Sergiy I Okovytyy

List of Publications by Year
in descending order

63	765	623734	580821
papers	citations	14 h-index	25 g-index

69	69	69	772
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Catalytic enantioselective synthesis of indanes by a cation-directed 5-endo-trig cyclization. Nature Chemistry, 2015, 7, 171-177.	13.6	87
2	The Mechanism of Unimolecular Decomposition of 2,4,6,8,10,12-Hexanitro-2,4,6,8,10,12-hexaazaisowurtzitane. A Computational DFT Study. Journal of Physical Chemistry A, 2005, 109, 2964-2970.	2.5	75
3	An analysis of stable forms of CL-20: A DFT study of conformational transitions, infrared and Raman spectra. Journal of Molecular Structure, 2007, 843, 14-25.	3.6	72
4	DFT M06-2X investigation of alkaline hydrolysis of nitroaromatic compounds. Chemosphere, 2012, 88, 635-643.	8.2	49
5	Comprehensive Investigations of Kinetics of Alkaline Hydrolysis of TNT (2,4,6-Trinitrotoluene), DNT (2,4-Dinitrotoluene), and DNAN (2,4-Dinitroanisole). Environmental Science & Technology, 2014, 48, 10465-10474.	10.0	47
6	A reinvestigation of the mechanism of epoxidation of alkenes by peroxy acids. A CASSCF and UQCISD study. Tetrahedron Letters, 2002, 43, 4215-4219.	1.4	29
7	Novel physically adapted STO^{##}â€3G basis sets. Efficiency for prediction of secondâ€order electric and magnetic properties of aromatic hydrocarbons. International Journal of Quantum Chemistry, 2012, 112, 2444-2449.	2.0	23
8	Computational Study of the Aminolysis of Anhydrides: Effect of the Catalysis to the Reaction of Succinic Anhydride with Methylamine in Gas Phase and Nonpolar Solution. Journal of Physical Chemistry A, 2008, 112, 5224-5235.	2.5	21
9	Prediction of CL-20 chemical degradation pathways, theoretical and experimental evidence for dependence on competing modes of reaction. SAR and QSAR in Environmental Research, 2005, 16, 495-515.	2.2	19
10	DFT Study on Tautomerism of Dihydroâ€2Hâ€1,5â€benzodiazepinâ€2â€ones and Dihydroâ€2Hâ€1,5â€benzodiazepineâ€2â€thiones. European Journal of Organic Chemistry, 2010, 2010, 280-291.	2.4	19
11	Hydrazinolysis of 3-R-[1,2,4]Triazino[2,3-c]quinazolin-2-ones. Synthetic and Theoretical Aspects. Journal of Physical Chemistry A, 2014, 118, 1895-1905.	2.5	18
12	In silico kinetics of alkaline hydrolysis of 1,3,5-trinitro-1,3,5-triazinane (RDX): M06-2X investigation. Environmental Sciences: Processes and Impacts, 2017, 19, 388-394.	3.5	18
13	Ligandâ€Mediated Regioselective Rhodiumâ€Catalyzed Benzotriazoleâ€“Allene Coupling: Mechanistic Exploration and Quantum Chemical Analysis. Chemistry - A European Journal, 2020, 26, 2342-2348.	3.3	16
14	An Investigation of the17O NMR Chemical Shifts in Oxiranes Using Magnetically Corrected Basis Sets. Journal of Physical Chemistry A, 2002, 106, 4176-4180.	2.5	15
15	Reactions of Alicyclic Epoxy Compounds with Nitrogen-Containing Nucleophiles. Russian Journal of Organic Chemistry, 2004, 40, 1-34.	0.8	15
16	Origin of Substituent Effect on Tautomeric Behavior of 1,2,4-Triazole Derivatives: Combined Spectroscopic and Theoretical Study. Journal of Physical Chemistry A, 2016, 120, 10116-10122.	2.5	14
17	In Silico Alkaline Hydrolysis of Octahydro-1,3,5,7-tetranitro-1,3,5,7-tetrazocine: Density Functional Theory Investigation. Environmental Science & Technology, 2016, 50, 10039-10046.	10.0	14
18	Novel xanthene push-pull chromophores and luminophores: Synthesis and study of their spectral properties. Tetrahedron, 2017, 73, 7159-7168.	1.9	14

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19	The performance of the new 6-31G## basis set: Molecular structures and vibrational frequencies of transition metal carbonyls. Journal of Computational Chemistry, 2007, 28, 778-782.	3.3	12
20	Are 1,5- and 1,7-dihydrodiimidazo[4,5-b:4â€²,5â€²-e]pyrazine the main products of 2,4,6,8,10,12-hexanitro-2,4,6,8,10,12-hexaazaisowurtzitane (CL-20) alkaline hydrolysis? A DFT study of vibrational spectra. Journal of Molecular Structure, 2006, 794, 288-302.	3.6	11
21	Azabrendanes IV. Synthesis and characterization of N-(alkyl- and) Tj ETQq1 1 0.784314 rgBT /Overlock 10 Tf 50 662 Td (benzyl)sulfonyl)	1.9	11
22	Alkaline hydrolysis of hexahydro-1,3,5-trinitro-1,3,5-triazine: M06-2X investigation. Chemosphere, 2015, 134, 31-38.	8.2	11
23	New insight on the mechanism of 2-oxabicyclobutane fragmentation. A high-level ab initio study. Tetrahedron, 2001, 57, 1509-1513.	1.9	10
24	Ethanolysis of N-substituted norbornane epoxyimides: Discovery of diverse pathways depending on substituent's character. Organic and Biomolecular Chemistry, 2010, 8, 2142-57.	2.8	9
25	A Counterionâ€Directed Approach to the Dielsâ€“Alder Paradigm: Cascade Synthesis of Tricyclic Fused Cyclopropanes. Angewandte Chemie - International Edition, 2016, 55, 13813-13817.	13.8	9
26	QSPR modeling of optical rotation of amino acids using specific quantum chemical descriptors. Journal of Molecular Modeling, 2018, 24, 59.	1.8	8
27	Reactions of alicyclic epoxy compounds with oxygen-centered nucleophiles. Russian Journal of Organic Chemistry, 2006, 42, 307-337.	0.8	7
28	Synthesis and characterization of sulfolane-based amino alcohols: A combined experimental and computational study. Journal of Molecular Structure, 2018, 1157, 149-158.	3.6	7
29	Is 2-oxabicyclobutane formed during the reaction of peroxyacids with cyclopropene? A high-level ab initio study. Tetrahedron, 2002, 58, 8751-8758.	1.9	6
30	Theoretical Study of Mechanism of 2,3-Dihydro-1,5-benzodiazepin-2-ones Hydrazinolysis. Journal of Physical Chemistry A, 2009, 113, 1475-1480.	2.5	6
31	Accurate calculations of second-order electric and magnetic properties: Two ways of physically justified modifications of basis sets. Chemical Physics, 2010, 372, 67-71.	1.9	6
32	Interaction of 3â€(2â€Aminophenyl)â€6â€R¹â€1,2,4â€triazinâ€5â€ones with Acylating Reagents: An Efficient Method for Preparation of 6â€Substituted 3â€R¹â€2Hâ€[1,2,4]triazino[2,3â€c]quinazolinâ€2â€ones. Journal of Heterocyclic Chemistry, 2016, 53, 776-783.	2.6	6
33	Synthesis, Tautomerism, and Antiradical Activity of Novel Pteridinetrione Derivatives. Journal of Heterocyclic Chemistry, 2018, 55, 1033-1041.	2.6	6
34	Use of dye aggregation phenomenon for spectrophotometric and SIA-LAV determination of bismuth(III) as a specific ion association complex between tetraiodobismuthate and Astra Phloxine. Journal of Molecular Structure, 2022, 1251, 132015.	3.6	6
35	Theoretical Study of Alkaline Methanolysis of Alicyclic Epoxy Derivatives. Russian Journal of Organic Chemistry, 2001, 37, 345-350.	0.8	5
36	A New Approach for Calculations of the Second-Order Magnetic Properties:Â Magnetic Susceptibility. Journal of Physical Chemistry A, 2004, 108, 4930-4933.	2.5	5

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37	Comprehensive DFT and MP2 Level Investigations of Reaction of 2,3-Dihydro-1,5-benzodiazepine-2-thiones with Hydrazine. Journal of Physical Chemistry A, 2009, 113, 11376-11381.	2.5	5
38	Role of Singlet Oxygen in the Degradation of Selected Insensitive Munitions Compounds: A Comprehensive, Quantum Chemical Investigation. Journal of Physical Chemistry A, 2019, 123, 7597-7608.	2.5	5
39	Title is missing!. Russian Journal of Organic Chemistry, 2001, 37, 1564-1569.	0.8	4
40	Synthesis, Structure, and Derivatives of endo-4-Aminomethyltetracyclo[6.2.1.13,6.02,7]dodec-9-ene. Russian Journal of Organic Chemistry, 2004, 40, 1080-1091.	0.8	4
41	Dimethyl Acetylenedicarboxylate in Reactions with Substituted 3â€(2â€aminophenyl)â€6â€R 1 â€1,2,4â€triazinâ€5â€(2 H) Tj ETQq1 1 0 2038-2042.	2.6	4
42	Reactions of 2Ð(4Ð)-chromenes with dinucleophiles: one-step synthesis of 2-(1H-(bi)pyrazol-3-yl)- and 2-(1,4(5)-(benzo)diazepin-4-yl)phenols. Chemistry of Heterocyclic Compounds, 2018, 54, 859-867.	1.2	4
43	Catalytic role of solvated electron in the spontaneous degradation of insensitive munition compounds: computational chemistry investigation. Structural Chemistry, 2021, 32, 521-527.	2.0	4
44	CL-20 photodecomposition: Ab initio foundations for identification of products. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2008, 71, 230-237.	3.9	3
45	A Counterionâ€Directed Approach to the Dielsâ€“Alder Paradigm: Cascade Synthesis of Tricyclic Fused Cyclopropanes. Angewandte Chemie, 2016, 128, 14017-14021.	2.0	3
46	Copper Crystallization from Aqueous Solution: Initiation and Evolution of the Polynuclear Clusters. Journal of Cluster Science, 2017, 28, 2517-2528.	3.3	3
47	Ð¡Ñ€ÑƒÐºÑ‚ÑƒÑ€Ð° Ñ– Ð¾ÐºÐ¸ÑĐ»ÑŽÐ²Ð°Ð»ÑŒÐ½Ð¾-Ð²Ñ–Ð´Ð½Ð¾Ð²Ð½Ñ– Ð²Ð»Ð°ÑÑ‚Ð¸Ð²Ð¾ÑÑ‚Ñ– 2,4,6,8,10,12-Ð³ÐµÐºÑ 23, 1.	0.1	3
48	Epoxidation of 1-Substituted 3-Cyclohexenes. Theoretical and Experimental Investigation. Russian Journal of Organic Chemistry, 2002, 38, 160-164.	0.8	2
49	Identification of the stereoisomers of tetrahydroindene diepoxide by the 1H and 13C NMR characteristics: A combined experimental and theoretical study. Computational and Theoretical Chemistry, 2005, 730, 125-132.	1.5	2
50	Azabrendanes V. Synthesis and reactions of stereoisomeric exo- and endo-5-aminomethylbicyclo[2.2.1]hept-2-ene-based ureas. Open Chemistry, 2008, 6, 161-174.	1.9	2
51	Experimental and theoretical study on the reaction of bicyclo[2.2.1]hept-5-en-endo-2-ylmethanamine with glycidyl ethers. Russian Journal of Organic Chemistry, 2011, 47, 74-82.	0.8	2
52	Accurate calculations of dynamic first hyperpolarizability: Construction of physically justified slaterâ€type basis sets. International Journal of Quantum Chemistry, 2014, 114, 689-695.	2.0	2
53	Ð†ÐŕÐµÐ½Ð¸Ð¸Ñ–Ñ–Ð¼Ð°Ñ†Ñ–Ñ•N-Ð¼ÐµÑ‚Ð¸Ð»-4-Ñ‚Ð¾Ð»Ñ–Ð»-1-(4-Ð±Ñ€Ð¾Ð¼Ð¾Ð¼Ð¾Ð½Ð°Ñ„Ñ‚Ð¸Ð»)Ð°Ð¼Ñ–Ð½Ñƒ Ñ‚Ð° N-Ñ„	0.8	2
54	New Tricyclic Amides. Synthesis, Structure, and Oxidation with Peroxyphthalic Acid. Russian Journal of Organic Chemistry, 2005, 41, 816-824.	0.8	1

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55	Efficient approach for exploring the multiple-channel bimolecular interactions of conformationally flexible reagents. Epoxide ring opening reaction. Structural Chemistry, 2021, 32, 581-589.	2.0	1
56	Structure and redox properties of hexahydro-1,3,5-trinitro-1,3,5-triazine (RDX) and octahydro-1,3,5,7-tetranitro-1,3,5,7-tetrazocine (HMX) adsorbed on a silica surface. A DFT M05 computational study. VÃ¬snik DnÃ¬propetrovsÊ¹kogo UnÃ¬versitetu: SerÃ¬Ã¢ HÃ¬mÃ¬Ã¢, 2017, 25, 1-8.	0.1	1
57	Ð”Ð²Ð¾Ñ…ÐµÐ»ÐµÐºÑ‚Ñ€Ð¾Ð½Ð½Ð¾Ð¹ Ð²Ñ–Ð´Ð½Ð¾Ð²Ð»ÐµÐ½Ð½Ñ•Ð½Ñ–Ñ‚Ñ€Ð¾Ð°Ñ€Ð¾Ð¼Ð°Ñ‚Ð¸Ñ‡Ð½Ð¸Ñ…	0.1	1
58	Quantum-Chemical Investigation of Epoxidic Compounds Transformation. Application for In Vitro and In Vivo Processes Modeling. Challenges and Advances in Computational Chemistry and Physics, 2014, , 295-323.	0.6	0
59	A density functional theory investigation of degradation of Nitroguanidine in the photoactivated triplet state. Journal of Molecular Modeling, 2019, 25, 372.	1.8	0
60	Application of Computational Approaches to Analysis of Multistep Chemical Reactions of Energetic Materials: Hydrolysis of Hexahydro-1,3,5-Trinitro-1,3,5-Triazine (RDX) and Octahydro-1,3,5,7-Tetranitro-1,3,5,7-Tetrazocine(HMX). , 2022, , 215-232.		0
61	Ð¢Ð°Ñƒ Ñ‚Ð¾Ð¼Ð¸Ñ•Ñ–Ñ•4-Ð³Ñ–Ð´Ñ€Ð°Ð·Ð¸Ð½Ñ…Ñ–Ð½Ð°Ð·Ð¾Ð»Ñ–Ð½Ñ–Ð², Ð¯Ð¾Ð»Ð¾Ð²Ñ–Ð¹	0.1	0
62	Ð¡Ñ‚ÐµÑ€Ð¾Ñ…Ñ–Ð¼Ñ•ÐµÐ¿Ð¾ÐºÑ•Ð¸Ð´Ñƒ Ñƒ Ð²Ñ–Ð´Ð½Ð¾Ñ•Ð½Ñ–Ð¹ Ð³ÐµÐ¿Ñ‚Ð°Ñ†Ð¸ÐºÐ»Ð¾ [2.2.1]Ð³ÐµÐ¿Ñ‚Ð°Ð½-Ñ”Ð½Ð¾Ð²Ð¸Ñ… Ñ‚Ð°Ñ—Ñ… 7-s	0.1	0
63	Probability of reaction pathways of amine with epoxides in the reagent ratio of 1:1 and 1:2. Structural Chemistry, 0, , .	2.0	0