	Density Matrix Analysis, Simulation, and Measurements of Electronic Absorption and Fluorescence Spectra of Spirobifluorenes. <i>Journal of Physical Chemistry A</i> , 2006, 110, 1775-1782.	2.5	9
62	The experimental and theoretical characterisation of the phenyl-perfluorophenyl π - π and hydrogen bond interactions in the aldimine co-crystal. <i>Chemical Physics</i> , 2006, 326, 271-280.	1.9	9
63	Theoretical Study of the Relations between Structure and Photophysical Properties of Model Oligofluorenes with Central Keto Defect. <i>Journal of Physical Chemistry A</i> , 2009, 113, 14141-14149.	2.5	9
64	Photoinduced processes of 3-substituted 6-fluoro-1,4-dihydro-4-oxoquinoline derivatives: A theoretical and spectroscopic study. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2010, 211, 47-58.	3.9	9
65	Alternative charge stabilisation and a changing reactivity of 1,3,5-triazine based starburst compounds as studied by in situ ESR/UV-vis-NIR spectroelectrochemistry. <i>Electrochemistry Communications</i> , 2010, 12, 513-516.	4.7	9
66	On the geometrical structure and spectral properties of pyrene monomer and sterically constrained intramolecular pyrene dimers. <i>Chemical Physics</i> , 2010, 377, 123-131.	1.9	9
67	Regioregular electrochromic polymers based on thienyl derivatives of fluorescent pyrene monomers: Optical properties, spectroelectrochemistry and quantum chemical study. <i>Electrochimica Acta</i> , 2014, 122, 57-65.	5.2	9
68	Relativistic effects in HgHe and HgXe CCSD(T) ground state potential curves. Low-density viscosity simulations of Hg:Xe mixture. <i>Journal of Computational Chemistry</i> , 2011, 32, 356-367.	3.3	8
69	On the geometry, electrical properties and optical spectra of spirobifluorene type molecules. <i>Journal of Molecular Structure</i> , 2004, 699, 93-99.	3.6	7
70	Thermochromism of bithiophenes and internal aromatic chain rotation. <i>Computational and Theoretical Chemistry</i> , 2007, 820, 35-39.	1.5	7
71	Theoretical study of structural and optical properties of regioregular head-to-tail oligo (3-n-octylthiophene) and related star molecules. <i>Computational and Theoretical Chemistry</i> , 2009, 910, 104-111.	1.5	7
72	Effects of the CN and NH ₂ substitutions on the geometrical and optical properties of model vinylfluorenes, based on DFT calculations. <i>Computational and Theoretical Chemistry</i> , 2010, 939, 75-81.	1.5	7

#	ARTICLE	IF	CITATIONS
73	On the Electrochemistry and Spectroelectrochemistry of Small Model Star-Shaped Compounds: 1,3,5-Triaryl-1-Methoxybenzenes and 2,4,6-Triaryl-1,3,5-Trimethoxybenzenes. <i>ChemPhysChem</i> , 2012, 13, 1 2322-2330.	3.1	7
74	Intermolecular and intramolecular coupling in charged monosubstituted hexapyrrolylbenzenes. <i>Electrochimica Acta</i> , 2007, 52, 7885-7894.	5.2	6
75	Charged states in diphenylamino endcapped thiophenes with a 1,4-phenylene core: In situ electron spin resonance/ultraviolet-visible near infrared and nuclear magnetic resonance spectroelectrochemistry and quantum chemical study. <i>Electrochimica Acta</i> , 2013, 110, 670-680.	5.2	6
76	The synthesis and examination of spectral properties of some 2,2-bithienyl derivatives with carbonyl-containing substituents. <i>Synthetic Metals</i> , 2013, 165, 17-26.	3.9	6
77	Solvent effect on the anodic oxidation of tannic acids: EPR/UV-Vis spectroelectrochemical and DFT theoretical study. <i>Journal of Solid State Electrochemistry</i> , 2015, 19, 2533-2544.	2.5	6
78	Radical anions of quinoxalines (an in situ electron paramagnetic resonance spectroelectrochemical) <i>Tj ETQq0 0 0 rgBT /Overlock 10 Tf 5</i>	2.5	6
79	Theoretical and experimental study of model oligothiophenes containing 1-methylene-2-(perfluorophenyl)hydrazine terminal unit. <i>Synthetic Metals</i> , 2016, 219, 83-92.	3.9	6
80	Electronic structure and charge-transport properties of symmetric linear condensed bis-benzothiadiazole derivatives. <i>Journal of Molecular Structure</i> , 2019, 1175, 297-306.	3.6	6
81	On the optical properties of fluoranthenopyracylene ladder type molecule series. <i>Synthetic Metals</i> , 2007, 157, 214-221.	3.9	5
82	Ab initio calculation of structure and transport properties of He _n X (X = Zn, Cd, Hg) van der Waals complexes. <i>Journal of Computational Chemistry</i> , 2012, 33, 767-778.	3.3	5
83	Substitution and torsional effects on the energetics of homolytic N-H bond cleavage in diphenylamines. <i>Polymer Degradation and Stability</i> , 2015, 114, 37-44.	5.8	5
84	Thermodynamics of radical scavenging of symmetric carotenoids and their charged species. <i>Food Chemistry</i> , 2018, 268, 542-549.	8.2	5
85	Theoretical comparative study of promising semiconducting aromatic molecules and their fluorinated counterparts. <i>Synthetic Metals</i> , 2020, 260, 116263.	3.9	5
86	On the NH and CH acidities of toluidine isomers: theoretical description and practical consequences for the synthesis of certain aniline dyes. <i>Coloration Technology</i> , 2021, 137, 389-398.	1.5	5
87	On the Structure and Physical Origin of the Weak Interaction Between H and CO. <i>Collection of Czechoslovak Chemical Communications</i> , 2004, 69, 1-12.	1.0	4
88	Density functional study of structural and opto-electronical properties of fluoranthenopyracylene oligomers in their neutral and oxidized forms. <i>Computational and Theoretical Chemistry</i> , 2006, 776, 69-75.	1.5	4
89	Structural Changes in 2-Diarylthiophene-Substituted Starburst Compounds upon Charging: A Theoretical and Spectroelectrochemical Study. <i>ChemPhysChem</i> , 2008, 9, 2501-2509.	2.1	4
90	Experimental and Theoretical Study of Model Ladder Fluoranthenopyracylene with Two-Dimensional π -Conjugation upon Charging: Structure and Optical Properties. <i>Journal of Physical Chemistry C</i> , 2008, 112, 3949-3958.	3.1	4

#	ARTICLE	IF	CITATIONS
91	Anodic oxidation of selenadiazoloquinolones in alkaline media. <i>Magnetic Resonance in Chemistry</i> , 2011, 49, 168-174.	1.9	4
92	Photoinduced decarboxylation of 9-oxo-9,9-dihydro[1,2,5]selenadiazolo[3,4-f]quinoline-8-carboxylic acid. <i>Journal of Physical Organic Chemistry</i> , 2012, 25, 643-648.	0.8	4
93	Substitution effect on the intermolecular halogen and hydrogen bonds of the π -bonded fluorinated pyridine- π -XY/HX complexes ($XY = F_2, Cl_2, ClF, HX = HF, HCl$). <i>International Journal of Quantum Chemistry</i> , 2014, 114, 869-878.	0.8	4
94	Conversion of hydrazides into N,N'-diacylhydrazines in the presence of a ruthenium(ii)-arene complex. <i>New Journal of Chemistry</i> , 2017, 41, 6857-6865.	2.8	4
95	Polyradical PROXYL/TEMPO-Derived Amides: Synthesis, Physicochemical Studies, DFT Calculations, and Antimicrobial Activity. <i>ChemPlusChem</i> , 2017, 82, 1326-1340.	2.8	4
96	Manifestation of copper coordination sphere plasticity in $[Cu_2(2\text{-bromopropionato})_4]_n$ and $[Cu_2(3\text{-bromopropionato})_4(H_2O)_2]$. <i>Inorganica Chimica Acta</i> , 2018, 479, 106-112.	2.4	4
97	Tuning Redox Properties and Self-Assembly of Thienoacene-Extended Tetrathiafulvalenes. <i>ChemPlusChem</i> , 2019, 84, 1279-1287.	2.8	4
98	On the Viscosity and Physical Origin of Stability of Weakly Bound Complexes CdZn, HgZn and HgCd. <i>Collection of Czechoslovak Chemical Communications</i> , 2007, 72, 363-378.	1.0	4
99	Theoretical study of a series of phenol derivatives: molecular properties vs. cytotoxicity. <i>Acta Chimica Slovaca</i> , 2017, 10, 91-95.	0.8	4
100	B3LYP Study of 3-hydroxynaphthalene-2-carboxanilide para-derivatives. <i>Acta Chimica Slovenica</i> , 2018, 65, 23-33.	0.6	4
101	Nature of interaction energy anisotropy in the $Li(2S) \cdots HF$ ($\infty X1\ddagger+$) van der Waals complex. A theoretical study. <i>Theoretical Chemistry Accounts</i> , 2003, 109, 316-325.	1.4	3
102	On the structure and physical origin of the interaction in $H_2 \cdots Cl^+$ and $H_2 \cdots Br^+$ van der Waals anion complexes. <i>Journal of Chemical Physics</i> , 2004, 121, 5852-5859.	3.0	3
103	Quantum chemical and experimental study of 1,2,4-trihydroxy-para-menthane. <i>Journal of Molecular Structure</i> , 2013, 1049, 494-501.	3.6	3
104	Chelates of 3- and 5-hydroxyflavone: Quantum chemical study. <i>Chemical Physics Letters</i> , 2021, 762, 138142.	2.6	3
105	On the diffusion coefficients and stability of van der Waals complex $Hg \cdots N_2$. <i>International Journal of Quantum Chemistry</i> , 2008, 108, 2150-2158.	2.0	2
106	Semiempirical Molecular Dynamics Study of Empty C_{82} Fullerene in Neutral and Charged Forms: Geometrical and Spectroscopic Characterization. <i>Journal of Physical Chemistry C</i> , 2009, 113, 19658-19663.	3.1	2
107	On the applicability of the molecular dynamics SCC-DFTB treatment on optical spectra simulations for thiophene and phenyl containing oligomers. <i>Computational and Theoretical Chemistry</i> , 2012, 999, 55-65.	2.5	2
108	Combined Spectroelectrochemical and Theoretical Study of Electron-Rich Dendritic 2,5-Diaminothiophene Derivatives: N,N'-Tetrakis-(4-diphenylamino-phenyl)-thiophene-2,5-diamine. <i>Journal of Physical Chemistry A</i> , 2013, 117, 6702-6711.	2.5	2

#	ARTICLE	IF	CITATIONS
109	Electronic structure and spectroscopic properties of (2S,3S)-2,3-diphenyl-5,6-diheteroaryl-2,3-dihydropyrazines and their model oligomers. <i>Synthetic Metals</i> , 2015, 199, 319-328.	3.9	2
110	Theoretical and experimental study of donor-bridge-acceptor system: model 2-[5-(9H-fluoren-9-ylidene)methyl]thiophen-2-yl]-1,3,4-oxadiazole derivatives. <i>Monatshefte für Chemie</i> , 2016, 147, 2103-2112.	1.8	2
111	Water liquid-vapor equilibrium by molecular dynamics: Alternative equilibrium pressure estimation. <i>Acta Chimica Slovaca</i> , 2016, 9, 36-43.	0.8	2
112	Thermodynamic prediction of proton and hydrogen atom abstraction in dehydroascorbic acid and its bicyclic form. <i>Acta Chimica Slovaca</i> , 2021, 14, 32-37.	0.8	2
113	The computational analysis and modelling of substitution effects on hydrolysis of formanilides in acidic aqueous solutions. <i>Chemical Physics Letters</i> , 2017, 687, 66-72.	2.6	2
114	On local aromaticity of selected model aza-[n]circulenes (n = 6, 7, 8 and 9): Density functional theoretical study. <i>Acta Chimica Slovaca</i> , 2019, 12, 70-81.	0.8	2
115	Theoretical modeling of optical spectra of N(1) and N(10) substituted lumichrome derivatives. <i>Acta Chimica Slovaca</i> , 2020, 13, 1-9.	0.8	2
116	Ab initio Study of the Li-CO van der Waals Complex. <i>Collection of Czechoslovak Chemical Communications</i> , 2003, 68, 35-46.	1.0	1
117	Theoretical Study of H ₂ ...I ⁻ van der Waals Anion Complex. <i>Collection of Czechoslovak Chemical Communications</i> , 2005, 70, 797-810.	1.0	1
118	Ab initio study of Hg(1S0)â ⁻ van der Waals complex. <i>Chemical Physics</i> , 2008, 349, 32-36.	1.9	1
119	Theoretical Study of the vdW Complex Cdâ ⁺ â ⁻ N ₂ . <i>Collection of Czechoslovak Chemical Communications</i> , 2008, 73, 1357-1371.	1.0	1
120	Ab initio X ¹⁰ +ground state potential curves of Pbâ ⁻ RG dimers (RG = He, Ne, Ar) including spinâ ⁺ orbit effects. Simulation of diffusion coefficients. <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 18519.	2.8	1
121	Theoretical study of the substituent effect on the hydrogen atom transfer mechanism of meta- and para-substituted benzenetelluroles. <i>Computational and Theoretical Chemistry</i> , 2016, 1079, 64-69.	2.5	1
122	The structural analysis and modelling of ring substituent effect for the ortho-derivatives of 1-hydroxynaphthalene-2-carboxanilides and 2-hydroxynaphthalene-1-carboxanilides. <i>Journal of Molecular Structure</i> , 2017, 1144, 473-481.	3.6	1
123	Adamantane Substitution Effects on Crystallization and Electrooptical Properties of Epindolidione and Quinacridone Dyes. <i>ChemPhotoChem</i> , 0, , .	3.0	1
124	THEORETICAL STUDY OF PRIMARY ANTIOXIDANT ACTION THERMODYNAMICS. <i>Journal of the Serbian Society for Computational Mechanics</i> , 2017, 11, 130-138.	0.4	1
125	Quantum chemical study of electron structure and charge transport properties of symmetric acenequinones. <i>Acta Chimica Slovaca</i> , 2018, 11, 83-93.	0.8	1
126	Electronic Excitations in a Ladder Type Fluoranthenopyracylene in its Neutral and Charged States: A Theoretical and Experimental Study. <i>Zeitschrift für Physikalische Chemie</i> , 2007, 221, 911-928.	2.8	0

#	ARTICLE	IF	CITATIONS
127	The synthesis and electron structure of oligothiophenes terminated with (10H-anthracen-9-one) methylene chromophores. <i>Synthetic Metals</i> , 2009, 159, 604-612.	3.9	0
128	5,7,8,10,15,17,18,20-Octaphenyl-21,23-dithiaporphyrin: synthesis, structure and spectroelectrochemistry. <i>Journal of Solid State Electrochemistry</i> , 2015, 19, 123-134.	2.5	0
129	Theoretical study of lumichrome, 1-methyl-lumichrome and lumiflavin binding ability with thymine. <i>Acta Chimica Slovaca</i> , 2021, 14, 7-13.	0.8	0
130	On the energetics of radical adduct formation of OH [•] with phenol analogs and aniline. <i>Acta Chimica Slovaca</i> , 2022, 15, 12-17.	0.8	0