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	Understanding the Reactivity of Captodative Ethylenes in Polar Cycloaddition Reactions. A Theoretical Study. Journal of Organic Chemistry, 2008, 73, 4615-4624.	1.7	846
2	Quantitative characterization of the global electrophilicity power of common diene/dienophile pairs in Dielsâ€“Alder reactions. Tetrahedron, 2002, 58, 4417-4423.	1.0	832
3	Applications of the Conceptual Density Functional Theory Indices to Organic Chemistry Reactivity. Molecules, 2016, 21, 748.	1.7	795
4	Understanding the local reactivity in polar organic reactions through electrophilic and nucleophilic Parr functions. RSC Advances, 2013, 3, 1486-1494.	1.7	628
5	A new Câ€“C bond formation model based on the quantum chemical topology of electron density. RSC Advances, 2014, 4, 32415-32428.	1.7	473
6	The nucleophilicity N index in organic chemistry. Organic and Biomolecular Chemistry, 2011, 9, 7168.	1.5	449
7	Understanding the mechanism of polar Dielsâ€“Alder reactions. Organic and Biomolecular Chemistry, 2009, 7, 3576.	1.5	427
8	A further exploration of a nucleophilicity index based on the gas-phase ionization potentials. Computational and Theoretical Chemistry, 2008, 865, 68-72.	1.5	367
9	Quantitative Characterization of the Local Electrophilicity of Organic Molecules. Understanding the Regioselectivity on Dielsâ^'Alder Reactions. Journal of Physical Chemistry A, 2002, 106, 6871-6875.	1.1	357
10	Molecular Electron Density Theory: A Modern View of Reactivity in Organic Chemistry. Molecules, 2016, 21, 1319.	1.7	324
11	Quantitative characterization of the global electrophilicity pattern of some reagents involved in 1,3-dipolar cycloaddition reactions. Tetrahedron, 2003, 59, 3117-3125.	1.0	301
12	Understanding the Participation of Quadricyclane as Nucleophile in Polar [2Ïƒ + 2Ïƒ + 2Ï€] Cycloadditions toward Electrophilic Ï€ Molecules. Journal of Organic Chemistry, 2008, 73, 8791-8799.	1.7	220
13	A condensed-to-atom nucleophilicity index. An application to the director effects on the electrophilic aromatic substitutions. Computational and Theoretical Chemistry, 2009, 895, 86-91.	1.5	199
14	New Highly Asymmetric Henry Reaction Catalyzed by Cu^{II} and a C₁â€Symmetric Aminopyridine Ligand, and Its Application to the Synthesis of Miconazole. Chemistry - A European Journal, 2008, 14, 4725-4730.	1.7	177
15	Unravelling the Mysteries of the [3+2] Cycloaddition Reactions. European Journal of Organic Chemistry, 2019, 2019, 267-282.	1.2	171
16	Understanding Reaction Mechanisms in Organic Chemistry from Catastrophe Theory Applied to the Electron Localization Function Topology. Journal of Physical Chemistry A, 2008, 112, 7128-7136.	1.1	165
17	A theoretical study on the regioselectivity of 1,3-dipolar cycloadditions using DFT-based reactivity indexes. Tetrahedron, 2004, 60, 11503-11509.	1.0	150
18	The Joint Use of Catastrophe Theory and Electron Localization Function to Characterize Molecular Mechanisms. A Density Functional Study of the Dielsâ^'Alder Reaction between Ethylene and 1,3-Butadiene. Journal of Physical Chemistry A, 2003, 107, 6014-6024.	1.1	149

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19	Influence of Reactant Polarity on the Course of the Inverse-Electron-Demand Dielsâ^'Alder Reaction. A DFT Study of Regio- and Stereoselectivity, Presence of Lewis Acid Catalyst, and Inclusion of Solvent Effects in the Reaction between Nitroethene and Substituted Ethenes. Journal of Organic Chemistry, 1999, 64, 5867-5875.	1.7	136
20	Global and local reactivity indices for electrophilic/nucleophilic free radicals. Organic and Biomolecular Chemistry, 2013, 11, 4350.	1.5	136
21	New Findings on the Dielsâ^'Alder Reactions. An Analysis Based on the Bonding Evolution Theory. Journal of Physical Chemistry A, 2006, 110, 13939-13947.	1.1	128
22	Understanding the High Reactivity of the Azomethine Ylides in [3 + 2] Cycloaddition Reactions. Letters in Organic Chemistry, 2010, 7, 432-439.	0.2	127
23	Origin of the Synchronicity on the Transition Structures of Polar Dielsâ^'Alder Reactions. Are These Reactions [4 + 2] Processes?. Journal of Organic Chemistry, 2003, 68, 3884-3890.	1.7	119
24	On the nature of Parr functions to predict the most reactive sites along organic polar reactions. Chemical Physics Letters, 2013, 582, 141-143.	1.2	116
25	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
26	Chapter 9 The electrophilicity index in organic chemistry. Theoretical and Computational Chemistry, 2007, , 139-201.	0.2	101
27	An Understanding of the Electrophilic/Nucleophilic Behavior of Electro-Deficient 2,3-Disubstituted 1,3-Butadienes in Polar Dielsâ^'Alder Reactions. A Density Functional Theory Study. Journal of Physical Chemistry A, 2008, 112, 4046-4053.	1.1	100
28	Understanding the mechanisms of [3+2] cycloaddition reactions. The pseudoradical versus the zwitterionic mechanism. Tetrahedron, 2014, 70, 1267-1273.	1.0	95
29	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
30	Density functional theory study of the mechanism of the proline-catalyzed intermolecular aldol reaction. Theoretical Chemistry Accounts, 2002, 108, 232-239.	0.5	93
31	Toward an Understanding of the Unexpected Regioselective Hetero-Dielsâ^'Alder Reactions of Asymmetric Tetrazines with Electron-Rich Ethylenes: A DFT Study. Journal of Organic Chemistry, 2009, 74, 2726-2735.	1.7	92
32	Enhancing Reactivity of Carbonyl Compounds via Hydrogen-Bond Formation. A DFT Study of the Hetero-Dielsâ^'Alder Reaction between Butadiene Derivative and Acetone in Chloroform. Journal of Organic Chemistry, 2003, 68, 8662-8668.	1.7	91
33	Understanding the Electronic Reorganization along the Nonpolar [3 + 2] Cycloaddition Reactions of Carbonyl Ylides.. Journal of Organic Chemistry, 2011, 76, 373-379.	1.7	89
34	Understanding the mechanism of non-polar Dielsâ€"Alder reactions. A comparative ELF analysis of concerted and stepwise diradical mechanisms. Organic and Biomolecular Chemistry, 2010, 8, 5495.	1.5	85
35	Density Functional Theory Study of the Cycloaddition Reaction of Furan Derivatives with Maskedo-Benzoquinones. Does the Furan Act as a Dienophile in the Cycloaddition Reaction?. Journal of Organic Chemistry, 2002, 67, 959-965.	1.7	84
36	Reactivity of the carbonâ€"carbon double bond towards nucleophilic additions. A DFT analysis. Tetrahedron, 2004, 60, 6585-6591.	1.0	84

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37	A density functional theory study for the Dielsâ€“Alder reaction between N-acyl-1-aza-1,3-butadienes and vinylamines. Lewis acid catalyst and solvent effects. Tetrahedron, 2002, 58, 3765-3774.	1.0	81
38	Electronic Contributions to the Ïƒpparameter of the Hammett Equation. Journal of Organic Chemistry, 2003, 68, 6060-6062.	1.7	80
39	Describing the Molecular Mechanism of Organic Reactions by Using Topological Analysis of Electronic Localization Function. Current Organic Chemistry, 2011, 15, 3566-3575.	0.9	79
40	Understanding the kinetic solvent effects on the 1,3â€dipolar cycloaddition of benzonitrile Nâ€oxide: a DFT study. Journal of Physical Organic Chemistry, 2011, 24, 611-618.	0.9	79
41	Density Functional Theory Study for the Cycloaddition of 1,3-Butadienes with Dimethyl Acetylenedicarboxylate. Polar Stepwise vs Concerted Mechanisms. Journal of Physical Chemistry A, 2002, 106, 952-961.	1.1	77
42	A Molecular Electron Density Theory Study of the Reactivity of Azomethine Imine in [3+2] Cycloaddition Reactions. Molecules, 2017, 22, 750.	1.7	76
43	Theoretical Study of the 1,3-Dipolar Cycloaddition Reactions of Azomethine Ylides. A DFT Study of Reaction between Trifluoromethyl Thiomethyl Azomethine Ylide and Acronitrile. Journal of Organic Chemistry, 1999, 64, 3922-3929.	1.7	71
44	An Analysis of the Regioselectivity of 1,3â€Dipolar Cycloaddition Reactions of Benzonitrile Nâ€Oxides Based on Global and Local Electrophilicity and Nucleophilicity Indices. European Journal of Organic Chemistry, 2009, 2009, 3036-3044.	1.2	71
45	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
46	Understanding local electrophilicity/nucleophilicity activation through a single reactivity difference index. Organic and Biomolecular Chemistry, 2012, 10, 2855.	1.5	68
47	A DFT analysis of the participation of zwitterionic TACs in polar [3+2] cycloaddition reactions. Tetrahedron, 2014, 70, 4519-4525.	1.0	68
48	Stereoselective 1,3-Dipolar Cycloadditions of a Chiral Nitrone Derived from Erythrulose. An Experimental and DFT Theoretical Study. Journal of Organic Chemistry, 2000, 65, 7000-7009.	1.7	67
49	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
50	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
51	A DFT study of the Huisgen 1,3-dipolar cycloaddition between hindered thiocarbonyl ylides and tetracyanoethylene. Tetrahedron, 2004, 60, 5053-5058.	1.0	63
52	Complementarity of reaction force and electron localization function analyses of asynchronicity in bond formation in Dielsâ€“Alder reactions. Physical Chemistry Chemical Physics, 2014, 16, 6726.	1.3	62
53	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
54	Toward an Understanding of Molecular Mechanism of Domino Cycloadditions. Density Functional Theory Study of the Reaction between Hexafluorobut-2-yne andN,Nâ€˜-Dipyrrolylmethane. Journal of the American Chemical Society, 1998, 120, 1617-1618.	6.6	60

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55	Understanding the mechanism of the N-heterocyclic carbene-catalyzed ring-expansion of 4-formyl-Î²-lactams to succinimide derivatives. Tetrahedron, 2009, 65, 3432-3440.	1.0	59
56	A DFT study of the polar Dielsâ€“Alder reaction between 4-aza-6-nitrobenzofuroxan and cyclopentadiene. Tetrahedron, 2005, 61, 7359-7365.	1.0	57
57	1,3-Dipolar Cycloadditions of Electrophilically Activated Benzonitrile N-Oxides. Polar Cycloaddition versus Oxime Formation. Journal of Organic Chemistry, 2006, 71, 9319-9330.	1.7	56
58	Understanding the mechanism of stereoselective synthesis of cyclopentenes via N-heterocyclic carbene catalyzed reactions of enals with enones. Organic and Biomolecular Chemistry, 2010, 8, 4884.	1.5	56
59	Understanding the mechanism of the Povarov reaction. A DFT study. RSC Advances, 2014, 4, 25268.	1.7	54
60	Understanding the origin of the asynchronicity in bond-formation in polar cycloaddition reactions. A DFT study of the 1,3-dipolar cycloaddition reaction of carbonyl ylides with 1,2-benzoquinones. RSC Advances, 2012, 2, 1334-1342.	1.7	53
61	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
62	Synthesis of (+)-podocarp-8(14)-en-13-one and methyl-(+)-13-oxo-podocarp-8(14)-en-18-oate from abietic acid. Tetrahedron, 1985, 41, 4937-4940.	1.0	52
63	Understanding the regioselectivity in hetero Dielsâ€“Alder reactions. AnÂELF analysis of the reaction between nitrosoethylene and 1-vinylpyrrolidine. Tetrahedron, 2013, 69, 107-114.	1.0	52
64	Theoretical Study of the Gas Phase Decomposition of Glycolic, Lactic, and 2-Hydroxyisobutyric Acids. Journal of the American Chemical Society, 1997, 119, 6415-6422.	6.6	51
65	A Theoretical Study of the Molecular Mechanism of the Reaction betweenN,N-Dimethylmethyleneammonium Cation and Cyclopentadiene. Journal of Organic Chemistry, 2001, 66, 3211-3214.	1.7	51
66	Origin of the synchronicity in bond formation in polar Dielsâ€“Alder reactions: an ELF analysis of the reaction between cyclopentadiene and tetracyanoethylene. Organic and Biomolecular Chemistry, 2012, 10, 3841.	1.5	51
67	Toward an Understanding of the Molecular Mechanism of the Reaction between 1-Methylpyrrole and Dimethyl Acetylenedicarboxylate. An ab Initio Study. Journal of Organic Chemistry, 1998, 63, 9183-9189.	1.7	50
68	Density functional theory study of the Lewis acid-catalyzed Diels-Alder reaction of nitroalkenes with vinyl ethers using aluminum derivatives. Journal of Physical Organic Chemistry, 2002, 15, 660-666.	0.9	50
69	Why do Electron-Deficient Dienes React Rapidly in Diels?Alder Reactions with Electron-Deficient Ethylenes? A Density Functional Theory Analysis. European Journal of Organic Chemistry, 2004, 2004, 4788-4793.	1.2	49
70	A Combined Experimental and Theoretical Study of the Polar [3 + 2] Cycloaddition of Electrophilically Activated Carbonyl Ylides with Aldehydes and Imines. Journal of Organic Chemistry, 2009, 74, 2120-2133.	1.7	49
71	Towards an intrinsic nucleofugality scale: The leaving group (LG) ability in CH3LG model system. Chemical Physics Letters, 2006, 420, 95-99.	1.2	48
72	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

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73	Nonlocal (Pair Site) Reactivity from Second-Order Static Density Response Function:â€‰Gas- and Solution-Phase Reactivity of the Acetaldehyde Enolate as a Test Case. Journal of Physical Chemistry A, 1999, 103, 1367-1375.	1.1	46
74	Photoreaction between 2-Benzoylthiophene and Phenol or Indole. Journal of Organic Chemistry, 2003, 68, 5104-5113.	1.7	46
75	A comparative analysis of the electrophilicity of organic molecules between the computed IPs and EAs and the HOMO and LUMO energies. Chemical Physics Letters, 2007, 438, 341-345.	1.2	46
76	Understanding the cooperative NHC/LA catalysis for stereoselective annulation reactions with homoenolates. A DFT study. Organic and Biomolecular Chemistry, 2011, 9, 6616.	1.5	45
77	Why Do Five-Membered Heterocyclic Compounds Sometimes Not Participate in Polar Dielsâ€“Alder Reactions?. Journal of Organic Chemistry, 2013, 78, 2462-2471.	1.7	45
78	Theoretical Study of the Elimination Kinetics of Carboxylic Acid Derivatives in the Gas Phase. Decomposition of 2-Chloropropionic Acid. Journal of Physical Chemistry A, 1997, 101, 1859-1865.	1.1	44
79	Biosynthesis of the Brevianamides. Anab InitioStudy of the Biosynthetic Intramolecular Dielsâ€Alder Cycloaddition. Journal of Organic Chemistry, 1997, 62, 1662-1667.	1.7	44
80	Towards an Understanding of the Polar Dielsâ€“Alder Reactions of Nitrosoalkenes with Enamines: A Theoretical Study. European Journal of Organic Chemistry, 2006, 2006, 2570-2580.	1.2	44
81	Nature of the ringâ€closure process along the rearrangement of octaâ€1,3,5,7â€tetraene to cyclooctaâ€1,3,5â€triene from the perspective of the electron localization function and catastrophe theory. Journal of Computational Chemistry, 2012, 33, 748-756.	1.5	44
82	Toward an Understanding of the Catalytic Role of Hydrogen-Bond Donor Solvents in the Hetero-Dielsâ€Alder Reaction between Acetone and Butadiene Derivative. Journal of Physical Chemistry A, 2005, 109, 10438-10444.	1.1	43
83	A Theoretical Study of the Reaction between Cyclopentadiene and Protonated Imine Derivatives:Â A Shift from a Concerted to a Stepwise Molecular Mechanism. Journal of Organic Chemistry, 2001, 66, 6151-6157.	1.7	41
84	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
85	Studies on the Biosynthesis of Paraherquamide A and VM99955. A Theoretical Study of Intramolecular Dielsâ€Alder Cycloaddition. Journal of Organic Chemistry, 2003, 68, 2895-2902.	1.7	40
86	Lewis Acid-Catalyzed [4 + 3] Cycloaddition of 2-(Trimethyl Silyloxy)acrolein with Furan. Insight on the Nature of the Mechanism from a DFT Analysis. Organic Letters, 2003, 5, 4117-4120.	2.4	39
87	Ring Expansion versus Cyclization in 4â€Oxoazetidineâ€2â€carbaldehydes Catalyzed by Molecular Iodine: Experimental and Theoretical Study in Concert. Advanced Synthesis and Catalysis, 2010, 352, 1688-1700.	2.1	39
88	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
89	Toward an understanding of the 1,3-dipolar cycloaddition between diphenylnitrone and a maleimide:bisamide complex. A DFT analysis of the reactivity of symmetrically substituted dipolarophiles. Computational and Theoretical Chemistry, 2007, 811, 125-133.	1.5	38
90	The domino reaction between 4,6-dinitrobenzofuroxan and cyclopentadiene. Insights on the nature of the molecular mechanism. Computational and Theoretical Chemistry, 2004, 709, 45-52.	1.5	37

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91	Density functional theory study of the 5-pyrrolidin-2-yltetrazole-catalyzed aldol reaction. Tetrahedron: Asymmetry, 2005, 16, 2764-2770.	1.8	37
92	Understanding the role of the Lewis acid catalyst on the 1,3-dipolar cycloaddition of N-benzylideneaniline N-oxide with acrolein: a DFT study. Tetrahedron, 2007, 63, 4464-4471.	1.0	37
93	Triplet Reactivity and Regio-/Stereoselectivity in the Macrocyclization of Diastereomeric Ketoprofenâ˜Quencher ConjugatesviaRemote Hydrogen Abstractions. Journal of the American Chemical Society, 2007, 129, 7407-7420.	6.6	36
94	Understanding the polar mechanism of the ene reaction. A DFT study. Organic and Biomolecular Chemistry, 2014, 12, 7581-7590.	1.5	36
95	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
96	The carbenoid-type reactivity of simplest nitrile imine from a molecular electron density theory perspective. Tetrahedron, 2019, 75, 1961-1967.	1.0	36
97	A DFT study of the Dielsâ€“Alder reaction between methyl acrolein derivatives and cyclopentadiene. Understanding the effects of Lewis acids catalysts based on sulfur containing boron heterocycles. Tetrahedron, 2006, 62, 5502-5509.	1.0	35
98	Understanding the Mechanism of the Intramolecular Stetter Reaction. A DFT Study. Molecules, 2012, 17, 1335-1353.	1.7	34
99	Unveiling the Lewis Acid Catalyzed Dielsâ€“Alder Reactions Through the Molecular Electron Density Theory. Molecules, 2020, 25, 2535.	1.7	34
100	Theoretical Study of the Reaction of Dimethyl Acetylenedicarboxylate with 1-Methyl-2-(1-substituted) Tj ETQq0 0 0 rgBT /Overlock 10 Tf	1.0	33
101	Theoretical study of the solvent effects on the mechanisms of addition of dimethyl acetylenedicarboxylate to 1-methyl-2-vinylpyrrole. Tetrahedron, 1996, 52, 10693-10704.	1.0	33
102	Comparative theoretical study of transition structures, barrier heights, and reaction energies for the intramolecular tautomerization in acetaldehyde/vinyl alcohol and acetaldimine/vinylamine systems. International Journal of Quantum Chemistry, 1998, 66, 9-24.	1.0	33
103	A DFT Characterization of the Mechanism for the Cycloaddition Reaction between 2-Methylfuran and Acetylenedicarboxylic Acid. Journal of Physical Chemistry A, 1999, 103, 11425-11430.	1.1	33
104	Theoretical Study of the Mechanisms for the Alkoxyacetic Acids Decomposition. Journal of Physical Chemistry A, 1999, 103, 3935-3943.	1.1	33
105	Effect of electron-withdrawing substituents on the electrophilicity of carbonyl carbons. Tetrahedron, 2005, 61, 417-422.	1.0	33
106	A combined experimental and theoretical study of the thermal cycloaddition of aryl azides with activated alkenes. Organic and Biomolecular Chemistry, 2011, 9, 4295.	1.5	33
107	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
108	On Transition Structures for Hydride Transfer Step: A Theoretical Study of the Reaction Catalyzed by Dihydrofolate Reductase Enzyme. Bioorganic Chemistry, 1996, 24, 10-18.	2.0	32

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109	Ab InitioStudy of Stereo- and Regioselectivity in the Dielsâ^'Alder Reaction between 2-Phenylcyclopentadiene and Î±-(Methylthio)acrylonitrile. Journal of Organic Chemistry, 1997, 62, 1775-1778.	1.7	32
110	Potential energy surface for the decomposition of mandelic acid. Chemical Physics Letters, 1997, 274, 422-428.	1.2	32
111	A DFT study for the regioselective 1,3-dipolar cycloadditions of nitrile N-oxides toward alkynylboronates. Tetrahedron, 2003, 59, 9167-9171.	1.0	32
112	Toward an Understanding of the Acceleration of Dielsâ^'Alder Reactions by a Pseudo-intramolecular Process Achieved by Molecular Recognition. A DFT Study. Journal of Organic Chemistry, 2007, 72, 4220-4227.	1.7	32
113	A DFT study of the asymmetric (S)-5-(pyrrolidin-2-yl)-1H-tetrazole catalyzed Michael addition of carbonyl compounds to nitroalkenes. Tetrahedron: Asymmetry, 2007, 18, 157-164.	1.8	32
114	Experimental and theoretical study on the substitution reactions of aryl 2,4-dinitrophenyl carbonates with quinuclidines. Tetrahedron, 2006, 62, 2555-2562.	1.0	31
115	Understanding the regio- and chemoselective polar [3+2] cycloaddition of the Padwa carbonyl ylides with Î±-methylene ketones. A DFT study. Tetrahedron, 2009, 65, 4644-4651.	1.0	31
116	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
117	Stereoselection Parameters and Theoretical Model in the Enantioselective Protonation of Enolates with Î±-Sulfinyl Alcohols. Journal of Organic Chemistry, 1998, 63, 9342-9347.	1.7	30
118	Polar [3 + 2] cycloaddition of ketones with electrophilically activated carbonyl ylides. Synthesis of spirocyclic dioxolane indolinones. Organic and Biomolecular Chemistry, 2008, 6, 3144.	1.5	30
119	Experimental and Theoretical Studies on the Radical-Cation-Mediated Imino-Dielsâ€"Alder Reaction. Organic Letters, 2011, 13, 5116-5119.	2.4	30
120	Controlled Rearrangement of Lactamâ€Tethered Allenols with Brominating Reagents: A Combined Experimental and Theoretical Study on Î±â€•versus Î²â€Keto Lactam Formation. Chemistry - A European Journal, 2011, 17, 11559-11566.	1.7	30
121	A DFT study on the NHC catalysed Michael addition of enols to Î±,Î²-unsaturated acyl-azoliums. A base catalysed Câ€"C bond-formation step. Organic and Biomolecular Chemistry, 2014, 12, 895-904.	1.5	30
122	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
123	Remarkable effect of lithium bromide in the enantioselective protonation with Î±-sulfinyl alcohols. Tetrahedron Letters, 1998, 39, 3277-3280.	0.7	29
124	Diastereomeric Differentiation in the Quenching of Excited States by Hydrogen Donors. Angewandte Chemie - International Edition, 2003, 42, 2531-2534.	7.2	29
125	Ï€-Strain-Induced Electrophilicity in Small Cycloalkynes: A DFT Analysis of the Polar Cycloaddition of Cyclopentyne towards Enol Ethers. European Journal of Organic Chemistry, 2006, 2006, 498-506.	1.2	28
126	A DFT Study of the [3 + 2] versus [4 + 2] Cycloaddition Reactions of 1,5,6-Trimethylpyrazinium-3-olate with Methyl Methacrylate. Journal of Organic Chemistry, 2013, 78, 1621-1629.	1.7	28

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127	A DFT Study of Interâ€•and Intramolecular Aryne Ene Reactions. European Journal of Organic Chemistry, 2015, 2015, 2826-2834.	1.2	28
128	Understanding the Nature of the Molecular Mechanisms Associated with the Competitive Lewis Acid Catalyzed[4+2] and[4+3] Cycloadditions between Arylidenoxazolone Systems and Cyclopentadiene: A DFT Analysis. Chemistry - A European Journal, 2004, 10, 4742-4749.	1.7	27
129	Mechanistic details of the domino reaction of nitronaphthalenes with the electron-rich dienes. A DFT study. Computational and Theoretical Chemistry, 2008, 853, 68-76.	1.5	27
130	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
131	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
132	Electronic fluxes during dielsâ€alder reactions involving 1,2â€benzoquinones: mechanistic insights from the analysis of electron localization function and catastrophe theory. Journal of Computational Chemistry, 2012, 33, 2400-2411.	1.5	26
133	The mechanism of ionic Dielsâ€“Alder reactions. A DFT study of the oxa-Povarov reaction. RSC Advances, 2014, 4, 16567-16577.	1.7	26
134	Polar Dielsâ€“Alder reactions using electrophilic nitrobenzothiophenes. A combined experimental and DFT study. Journal of Molecular Structure, 2015, 1079, 47-53.	1.8	26
135	A combined experimental and theoretical study of the unimolecular elimination kinetics of 2-alkoxypropionic acids in the gas phase. Chemical Physics, 1999, 246, 1-12.	0.9	25
136	A DFT Study of the Domino Inter [4 + 2]/Intra [3 + 2] Cycloaddition Reactions of Nitroalkenes with Enol Ethers. Journal of Organic Chemistry, 2000, 65, 1076-1083.	1.7	25
137	DFT Study of the Molecular Mechanism of Lewis Acid Induced [4 + 3] Cycloadditions of 2-Alkylacroleins with Cyclopentadiene. Journal of Organic Chemistry, 2009, 74, 5934-5940.	1.7	25
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