Saeedreza Emamian

List of Publications by Year
in descending order

45	1,182	686830 13	395343 33
papers	citations	h-index	g-index

45	45	45	1034
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	A molecular electron density theory study on the Chichibabin reaction: The origin of regioselectivity. Journal of Molecular Graphics and Modelling, 2022, 116, 108240.	1.3	7
2	Exploring influence of fluorine substitution on the strength and nature of halogen bond between iodobenzene and hydrogen cyanide. Journal of Physical Organic Chemistry, 2021, 34, e4213.	0.9	3
3	Shedding light on the energetics, regioselectivity, stereoselectivity, and mechanistic aspects of [3 + 2] cycloaddition reaction between azomethine imines and 2â€sulfolene through molecular electron density theory. Journal of Physical Organic Chemistry, 2020, 33, e4042.	0.9	3
4	A Study of the Effects of the Lewis Acid Catalysts on Oxaâ€Dielsâ€Alder Reactions through Molecular Electron Density Theory. ChemistrySelect, 2020, 5, 5341-5348.	0.7	6
5	Regio- and stereochemistry in the aza-Dielsâ€“Alder reaction of an azoalkene with furan and 2,3-dihydrofuran: a molecular electron density theory study. Structural Chemistry, 2020, 31, 2161-2170.	1.0	6
6	Hexamethylphosphanetriamineâ€mediated aziridination of imines with alphaâ€ketoesters: A molecular electron density theory study. Journal of Physical Organic Chemistry, 2020, 33, e4058.	0.9	6
7	Stereoselective Cyclopropanation of Arylmethylidenemalononitriles by 2,6-Dimethylquinoline: A Molecular Electron Density Theory Study. Russian Journal of Organic Chemistry, 2020, 56, 2171-2178.	0.3	0
8	Exploring Nature and Predicting Strength of Hydrogen Bonds: A Correlation Analysis Between Atomsâ€inâ€Molecules Descriptors, Binding Energies, and Energy Components of Symmetryâ€Adapted Perturbation Theory. Journal of Computational Chemistry, 2019, 40, 2868-2881.	1.5	678
9	Stereoselective cyclopropanation of olefins through ammonium ylides: A molecular electron density theory study. Journal of Physical Organic Chemistry, 2019, 32, e4008.	0.9	3
10	Understanding the domino reactions of alkyne-tethered N-tosylhydrazones yielding fused polycyclic pyrazoles. An MEDT study. Tetrahedron, 2019, 75, 2807-2816.	1.0	4
11	Copper(<scp>i</scp>)-catalyzed asymmetric aza Dielsâ€“Alder reactions of azoalkenes toward fulvenes: a molecular electron density theory study. New Journal of Chemistry, 2019, 43, 4765-4776.	1.4	21
12	Aziridination of Aromatic Aldimines Through Stabilized Ammonium Ylides: A Molecular Electron Density Theory Study. European Journal of Organic Chemistry, 2019, 2019, 1605-1613.	1.2	4
13	[3 + 2] cycloaddition reaction ofN,Nâ€²cyclic azomethine imines toward highly electronâ€deficient nitroalkenes: A molecular electron density theory study. Journal of Physical Organic Chemistry, 2019, 32, e3925.	0.9	4
14	Participation of furoxancarbonitrile oxide in [3+2] cycloaddition reaction toward Câ€“N triple bond: a Molecular Electron Density Theory study of regioselectivity and mechanistic aspect. Structural Chemistry, 2019, 30, 317-326.	1.0	7
15	[3+2] cycloaddition reaction between CF3-substituted thiocarbonyl ylides and thioketones: Exploration of regioselectivity and mechanistic aspects using Molecular Electron Density Theory. Journal of Fluorine Chemistry, 2018, 209, 14-22.	0.9	10
16	A molecular electron density theory study of the chemo- and regioselective [3â€¯+â€¯2] cycloaddition reactions between trifluoroacetonitrile N-oxide and thioketones. Chemical Physics, 2018, 501, 128-137.	0.9	11
17	A molecular electron density theory study on the [3+2] cycloaddition reaction of thiocarbonyl ylides with hetaryl thioketones. New Journal of Chemistry, 2018, 42, 11819-11830.	1.4	7
18	Toward understanding regioselectivity and molecular mechanism in the synthesis of CF 2 H-containing 2-pyrazolines: A molecular electron-density theory study. Journal of Fluorine Chemistry, 2017, 199, 77-91.	0.9	13

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19	A DFT computational study on the molecular mechanism of reaction between pyridinium salts and Ï€-deficient ethylenes: Why furan derivatives are formed instead of feasible cyclopropane derivatives and [3 + 2] cycloadducts?. Computational and Theoretical Chemistry, 2017, 1114, 87-100.	1.1	6
20	A Molecular Electron Density Theory Study of [3+2] Cycloaddition Reaction between Azomethine Ylides and Electronâ€Deficient Nitroalkenes. ChemistrySelect, 2017, 2, 4193-4203.	0.7	10
21	Understanding the domino reaction between 1-diazopropan-2-one and 1,1-dinitroethylene. A molecular electron density theory study of the [3 + 2] cycloaddition reactions of diazoalkanes with electron-deficient ethylenes. RSC Advances, 2017, 7, 15586-15595.	1.7	19
22	Understanding the molecular mechanism of the [3â€‰+â€‰2] cycloaddition reaction of benzonitrile oxide toward electronâ€rich Nâ€vinylpyrrole: a DFT study. Journal of Physical Organic Chemistry, 2016, 29, 368-376.	0.9	14
23	Conformational stability, barriers to internal rotations, and normal coordinate analysis of acetone and its2H-isotopomers. Canadian Journal of Chemistry, 2016, 94, 818-826.	0.6	5
24	How the mechanism of a [3 + 2] cycloaddition reaction involving a stabilized N-lithiated azomethine ylide toward a Ï€-deficient alkene is changed to stepwise by solvent polarity? What is the origin of its regio- and endo stereospecificity? A DFT study using NBO, QTAIM, and NCI analyses. RSC Advances, 2016, 6, 75299-75314.	1.7	20
25	Understanding the stereoselectivity in BrÃ¸nsted acid catalysed Povarov reactions generating cis/trans CF₃-substituted tetrahydroquinolines: a DFT study. RSC Advances, 2016, 6, 17064-17073.	1.7	17
26	Conformational analysis, structure, and normal coordinate analysis of vibrational spectra of hexafluoroacetone. A density functional theory study. Journal of Fluorine Chemistry, 2016, 184, 65-71.	0.9	10
27	Understanding the molecular mechanism and regioselectivity in the synthesis of celecoxib via a domino reaction: A DFT study. Journal of Molecular Graphics and Modelling, 2015, 60, 155-161.	1.3	7
28	Generation of a substituted 1,2,4-thiadiazole ring via the [3+2] cycloaddition reaction of benzonitrile sulfide toward trichloroacetonitrile. A DFT study of the regioselectivity and of the molecular mechanism. Comptes Rendus Chimie, 2015, 18, 1277-1283.	0.2	9
29	Ionic Dielsâ€“Alder reaction of 3-bromofuran toward the highly electron deficient cyclobuteniminium cation: a regio- and stereoselectivity, and molecular mechanism study using DFT. RSC Advances, 2015, 5, 98538-98548.	1.7	6
30	Understanding the domino reaction between 3-chloroindoles and methyl coumalate yielding carbazoles. A DFT study. Organic and Biomolecular Chemistry, 2015, 13, 2034-2043.	1.5	15
31	Can the high reactivity of azomethine betaines in [3Â+ 2] cycloaddition reactions be explained using singlet-diradical character descriptors? What molecular mechanism is actually involved in these cycloadditions?. RSC Advances, 2015, 5, 62248-62259.	1.7	18
32	Understanding the regioselectivity and molecular mechanism in the synthesis of isoxazoles containing pentafluorosulfanyl substitution via a [3+2] cycloaddition reaction: A DFT study. Journal of Fluorine Chemistry, 2015, 178, 165-172.	0.9	28
33	Polar Dielsâ€“Alder reaction of isoprene toward 2-bromocyclobutenone followed by a subsequent sodium hydroxide-assisted ring contraction reaction. A regio- and stereoselectivity and molecular mechanism study using DFT. New Journal of Chemistry, 2015, 39, 9525-9534.	1.4	12
34	Understanding the molecular mechanism in a regiospecific [3 + 2] cycloaddition reaction including Câ€“O and Câ€“S interactions: an ELF topological analysis. RSC Advances, 2015, 5, 72959-72970.	1.7	19
35	Tautomerism in pyridazin-3(2H)-one: A theoretical study using implicit/explicit solvation models. Journal of Molecular Graphics and Modelling, 2014, 49, 47-54.	1.3	23
36	Mechanism and regioselectivity of 1,3-dipolar cycloaddition reactions of sulphur-centred dipoles with furan-2,3-dione: A theoretical study using DFT. Journal of Chemical Sciences, 2014, 126, 293-302.	0.7	10

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37	Understanding the mechanisms of [3+2] cycloaddition reactions. The pseudoradical versus the zwitterionic mechanism. Tetrahedron, 2014, 70, 1267-1273.	1.0	95
38	Comparative Investigation of the Stabilities of Indene and Isoindene and the Their Heteroanalogs (N,O,S) Using Computational Methods. Phosphorus, Sulfur and Silicon and the Related Elements, 2014, 189, 1367-1377.	0.8	1
39	Theoretical study of intramolecular hydrogen bonding in the halo derivatives of 1-amino-3-imino-prop-1-ene. Journal of Chemical Sciences, 2013, 125, 939-948.	0.7	23
40	DFT Study of NBO, NICS and ¹⁴N NQR Parameters of Guanine Tautomers in the Gas Phase. Zeitschrift Fur Physikalische Chemie, 2012, 226, 47-57.	1.4	3
41	Mechanism and Regioselectivity of the 1,3-Dipolar Cycloaddition of Methyleneamine N-Oxide with Cyclopent-3-Ene-1,2-Dione and its Aza, Oxa and Thia Analogues: A Dft Approach. Progress in Reaction Kinetics and Mechanism, 2012, 37, 90-102.	1.1	3
42	Mechanism and regioselectivity of the 1,3â€dipolar cycloaddition of thiocarbonyl Sâ€imide with cyclopentâ€3â€eneâ€1,2â€dione and methoxyethene: a density functional theory approach. Journal of Physical Organic Chemistry, 2012, 25, 748-753.	0.9	3
43	Kinetic and thermodynamic study of the substituent effect on the amino-Claisen rearrangement ofpara-substitutedN-allyl-N-arylamine: a Hammett study via DFT. Molecular Simulation, 2010, 36, 978-985.	0.9	5
44	Structure and vibrational assignment of the enol form of 1-chloro-1,1-difluoro-pentane-2,4-dione. Journal of Molecular Structure, 2008, 878, 10-21.	1.8	8
45	A comprehensive theoretical analysis on the intermolecular hydrogen bond interactions with the Lewis bases having multiple hydrogen bonding ability. Journal of Physical Organic Chemistry, 0, , .	0.9	0