Luis R Domingo

List of Publications by Year
in descending order

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359 papers	15,861 citations	26567 56 h-index	24179 110 g-index
386 all docs	386 docs citations	386 times ranked	5959 citing authors

#	Article	IF	Citations
1	Synthesis and anti-Cancer Activity of a New Hybrid Based Spirooxindole-Pyrrolidine -Thiochromene Scaffolds via [3â€‰+â€‰2] Cycloaddition Reaction: Computational Investigation. Polycyclic Aromatic Compounds, 2023, 43, 2302-2320.	1.4	3
2	A Molecular Electron Density Theory Study of the Lewis Acid Catalyzed [3+2] Cycloaddition Reactions of Nitrones with Nucleophilic Ethylenes. European Journal of Organic Chemistry, 2022, 2022, .	1.2	21
3	Understanding the higherâ€“order cycloaddition reactions of heptafulvene, tropone, and its nitrogen derivatives, with electrophilic and nucleophilic ethylenes inside the molecular electron density theory. New Journal of Chemistry, 2022, 46, 11520-11530.	1.4	4
4	Unveiling the cbâ€type Intramolecular [3+2] Cycloaddition Reactions of Fluorinated Azomethine Ylides to Ester Carbonyls with a Molecular Electron Density Theory Perspective. ChemistrySelect, 2022, 7, .	0.7	1
5	A Molecular Electron Density Theory Study of the [3+2] Cycloaddition Reaction of Pseudo(mono)radical Azomethine Ylides with Phenyl Vinyl Sulphone. Organics, 2022, 3, 122-136.	0.6	10
6	Does Cr(CO) ₃ Really behave as Catalyst in the Dielsâ€Alder Reaction of Styrene with Cyclopentadiene? A Molecular Electron Density Theory Study. ChemistrySelect, 2022, 7, .	0.7	3
7	Divulging the various chemical reactivity of trifluoromethyl-4-vinyl-benzene as well as methyl-4-vinyl-benzene in [3+2] cycloaddition reactions. Journal of Molecular Graphics and Modelling, 2021, 102, 107760.	1.3	10
8	A molecular electron density theory study for [3â€‰+â€‰2] cycloaddition reactions of<scp>1â€pyrroline</scp>â€1â€oxide with disubstituted acetylenes leading to bicyclic 4â€isoxazolines. International Journal of Quantum Chemistry, 2021, 121, e26503.	1.0	11
9	Unveiling the Unexpected Reactivity of Electrophilic Diazoalkanes in [3+2] Cycloaddition Reactions within Molecular Electron Density Theory. Chemistry, 2021, 3, 74-93.	0.9	9
10	Mpro-SARS-CoV-2 Inhibitors and Various Chemical Reactivity of 1-Bromo- and 1-Chloro-4-vinylbenzene in [3 + 2] Cycloaddition Reactions. Organics, 2021, 2, 1-16.	0.6	16
11	Quasi-RRHO approximation and DFT study for understanding the mechanism and kinetics of nitration reaction of benzonitrile with nitronium ion. Computational and Theoretical Chemistry, 2021, 1199, 113209.	1.1	5
12	Unveiling the Chemoâ€and Regioselectivity of the [3+2] Cycloaddition Reaction between 4â€Chlorobenzonitrile Oxide and Î²â€Aminocinnamonitrile with a MEDT Perspective**. ChemistrySelect, 2021, 6, 4521-4532.	0.7	14
13	Unveiling the Ionic Dielsâ€“Alder Reactions within the Molecular Electron Density Theory. Molecules, 2021, 26, 3638.	1.7	3
14	Unveiling the Different Reactivity of Bent and Linear Three-Atom-Components Participating in [3 + 2] Cycloaddition Reactions. Organics, 2021, 2, 274-286.	0.6	6
15	Closer Investigation of the Kinetics and Mechanism of Spirovinylcyclopropyl Oxindole Reaction with 3Î£â€“g-O2 by Topological Approaches and Unraveling the Role of the I2 Catalyst. Journal of Physical Chemistry A, 2021, 125, 6913-6926.	1.1	1
16	Understanding the Participation of Fluorinated Azomethine Ylides in Carbenoid-Type [3 + 2] Cycloaddition Reactions with Ynal Systems: A Molecular Electron Density Theory Study. Journal of Organic Chemistry, 2021, 86, 12644-12653.	1.7	17
17	Unveiling the Intramolecular Ionic Dielsâ€“Alder Reactions within Molecular Electron Density Theory. Chemistry, 2021, 3, 834-853.	0.9	0
18	Understanding the different reactivity of (Z)- and (E)-Î²-nitrostyrenes in [3+2] cycloaddition reactions. An MEDT study. RSC Advances, 2021, 11, 9698-9708.	1.7	7

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19	Unveiling the regioselectivity in electrophilic aromatic substitution reactions of deactivated benzenes through molecular electron density theory. New Journal of Chemistry, 2021, 45, 13626-13638.	1.4	10
20	On the Catalytic Effects of the Thiazolium Salt in the Oxa-Diel-Alder Reaction between Benzaldehyde and Danishefskyâ€™s Diene: A Molecular Electron Density Theory Study. Organic and Biomolecular Chemistry, 2021, 19, 9306-9317.	1.5	0
21	Unveiling the Substituent Effects in the Stereochemistry of [3+2] Cycloaddition Reactions of Arylâ€•and Alkyldiazomethylphosphonates with Norbornadiene within a MEDT Perspective. ChemistrySelect, 2021, 6, 10722-10733.	0.7	12
22	Theoretical Studies on the Mechanism of the Formation of Cyclopentadienes and Dihydropyridazines. ChemistrySelect, 2021, 6, 9806-9813.	0.7	0
23	Straightforward Regio- and Diastereoselective Synthesis, Molecular Structure, Intermolecular Interactions and Mechanistic Study of Spirooxindole-Engrafted Rhodanine Analogs. Molecules, 2021, 26, 7276.	1.7	12
24	A molecular electron density theory study of the higher-order cycloaddition reactions of tropone with electron-rich ethylenes. The role of the Lewis acid catalyst in the mechanism and pseudocyclic selectivity. New Journal of Chemistry, 2021, 46, 294-308.	1.4	4
25	Design, Synthesis, Chemical and Biochemical Insights Into Novel Hybrid Spirooxindole-Based p53-MDM2 Inhibitors With Potential Bcl2 Signaling Attenuation. Frontiers in Chemistry, 2021, 9, 735236.	1.8	22
26	Synthesis of Spirooxindole Analogs Tethered Pyrazole Scaffold as Acetylcholinesterase Inhibitors. ChemistrySelect, 2021, 6, 14039-14053.	0.7	9
27	A molecular electron density theory study of the enhanced reactivity of aza aromatic compounds participating in Dielsâ€“Alder reactions. Organic and Biomolecular Chemistry, 2020, 18, 292-304.	1.5	24
28	Unveiling the Reactivity of Cyclic Azomethine Ylides in [3+2] Cycloaddition Reactions within the Molecular Electron Density Theory. European Journal of Organic Chemistry, 2020, 2020, 5938-5948.	1.2	48
29	Unveiling the high reactivity of strained dibenzocyclooctyne in [3 + 2] cycloaddition reactions with diazoalkanes through the molecular electron density theory. Journal of Physical Organic Chemistry, 2020, 33, e4100.	0.9	21
30	Calculation of the rate constants for hydrogen abstraction reactions by Hydroperoxyl radical from Methanol, and the investigation of stability of CH3OH.HO2 complex. Computational and Theoretical Chemistry, 2020, 1190, 113010.	1.1	1
31	Understanding the Origin of the Regioselectivity in Non-Polar [3+2] Cycloaddition Reactions through the Molecular Electron Density Theory. Organics, 2020, 1, 19-35.	0.6	12
32	Unveiling the high reactivity of benzyne in the formal [3+2] cycloaddition reactions towards thioamides through the Molecular Electron Density Theory. Tetrahedron, 2020, 76, 131458.	1.0	11
33	Unravelling the strain-promoted [3+2] cycloaddition reactions of phenyl azide with cycloalkynes from the molecular electron density theory perspective. New Journal of Chemistry, 2020, 44, 13633-13643.	1.4	30
34	Understanding the Influence of the Trifluoromethyl Group on the Selectivities of the [3+2] Cycloadditions of Thiocarbonyl Sâ€•methanides with Î±,Î²â€Unsaturated Ketones. A MEDT study. ChemistrySelect, 2020, 5, 12791-12806.	0.7	4
35	Lithium Cation-Catalyzed Benzene Dielsâ€“Alder Reaction: Insights on the Molecular Mechanism Within the Molecular Electron Density Theory. Journal of Organic Chemistry, 2020, 85, 13121-13132.	1.7	13
36	Unraveling the kinetics and molecular mechanism of gas phase pyrolysis of cubane to [8]annulene. RSC Advances, 2020, 10, 32730-32739.	1.7	2

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37	Deciphering the Mechanism of Silver Catalysis of â€œClickâ€•Chemistry in Water by Combining Experimental and MEDT Studies. Catalysts, 2020, 10, 956.	1.6	18
38	Understanding the Reactivity of Trimethylsilyldiazoalkanes Participating in [3+2] Cycloaddition Reactions towards Diethylfumarate with a Molecular Electron Density Theory Perspective. Organics, 2020, 1, 3-18.	0.6	13
39	Atmospheric Oxidation Reactions of Methyl Salicylate as Green Leaf Volatiles by OH Radical: Theoretical Kinetics and Mechanism. ChemistrySelect, 2020, 5, 12535-12547.	0.7	2
40	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
41	Unveiling the Lewis Acid Catalyzed Dielsâ€“Alder Reactions Through the Molecular Electron Density Theory. Molecules, 2020, 25, 2535.	1.7	34
42	Unveiling the Different Chemical Reactivity of Diphenyl Nitrilimine and Phenyl Nitrile Oxide in [3+2] Cycloaddition Reactions with (R)-Carvone through the Molecular Electron Density Theory. Molecules, 2020, 25, 1085.	1.7	27
43	A molecular electron density theory study of the [3â€‰+â€‰2] cycloaddition reaction of 1,4-diphosphorinium-3-olates with methyl acrylate and methyl methacrylate. Theoretical Chemistry Accounts, 2020, 139, 1.	0.5	1
44	A molecular electron density theory study of the Grignard reagentâ€mediated regioselective direct synthesis of 1,5â€disubstitutedâ€1,2,3â€triazoles. Journal of Physical Organic Chemistry, 2020, 33, e4062.	0.9	20
45	A molecular electron density theory investigation of the molecular mechanism, regioselectivity, stereoselectivity and chemoselectivity of cycloaddition reaction between acetonitrile N-oxide and 2,5-dimethyl-2H-[1,2,3]diazarsole. Theoretical Chemistry Accounts, 2020, 139, 1.	0.5	21
46	Unravelling the kinetics and molecular mechanism of the degenerate Cope rearrangement of bullvalene. New Journal of Chemistry, 2020, 44, 6543-6552.	1.4	8
47	A molecular electron density theory study of the participation of tetrazines in aza-Dielsâ€“Alder reactions. RSC Advances, 2020, 10, 15394-15405.	1.7	94
48	A Close Look to the Oxaphosphetane Formation along the Wittig Reaction: A [2+2] Cycloaddition?. Journal of Organic Chemistry, 2020, 85, 6675-6686.	1.7	31
49	A molecular electron density theory (MEDT) study of the role of halogens (X₂=) Tj ETQq1 1 0.784314 rgBT /Overlock 10 Tf reactions. New Journal of Chemistry, 2020, 44, 19002-19012.	1.4	8
50	Molecular Electron Density Theory: A New Theoretical Outlook on Organic Chemistry. Frontiers in Computational Chemistry, 2020, , 174-227.	0.1	18
51	An investigation of the molecular mechanism, chemoselectivity and regioselectivity of cycloaddition reaction between acetonitrile N-Oxide and 2,5-dimethyl-2H-[1,2,3]diazaphosphole: a MEDT study. Journal of Chemical Sciences, 2019, 131, 1.	0.7	15
52	Are one-step aromatic nucleophilic substitutions of non-activated benzenes concerted processes?. Organic and Biomolecular Chemistry, 2019, 17, 8185-8193.	1.5	11
53	Clicking Azides and Alkynes with Poly(pyrazolyl)borate-Copper(I) Catalysts: An Experimental and Computational Study. Catalysts, 2019, 9, 687.	1.6	8
54	A molecular electron density theory study of the mechanism, chemo- and stereoselectivity of the epoxidation reaction ofR-carvone with peracetic acid. RSC Advances, 2019, 9, 28500-28509.	1.7	15

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55	Site-selectivity control in hetero-Dielsâ€“Alder reactions of methylidene derivatives of lawsone through modification of the reactive carbonyl group: an experimental and theoretical study. Organic and Biomolecular Chemistry, 2019, 17, 692-702.	1.5	4
56	Unveiling the high reactivity of cyclohexynes in [3 + 2] cycloaddition reactions through the molecular electron density theory. Organic and Biomolecular Chemistry, 2019, 17, 498-508.	1.5	11
57	A molecular electron density theory study of the insertion of CO into frustrated Lewis pair boron-amidines: a [4 + 1] cycloaddition reaction. Dalton Transactions, 2019, 48, 9214-9224.	1.6	4
58	On the nature of organic electron density transfer complexes within molecular electron density theory. Organic and Biomolecular Chemistry, 2019, 17, 6478-6488.	1.5	12
59	An MEDT study of the mechanism and selectivities of the [3+2] cycloaddition reaction of tomentosin with benzonitrile oxide. International Journal of Quantum Chemistry, 2019, 119, e25980.	1.0	21
60	A molecular electron density theory study of the Lewis acidâ€“catalyzed decomposition reaction of nitroethyl benzoate using aluminum derivatives. Journal of Physical Organic Chemistry, 2019, 32, e3938.	0.9	17
61	Understanding the domino reactions of alkyne-tethered N-tosylhydrazones yielding fused polycyclic pyrazoles. An MEDT study. Tetrahedron, 2019, 75, 2807-2816.	1.0	4
62	The carbenoid-type reactivity of simplest nitrile imine from a molecular electron density theory perspective. Tetrahedron, 2019, 75, 1961-1967.	1.0	36
63	A Molecular Electron Density Theory Study of the Chemoselectivity, Regioselectivity, and Diastereofacial Selectivity in the Synthesis of an Anticancer Spiroisoxazoline derived from Î±-Santonin. Molecules, 2019, 24, 832.	1.7	39
64	A Molecular Electron Density Theory Study of the Synthesis of Spirobipyrazolines through the Domino Reaction of Nitrilimines with Allenoates. Molecules, 2019, 24, 4159.	1.7	11
65	Understanding the Mechanism of Nitrobenzene Nitration with Nitronium Ion: A Molecular Electron Density Theory Study. ChemistrySelect, 2019, 4, 13313-13319.	0.7	13
66	Unravelling the Mysteries of the [3+2] Cycloaddition Reactions. European Journal of Organic Chemistry, 2019, 2019, 267-282.	1.2	171
67	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
68	Structure, Reactivity, Nonlinear Optical Properties and Vibrational Study of 5-Thioxo-1,4-thiazaolidin-3-one and 5-thioxo-1,4,2-thiazasilolidin-3-one (Silicon vs. Carbon). A DFT Study. Silicon, 2019, 11, 2135-2147.	1.8	2
69	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
70	A molecular electron density theory study of the [3Â+Â2] cycloaddition reaction between an azomethine imine and electron deficient ethylenes. Journal of Physical Organic Chemistry, 2018, 31, e3830.	0.9	22
71	Understanding the mechanism and regioselectivity of the copper(<scp>i</scp>) catalyzed [3 + 2] cycloaddition reaction between azide and alkyne: a systematic DFT study. RSC Advances, 2018, 8, 7670-7678.	1.7	67
72	Experimental and Theoretical MEDT Study of the Thermal [3+2] Cycloaddition Reactions of Aryl Azides with Alkyne Derivatives. ChemistrySelect, 2018, 3, 1215-1223.	0.7	12

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73	A Molecular Electron Density Theory Study of the Reactivity and Selectivities in [3 + 2] Cycloaddition Reactions of C,N-Dialkyl Nitrones with Ethylene Derivatives. Journal of Organic Chemistry, 2018, 83, 2182-2197.	1.7	102
74	A combined experimental and theoretical study of the thermal [3+2] cycloaddition of carbonyl ylides with activated alkenes. Journal of Molecular Structure, 2018, 1157, 276-287.	1.8	9
75	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
76	The Mysticism of Pericyclic Reactions: A Contemporary Rationalisation of Organic Reactivity Based on Electron Density Analysis. European Journal of Organic Chemistry, 2018, 2018, 1107-1120.	1.2	69
77	Does a fluorinated Lewis acid catalyst change the molecular mechanism of the decomposition process of nitroethyl carboxylates?. Research on Chemical Intermediates, 2018, 44, 325-337.	1.3	15
78	Molecular Electron Density Theory Study of Fused Regioselectivity in the Intramolecular [3+2] Cycloaddition Reaction of Cyclic Nitrones. ChemistrySelect, 2018, 3, 5412-5420.	0.7	16
79	[3+2] Cycloaddition Reaction of Câ€Phenylâ€Nâ€methyl Nitrone to Acyclicâ€Olefinâ€Bearing Electronâ€Donating Substituent: A Molecular Electron Density Theory Study. ChemistrySelect, 2018, 3, 8373-8380.	0.7	21
80	DFT exploration of [3 + 2] cycloaddition reaction of 1H-phosphorinium-3-olate and 1-methylphosphorinium-3-olate with methyl methacrylate. RSC Advances, 2018, 8, 27406-27416.	1.7	7
81	A Molecular Electron Density Theory Study of the Role of the Copper Metalation of Azomethine Ylides in [3 + 2] Cycloaddition Reactions. Journal of Organic Chemistry, 2018, 83, 10959-10973.	1.7	41
82	A Molecular Electron Density Theory Study of the Competitiveness of Polar Dielsâ€“Alder and Polar Alder-ene Reactions. Molecules, 2018, 23, 1913.	1.7	13
83	A molecular electron density theory study of the [3 + 2] cycloaddition reaction of nitrones with ketenes. Organic and Biomolecular Chemistry, 2017, 15, 1618-1627.	1.5	33
84	How does the global electron density transfer diminish activation energies in polar cycloaddition reactions? A Molecular Electron Density Theory study. Tetrahedron, 2017, 73, 1718-1724.	1.0	65
85	Steric interactions controlling the syn diastereofacial selectivity in the [3Â+Â2] cycloaddition reaction between acetonitrile oxide and 7-oxanorborn-5-en-2-ones: A molecular electron density theory study. Journal of Physical Organic Chemistry, 2017, 30, e3710.	0.9	23
86	Understanding the reaction mechanism of the Lewis acid (MgBr2)-catalysed [3+2] cycloaddition reaction between C-methoxycarbonyl nitrone and 2-propen-1-ol: a DFT study. Theoretical Chemistry Accounts, 2017, 136, 1.	0.5	9
87	A molecular electron density theory study of the [3 + 2] cycloaddition reaction of nitrones with strained allenes. RSC Advances, 2017, 7, 26879-26887.	1.7	19
88	Copper(I)-catalysed regioselective synthesis of pyrazolo[5,1-c]-1,2,4-triazoles: A DFT mechanistic study. Tetrahedron, 2017, 73, 4653-4662.	1.0	5
89	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
90	Understanding the Intramolecular Dielsâ€Alder Reactions of Nâ€Substituted Nâ€Allylâ€Furfurylamines: An MEDT Study. ChemistrySelect, 2017, 2, 9736-9743.	0.7	2

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91	Understanding the mechanism of the decomposition reaction of nitroethyl benzoate through the Molecular Electron Density Theory. Theoretical Chemistry Accounts, 2017, 136, 1.	0.5	13
92	A DFT Study of the Conversion of Ptaquiloside, a Bracken Fern Carcinogen, to Pterosin B in Neutral and Acidic Aqueous Medium. ChemistrySelect, 2017, 2, 8178-8186.	0.7	1
93	A molecular electron density theory study of [3Â+Â2] cycloaddition reactions of chiral azomethine ylides with Î²-nitrostyrene. Theoretical Chemistry Accounts, 2017, 136, 1.	0.5	21
94	Understanding the reactivity and regioselectivity of [3â€‰+â€‰2] cycloaddition reactions between substituted nitrile oxides and methyl acrylate. A molecular electron density theory study. International Journal of Quantum Chemistry, 2017, 117, e25451.	1.0	27
95	Nitropyrroles, Diels-Alder reactions assisted by microwave irradiation and solvent effect. An experimental and theoretical study. Journal of Molecular Structure, 2017, 1147, 155-160.	1.8	13
96	Electrophilic activation of CO2 in cycloaddition reactions towards a nucleophilic carbenoid intermediate: new defying insights from the Molecular Electron Density Theory. Theoretical Chemistry Accounts, 2017, 136, 1.	0.5	11
97	A DFT study of the mechanism and selectivities of the [3Â+Â2] cycloaddition reaction between 3â€(benzylideneamino)oxindole and transâ€Î²â€nitrostyrene. Journal of Physical Organic Chemistry, 2017, 30, e3637.	0.9	22
98	A Molecular Electron Density Theory Study of the Reactivity of Azomethine Imine in [3+2] Cycloaddition Reactions. Molecules, 2017, 22, 750.	1.7	76
99	A Theoretical Study of the Relationship between the Electrophilicity Ï‰ Index and Hammett Constant Ïƒp in [3+2] Cycloaddition Reactions of Aryl Azide/Alkyne Derivatives. Molecules, 2016, 21, 1434.	1.7	13
100	Applications of the Conceptual Density Functional Theory Indices to Organic Chemistry Reactivity. Molecules, 2016, 21, 748.	1.7	795
101	Molecular Electron Density Theory: A Modern View of Reactivity in Organic Chemistry. Molecules, 2016, 21, 1319.	1.7	324
102	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
103	[3+2] Cycloaddition reaction of 1H-phosphorinium-3-olate and 1-methylphosphorinium-3-olate with methyl acrylate: A DFT study. Computational and Theoretical Chemistry, 2016, 1087, 36-47.	1.1	2
104	An MEDT study of the carbenoid-type [3 + 2] cycloaddition reactions of nitrile ylides with electron-deficient chiral oxazolidinones. Organic and Biomolecular Chemistry, 2016, 14, 10427-10436.	1.5	15
105	Intrinsic relative nucleophilicity of indoles. Theoretical Chemistry Accounts, 2016, 135, 1.	0.5	7
106	A DFT study of the mechanism of NHC catalysed annulation reactions involving Î±,Î²-unsaturated acyl azoliums and Î²-naphthol. Organic and Biomolecular Chemistry, 2016, 14, 8338-8345.	1.5	11
107	Aromaticity in Pericyclic Transition State Structures? A Critical Rationalisation Based on the Topological Analysis of Electron Density. ChemistrySelect, 2016, 1, 6026-6039.	0.7	18
108	A DFT study of [3 + 2] cycloaddition reactions of an azomethine imine with N-vinyl pyrrole and N-vinyl tetrahydroindole. Journal of Molecular Graphics and Modelling, 2016, 70, 296-304.	1.3	17

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109	Understanding the carbenoid-type reactivity of nitrile ylides in [3+2] cycloaddition reactions towards electron-deficient ethylenes: a molecular electron density theory study. Theoretical Chemistry Accounts, 2016, 135, 1.	0.5	23
110	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
111	Theoretical study of the regio- and stereoselectivity of the intramolecular Povarov reactions yielding 5H-chromeno[2,3-c] acridine derivatives. RSC Advances, 2016, 6, 15759-15769.	1.7	10
112	Understanding the [2n+2n] reaction mechanism between a carbenoid intermediate and CO₂. Molecular Physics, 2016, 114, 1374-1391.	0.8	20
113	A new model for Câ€“C bond formation processes derived from the Molecular Electron Density Theory in the study of the mechanism of [3+2] cycloaddition reactions of carbenoid nitrile ylides with electron-deficient ethylenes. Tetrahedron, 2016, 72, 1524-1532.	1.0	62
114	Analysis of mebendazole binding to its target biomolecule by laser flash photolysis. Journal of Photochemistry and Photobiology B: Biology, 2016, 155, 1-6.	1.7	7
115	Diels-Alderase Catalyzing the Cyclization Step in the Biosynthesis of Spinosyn A. , 2015, , 169-201.		0
116	Synthesis, molecular structure and stability of fused bicyclic Î”4-1,2,4-oxadiazoline Pt(II) complexes. Polyhedron, 2015, 98, 55-63.	1.0	7
117	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
118	Efficient Synthesis of 5â€Chalcogenylâ€1,3â€oxazinâ€2â€ones by Chalcogenâ€Mediated Yneâ€“Carbamate Cyclisation: An Experimental and Theoretical Study. European Journal of Organic Chemistry, 2015, 2015, 1020-1027.	1.2	16
119	A mechanistic study of the participation of azomethine ylides and carbonyl ylides in [3+2] cycloaddition reactions. Tetrahedron, 2015, 71, 1050-1057.	1.0	24
120	A DFT study of the ionic [2+2] cycloaddition reactions of keteniminium cations with terminal acetylenes. Tetrahedron, 2015, 71, 2421-2427.	1.0	24
121	A bonding evolution theory study of the mechanism of [3+2] cycloaddition reactions of nitrones with electron-deficient ethylenes. RSC Advances, 2015, 5, 58464-58477.	1.7	53
122	A DFT study of the role of the Lewis acid catalysts in the [3 + 2] cycloaddition reaction of the electrophilic nitrone isomer of methyl glyoxylate oxime with nucleophilic cyclopentene. RSC Advances, 2015, 5, 64098-64105.	1.7	22
123	A DFT Study of Interâ€and Intramolecular Aryne Ene Reactions. European Journal of Organic Chemistry, 2015, 2015, 2826-2834.	1.2	28
124	A computational and conceptual DFT study on the mechanism of hydrogen activation by novel frustrated Lewis pairs. Physical Chemistry Chemical Physics, 2015, 17, 10715-10725.	1.3	20
125	Understanding the role of the trifluoromethyl group in reactivity and regioselectivity in [3+2] cycloaddition reactions of enol acetates with nitrones. A DFT study. Journal of Molecular Modeling, 2015, 21, 104.	0.8	5
126	A Combined Experimental and Theoretical Study of the Ammonium Bifluoride Catalyzed Regioselective Synthesis of Quinoxalines and Pyrido[2,3-b]pyrazines. Synthesis, 2015, 47, 2680-2689.	1.2	21

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127	Unravelling the mechanism of the ketene-imine Staudinger reaction. An ELF quantum topological analysis. RSC Advances, 2015, 5, 37119-37129.	1.7	23
128	Understanding the participation of 3-nitropyridine in polar Dielsâ€“Alder reactions. A DFT study. Computational and Theoretical Chemistry, 2015, 1072, 37-42.	1.1	13
129	A DFT study of the mechanism of BrÃ¸nsted acid catalysed Povarov reactions. Tetrahedron, 2015, 71, 9339-9345.	1.0	18
130	Understanding the high reactivity of carbonyl compounds towards nucleophilic carbenoid intermediates generated from carbene isocyanides. RSC Advances, 2015, 5, 84797-84809.	1.7	21
131	Non-classical CHâ‹¯O hydrogen-bond determining the regio- and stereoselectivity in the [3 + 2] cycloaddition reaction of (Z)-C-phenyl-N-methylnitrone with dimethyl 2-benzylidenecyclopropane-1,1-dicarboxylate. A topological electron-density study. RSC Advances, 2015, 5, 99299-99311.	1.7	36
132	Polar Dielsâ€“Alder reactions using electrophilic nitrobenzothiophenes. A combined experimental and DFT study. Journal of Molecular Structure, 2015, 1079, 47-53.	1.8	26
133	WHY DIELS-ALDER REACTIONS ARE NON-CONCERTED PROCESSES. Journal of the Chilean Chemical Society, 2014, 59, 2615-2618.	0.5	11
134	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
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