

Sonia Ilieva

List of Publications by Year in descending order

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361413

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docs citations

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1072
citing authors

#	ARTICLE	IF	CITATIONS
1	Hydrogen bonding as a probe of electron density Variations: Substituted pyridines. <i>Chemical Physics Letters</i> , 2022, 791, 139378.	2.6	3
2	Theoretical Modeling of Absorption and Fluorescent Characteristics of Cyanine Dyes. <i>Photochem</i> , 2022, 2, 202-216.	2.2	5
3	Mini-Review on Structure-Reactivity Relationship for Aromatic Molecules: Recent Advances. <i>ACS Omega</i> , 2022, 7, 8199-8208.	3.5	2
4	Hydrogen bonding probes electron density variations at the basic center in substituted alkyl benzoates: Theory and experiment. <i>Journal of Physical Organic Chemistry</i> , 2021, 34, e4258.	1.9	3
5	Ca ²⁺ /Sr ²⁺ Selectivity in Calcium-Sensing Receptor (CaSR): Implications for Strontium's Anti-Osteoporosis Effect. <i>Biomolecules</i> , 2021, 11, 1576.	4.0	19
6	Electric field influence on the helical structure of peptides: insights from DFT/PCM computations. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 16198-16206.	2.8	8
7	Atomic Charges in Describing Properties of Aromatic Molecules. <i>Journal of Organic Chemistry</i> , 2019, 84, 1908-1915.	3.2	35
8	How an electric field can modulate the metal ion selectivity of protein binding sites: insights from DFT/PCM calculations. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 24633-24640.	2.8	19
9	Assembly of New Merocyanine Chromophores with a 1,8-Naphthalimide Core by a New Method for the Synthesis of the Methine Function. <i>Australian Journal of Chemistry</i> , 2015, 68, 1399.	0.9	4
10	Do π -Conjugative Effects Facilitate SN ₂ Reactions?. <i>Journal of the American Chemical Society</i> , 2014, 136, 3118-3126.	13.7	20
11	Experimental Measurement and Theory of Substituent Effects in π -Hydrogen Bonding: Complexes of Substituted Phenols with Benzene. <i>Journal of Organic Chemistry</i> , 2014, 79, 6823-6831.	3.2	23
12	Synthesis, structural analysis and application of a series of solid-state fluorochromes' aryl hydrazones of 4-hydrazino-N-hexyl-1,8-naphthalimide. <i>Tetrahedron</i> , 2013, 69, 712-721.	1.9	6
13	Does the Molecular Electrostatic Potential Reflect the Effects of Substituents in Aromatic Systems?. <i>Chemistry - A European Journal</i> , 2013, 19, 5149-5155.	3.3	35
14	Aminolysis of Phenyl N-Phenylcarbamate via an Isocyanate Intermediate: Theory and Experiment. <i>Journal of Organic Chemistry</i> , 2013, 78, 6440-6449.	3.2	23
15	Structure-reactivity relationships for aromatic molecules: electrostatic potentials at nuclei and electrophile affinity indices. <i>Wiley Interdisciplinary Reviews: Computational Molecular Science</i> , 2013, 3, 37-55.	14.6	31
16	Initiation of ring-opening polymerization of lactide: The effect of metal alkoxide catalyst. <i>Computational and Theoretical Chemistry</i> , 2012, 995, 8-16.	2.5	24
17	The nature of intramolecular interactions determining the ρ constants for aromatic systems. <i>Journal of Molecular Structure</i> , 2012, 1023, 31-36.	3.6	2
18	Rationalizing IR intensities in terms of electronic parameters. <i>Journal of Molecular Structure</i> , 2012, 1009, 69-73.	3.6	1

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19	Experimental and theoretical study on the absorption and fluorescence properties of substituted aryl hydrazones of 1,8-naphthalimide. <i>Physical Chemistry Chemical Physics</i> , 2011, 13, 18530.	2.8	35
20	Reactivity of phenyl <i>N</i> -phenylcarbamates in the alkaline hydrolysis reaction. <i>Journal of Physical Organic Chemistry</i> , 2011, 24, 1166-1171.	1.9	6
21	Computational evaluation of σ_{F} and σ_{R} substituent constants. <i>Journal of Molecular Structure</i> , 2010, 976, 427-430.	3.6	13
22	The origin of diastereoselectivity in the Michael addition reaction: a computational study of the interaction between CH-acidic Schiff base and α,β -unsaturated ketones. <i>Tetrahedron</i> , 2010, 66, 5168-5172.	1.9	6
23	Communication: Energetics of reaction pathways for reactions of ethenol with the hydroxyl radical: The importance of internal hydrogen bonding at the transition state. <i>Journal of Chemical Physics</i> , 2010, 133, 021102.	3.0	24
24	The mechanism of alkaline hydrolysis of amides: a comparative computational and experimental study of the hydrolysis of <i>N</i> -methylacetamide, <i>N</i> -methylbenzamide, and acetanilide. <i>Journal of Physical Organic Chemistry</i> , 2009, 22, 619-631.	1.9	31
25	Reactivity of acetanilides in the alkaline hydrolysis reaction: theory vs. experiment. <i>Molecular Physics</i> , 2009, 107, 1187-1192.	1.7	15
26	Predicting Reactivities of Organic Molecules. Theoretical and Experimental Studies on the Aminolysis of Phenyl Acetates. <i>Journal of Physical Chemistry A</i> , 2008, 112, 6700-6707.	2.5	66
27	QSAR analysis of 1,4-dihydro-4-oxo-1-(2-thiazolyl)-1,8-naphthyridines with anticancer activity. <i>European Journal of Medicinal Chemistry</i> , 2007, 42, 1184-1192.	5.5	65
28	An Efficient Computational Approach for the Evaluation of Substituent Constants. <i>Journal of Organic Chemistry</i> , 2006, 71, 6382-6387.	3.2	105
29	Conformation of some biologically active aromatic ureas. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2005, 61, 1321-1326.	3.9	3
30	Mechanism of the Aminolysis of Methyl Benzoate: A Computational Study. <i>Journal of Physical Chemistry A</i> , 2005, 109, 11470-11474.	2.5	41
31	Quantitative Structure-Activity Relationship Analysis of the Substituent Effects on the Binding Affinity of Derivatives of Trimetazidine. <i>Arzneimittelforschung</i> , 2004, 54, 9-14.	0.4	5
32	Computational study of the alkaline hydrolysis of acetanilide. <i>Computational and Theoretical Chemistry</i> , 2004, 681, 105-112.	1.5	13
33	Computational Study of the Reactivity of <i>N</i> -Phenylacetamides in the Alkaline Hydrolysis Reaction. <i>Journal of Physical Chemistry A</i> , 2004, 108, 11457-11462.	2.5	61
34	Reactivity descriptors for the hydrogen bonding ability of aliphatic alcohols. <i>Journal of Molecular Structure</i> , 2003, 657, 317-324.	3.6	4
35	Computational study of the general base catalysed aminolysis of 2-benzoxazolinone. <i>Computational and Theoretical Chemistry</i> , 2003, 633, 49-55.	1.5	9
36	Electrostatic potential at nuclei as a reactivity index in hydrogen bond formation. Complexes of ammonia with $\text{C}=\text{H}$, $\text{N}=\text{H}$ and $\text{O}=\text{H}$ proton donor molecules. <i>Computational and Theoretical Chemistry</i> , 2003, 637, 73-80.	1.5	20

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37	Computational Study of the Aminolysis of Esters. The Reaction of Methylformate with Ammonia. Journal of Organic Chemistry, 2003, 68, 1496-1502.	3.2	87
38	Computational Study of the Aminolysis of 2-Benzoxazolinone. Journal of Organic Chemistry, 2003, 68, 3406-3412.	3.2	27
39	On the Origin of Higher Rotational Barriers in Thioamides than in Amides. Remote Substituent Effects on the Conformational Stability of the Thioamide Group in Thioacetanilides. Journal of Physical Chemistry A, 2003, 107, 5854-5861.	2.5	26
40	Theory Supplemented by Experiment. Electronic Effects on the Rotational Stability of the Amide Group in p-Substituted Acetanilides. Journal of Organic Chemistry, 2002, 67, 6210-6215.	3.2	27
41	Electrostatic Potential at Atomic Sites as a Reactivity Descriptor for Hydrogen Bonding. Complexes of Monosubstituted Acetylenes and Ammonia. Journal of Physical Chemistry A, 2002, 106, 11801-11805.	2.5	75
42	Ab initio molecular orbital study of the conformation of amide group: o-methylformanilide. Journal of Molecular Structure, 1999, 476, 151-156.	3.6	8
43	Creation of intensity theory in vibrational spectroscopy: Key role of ab initio quantum mechanical calculations. International Journal of Quantum Chemistry, 1998, 70, 331-339.	2.0	4
44	Electrostatic Potential at Nuclei. , 0, , 87-122.		0
45	Electrostatic Potential at Nuclei. , 0, , 280-317.		0