Vassil B Delchev

List of Publications by Year
in descending order

54	372	932766 10	887659 17
papers	citations	h-index	g-index

54	54	54	438
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Comparison of the non-radiative decay mechanisms of 4-pyrimidinone and uracil: an ab initio study. Physical Chemistry Chemical Physics, 2010, 12, 5007.	1.3	61
2	The Keto-Enol Equilibrium of Pentane-2,4-dione Studied by ab initio Methods. Monatshefte FÃ¼r Chemie, 2001, 132, 339-348.	0.9	32
3	Comparative study of the relaxation mechanisms of the excited states of cytosine and isocytosine. Journal of Molecular Modeling, 2012, 18, 5133-5146.	0.8	30
4	DFT ab initio study of the keto-enol tautomerism of barbituric acid. Journal of Structural Chemistry, 2004, 45, 570-578.	0.3	28
5	Ab initio Study of the Keto-Enol Equilibriumof Malonaldehyde. Monatshefte FÃ¼r Chemie, 2000, 131, 99-105.	0.9	20
6	Comparative study of radiationless deactivation mechanisms in cytosine and 2,4-diaminopyrimidine. Journal of Photochemistry and Photobiology A: Chemistry, 2016, 321, 266-274.	2.0	12
7	Theoretical investigation of the intermolecular H-bonding and proton transfer in cytosine assisted by water and methanol. Monatshefte FÃ¼r Chemie, 2009, 140, 1381-1394.	0.9	11
8	Computational (DFT and TD DFT) study of the electron structure of the tautomers/conformers of uridine and deoxyuridine and the processes of intramolecular proton transfers. Journal of Molecular Modeling, 2010, 16, 749-757.	0.8	11
9	DFT study of the gas phase proton transfer in guanine assisted by water, methanol, and hydrogen peroxide. Journal of Molecular Modeling, 2006, 12, 229-236.	0.8	10
10	Theoretical study of the excited-state reaction paths of the OH and NH dissociation processes in barbituric acid. Monatshefte FÃ¼r Chemie, 2012, 143, 1141-1150.	0.9	10
11	Electron and Geometry Structure of Hydrogen-Bonded Complexes of Guanine with One Molecule Methanol. A DFT Level Study. Monatshefte FÃ¼r Chemie, 2004, 135, 1373-1387.	0.9	9
12	Ab initio Study of Malonaldehyde Rotamers. Monatshefte FÃ¼r Chemie, 2000, 131, 107-115.	0.9	8
13	Hydrogen Bonded Complexes of Acetylacetone and Methanol: HF and DFT level Study. Monatshefte FÃ¼r Chemie, 2004, 135, 249-260.	0.9	8
14	Investigation of the intermolecular proton transfer in the supersystems adenine-methanol/ethanol/i-propanol: MP2 and DFT levels study. Journal of Molecular Modeling, 2007, 13, 1001-1008.	0.8	8
15	Theoretical investigation (DFT and MP2) of the intermolecular proton transfer in the supersystems uracil-(H2O) n and uracil-(CH3OH) n (n = 1, 2). Monatshefte FÃ¼r Chemie, 2008, 139, 349-362.	0.9	8
16	Solvent influence on the excited states of the oxo form of barbituric acid and the mechanisms of the out-of-plane non-radiative elongation of the NH bond: A comparative theoretical and experimental study. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2014, 125, 384-390.	2.0	8
17	Experimental and theoretical study of the excited-state tautomerism of 6-azauracil in water surroundings. Chemical Physics, 2018, 515, 663-671.	0.9	8
18	Theoretical study of the hydrogen-bonded complexes serotoninâ€“water/hydrogen peroxide. Journal of Molecular Modeling, 2006, 12, 272-280.	0.8	7

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19	Theoretical study of the intermolecular H-bonding and intermolecular proton transfer between isocytosine tautomeric forms and R,S-lactic acid. Journal of Molecular Modeling, 2006, 13, 19-28.	0.8	6
20	An ab initio Study of the Rotamers and Rotations of Propane-1,3-dial by DFT and SCF Calculations. Monatshefte FÃ¼r Chemie, 2001, 132, 223-233.	0.9	5
21	A DFT Study of Electron Structure, Geometry, and Keto?Enol Tautomerism of 3-Oxopropionyl Halogenides. Monatshefte FÃ¼r Chemie, 2004, 135, 371-384.	0.9	5
22	Excited-state deactivation of the monohydrated complexes of cytosine, uracil, and thymine through S0/S1 conical intersections. Monatshefte FÃ¼r Chemie, 2012, 143, 763-770.	0.9	5
23	Ab initio study of the cyclodimerization of uracil through butane-like and oxetane-like conical intersections. Journal of Photochemistry and Photobiology A: Chemistry, 2013, 271, 1-7.	2.0	4
24	New platinum(II) complexes of cycloalkanespiro-5-(2-thiohydantoins). Synthesis and quantum chemical investigation. Acta Chimica Slovenica, 2015, 62, 225-32.	0.2	4
25	Investigation of the mechanisms of photo-induced formation of cyclobutane dimers of cytosine and 2,4-diaminopyrimidine. Journal of Molecular Modeling, 2016, 22, 230.	0.8	4
26	Selection of a quantum-chemical method and basis set for optimization of the complex ion Cu(H2O)+. Journal of Structural Chemistry, 2006, 47, 979-984.	0.3	3
27	â€œFace-to-backâ€•photo-cyclodimerization of the malonaldehyde enol form with the strong intramolecular H-bond: A TD DFT theoretical study. Computational and Theoretical Chemistry, 2010, 958, 101-105.	1.5	3
28	The shape of the conical intersections of monohydrated pyrimidine bases cytosine, uracil, and thymine: a theoretical study. Monatshefte FÃ¼r Chemie, 2011, 142, 251-260.	0.9	3
29	NXO beta structure mimicry: an ultrashort turn/hairpin mimic that folds in water. RSC Advances, 2014, 4, 21351-21360.	1.7	3
30	Extraction-spectrophotometric and theoretical (Hartree-Fock) investigations of a ternary complex of iron(II) with 4-nitrocatechol and 2,3,5-triphenyl-2H-tetrazolium. Russian Journal of General Chemistry, 2015, 85, 1945-1951.	0.3	3
31	An extraction-chromogenic system for vanadium(IV,V) based on 2,3-dihydroxynaphtahlene. Open Chemistry, 2016, 14, 197-205.	1.0	3
32	Specific features of tetranitrotetrazolium blue chloride as an extraction reagent for iron(III). Russian Journal of General Chemistry, 2016, 86, 1167-1176.	0.3	3
33	Extraction-Spectrophotometric and Theoretical Studies on a Ternary Complex Obtained from Vanadium(V) and 4-Nitrocatechol. Russian Journal of Inorganic Chemistry, 2021, 66, 1880-1886.	0.3	3
34	Spectrophotometric Determination of Molybdenum(VI) as a Ternary Complex with 4-Nitrocatechol and Benzalkonium Chloride. Molecules, 2022, 27, 1217.	1.7	3
35	H-bonded complexes between acetylacetone and two molecules of methanol: HF and DFT level study. Journal of Molecular Modeling, 2005, 11, 474-480.	0.8	2
36	DFT study of oxaloacetic acid condensation â€” The first step of the citric acid cycle. Journal of Structural Chemistry, 2007, 48, 615-622.	0.3	2

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37	Ground state intermolecular proton transfer in the supersystems thymineâ€“(H2O)n and thymineâ€“(CH3OH)n, nâ€‰=â€‰1,2: a theoretical study. Journal of Molecular Modeling, 2009, 15, 411-419.	0.8	2
38	Ground- and excited-state stability of the conformers of 3,5-dinitrocatechol and its complexes with W(VI) and V(V): combined theoretical and experimental study. Journal of Molecular Modeling, 2014, 20, 2549.	0.8	2
39	Phototransformations in m-aminophenol: A theoretical and experimental study. Journal of Molecular Structure, 2017, 1141, 6-11.	1.8	2
40	Phototautomerism of Isocytosine in a Water Medium: Theoretical and Experimental Study. Journal of Structural Chemistry, 2019, 60, 898-908.	0.3	2
41	Excited-state photocycodimerization of 6-azauracil to oxazetidine cyclodimer: A mechanism elucidation in water surroundings. Journal of Molecular Structure, 2020, 1205, 127571.	1.8	2
42	CRYSTAL STRUCTURE AND PHOTOCHEMISTRY OF 5-AZACYTOSINE: EXPERIMENTAL AND THEORETICAL STUDY. Journal of Structural Chemistry, 2022, 63, 319-330.	0.3	2
43	Photoinduced conformational transformation of the hydroxy form of uridine and deoxyuridine and hydrogen detachment in oxo and hydroxy tautomers of the compounds: a computational study. Monatshefte FÃ¼r Chemie, 2010, 141, 1153-1157.	0.9	1
44	Excited-state relaxation paths of oxo/hydroxy and N9H/N7H tautomers of guanine: a CC2 theoretical study. Journal of Molecular Modeling, 2013, 19, 2299-2308.	0.8	1
45	Comparative study of the OÂ·Â·Â·HÂ·Â·Â·O proton transfer in the enol form of a single acetylacetone molecule and acetylacetone incorporated in Î²-cyclodextrin: a theoretical investigation. Monatshefte FÃ¼r Chemie, 2013, 144, 1153-1158.	0.9	1
46	Excitedâ€state deactivation channels via internal conversions in two position isomers of hydroxyâ€methylâ€pyridine: a theoretical study. Journal of Physical Organic Chemistry, 2015, 28, 681-689.	0.9	1
47	Phototransformations of quinaldic acid: Theoretical and experimental study. Journal of Molecular Structure, 2017, 1127, 23-30.	1.8	1
48	Complex formation in a liquid-liquid extraction-chromogenic system for vanadium(IV). Open Chemistry, 2019, 17, 599-608.	1.0	1
49	Photo-induced Dissociation of the N1â€“H Bond in the Imino Tautomers of Isocytosine in Water Medium. Croatica Chemica Acta, 2020, 93, .	0.1	1
50	Gas phase ionization of 1,3-propanedial tautomeric forms: A theoretical study. Journal of Structural Chemistry, 2005, 46, 409-416.	0.3	0
51	Photoinduced disruption of the strong intramolecular H-bond in the enol form of acetylacetone: Mechanisms of radiationless decay. Computational and Theoretical Chemistry, 2011, 967, 152-159.	1.1	0
52	Conical intersections S₀/S₁ of thymine mediating the non-radiative photodestruction of cyclobutane dimers: a CASSCF level study. Proceedings of SPIE, 2017, , .	0.8	0
53	Photoinduced phenomena in water solution of melamine explaining the photostability of the compound. Journal of Molecular Modeling, 2021, 27, 196.	0.8	0
54	Photoinduced Phenomena in 6,6â€™-Dibromoindigo (Tyrian Purple): a Theoretical Study. Croatica Chemica Acta, 2020, 93, .	0.1	0