

JosÃ© A SÃ¡ez

List of Publications by Year in descending order

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52
papers

2,659
citations

201385

27
h-index

182168

51
g-index

55
all docs

55
docs citations

55
times ranked

1989
citing authors

#	ARTICLE	IF	CITATIONS
1	Understanding the local reactivity in polar organic reactions through electrophilic and nucleophilic Parr functions. <i>RSC Advances</i> , 2013, 3, 1486-1494.	1.7	628
2	Understanding the mechanism of polar Diels-Alder reactions. <i>Organic and Biomolecular Chemistry</i> , 2009, 7, 3576.	1.5	427
3	Understanding the Participation of Quadricyclane as Nucleophile in Polar $[2i^f + 2i^f + 2i^e]$ Cycloadditions toward Electrophilic i^e Molecules. <i>Journal of Organic Chemistry</i> , 2008, 73, 8791-8799.	1.7	220
4	Toward an Understanding of the Unexpected Regioselective Hetero-Diels-Alder Reactions of Asymmetric Tetrazines with Electron-Rich Ethylenes: A DFT Study. <i>Journal of Organic Chemistry</i> , 2009, 74, 2726-2735.	1.7	92
5	Understanding the Electronic Reorganization along the Nonpolar $[3 + 2]$ Cycloaddition Reactions of Carbonyl Ylides. <i>Journal of Organic Chemistry</i> , 2011, 76, 373-379.	1.7	89
6	1,3-Dipolar Cycloadditions of Electrophilically Activated Benzonitrile N-Oxides. Polar Cycloaddition versus Oxime Formation. <i>Journal of Organic Chemistry</i> , 2006, 71, 9319-9330.	1.7	56
7	Understanding the mechanism of the Povarov reaction. A DFT study. <i>RSC Advances</i> , 2014, 4, 25268.	1.7	54
8	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. <i>RSC Advances</i> , 2012, 2, 1334-1342.	1.7	53
9	Understanding the regioselectivity in hetero Diels-Alder reactions. An ELF analysis of the reaction between nitrosoethylene and 1-vinylpyrrolidine. <i>Tetrahedron</i> , 2013, 69, 107-114.	1.0	52
10	Origin of the synchronicity in bond formation in polar Diels-Alder reactions: an ELF analysis of the reaction between cyclopentadiene and tetracyanoethylene. <i>Organic and Biomolecular Chemistry</i> , 2012, 10, 3841.	1.5	51
11	A Combined Experimental and Theoretical Study of the Polar $[3 + 2]$ Cycloaddition of Electrophilically Activated Carbonyl Ylides with Aldehydes and Imines. <i>Journal of Organic Chemistry</i> , 2009, 74, 2120-2133.	1.7	49
12	A comparative analysis of the electrophilicity of organic molecules between the computed IPs and EAs and the HOMO and LUMO energies. <i>Chemical Physics Letters</i> , 2007, 438, 341-345.	1.2	46
13	Supramolecular hydrogels for enzymatically triggered self-immolative drug delivery. <i>Tetrahedron</i> , 2010, 66, 2614-2618.	1.0	46
14	Selective catechol-triggered supramolecular gel disassembly. <i>Chemical Communications</i> , 2010, 46, 7996.	2.2	42
15	Stereoisomerization of β -Hydroxy- α -sulfonyl- γ -butyrolactones Controlled by Two Concomitant 1,4-Type Nonbonded Sulfur-Oxygen Interactions As Analyzed by X-ray Crystallography. <i>Journal of Organic Chemistry</i> , 2010, 75, 5888-5894.	1.7	40
16	Lewis Acid-Catalyzed $[4 + 3]$ Cycloaddition of 2-(Trimethyl Silyloxy)acrolein with Furan. Insight on the Nature of the Mechanism from a DFT Analysis. <i>Organic Letters</i> , 2003, 5, 4117-4120.	2.4	39
17	Toward an understanding of the 1,3-dipolar cycloaddition between diphenylnitrene and a maleimide:bisamide complex. A DFT analysis of the reactivity of symmetrically substituted dipolarophiles. <i>Computational and Theoretical Chemistry</i> , 2007, 811, 125-133.	1.5	38
18	Understanding the Mechanism of the Intramolecular Stetter Reaction. A DFT Study. <i>Molecules</i> , 2012, 17, 1335-1353.	1.7	34

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19	A combined experimental and theoretical study of the thermal cycloaddition of aryl azides with activated alkenes. <i>Organic and Biomolecular Chemistry</i> , 2011, 9, 4295.	1.5	33
20	A DFT study for the regioselective 1,3-dipolar cycloadditions of nitrile N-oxides toward alkynylboronates. <i>Tetrahedron</i> , 2003, 59, 9167-9171.	1.0	32
21	Toward an Understanding of the Acceleration of Diels-Alder Reactions by a Pseudo-intramolecular Process Achieved by Molecular Recognition. A DFT Study. <i>Journal of Organic Chemistry</i> , 2007, 72, 4220-4227.	1.7	32
22	Experimental and theoretical study on the substitution reactions of aryl 2,4-dinitrophenyl carbonates with quinuclidines. <i>Tetrahedron</i> , 2006, 62, 2555-2562.	1.0	31
23	Polar [3 + 2] cycloaddition of ketones with electrophilically activated carbonyl ylides. Synthesis of spirocyclic dioxolane indolinones. <i>Organic and Biomolecular Chemistry</i> , 2008, 6, 3144.	1.5	30
24	Molecular recognition through divalent interactions with a self-assembled fibrillar network of a supramolecular organogel. <i>Organic and Biomolecular Chemistry</i> , 2008, 6, 4378.	1.5	30
25	A DFT study on the NHC catalysed Michael addition of enols to α,β -unsaturated acyl-azoliums. A base catalysed C-C bond-formation step. <i>Organic and Biomolecular Chemistry</i> , 2014, 12, 895-904.	1.5	30
26	Photophysical properties of 5-substituted 2-thiopyrimidines. <i>Photochemical and Photobiological Sciences</i> , 2013, 12, 1460-1465.	1.6	28
27	A DFT Study of the [3 + 2] versus [4 + 2] Cycloaddition Reactions of 1,5,6-Trimethylpyrazinium-3-olate with Methyl Methacrylate. <i>Journal of Organic Chemistry</i> , 2013, 78, 1621-1629.	1.7	28
28	DFT Study of the Molecular Mechanism of Lewis Acid Induced [4 + 3] Cycloadditions of 2-Alkylacroleins with Cyclopentadiene. <i>Journal of Organic Chemistry</i> , 2009, 74, 5934-5940.	1.7	25
29	Understanding C-C bond formation in polar reactions. An ELF analysis of the Friedel-Crafts reaction between indoles and nitroolefins. <i>RSC Advances</i> , 2013, 3, 7520.	1.7	23
30	Unravelling the mechanism of the ketene-imine Staudinger reaction. An ELF quantum topological analysis. <i>RSC Advances</i> , 2015, 5, 37119-37129.	1.7	23
31	An ELF analysis of the C-C bond formation step in the N-heterocyclic carbene-catalyzed hydroacylation of unactivated C=C double bonds. <i>RSC Advances</i> , 2012, 2, 7127.	1.7	21
32	Experimental and theoretical investigations for the tandem alkylation-isomerization reactions between unsaturated carboxylic acids and allyl halides. <i>Tetrahedron</i> , 2003, 59, 6233-6239.	1.0	20
33	Lewis acid induced [4+3] cycloadditions of 2-silyloxyacroleins. Insights on the mechanism from a DFT analysis. <i>Tetrahedron</i> , 2005, 61, 7538-7545.	1.0	20
34	Understanding the formation of [3+2] and [2+4] cycloadducts in the Lewis acid catalysed reaction between methyl glyoxylate oxime and cyclopentadiene: a theoretical study. <i>RSC Advances</i> , 2013, 3, 447-457.	1.7	20
35	Study of the stereoselectivity of the nucleophilic epoxidation of 3-hydroxy-2-methylene esters. <i>Tetrahedron</i> , 2014, 70, 97-102.	1.0	20
36	Understanding the Bond Formation in Hetero-Diels-Alder Reactions. An ELF Analysis of the Reaction of Nitroethylene with Dimethylvinylamine. <i>Current Organic Chemistry</i> , 2012, 16, 2343-2351.	0.9	19

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37	Solvent-free construction of self-assembled 1D nanostructures from low-molecular-weight organogelators: sublimation vs. gelation. <i>Soft Matter</i> , 2009, 5, 3727.	1.2	18
38	Understanding the domino reaction between 3-chloroindoles and methyl coumalate yielding carbazoles. A DFT study. <i>Organic and Biomolecular Chemistry</i> , 2015, 13, 2034-2043.	1.5	15
39	Understanding the selectivity in the formation of β -lactams vs. γ -lactams in the Staudinger reactions of chloro-cyan-ketene with unsaturated imines. A DFT study. <i>RSC Advances</i> , 2014, 4, 58559-58566.	1.7	14
40	Ring splitting of azetidin-2-ones via radical anions. <i>Organic and Biomolecular Chemistry</i> , 2012, 10, 7928.	1.5	13
41	Experimental and theoretical study of the [3 + 2] cycloaddition of carbonyl ylides with alkynes. <i>Organic and Biomolecular Chemistry</i> , 2012, 10, 8434.	1.5	12
42	Protection against chemical submission: naked-eye detection of β -hydroxybutyric acid (GHB) in soft drinks and alcoholic beverages. <i>Chemical Communications</i> , 2020, 56, 12600-12603.	2.2	12
43	A DFT study for the formation of imidazo[1,2-c]pyrimidines through an intramolecular Michael addition. <i>Tetrahedron</i> , 2006, 62, 10408-10416.	1.0	9
44	Formation of pyrazolo[1,3,4-c]thiadiazoles through 1,3-dipolar cycloadditions of 3-thioxo-1,2,4-triazepin-5-one with nitrilimines: an experimental and computational study. <i>Journal of Physical Organic Chemistry</i> , 2009, 22, 31-41.	0.9	8
45	Oxetane Ring Enlargement through Nucleophilic Trapping of Radical Cations by Acetonitrile. <i>Organic Letters</i> , 2012, 14, 5700-5703.	2.4	8
46	Cycloreversion of β -lactams via photoinduced electron transfer. <i>Organic and Biomolecular Chemistry</i> , 2014, 12, 8428-8432.	1.5	8
47	Azo-hydrazo conversion via [1,5]-hydrogen shifts. A combined experimental and theoretical study. <i>Tetrahedron</i> , 2012, 68, 6902-6907.	1.0	7
48	Heteroditopic chemosensor to detect β -hydroxybutyric acid (GHB) in soft drinks and alcoholic beverages. <i>Analyst</i> , The, 2021, 146, 5601-5609.	1.7	5
49	Spermine and Spermidine Detection through Restricted Intramolecular Rotations in a Tetraphenylethylene Derivative. <i>Chemosensors</i> , 2022, 10, 8.	1.8	5
50	Theoretical study on the molecular mechanism of the [5 + 2] vs. [4 + 2] cyclization mediated by Lewis acid in the quinone system. <i>Organic and Biomolecular Chemistry</i> , 2013, 11, 8357.	1.5	2
51	Isomerization and Redox Tuning: Reorganizing the Maya Blue Puzzle from Synthetic, Spectral, and Electrochemical Issues. <i>Journal of Physical Chemistry C</i> , 2021, 125, 26188-26200.	1.5	2
52	Diels-Alderase Catalyzing the Cyclization Step in the Biosynthesis of Spinosyn A. , 2015, , 169-201.		0