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 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
2	Perfluorobicyclo[2.2.0]hex-1(4)-ene as unique partner for Dielsâ€“Alder reactions with benzene: a density functional theory study. Theoretical Chemistry Accounts, 2021, 140, 1.	0.5	6
3	Are There Only Fold Catastrophes in the Dielsâ€“Alder Reaction Between Ethylene and 1,3-Butadiene?. Journal of Physical Chemistry A, 2021, 125, 5152-5165.	1.1	19
4	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
5	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
6	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
7	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
8	Unveiling the Lewis Acid Catalyzed Dielsâ€“Alder Reactions Through the Molecular Electron Density Theory. Molecules, 2020, 25, 2535.	1.7	34
9	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
10	Are one-step aromatic nucleophilic substitutions of non-activated benzenes concerted processes?. Organic and Biomolecular Chemistry, 2019, 17, 8185-8193.	1.5	11
11	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
12	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
13	Effect of the exchangeâ€“correlation functional on the synchronicity/nonsynchronicity in bond formation in Dielsâ€“Alder reactions: a reaction force constant analysis. Physical Chemistry Chemical Physics, 2019, 21, 7412-7428.	1.3	31
14	Reaction Electronic Flux Perspective on the Mechanism of the Zimmerman Di-Ï€-methane Rearrangement. Journal of Organic Chemistry, 2018, 83, 5969-5974.	1.7	11
15	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
16	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
17	On the electron flow sequence driving the hydrometallation of acetylene by lithium hydride. Journal of Molecular Modeling, 2018, 24, 305.	0.8	5
18	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

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19	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
20	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
21	Effect of Lewis acid bulkiness on the stereoselectivity of Dielsâ€“Alder reactions between acyclic dienes and Î±,Î²-enals. Organic Chemistry Frontiers, 2017, 4, 1390-1399.	2.3	29
22	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
23	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
24	Applications of the Conceptual Density Functional Theory Indices to Organic Chemistry Reactivity. Molecules, 2016, 21, 748.	1.7	795
25	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
26	Intrinsic relative nucleophilicity of indoles. Theoretical Chemistry Accounts, 2016, 135, 1.	0.5	7
27	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
28	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
29	Understanding the [2n+2n] reaction mechanism between a carbenoid intermediate and CO₂. Molecular Physics, 2016, 114, 1374-1391.	0.8	20
30	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
31	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
32	A DFT study of the ionic [2+2] cycloaddition reactions of keteniminium cations with terminal acetylenes. Tetrahedron, 2015, 71, 2421-2427.	1.0	24
33	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
34	Understanding the thermal dehydrochlorination reaction of 1-chlorohexane. Revealing the driving bonding pattern at the planar catalytic reaction center. RSC Advances, 2015, 5, 62946-62956.	1.7	9
35	A DFT Study of Interâ€•and Intramolecular Aryne Ene Reactions. European Journal of Organic Chemistry, 2015, 2015, 2826-2834.	1.2	28
36	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

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37	Understanding the high reactivity of carbonyl compounds towards nucleophilic carbenoid intermediates generated from carbene isocyanides. RSC Advances, 2015, 5, 84797-84809.	1.7	21
38	The mechanism of ionic Dielsâ€“Alder reactions. A DFT study of the oxa-Povarov reaction. RSC Advances, 2014, 4, 16567-16577.	1.7	26
39	A quantum chemical topological analysis of the Câ€“C bond formation in organic reactions involving cationic species. Physical Chemistry Chemical Physics, 2014, 16, 14108.	1.3	15
40	Understanding the polar mechanism of the ene reaction. A DFT study. Organic and Biomolecular Chemistry, 2014, 12, 7581-7590.	1.5	36
41	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
42	A DFT analysis of the participation of zwitterionic TACs in polar [3+2] cycloaddition reactions. Tetrahedron, 2014, 70, 4519-4525.	1.0	68
43	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
44	Understanding Câ€“C bond formation in polar reactions. An ELF analysis of the Friedelâ€“Crafts reaction between indoles and nitroolefins. RSC Advances, 2013, 3, 7520.	1.7	23
45	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
46	Intrinsic Relative Scales of Electrophilicity and Nucleophilicity. Journal of Physical Chemistry A, 2013, 117, 2636-2643.	1.1	19
47	Theoretical investigation of the selectivity in intramolecular cyclizations of some 2â€™â€“aminochalcones to dihydroquinolinâ€“8â€“ones and indolinâ€“3â€“ones. Journal of Molecular Modeling, 2013, 19, 3611-3618.	0.8	6
48	Understanding the local reactivity in polar organic reactions through electrophilic and nucleophilic Parr functions. RSC Advances, 2013, 3, 1486-1494.	1.7	628
49	The reaction force constant as an indicator of synchronicity/nonsynchronicity in [4+2] cycloaddition processes. Physical Chemistry Chemical Physics, 2013, 15, 7311.	1.3	53
50	Global and local reactivity indices for electrophilic/nucleophilic free radicals. Organic and Biomolecular Chemistry, 2013, 11, 4350.	1.5	136
51	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
52	Isoelectronic and isolobal O, CH₂, CH₃⁺and BH₃as electron pairs; similarities between molecular and solid-state chemistry. Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials, 2013, 69, 163-175.	0.5	5
53	Isoelectronic and isolobal O, CH₂, CH₃⁺and BH₃as electron pairs; similarities between molecular and solid-state chemistry. Acta Crystallographica Section B: Structural Science, 2013, 69, 163-175.	1.8	0
54	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

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55	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
56	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
57	Oxygenation of the phenylhalocarbenes. Are they spin-allowed or spin-forbidden reactions?. Journal of Molecular Modeling, 2012, 18, 2813-2821.	0.8	3
58	Intrinsic electronic reorganization energy in the electron transfer from substituted N,N-dimethylanilines to phthalimide N-oxyl radical. Chemical Physics Letters, 2012, 534, 67-71.	1.2	4
59	The nucleophilicity N index in organic chemistry. Organic and Biomolecular Chemistry, 2011, 9, 7168.	1.5	449
60	Theoretical Analysis of Substituted Diels - Alder Reagents to Determine the Polar or Non Polar Character of the Reaction. Letters in Organic Chemistry, 2011, 8, 88-94.	0.2	6
61	Global and local reactivity of N-heterocyclic carbenes with boron and phosphorus atoms: An analysis based on spin polarized density functional framework. Computational and Theoretical Chemistry, 2010, 943, 110-114.	1.5	7
62	Understanding the High Reactivity of the Azomethine Ylides in [3 + 2] Cycloaddition Reactions. Letters in Organic Chemistry, 2010, 7, 432-439.	0.2	127
63	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
64	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
65	The mechanism of double proton transfer in dimers of uracil and 2â€thiouracilâ€”The reaction force perspective. Journal of Computational Chemistry, 2009, 30, 389-398.	1.5	26
66	Further relationships between theoretical and experimental models of electrophilicity and nucleophilicity. Computational and Theoretical Chemistry, 2009, 901, 145-152.	1.5	34
67	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
68	A comparison between theoretical and experimental models of electrophilicity and nucleophilicity. Computational and Theoretical Chemistry, 2009, 896, 73-79.	1.5	56
69	On the Nucleophilicity of Boryllithium Compounds. A Theoretical Study. Journal of Physical Chemistry A, 2009, 113, 6812-6817.	1.1	15
70	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
71	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
72	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

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73	Universal mathematical identities in density functional theory: Results from three different spin-resolved representations. Journal of Chemical Physics, 2008, 128, 204108.	1.2	66
74	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
75	Understanding the Reactivity of Captodative Ethylenes in Polar Cycloaddition Reactions. A Theoretical Study. Journal of Organic Chemistry, 2008, 73, 4615-4624.	1.7	846
76	Dual descriptors within the framework of spin-polarized density functional theory. Journal of Chemical Physics, 2008, 129, 064117.	1.2	47
77	Chapter 9 The electrophilicity index in organic chemistry. Theoretical and Computational Chemistry, 2007, , 139-201.	0.2	101
78	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
79	A theoretical scale for pericyclic and pseudopericyclic reactions. Chemical Physics Letters, 2007, 443, 136-140.	1.2	27
80	Global and local reactivity of simple substituted nitrenes and phosphinidenes within the spin-polarized density functional theory framework. Chemical Physics Letters, 2007, 448, 273-279.	1.2	10
81	Relationship between basicity and nucleophilicity. Journal of Physical Organic Chemistry, 2007, 20, 1050-1057.	0.9	32
82	Understanding the chemical reactivity of phenylhalocarbene systems: an analysis based on the spin-polarized density functional theory. Theoretical Chemistry Accounts, 2007, 118, 325-335.	0.5	16
83	Definition of a Nucleophilicity Scale. Journal of Physical Chemistry A, 2006, 110, 8181-8187.	1.1	116
84	Hardness and softness kernels, and related indices in the spin polarized version of density functional theory. Chemical Physics Letters, 2006, 419, 37-43.	1.2	15
85	Towards an intrinsic nucleofugality scale: The leaving group (LG) ability in CH3LG model system. Chemical Physics Letters, 2006, 420, 95-99.	1.2	48
86	Nucleophilicity scale for n- and Ï€-nucleophiles. Chemical Physics Letters, 2006, 427, 421-425.	1.2	34
87	Electrophilicity and spin polarization of simple substituted silylenes. Chemical Physics Letters, 2006, 431, 210-215.	1.2	24
88	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
89	Philicity indices within the spin-polarized density-functional theory framework. Journal of Chemical Physics, 2006, 124, 044105.	1.2	35
90	Effect of electron-withdrawing substituents on the electrophilicity of carbonyl carbons. Tetrahedron, 2005, 61, 417-422.	1.0	33

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91	Condensed-to-atoms electronic Fukui functions within the framework of spin-polarized density-functional theory. Journal of Chemical Physics, 2005, 123, 114107.	1.2	82
92	Empirical Energyâ^'Density Relationships Applied to the Analysis of the Basicity of Strong Organic Superbases. Journal of Physical Chemistry A, 2005, 109, 10068-10076.	1.1	17
93	Relationship between local electrophilicity and rate coefficients for the hydrolysis of carbenium ions. Tetrahedron, 2005, 61, 889-895.	1.0	26
94	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. Journal of Physical Organic Chemistry, 2005, 18, 1161-1168.	0.9	11
95	A DFT Analysis of the Strain-Induced Regioselective[2+2]Cycloaddition of Benzyne Possessing Fused Four-Membered Ring. Letters in Organic Chemistry, 2005, 2, 68-73.	0.2	15
96	Exploring Two-State Reactivity Pathways in the Cycloaddition Reactions of Triplet Methylene. Journal of Physical Chemistry A, 2005, 109, 4178-4184.	1.1	10
97	Reactivity of the carbonâ€"carbon double bond towards nucleophilic additions. A DFT analysis. Tetrahedron, 2004, 60, 6585-6591.	1.0	84
98	A theoretical study on the regioselectivity of 1,3-dipolar cycloadditions using DFT-based reactivity indexes. Tetrahedron, 2004, 60, 11503-11509.	1.0	150
99	Relationship between Superelectrophilicity and the Electrophilicity Index of Isolated Species. Journal of Organic Chemistry, 2004, 69, 5048-5053.	1.7	13
100	ON THE REDUCTION OF 4-OXO-4H-BENZOPYRAN-3-CARBALDEHYDES: GLOBAL AND LOCAL ELECTROPHILICITY PATTERNSÂ‡. Journal of the Chilean Chemical Society, 2004, 49, .	0.5	7
101	QUANTITATIVE REPRESENTATION OF REACTIVITY, SELECTIVITY AND SITE ACTIVATION CONCEPTS IN ORGANIC CHEMISTRY@. Journal of the Chilean Chemical Society, 2004, 49, .	0.5	8
102	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
103	Origin of the Synchronicity on the Transition Structures of Polar Dielsâ€"Alder Reactions. Are these Reactions [4 + 2] Processes?. ChemInform, 2003, 34, no.	0.1	0
104	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
105	Global and Local Electrophilicity Patterns of Diazonium Ions and Their Reactivity toward Ï€-Nucleophiles. Journal of Organic Chemistry, 2003, 68, 5886-5889.	1.7	31
106	Theoretical Evaluation of the Global and Local Electrophilicity Patterns of Singlet Carbenes. Journal of Physical Chemistry A, 2003, 107, 522-525.	1.1	44
107	Electronic Contributions to the Ïƒp Parameter of the Hammett Equation. Journal of Organic Chemistry, 2003, 68, 6060-6062.	1.7	80
108	Spin-Philicity and Spin-Donicity as Auxiliary Concepts To Quantify Spin-Catalysis Phenomena. Journal of Physical Chemistry A, 2002, 106, 5353-5357.	1.1	50

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109	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
110	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
111	Comparison between Experimental and Theoretical Scales of Electrophilicity in Benzhydryl Cations. Journal of Organic Chemistry, 2002, 67, 4747-4752.	1.7	133
112	Comparison between Experimental and Theoretical Scales of Electrophilicity Based on Reactivity Indexes. Journal of Physical Chemistry A, 2002, 106, 3964-3966.	1.1	35
113	Theoretical study of the trans-N2H2â†'cis-N2H2 and F2S2â†'FSSF reactions in gas and solution phases.. Computational and Theoretical Chemistry, 2002, 580, 171-182.	1.5	28
114	Quantitative characterization of the global electrophilicity power of common diene/dienophile pairs in Dielsâ€"Alder reactions. Tetrahedron, 2002, 58, 4417-4423.	1.0	832
115	Theoretical Study of the Effect of the Substituents on the Gas Phase Acidity of Alcohols and Silanols. Journal of Physical Chemistry A, 2001, 105, 6182-6186.	1.1	16
116	Solvent Effects on Electrophilicity. Journal of the American Chemical Society, 2001, 123, 5527-5531.	6.6	73
117	Ab Initio SCF and DFT Studies on Solvent Effects on Intramolecular Rearrangement Reactions. Journal of Physical Chemistry A, 2001, 105, 4272-4283.	1.1	67
118	Theoretical analysis of some substituted imine-enamine tautomerism. Theoretical Chemistry Accounts, 2001, 105, 422-430.	0.5	28
119	On the condensed Fukui function. Journal of Chemical Physics, 2000, 113, 2544-2551.	1.2	345
120	Characterization of Keto-Enol Tautomerism of Acetyl Derivatives from the Analysis of Energy, Chemical Potential, and Hardness. Journal of Physical Chemistry A, 2000, 104, 1557-1562.	1.1	53
121	Global and Local Analysis of the Gas-Phase Acidity of Haloacetic Acids. Journal of Physical Chemistry A, 2000, 104, 5882-5887.	1.1	24
122	Empirical Energyâ^'Density Relationships for the Analysis of Substituent Effects in Chemical Reactivity. Journal of the American Chemical Society, 2000, 122, 4756-4762.	6.6	92
123	A Semiquantitative Description of Electrostatics and Polarization Substituent Effects: Gas-Phase Acidâ^'Base Equilibria as Test Cases. Journal of Physical Chemistry A, 2000, 104, 11993-11998.	1.1	17
124	A direct evaluation of regional Fukui functions in molecules. Chemical Physics Letters, 1999, 304, 405-413.	1.2	420
125	Sites of protonation of N 2-substituted N 1, N 1-dimethyl formamidines from regional reactivity indices. Computational and Theoretical Chemistry, 1999, 493, 267-273.	1.5	13
126	Basicity and solvent effects on hydrogen bonding in NR3ï¿½ï¿½HCOOH (R=H, CH3) model systems. International Journal of Quantum Chemistry, 1999, 74, 387-394.	1.0	4

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127	HSAB Analysis of Charge Transfer in the Gas-Phase Acidâ"Base Equilibria of Alkyl-Substituted Alcohols. Journal of Physical Chemistry A, 1999, 103, 11246-11249.	1.1	24
128	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
129	A theoretical analysis of the gas-phase protonation of hydroxylamine, methyl-derivatives and aliphatic amino acids. Chemical Physics Letters, 1998, 293, 239-244.	1.2	42
130	Theory of non-local (pair site) reactivity from model static-density response functions. Theoretical Chemistry Accounts, 1998, 99, 183-191.	0.5	17
131	Relationship between solvation energy, chemical potential and hardness variations. Computational and Theoretical Chemistry, 1997, 390, 169-175.	1.5	9
132	Relationship between the electronic chemical potential and proton transfer barriers. Chemical Physics Letters, 1997, 269, 419-427.	1.2	24
133	Solvation energies from the linear response function of density functional theory. Chemical Physics Letters, 1996, 260, 236-242.	1.2	22
134	Analysis of gas phase proton transfer using density functional theory. The H2O â‹¯ HX (Xî—»F, Cl and OH) system. Chemical Physics Letters, 1996, 256, 15-20.	1.2	10
135	Electrostatic and Non-Electrostatic Contributions to Hydrogen Bonding and Proton Transfer in Solution Phase. The Journal of Physical Chemistry, 1996, 100, 19326-19332.	2.9	5
136	A density functional theory formulation of the reaction field model of solvent effects. International Journal of Quantum Chemistry, 1995, 56, 433-444.	1.0	10