JosÃ© JoaquÃn Quirante SÃ¡nchez

List of Publications by Year
in descending order

32 papers	343 citations	840776 11 h-index	888059 17 g-index
33 all docs	33 docs citations	33 times ranked	426 citing authors

#	Article	IF	Citations
1	Raman Spectroscopy Shows Interchain through Space Charge Delocalization in a Mixed Valence Oligothiophene Cation and in Its Ï€-Dimeric Biradicaloid Dication. Journal of the American Chemical Society, 2008, 130, 14028-14029.	13.7	36
2	Molecular conformations and harmonic force field of 1,3,5-benzenetriol molecule from ab initio and density functional theory investigations. Computational and Theoretical Chemistry, 1997, 390, 139-148.	1.5	30
3	Rationalizing the Catalytic Activity of Copper in the Cycloaddition of Azide and Alkynes (CuAAC) with the Topology of â^‡²Ï(r) and â^‡â^‡²Ï(r). Journal of Physical Chemistry B, 2015, 119, 1243-1258.	2.6	28
4	Rearrangement of azirine intermediates to nitriles: Theoretical study of cleavage of 3,4-dihydro-1aH-azirine[2,3-c]pyrrol-2-one to cyanoketene-formaldimine complex. Journal of Computational Chemistry, 1998, 19, 912-922.	3.3	26
5	Hybrid Organic Semiconductors Including Chalcogen Atoms in Ï€-Conjugated Skeletons. Tuning of Optical, Redox, and Vibrational Properties by Heavy Atom Conjugation. Journal of Physical Chemistry A, 2006, 110, 7422-7430.	2.5	25
6	Pericyclic versus Pseudopericyclic Reactions. What the Laplacian of the Charge Density, â^‡²Ï(r), Has To Say about It? The Case of Cycloaddition Reactions. Journal of Physical Chemistry A, 2008, 112, 8164-8178.	2.5	22
7	Influence of the Incorporation of Basic or Amphoteric Oxides on the Performance of Cu-Based Catalysts Supported on Sepiolite in Furfural Hydrogenation. Catalysts, 2019, 9, 315.	3.5	18
8	Ni supported on sepiolite catalysts for the hydrogenation of furfural to value-added chemicals: influence of the synthesis method on the catalytic performance. Topics in Catalysis, 2019, 62, 535-550.	2.8	16
9	The vinylcyclopropane rearrangement: An AM1 study. Computational and Theoretical Chemistry, 1990, 204, 193-200.	1.5	13
10	Structure, polarized micro-Raman and FT-IR spectra, and ab initio calculations of 1,2-dicyanobenzene. The Journal of Physical Chemistry, 1993, 97, 10561-10569.	2.9	13
11	On the regioselectivity of the mononuclear copper-catalyzed cycloaddition of azide and alkynes (CuAAC). A quantum chemical topological study. Journal of Molecular Modeling, 2014, 20, 2187.	1.8	13
12	Harmonic force filed for amino acid L-glutamine by MNDO semiempirical method. Journal of Molecular Structure, 1993, 294, 49-52.	3.6	8
13	Study of the bimolecular pyrolysis of acetic acid by the Austin Model 1 semi-empirical method. Journal of Analytical and Applied Pyrolysis, 1995, 31, 169-175.	5.5	8
14	Synthesis of tetrazole fused azepanes and quantum chemical topology study on the mechanism of the intramolecular cycloaddition reaction. RSC Advances, 2017, 7, 50367-50371.	3.6	8
15	AM1 study of the cycloaddition of singlet methylene to butadiene and the vinylcyclopropane rearrangement. Computational and Theoretical Chemistry, 1992, 254, 493-504.	1.5	7
16	Ab initio theoretical study of thiophene derivatives: 2-methylthiophene and 3-methylthiophene. Journal of Molecular Structure, 1997, 410-411, 311-314.	3.6	7
17	Competition between Wolff Rearrangement and 1,2-Hydrogen Shift in Î²-Oxy-Î±-ketocarbenes:â€‰ Electrostatic and Specific Solvent Effects. Journal of Physical Chemistry B, 1999, 103, 7145-7150.	2.6	7
18	Study of the Interconversion of Isomers of [16]annulene by the AM1 Method. Collection of Czechoslovak Chemical Communications, 1992, 57, 1-6.	1.0	7

#	Article	IF	Citations
19	Study of the interconversion of the isomers of 14-annulene by the AM1 method. Computational and Theoretical Chemistry, 1990, 204, 201-208.	1.5	6
20	Exploring the regioselectivity in the cycloaddition of azides to alkynes catalyzed by dinuclear copper clusters (Cu2AAC reaction) using the topologies of âˆ‡2 Ï•(r) and âˆ‡âˆ‡2 Ï•(r). Journal of Molecular Modeling, 2017, 23, 337.	1.8	6
21	Thermal Fragmentation of 3-Vinyloxetane:â€‰ A Quantum Chemical Study. Journal of Physical Chemistry A, 2003, 107, 2919-2928.	2.5	5
22	Quantum mechanical study and vibrational spectra of indazolium-3-carboxylate and its decarboxylation product, the N-heterocyclic carbene indazol-3-ylidene. Physical Chemistry Chemical Physics, 2009, 11, 341-348.	2.8	5
23	MINDO/3 study of the thermolysis of 2(3H)-furanone. Computational and Theoretical Chemistry, 1989, 183, 143-150.	1.5	4
24	Harmonic force field for the glycine molecule by semiempirical methods. Journal of Molecular Structure, 1992, 268, 249-261.	3.6	4
25	AM1 study of Wolff and 1,2-hydrogen shift rearrangements of Î²-oxy-Î±-Diazo carbonyl compounds. Theoretica Chimica Acta, 1996, 94, 13-22.	0.8	4
26	A Raman and Computational Study of Two Dithienyl Naphthodithiophenes:Â Synthesis and Characterization of New Polymers Showing Low Band Gap Optical and Electroactive Features. Journal of Physical Chemistry B, 2004, 108, 7611-7619.	2.6	4
27	Mindo/3 study of the thermolysis of vinylene carbonate. Computational and Theoretical Chemistry, 1988, 170, 233-237.	1.5	3
28	Theoretical ab initio study of the thermal decomposition of 3-cyclopentenone. Computational and Theoretical Chemistry, 1995, 330, 389-393.	1.5	3
29	An AM1 study of the molecules of [10]annulene and [12]annulene. Computational and Theoretical Chemistry, 1993, 287, 131-138.	1.5	2
30	Study of the thermal decomposition of 3-cyclopentenone by using the AM1 semiempirical method. Theoretica Chimica Acta, 1994, 89, 251-259.	0.8	2
31	The influence of protecting the hydroxyl group of Î²-oxy-Î±-diazo carbonyl compounds in the competition between Wolff rearrangement and [1,2]-hydrogen shift. Density functional theory study and topological analysis of the charge density. Theoretical Chemistry Accounts, 2000, 103, 423-430.	1.4	2
32	Thermolysis of 2-methyloxetane: a computational study. Theoretical Chemistry Accounts, 2011, 128, 327-339.	1.4	1