

# Patricia Perez

## List of Publications by Year in descending order

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136  
papers

10,179  
citations

46918

47  
h-index

34900

98  
g-index

138  
all docs

138  
docs citations

138  
times ranked

4174  
citing authors

#	ARTICLE	IF	CITATIONS
1	Understanding the Reactivity of Captodative Ethylenes in Polar Cycloaddition Reactions. A Theoretical Study. <i>Journal of Organic Chemistry</i> , 2008, 73, 4615-4624.	1.7	846
2	Quantitative characterization of the global electrophilicity power of common diene/dienophile pairs in Diels-Alder reactions. <i>Tetrahedron</i> , 2002, 58, 4417-4423.	1.0	832
3	Applications of the Conceptual Density Functional Theory Indices to Organic Chemistry Reactivity. <i>Molecules</i> , 2016, 21, 748.	1.7	795
4	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
5	The nucleophilicity N index in organic chemistry. <i>Organic and Biomolecular Chemistry</i> , 2011, 9, 7168.	1.5	449
6	A direct evaluation of regional Fukui functions in molecules. <i>Chemical Physics Letters</i> , 1999, 304, 405-413.	1.2	420
7	A further exploration of a nucleophilicity index based on the gas-phase ionization potentials. <i>Computational and Theoretical Chemistry</i> , 2008, 865, 68-72.	1.5	367
8	Quantitative Characterization of the Local Electrophilicity of Organic Molecules. Understanding the Regioselectivity on Diels-Alder Reactions. <i>Journal of Physical Chemistry A</i> , 2002, 106, 6871-6875.	1.1	357
9	On the condensed Fukui function. <i>Journal of Chemical Physics</i> , 2000, 113, 2544-2551.	1.2	345
10	Quantitative characterization of the global electrophilicity pattern of some reagents involved in 1,3-dipolar cycloaddition reactions. <i>Tetrahedron</i> , 2003, 59, 3117-3125.	1.0	301
11	A condensed-to-atom nucleophilicity index. An application to the director effects on the electrophilic aromatic substitutions. <i>Computational and Theoretical Chemistry</i> , 2009, 895, 86-91.	1.5	199
12	A theoretical study on the regioselectivity of 1,3-dipolar cycloadditions using DFT-based reactivity indexes. <i>Tetrahedron</i> , 2004, 60, 11503-11509.	1.0	150
13	Global and local reactivity indices for electrophilic/nucleophilic free radicals. <i>Organic and Biomolecular Chemistry</i> , 2013, 11, 4350.	1.5	136
14	Comparison between Experimental and Theoretical Scales of Electrophilicity in Benzhydryl Cations. <i>Journal of Organic Chemistry</i> , 2002, 67, 4747-4752.	1.7	133
15	Understanding the High Reactivity of the Azomethine Ylides in [3 + 2] Cycloaddition Reactions. <i>Letters in Organic Chemistry</i> , 2010, 7, 432-439.	0.2	127
16	Origin of the Synchronicity on the Transition Structures of Polar Diels-Alder Reactions. Are These Reactions [4 + 2] Processes?. <i>Journal of Organic Chemistry</i> , 2003, 68, 3884-3890.	1.7	119
17	Definition of a Nucleophilicity Scale. <i>Journal of Physical Chemistry A</i> , 2006, 110, 8181-8187.	1.1	116
18	On the nature of Parr functions to predict the most reactive sites along organic polar reactions. <i>Chemical Physics Letters</i> , 2013, 582, 141-143.	1.2	116

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19	A Molecular Electron Density Theory Study of the Reactivity and Selectivities in [3 + 2] Cycloaddition Reactions of <i>C</i> - <i>N</i> -Dialkyl Nitrones with Ethylene Derivatives. <i>Journal of Organic Chemistry</i> , 2018, 83, 2182-2197.	1.7	102
20	Chapter 9 The electrophilicity index in organic chemistry. <i>Theoretical and Computational Chemistry</i> , 2007, , 139-201.	0.2	101
21	An Understanding of the Electrophilic/Nucleophilic Behavior of Electro-Deficient 2,3-Disubstituted 1,3-Butadienes in Polar Diels-Alder Reactions. A Density Functional Theory Study. <i>Journal of Physical Chemistry A</i> , 2008, 112, 4046-4053.	1.1	100
22	A molecular electron density theory study of the participation of tetrazines in aza-Diels-Alder reactions. <i>RSC Advances</i> , 2020, 10, 15394-15405.	1.7	94
23	Empirical Energy-Density Relationships for the Analysis of Substituent Effects in Chemical Reactivity. <i>Journal of the American Chemical Society</i> , 2000, 122, 4756-4762.	6.6	92
24	Understanding the mechanism of non-polar Diels-Alder reactions. A comparative ELF analysis of concerted and stepwise diradical mechanisms. <i>Organic and Biomolecular Chemistry</i> , 2010, 8, 5495.	1.5	85
25	Reactivity of the carbon-carbon double bond towards nucleophilic additions. A DFT analysis. <i>Tetrahedron</i> , 2004, 60, 6585-6591.	1.0	84
26	Condensed-to-atoms electronic Fukui functions within the framework of spin-polarized density-functional theory. <i>Journal of Chemical Physics</i> , 2005, 123, 114107.	1.2	82
27	Electronic Contributions to the $\rho$ -Parameter of the Hammett Equation. <i>Journal of Organic Chemistry</i> , 2003, 68, 6060-6062.	1.7	80
28	Density Functional Theory Study for the Cycloaddition of 1,3-Butadienes with Dimethyl Acetylenedicarboxylate. Polar Stepwise vs Concerted Mechanisms. <i>Journal of Physical Chemistry A</i> , 2002, 106, 952-961.	1.1	77
29	Solvent Effects on Electrophilicity. <i>Journal of the American Chemical Society</i> , 2001, 123, 5527-5531.	6.6	73
30	An Analysis of the Regioselectivity of 1,3-Dipolar Cycloaddition Reactions of Benzonitrile <i>N</i> -Oxides Based on Global and Local Electrophilicity and Nucleophilicity Indices. <i>European Journal of Organic Chemistry</i> , 2009, 2009, 3036-3044.	1.2	71
31	The Mysticism of Pericyclic Reactions: A Contemporary Rationalisation of Organic Reactivity Based on Electron Density Analysis. <i>European Journal of Organic Chemistry</i> , 2018, 2018, 1107-1120.	1.2	69
32	A DFT analysis of the participation of zwitterionic TACs in polar [3+2] cycloaddition reactions. <i>Tetrahedron</i> , 2014, 70, 4519-4525.	1.0	68
33	Ab Initio SCF and DFT Studies on Solvent Effects on Intramolecular Rearrangement Reactions. <i>Journal of Physical Chemistry A</i> , 2001, 105, 4272-4283.	1.1	67
34	Universal mathematical identities in density functional theory: Results from three different spin-resolved representations. <i>Journal of Chemical Physics</i> , 2008, 128, 204108.	1.2	66
35	How does the global electron density transfer diminish activation energies in polar cycloaddition reactions? A Molecular Electron Density Theory study. <i>Tetrahedron</i> , 2017, 73, 1718-1724.	1.0	65
36	Complementarity of reaction force and electron localization function analyses of asynchronicity in bond formation in Diels-Alder reactions. <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 6726.	1.3	62

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37	A new model for C=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. <i>Tetrahedron</i> , 2016, 72, 1524-1532.	1.0	62
38	A comparison between theoretical and experimental models of electrophilicity and nucleophilicity. <i>Computational and Theoretical Chemistry</i> , 2009, 896, 73-79.	1.5	56
39	Characterization of Keto-Enol Tautomerism of Acetyl Derivatives from the Analysis of Energy, Chemical Potential, and Hardness. <i>Journal of Physical Chemistry A</i> , 2000, 104, 1557-1562.	1.1	53
40	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
41	The reaction force constant as an indicator of synchronicity/nonsynchronicity in [4+2] cycloaddition processes. <i>Physical Chemistry Chemical Physics</i> , 2013, 15, 7311.	1.3	53
42	A bonding evolution theory study of the mechanism of [3+2] cycloaddition reactions of nitrones with electron-deficient ethylenes. <i>RSC Advances</i> , 2015, 5, 58464-58477.	1.7	53
43	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
44	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
45	Spin-Philicity and Spin-Donicity as Auxiliary Concepts To Quantify Spin-Catalysis Phenomena. <i>Journal of Physical Chemistry A</i> , 2002, 106, 5353-5357.	1.1	50
46	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
47	Towards an intrinsic nucleofugality scale: The leaving group (LG) ability in CH3LG model system. <i>Chemical Physics Letters</i> , 2006, 420, 95-99.	1.2	48
48	Dual descriptors within the framework of spin-polarized density functional theory. <i>Journal of Chemical Physics</i> , 2008, 129, 064117.	1.2	47
49	Nonlocal (Pair Site) Reactivity from Second-Order Static Density Response Function: Gas- and Solution-Phase Reactivity of the Acetaldehyde Enolate as a Test Case. <i>Journal of Physical Chemistry A</i> , 1999, 103, 1367-1375.	1.1	46
50	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
51	Why Do Five-Membered Heterocyclic Compounds Sometimes Not Participate in Polar Diels-Alder Reactions?. <i>Journal of Organic Chemistry</i> , 2013, 78, 2462-2471.	1.7	45
52	Theoretical Evaluation of the Global and Local Electrophilicity Patterns of Singlet Carbenes. <i>Journal of Physical Chemistry A</i> , 2003, 107, 522-525.	1.1	44
53	A theoretical analysis of the gas-phase protonation of hydroxylamine, methyl-derivatives and aliphatic amino acids. <i>Chemical Physics Letters</i> , 1998, 293, 239-244.	1.2	42
54	A Molecular Electron Density Theory Study of the Role of the Copper Metalation of Azomethine Ylides in [3 + 2] Cycloaddition Reactions. <i>Journal of Organic Chemistry</i> , 2018, 83, 10959-10973.	1.7	41

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55	Understanding the polar mechanism of the ene reaction. A DFT study. <i>Organic and Biomolecular Chemistry</i> , 2014, 12, 7581-7590.	1.5	36
56	Comparison between Experimental and Theoretical Scales of Electrophilicity Based on Reactivity Indexes. <i>Journal of Physical Chemistry A</i> , 2002, 106, 3964-3966.	1.1	35
57	Philicity indices within the spin-polarized density-functional theory framework. <i>Journal of Chemical Physics</i> , 2006, 124, 044105.	1.2	35
58	Nucleophilicity scale for n- and $\pi$ -nucleophiles. <i>Chemical Physics Letters</i> , 2006, 427, 421-425.	1.2	34
59	Further relationships between theoretical and experimental models of electrophilicity and nucleophilicity. <i>Computational and Theoretical Chemistry</i> , 2009, 901, 145-152.	1.5	34
60	Unveiling the Lewis Acid Catalyzed Diels-Alder Reactions Through the Molecular Electron Density Theory. <i>Molecules</i> , 2020, 25, 2535.	1.7	34
61	Effect of electron-withdrawing substituents on the electrophilicity of carbonyl carbons. <i>Tetrahedron</i> , 2005, 61, 417-422.	1.0	33
62	Relationship between basicity and nucleophilicity. <i>Journal of Physical Organic Chemistry</i> , 2007, 20, 1050-1057.	0.9	32
63	Global and Local Electrophilicity Patterns of Diazonium Ions and Their Reactivity toward $\pi$ -Nucleophiles. <i>Journal of Organic Chemistry</i> , 2003, 68, 5886-5889.	1.7	31
64	Effect of the exchange-correlation functional on the synchronicity/nonsynchronicity in bond formation in Diels-Alder reactions: a reaction force constant analysis. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 7412-7428.	1.3	31
65	Effect of Lewis acid bulkiness on the stereoselectivity of Diels-Alder reactions between acyclic dienes and $\beta,\gamma$ -enals. <i>Organic Chemistry Frontiers</i> , 2017, 4, 1390-1399.	2.3	29
66	Theoretical analysis of some substituted imine-enamine tautomerism. <i>Theoretical Chemistry Accounts</i> , 2001, 105, 422-430.	0.5	28
67	Theoretical study of the trans-N <sub>2</sub> H <sub>2</sub> and cis-N <sub>2</sub> H <sub>2</sub> and F <sub>2</sub> S <sub>2</sub> and FSSF reactions in gas and solution phases.. <i>Computational and Theoretical Chemistry</i> , 2002, 580, 171-182.	1.5	28
68	$\pi$ -Strain-Induced Electrophilicity in Small Cycloalkynes: A DFT Analysis of the Polar Cycloaddition of Cyclopentyne towards Enol Ethers. <i>European Journal of Organic Chemistry</i> , 2006, 2006, 498-506.	1.2	28
69	A DFT Study of Inter- and Intramolecular Aryne Ene Reactions. <i>European Journal of Organic Chemistry</i> , 2015, 2015, 2826-2834.	1.2	28
70	A theoretical scale for pericyclic and pseudopericyclic reactions. <i>Chemical Physics Letters</i> , 2007, 443, 136-140.	1.2	27
71	Relationship between local electrophilicity and rate coefficients for the hydrolysis of carbenium ions. <i>Tetrahedron</i> , 2005, 61, 889-895.	1.0	26
72	The mechanism of double proton transfer in dimers of uracil and 2-thiouracil-The reaction force perspective. <i>Journal of Computational Chemistry</i> , 2009, 30, 389-398.	1.5	26

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73	The mechanism of ionic Diels-Alder reactions. A DFT study of the oxa-Povarov reaction. RSC Advances, 2014, 4, 16567-16577.	1.7	26
74	Relationship between the electronic chemical potential and proton transfer barriers. Chemical Physics Letters, 1997, 269, 419-427.	1.2	24
75	HSAB Analysis of Charge Transfer in the Gas-Phase Acid-Base Equilibria of Alkyl-Substituted Alcohols. Journal of Physical Chemistry A, 1999, 103, 11246-11249.	1.1	24
76	Global and Local Analysis of the Gas-Phase Acidity of Haloacetic Acids. Journal of Physical Chemistry A, 2000, 104, 5882-5887.	1.1	24
77	Electrophilicity and spin polarization of simple substituted silylenes. Chemical Physics Letters, 2006, 431, 210-215.	1.2	24
78	Solvent Effects on Global Reactivity Properties for Neutral and Charged Systems Using the Sequential Monte Carlo Quantum Mechanics Model. Journal of Physical Chemistry B, 2009, 113, 4314-4322.	1.2	24
79	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
80	A DFT study of the ionic [2+2] cycloaddition reactions of keteniminium cations with terminal acetylenes. Tetrahedron, 2015, 71, 2421-2427.	1.0	24
81	A molecular electron density theory study of the enhanced reactivity of aza aromatic compounds participating in Diels-Alder reactions. Organic and Biomolecular Chemistry, 2020, 18, 292-304.	1.5	24
82	Understanding C-C bond formation in polar reactions. An ELF analysis of the Friedel-Crafts reaction between indoles and nitroolefins. RSC Advances, 2013, 3, 7520.	1.7	23
83	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
84	Solvation energies from the linear response function of density functional theory. Chemical Physics Letters, 1996, 260, 236-242.	1.2	22
85	Understanding the high reactivity of carbonyl compounds towards nucleophilic carbenoid intermediates generated from carbene isocyanides. RSC Advances, 2015, 5, 84797-84809.	1.7	21
86	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
87	Understanding the [2n+2n] reaction mechanism between a carbenoid intermediate and CO <sub>2</sub> . Molecular Physics, 2016, 114, 1374-1391.	0.8	20
88	Understanding the Bond Formation in Hetero-Diels-Alder Reactions. An ELF Analysis of the Reaction of Nitroethylene with Dimethylvinylamine. Current Organic Chemistry, 2012, 16, 2343-2351.	0.9	19
89	Intrinsic Relative Scales of Electrophilicity and Nucleophilicity. Journal of Physical Chemistry A, 2013, 117, 2636-2643.	1.1	19
90	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

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91	Are There Only Fold Catastrophes in the Diels-Alder Reaction Between Ethylene and 1,3-Butadiene?. <i>Journal of Physical Chemistry A</i> , 2021, 125, 5152-5165.	1.1	19
92	Aromaticity in Pericyclic Transition State Structures? A Critical Rationalisation Based on the Topological Analysis of Electron Density. <i>ChemistrySelect</i> , 2016, 1, 6026-6039.	0.7	18
93	Theory of non-local (pair site) reactivity from model static-density response functions. <i>Theoretical Chemistry Accounts</i> , 1998, 99, 183-191.	0.5	17
94	A Semiquantitative Description of Electrostatics and Polarization Substituent Effects: Gas-Phase Acid-Base Equilibria as Test Cases. <i>Journal of Physical Chemistry A</i> , 2000, 104, 11993-11998.	1.1	17
95	Empirical Energy-Density Relationships Applied to the Analysis of the Basicity of Strong Organic Superbases. <i>Journal of Physical Chemistry A</i> , 2005, 109, 10068-10076.	1.1	17
96	Theoretical Study of the Effect of the Substituents on the Gas Phase Acidity of Alcohols and Silanols. <i>Journal of Physical Chemistry A</i> , 2001, 105, 6182-6186.	1.1	16
97	Understanding the chemical reactivity of phenylhalocarbene systems: an analysis based on the spin-polarized density functional theory. <i>Theoretical Chemistry Accounts</i> , 2007, 118, 325-335.	0.5	16
98	A DFT Analysis of the Strain-Induced Regioselective [2+2] Cycloaddition of Benzyne Possessing Fused Four-Membered Ring. <i>Letters in Organic Chemistry</i> , 2005, 2, 68-73.	0.2	15
99	Hardness and softness kernels, and related indices in the spin polarized version of density functional theory. <i>Chemical Physics Letters</i> , 2006, 419, 37-43.	1.2	15
100	On the Nucleophilicity of Boryllithium Compounds. A Theoretical Study. <i>Journal of Physical Chemistry A</i> , 2009, 113, 6812-6817.	1.1	15
101	A quantum chemical topological analysis of the C-C bond formation in organic reactions involving cationic species. <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 14108.	1.3	15
102	An MEDT study of the carbenoid-type [3 + 2] cycloaddition reactions of nitrile ylides with electron-deficient chiral oxazolidinones. <i>Organic and Biomolecular Chemistry</i> , 2016, 14, 10427-10436.	1.5	15
103	Sites of protonation of N 2-substituted N 1, N 1-dimethyl formamidines from regional reactivity indices. <i>Computational and Theoretical Chemistry</i> , 1999, 493, 267-273.	1.5	13
104	Relationship between Superelectrophilicity and the Electrophilicity Index of Isolated Species. <i>Journal of Organic Chemistry</i> , 2004, 69, 5048-5053.	1.7	13
105	A Molecular Electron Density Theory Study of the Competitiveness of Polar Diels-Alder and Polar Alder-ene Reactions. <i>Molecules</i> , 2018, 23, 1913.	1.7	13
106	Lithium Cation-Catalyzed Benzene Diels-Alder Reaction: Insights on the Molecular Mechanism Within the Molecular Electron Density Theory. <i>Journal of Organic Chemistry</i> , 2020, 85, 13121-13132.	1.7	13
107	Do substituents make any contribution to the formation of systems where the electronic effects seem to be neutralized? The case of the indigo dye formation. <i>Journal of Physical Organic Chemistry</i> , 2005, 18, 1161-1168.	0.9	11
108	Electrophilic activation of CO <sub>2</sub> in cycloaddition reactions towards a nucleophilic carbenoid intermediate: new defying insights from the Molecular Electron Density Theory. <i>Theoretical Chemistry Accounts</i> , 2017, 136, 1.	0.5	11

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109	Reaction Electronic Flux Perspective on the Mechanism of the Zimmerman Di- $\pi$ -methane Rearrangement. <i>Journal of Organic Chemistry</i> , 2018, 83, 5969-5974.	1.7	11
110	Are one-step aromatic nucleophilic substitutions of non-activated benzenes concerted processes?. <i>Organic and Biomolecular Chemistry</i> , 2019, 17, 8185-8193.	1.5	11
111	Unveiling the high reactivity of cyclohexynes in [3 + 2] cycloaddition reactions through the molecular electron density theory. <i>Organic and Biomolecular Chemistry</i> , 2019, 17, 498-508.	1.5	11
112	A density functional theory formulation of the reaction field model of solvent effects. <i>International Journal of Quantum Chemistry</i> , 1995, 56, 433-444.	1.0	10
113	Analysis of gas phase proton transfer using density functional theory. The H <sub>2</sub> O $\cdots$ HX (X = F, Cl and OH) system. <i>Chemical Physics Letters</i> , 1996, 256, 15-20.	1.2	10
114	Exploring Two-State Reactivity Pathways in the Cycloaddition Reactions of Triplet Methylene. <i>Journal of Physical Chemistry A</i> , 2005, 109, 4178-4184.	1.1	10
115	Global and local reactivity of simple substituted nitrenes and phosphinidenes within the spin-polarized density functional theory framework. <i>Chemical Physics Letters</i> , 2007, 448, 273-279.	1.2	10
116	Relationship between solvation energy, chemical potential and hardness variations. <i>Computational and Theoretical Chemistry</i> , 1997, 390, 169-175.	1.5	9
117	Understanding the thermal dehydrochlorination reaction of 1-chlorohexane. Revealing the driving bonding pattern at the planar catalytic reaction center. <i>RSC Advances</i> , 2015, 5, 62946-62956.	1.7	9
118	QUANTITATIVE REPRESENTATION OF REACTIVITY, SELECTIVITY AND SITE ACTIVATION CONCEPTS IN ORGANIC CHEMISTRY@. <i>Journal of the Chilean Chemical Society</i> , 2004, 49, .	0.5	8
119	Global and local reactivity of N-heterocyclic carbenes with boron and phosphorus atoms: An analysis based on spin polarized density functional framework. <i>Computational and Theoretical Chemistry</i> , 2010, 943, 110-114.	1.5	7
120	Intrinsic relative nucleophilicity of indoles. <i>Theoretical Chemistry Accounts</i> , 2016, 135, 1.	0.5	7
121	ON THE REDUCTION OF 4-OXO-4H-BENZOPYRAN-3-CARBALDEHYDES: GLOBAL AND LOCAL ELECTROPHILICITY PATTERNS. <i>Journal of the Chilean Chemical Society</i> , 2004, 49, .	0.5	7
122	Theoretical Analysis of Substituted Diels - Alder Reagents to Determine the Polar or Non Polar Character of the Reaction. <i>Letters in Organic Chemistry</i> , 2011, 8, 88-94.	0.2	6
123	Theoretical investigation of the selectivity in intramolecular cyclizations of some $\alpha$ -aminochalcones to dihydroquinolinones and indolinones. <i>Journal of Molecular Modeling</i> , 2013, 19, 3611-3618.	0.8	6
124	Perfluorobicyclo[2.2.0]hex-1(4)-ene as unique partner for Diels-Alder reactions with benzene: a density functional theory study. <i>Theoretical Chemistry Accounts</i> , 2021, 140, 1.	0.5	6
125	Electrostatic and Non-Electrostatic Contributions to Hydrogen Bonding and Proton Transfer in Solution Phase. <i>The Journal of Physical Chemistry</i> , 1996, 100, 19326-19332.	2.9	5
126	Isoelectronic and isolobal O, CH <sub>2</sub> , CH <sub>3</sub> <sup>+</sup> and BH <sub>3</sub> as electron pairs; similarities between molecular and solid-state chemistry. <i>Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials</i> , 2013, 69, 163-175.	0.5	5

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127	On the electron flow sequence driving the hydrometallation of acetylene by lithium hydride. <i>Journal of Molecular Modeling</i> , 2018, 24, 305.	0.8	5
128	Basicity and solvent effects on hydrogen bonding in $\text{NR}_3\text{i}^{-1/2}\text{i}^{-1/2}\text{i}^{-1/2}\text{HCOOH}$ (R=H, CH <sub>3</sub> ) model systems. <i>International Journal of Quantum Chemistry</i> , 1999, 74, 387-394.	1.0	4
129	Intrinsic electronic reorganization energy in the electron transfer from substituted N,N-dimethylanilines to phthalimide N-oxyl radical. <i>Chemical Physics Letters</i> , 2012, 534, 67-71.	1.2	4
130	A molecular electron density theory study of the insertion of CO into frustrated Lewis pair boron-amidines: a [4 + 1] cycloaddition reaction. <i>Dalton Transactions</i> , 2019, 48, 9214-9224.	1.6	4
131	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. <i>New Journal of Chemistry</i> , 2021, 46, 294-308.	1.4	4
132	Understanding the higher-order cycloaddition reactions of heptafulvene, tropone, and its nitrogen derivatives, with electrophilic and nucleophilic ethylenes inside the molecular electron density theory. <i>New Journal of Chemistry</i> , 2022, 46, 11520-11530.	1.4	4
133	Oxygenation of the phenylhalocarbenes. Are they spin-allowed or spin-forbidden reactions?. <i>Journal of Molecular Modeling</i> , 2012, 18, 2813-2821.	0.8	3
134	Origin of the Synchronicity on the Transition Structures of Polar Diels-Alder Reactions. Are these Reactions [4 + 2] Processes?. <i>ChemInform</i> , 2003, 34, no.	0.1	0
135	On the Catalytic Effects of the Thiazolium Salt in the Oxa-Diel-Alder Reaction between Benzaldehyde and Danishefsky's Diene: A Molecular Electron Density Theory Study. <i>Organic and Biomolecular Chemistry</i> , 2021, 19, 9306-9317.	1.5	0
136	Isoelectronic and isolobal O, CH <sub>2</sub> , CH <sub>3</sub> <sup>+</sup> and BH <sub>3</sub> as electron pairs; similarities between molecular and solid-state chemistry. <i>Acta Crystallographica Section B: Structural Science</i> , 2013, 69, 163-175.	1.8	0