Renato Contreras

List of Publications by Year
in descending order

148 papers	6,480 citations	109321 35 h-index	71685 76 g-index
149 all docs	149 docs citations	149 times ranked	4100 citing authors

#	Article	IF	Citations
1	Quantitative characterization of the global electrophilicity power of common diene/dienophile pairs in Dielsâ€“Alder reactions. Tetrahedron, 2002, 58, 4417-4423.	1.9	832
2	A direct evaluation of regional Fukui functions in molecules. Chemical Physics Letters, 1999, 304, 405-413.	2.6	420
3	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.	2.5	357
4	On the condensed Fukui function. Journal of Chemical Physics, 2000, 113, 2544-2551.	3.0	345
5	Quantitative characterization of the global electrophilicity pattern of some reagents involved in 1,3-dipolar cycloaddition reactions. Tetrahedron, 2003, 59, 3117-3125.	1.9	301
6	Quantum Mechanical Continuum Solvation Models for Ionic Liquids. Journal of Physical Chemistry B, 2012, 116, 9122-9129.	2.6	225
7	Sigmaâ€“pi separation of the electron localization function and aromaticity. Journal of Chemical Physics, 2004, 120, 1670-1673.	3.0	210
8	Self consistent field theory of solvent effects representation by continuum models: Introduction of desolvation contribution. Theoretica Chimica Acta, 1984, 65, 1-11.	0.8	166
9	A theoretical study on the regioselectivity of 1,3-dipolar cycloadditions using DFT-based reactivity indexes. Tetrahedron, 2004, 60, 11503-11509.	1.9	150
10	Comparison between Experimental and Theoretical Scales of Electrophilicity in Benzhydryl Cations. Journal of Organic Chemistry, 2002, 67, 4747-4752.	3.2	133
11	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.	3.2	119
12	Definition of a Nucleophilicity Scale. Journal of Physical Chemistry A, 2006, 110, 8181-8187.	2.5	116
13	A Theoretical Study on the Relationship between Nucleophilicity and Ionization Potentials in Solution Phase. Journal of Physical Chemistry A, 2003, 107, 5588-5593.	2.5	100
14	Empirical Energyâ^'Density Relationships for the Analysis of Substituent Effects in Chemical Reactivity. Journal of the American Chemical Society, 2000, 122, 4756-4762.	13.7	92
15	Woodwardâ^'Hoffmann Rule in the Light of the Principles of Maximum Hardness and Minimum Polarizability:Â DFT and Ab Initio SCF Studies. Journal of the American Chemical Society, 2000, 122, 348-351.	13.7	90
16	Reactivity of the carbonâ€“carbon double bond towards nucleophilic additions. A DFT analysis. Tetrahedron, 2004, 60, 6585-6591.	1.9	84
17	Electronic Contributions to the Ïƒ pParameter of the Hammett Equation. Journal of Organic Chemistry, 2003, 68, 6060-6062.	3.2	80
18	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.	2.5	77

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19	A proposal for a new local hardness as selectivity index. Chemical Physics Letters, 2004, 383, 181-187.	2.6	77
20	Solvent Effects on Electrophilicity. Journal of the American Chemical Society, 2001, 123, 5527-5531.	13.7	73
21	Structure-genotoxic activity relationships of pesticides: comparison of the results from several short-term assays. Mutation Research - Environmental Mutagenesis and Related Subjects Including Methodology, 1985, 147, 343-356.	0.4	71
22	Experimental and Theoretical Studies on the Nucleofugality Patterns in the Aminolysis and Phenolysis of S-Aryl O-Aryl Thiocarbonates. Journal of Organic Chemistry, 2009, 74, 9173-9179.	3.2	69
23	Comparison among Four Different Ways to Condense the Fukui Function. Journal of Physical Chemistry A, 2005, 109, 3220-3224.	2.5	67
24	On theSCF theory of continuum solvent effects representation: Introduction of local dielectric effects. International Journal of Quantum Chemistry, 1985, 27, 293-301.	2.0	61
25	Nucleophilicity Index from Perturbed Electrostatic Potentials. Journal of Physical Chemistry A, 2007, 111, 2442-2447.	2.5	59
26	Spin-Philicity and Spin-Donicity as Auxiliary Concepts To Quantify Spin-Catalysis Phenomena. Journal of Physical Chemistry A, 2002, 106, 5353-5357.	2.5	50
27	A Computational Study of the Protein-Ligand Interactions in CDK2 Inhibitors: Using Quantum Mechanics/Molecular Mechanics Interaction Energy as a Predictor of the Biological Activity. Biophysical Journal, 2007, 92, 430-439.	0.5	49
28	Mechanistic pathways of aromatic nucleophilic substitution in conventional solvents and ionic liquids. New Journal of Chemistry, 2014, 38, 2611-2618.	2.8	48
29	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.	2.5	46
30	Relationships between the Electrophilicity Index and Experimental Rate Coefficients for the Aminolysis of Thiolcarbonates and Dithiocarbonates. Journal of Organic Chemistry, 2005, 70, 1754-1760.	3.2	44
31	A theoretical analysis of the gas-phase protonation of hydroxylamine, methyl-derivatives and aliphatic amino acids. Chemical Physics Letters, 1998, 293, 239-244.	2.6	42
32	Gutmann's Donor Numbers Correctly Assess the Effect of the Solvent on the Kinetics of S_NAr Reactions in Ionic Liquids. Chemistry - A European Journal, 2016, 22, 13347-13351.	3.3	41
33	N-borane adducts of oxazolidines derived from ephedrine and pseudo- ephedrine. Study of stereochemistry by nuclear magnetic resonance. Tetrahedron, 1984, 40, 3829-3838.	1.9	40
34	A Density Functional Study of the Claisen Rearrangement of Allyl Aryl Ether, Allyl Arylamine, Allyl Aryl Thio Ether, and a Series of Meta-Substituted Molecules through Reactivity and Selectivity Profiles. Journal of Physical Chemistry A, 2002, 106, 11227-11233.	2.5	40
35	N-Heterocyclic carbene copper(<scp>i</scp>) complex-catalyzed synthesis of 2-aryl benzoxazoles and benzothiazoles. RSC Advances, 2016, 6, 82401-82408.	3.6	40
36	Group electrophilicity as a model of nucleofugality in nucleophilic substitution reactions. Chemical Physics Letters, 2006, 422, 340-344.	2.6	37

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37	Comparison between Experimental and Theoretical Scales of Electrophilicity Based on Reactivity Indexes. Journal of Physical Chemistry A, 2002, 106, 3964-3966.	2.5	35
38	Specific nucleophileâ€“electrophile interactions in nucleophilic aromatic substitutions. Organic and Biomolecular Chemistry, 2013, 11, 2302.	2.8	35
39	Some relationships within the nonlocal (pairâ€“site) chemical reactivity formalism of density functional theory. Journal of Chemical Physics, 2000, 113, 10861-10866.	3.0	33
40	Effect of electron-withdrawing substituents on the electrophilicity of carbonyl carbons. Tetrahedron, 2005, 61, 417-422.	1.9	33
41	The Chromophore Structure of the Cyanobacterial Phytochrome Cph1 As Predicted by Time-Dependent Density Functional Theory. Journal of Physical Chemistry B, 2008, 112, 16253-16256.	2.6	33
42	Relationship between nucleophilicity/electrophilicity indices and reaction mechanisms for the nucleophilic substitution reactions of carbonyl compounds. Journal of Physical Organic Chemistry, 2004, 17, 273-281.	1.9	32
43	Proton transfer in water polymers as a model for intime and solvent-separated ion pairs. The Journal of Physical Chemistry, 1984, 88, 1905-1908.	2.9	31
44	The Markovnikov Regioselectivity Rule in the Light of Site Activation Models. Journal of Physical Chemistry A, 2002, 106, 7844-7849.	2.5	31
45	Experimental and theoretical study on the substitution reactions of aryl 2,4-dinitrophenyl carbonates with quinuclidines. Tetrahedron, 2006, 62, 2555-2562.	1.9	31
46	Chemical Reactivity in the {N, NS, ν(r)} Space. Journal of Physical Chemistry A, 2003, 107, 3831-3835.	2.5	29
47	Time-Dependent DFT on Phytochrome Chromophores: A Way to the Right Conformer. Journal of Physical Chemistry Letters, 2010, 1, 796-801.	4.6	29
48	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.	2.4	28
49	The maximum hardness and minimum polarizability principles as the basis for the study of reaction profiles. Theoretical Chemistry Accounts, 2003, 110, 421-427.	1.4	26
50	Relationship between local electrophilicity and rate coefficients for the hydrolysis of carbenium ions. Tetrahedron, 2005, 61, 889-895.	1.9	26
51	On the variations of electronic chemical potential and chemical hardness induced by solvent effects. Chemical Physics Letters, 2006, 433, 54-57.	2.6	26
52	Empirical scale of nucleophilicity for substituted pyridines. Chemical Physics Letters, 2006, 422, 204-209.	2.6	25
53	Nucleofugality index in Î±-elimination reactions. Chemical Physics Letters, 2007, 439, 177-182.	2.6	25
54	Electrofugality index for benzhydryl derivatives. Chemical Physics Letters, 2007, 447, 375-378.	2.6	25

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55	Hydrogen Bond Contribution to Preferential Solvation in S_NAr Reactions. Journal of Physical Chemistry B, 2013, 117, 5908-5915.	2.6	25
56	Relationship between the electronic chemical potential and proton transfer barriers. Chemical Physics Letters, 1997, 269, 419-427.	2.6	24
57	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.	2.5	24
58	Global and Local Analysis of the Gas-Phase Acidity of Haloacetic Acids. Journal of Physical Chemistry A, 2000, 104, 5882-5887.	2.5	24
59	An unusual halogenated meroditerpenoid from Stypopodium flabelliforme: Studies by NMR spectroscopic and computational methods. Phytochemistry, 2009, 70, 1315-1320.	2.9	24
60	Reactivity Indices Profile: A Companion Tool of the Potential Energy Surface for the Analysis of Reaction Mechanisms. Nucleophilic Aromatic Substitution Reactions as Test Case. Journal of Organic Chemistry, 2013, 78, 1091-1097.	3.2	24
61	Topological analysis of the electron localization function applied to the study of the [1,3] sigmatropic shift of fluorine in 3-fluorpropene. Journal of Chemical Physics, 2001, 114, 23.	3.0	23
62	Experimental and theoretical study on the oxidation mechanism of dopamine in n-octyl pyridinium based ionic liquidsâ€“carbon paste modified electrodes. Electrochimica Acta, 2013, 111, 846-854.	5.2	23
63	Lewis Molecular Acidity of Ionic Liquids from Empirical Energyâ€“Density Models. Journal of Physical Chemistry B, 2013, 117, 1911-1920.	2.6	23
64	On the mechanism of CO2 electro-cycloaddition to propylene oxides. Journal of CO2 Utilization, 2016, 16, 114-120.	6.8	23
65	Solvation energies from the linear response function of density functional theory. Chemical Physics Letters, 1996, 260, 236-242.	2.6	22
66	The Bonding Nature of Some Simple Sigmatropic Transition States from the Topological Analysis of the Electron Localization Function. Journal of Physical Chemistry A, 2002, 106, 11533-11539.	2.5	22
67	Relationship between the electrophilicity of substituting agents and substrate selectivity in Friedelâ€“Crafts reactions. Tetrahedron, 2005, 61, 831-836.	1.9	22
68	Local hardness: An application to electrophilic additions. Chemical Physics Letters, 2007, 446, 170-175.	2.6	22
69	Changes in the S_NAr reaction mechanism brought about by preferential solvation. RSC Advances, 2015, 5, 99322-99328.	3.6	22
70	Electrophilicity of quinones and its relationship with hydride affinity. Chemical Physics Letters, 2009, 471, 168-173.	2.6	21
71	Quantitative characterization of group electrophilicity and nucleophilicity for intramolecular Dielsâ€“Alder reactions. Organic and Biomolecular Chemistry, 2010, 8, 3678.	2.8	21
72	Synthesis and characterization of poly (ionic liquid) derivatives of N-alkyl quaternized poly(4-vinylpyridine). Reactive and Functional Polymers, 2018, 124, 64-71.	4.1	20

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73	Local reactivity index defined through the density of states describes the basicity of alkaline-exchanged zeolites. Journal of Chemical Physics, 2002, 116, 4311-4316.	3.0	19
74	Solvent effects in ionic liquids: empirical linear energyâ€“density relationships. Physical Chemistry Chemical Physics, 2012, 14, 10041.	2.8	18
75	Theoretical insights into the E1cB/E2 mechanistic dichotomy of elimination reactions. Organic and Biomolecular Chemistry, 2019, 17, 9874-9882.	2.8	18
76	Theory of non-local (pair site) reactivity from model static-density response functions. Theoretical Chemistry Accounts, 1998, 99, 183-191.	1.4	17
77	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.	2.5	17
78	On the Catalytic Effect of Water in the Intramolecular Dielsâ€“Alder Reaction of Quinone Systems: A Theoretical Study. Molecules, 2012, 17, 13687-13703.	3.8	17
79	Global and Local Reactivity and Activation Patterns of HOOX (X = H, NO2, CO2-, SO3-) Peroxides with Solvent Effects. Journal of Physical Chemistry A, 2003, 107, 10098-10104.	2.5	16
80	A computational ONIOM model for the description of the H-bond interactions between NU2058 analogues and CDK2 active site. Chemical Physics Letters, 2009, 479, 149-155.	2.6	16
81	Phenomenological chemical reactivity theory for mobile electrons. Theoretical Chemistry Accounts, 2010, 126, 45-54.	1.4	16
82	Are Electrophilicity and Electrofugality Related Concepts? A Density Functional Theory Study. Organic Letters, 2011, 13, 822-824.	4.6	16
83	Effect of the nature of the nucleophile and solvent on an S_NAr reaction. New Journal of Chemistry, 2018, 42, 260-264.	2.8	16
84	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.	0.5	15
85	Hardness and softness kernels, and related indices in the spin polarized version of density functional theory. Chemical Physics Letters, 2006, 419, 37-43.	2.6	15
86	Homofugality: A new reactivity index describing the leaving group ability in homolytic substitution reactions. Chemical Physics Letters, 2006, 424, 437-442.	2.6	15
87	Site activation effects promoted by intramolecular hydrogen bond interactions in SNAr reactions. RSC Advances, 2014, 4, 30638-30643.	3.6	15
88	Theoretical study of lithium-fluoride and lithium-chloride ion pairs in aqueous solution. AnSCF-CNDO/2 approach including continuum solvent effects. International Journal of Quantum Chemistry, 1986, 30, 581-590.	2.0	14
89	Molecular modelling of lithium intercalation in. Journal of Physics Condensed Matter, 1997, 9, 3011-3021.	1.8	14
90	Two state reactivity mechanism for the rearrangement of hydrogen peroxynitrite to nitric acid. Chemical Physics Letters, 2008, 457, 216-221.	2.6	14

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91	Structureâ€“reactivity relationships for electrophilic sugars in interaction with nucleophilic biological targets. Bioorganic and Medicinal Chemistry, 2008, 16, 3184-3190.	3.0	14
92	Reactivity of benzohydrazide derivatives towards acetylation reaction. Experimental and theoretical studies. Chemical Physics Letters, 2010, 488, 86-89.	2.6	14
93	Bond Fukui Functions As Descriptor of the Electron Density Reorganization in Ï€ Conjugated Systems. Journal of Organic Chemistry, 2012, 77, 90-95.	3.2	14
94	Regional Electrophilic and Nucleophilic Fukui Functions Efficiently Highlight the Lewis Acidic/Basic Regions in Ionic Liquids. Journal of Physical Chemistry B, 2014, 118, 3696-3701.	2.6	14
95	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
96	A density functional theory analysis of the gas and solution phase isomerization reactions of MCN, (M) Tj ETQq0 0 0 rgBT /Overlock 10 T	1.5	12
97	Probing the hydride transfer process in the lumiflavineâ€“1-methylnicotinamide model system using group softness. Tetrahedron, 2004, 60, 4189-4196.	1.9	12
98	Theoretical Study on CDK2 Inhibitors Using a Global Softness Obtained from the Density of States. Journal of Physical Chemistry B, 2007, 111, 3293-3297.	2.6	12
99	Higher order derivatives for nuclear indexes in the framework of density functional theory. Journal of Chemical Physics, 2001, 115, 6822-6826.	3.0	11
100	Local reactivity index as descriptor of benzene adsorption in cluster models of exchanged zeolite-Y. Chemical Physics Letters, 2004, 383, 612-616.	2.6	11
101	Non-electrostatic components of short and strong hydrogen bonds induced by compression inside fullerenes. Chemical Physics Letters, 2010, 486, 119-122.	2.6	11
102	Permanent group effect on nucleofugality in aryl benzoates. Chemical Physics Letters, 2010, 498, 221-225.	2.6	11
103	Activation of Electrophile/Nucleophile Pair by a Nucleophilic and Electrophilic Solvation in a SNAr Reaction. Frontiers in Chemistry, 2018, 6, 509.	3.6	11
104	Energy-density relationships for the treatment of ion solvation within density-functional theory. Physical Review A, 1994, 49, 3439-3444.	2.5	10
105	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.	2.6	10
106	Exploring Two-State Reactivity Pathways in the Cycloaddition Reactions of Triplet Methylene. Journal of Physical Chemistry A, 2005, 109, 4178-4184.	2.5	10
107	Understanding the influence of Lewis acids in the regioselectivity of the Dielsâ€“Alder reactions of 2-methoxy-5-methyl-1,4-benzoquinone: A DFT study. Computational and Theoretical Chemistry, 2009, 902, 103-108.	1.5	10
108	Theoretical study of alkoxide ion solvation and its effect on the relative acidity of alcohols in DMSO. Chemical Physics Letters, 1986, 127, 169-171.	2.6	9

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109	A model for the charge capacity of 1T-TiS2 intercalated with Li. International Journal of Quantum Chemistry, 1995, 56, 819-823.	2.0	9
110	Relationship between solvation energy, chemical potential and hardness variations. Computational and Theoretical Chemistry, 1997, 390, 169-175.	1.5	9
111	Î²-Scission of thioimidoyl radicals (R1â€“Nâ€“CSâ€“R2): A theoretical scale of radical leaving group ability. Chemical Physics Letters, 2007, 443, 383-388.	2.6	9
112	On the Role of Short and Strong Hydrogen Bonds on the Mechanism of Action of a Model Chymotrypsine Active Site. Journal of Physical Chemistry A, 2009, 113, 5769-5772.	2.5	9
113	Lewis Acidity/Basicity Changes in Imidazolium Based Ionic Liquids Brought About by Impurities. Journal of Physical Chemistry B, 2015, 119, 13160-13166.	2.6	9
114	Methodological Issues in First-Principle Calculations of CH₃NH₃PbI₃ Perovskite Surfaces: Quantum Confinement and Thermal Motion. ACS Omega, 2020, 5, 29477-29491.	3.5	9
115	Understanding the stereoâ€•and regioselectivities of the polar Dielsâ€“Alder reactions between 2â€•acetylâ€•1,4â€•benzoquinone and methyl substituted 1,3â€•butadienes: a DFT study. Journal of Physical Organic Chemistry, 2009, 22, 578-584.	1.9	8
116	Kinetic and theoretical study on nucleofugality in the phenolysis of 3-nitrophenyl and 4-nitrophenyl 4-cyanophenyl thionocarbonates. Chemical Physics Letters, 2013, 572, 130-135.	2.6	8
117	Philicity and Fugality Scales for Organic Reactions. Advances in Chemistry, 2014, 2014, 1-13.	1.1	8
118	Mechanistic insights into the ANRORC-like rearrangement between methylhydrazine and 1,2,4-oxadiazole derivatives. Organic and Biomolecular Chemistry, 2015, 13, 9439-9444.	2.8	8
119	Solvent effect on a model SNAr reaction in ionic liquid/water mixtures at different compositions. New Journal of Chemistry, 2018, 42, 9645-9650.	2.8	8
120	Self-consistent reaction field calculations on the proton transfer in ammonia-formic acid systems as a model for hydrogen bonding in amino acids in solution. International Journal of Quantum Chemistry, 1988, 33, 41-52.	2.0	7
121	Wave function instabilities in the cisâ€“trans isomerization and singletâ€“triplet energy gaps in a pushâ€“pull compound. Journal of Chemical Physics, 2003, 119, 4112-4116.	3.0	7
122	Invariance of electrophilicity of independent fragments. Application to intramolecular Dielsâ€“Alder reactions. Chemical Physics Letters, 2010, 499, 272-277.	2.6	7
123	How Meaningful Is the Halogen Bonding in 1-Ethyl-3-methyl Imidazolium-Based Ionic Liquids for CO₂ Capture?. Journal of Physical Chemistry B, 2018, 122, 7907-7914.	2.6	7
124	Quantum mechanical calculation of thermodynamic functions of solvation of ammonium ions in water. Canadian Journal of Chemistry, 1985, 63, 1746-1749.	1.1	6
125	On the role of water in the hydrogen bond network in DESs: an ab initio molecular dynamics and quantum mechanical study on the ureaâ€“betaine system. Physical Chemistry Chemical Physics, 2021, 23, 1994-2004.	2.8	6
126	On theSCF theory of continuum solvent effects representation II. Quantum chemical calculation of thermodynamic properties of some acid-base equilibria in solution. International Journal of Quantum Chemistry, 1986, 30, 573-584.	2.0	5

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127	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
128	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.	2.0	4
129	Proton transport catalysis in intramolecular rearrangements: A density functional theory study. Chemical Physics Letters, 2008, 464, 271-275.	2.6	4
130	On the Principle of Spin Potential Equalization. Journal of Physical Chemistry A, 2009, 113, 1390-1396.	2.5	4
131	On the Gas-Phase Electronic Chemical Potential of Anions. Journal of Chemical Theory and Computation, 2009, 5, 2944-2949.	5.3	4
132	Endohedral Cluster of Li₁₀O with T_d Symmetry. Journal of Physical Chemistry A, 2009, 113, 13451-13456.	2.5	3
133	Predicting the reaction mechanism of nucleophilic substitutions at carbonyl and thiocarbonyl centres of esters and thioesters. Journal of Physical Organic Chemistry, 2012, 25, 1359-1364.	1.9	3
134	Quantitative characterization of the global philicity patterns of common diene/dienophile pairs in cycloaddition reactions II: the interacting pair model. Tetrahedron Letters, 2015, 56, 1767-1770.	1.4	3
135	Gutmannâ€™s Donor and Acceptor Numbers for Ionic Liquids and Deep Eutectic Solvents. Frontiers in Chemistry, 2022, 10, 861379.	3.6	3
136	REACTIVITY OF SULFUR(II) COMPOUNDS. CHEMICAL PROPERTIES AND FRONTIER MOLECULAR ORBITAL ANALYSIS. Phosphorus, Sulfur and Silicon and the Related Elements, 1991, 55, 219-228.	1.6	2
137	The electronic chemical potential as a basis for a cluster model approximation for intercalation of Li in 1T â€" TiS2. Computational and Theoretical Chemistry, 1995, 335, 161-166.	1.5	2
138	Hydrogen bonding and dissociation effects on the gas phase proton transfer reactions of ozone. Theoretical Chemistry Accounts, 1998, 99, 60-63.	1.4	2
139	Origins of the ANRORC reactivity in nitroimidazole derivatives. RSC Advances, 2016, 6, 25215-25221.	3.6	2
140	Inertia defects of urea. Journal of Molecular Structure, 1986, 142, 91-92.	3.6	1
141	Desolvation effects on the dissociation energy of diatomic molecules:Ab initio study of the dissociation of Li-F in polar media. Theoretica Chimica Acta, 1993, 86, 211-217.	0.8	1
142	Molecular modelling of the photoconduction mechanism by charged solitons intrans-polyacetylene: I. Molecular Engineering, 1996, 6, 229-237.	0.2	1
143	A DFT Study of the Regioselectivity in Intramolecular Diels-Alder Reactions with Formation of a Tricyclodecane Skeleton. Letters in Organic Chemistry, 2011, 8, 125-131.	0.5	1
144	Theoretical Basis for the Treatment of Solvent Effects in the Context of Density Functional Theory. , 2002, , 81-123.		1

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145	A Local Extension of the Electrophilicity Index Concept. Journal of the Mexican Chemical Society, 2017, 56, .	0.6	1
146	Origin of the Synchronicity on the Transition Structures of Polar Dielsâ€"Alder Reactions. Are these Reactions [4 + 2] Processes?. ChemInform, 2003, 34, no.	0.0	0
147	Microbial Transformation of Marine Halogenated Sesquiterpenes. Natural Product Communications, 2010, 5, 1934578X1000501.	0.5	0
148	Quantum mechanical and molecular dynamic approaches to describe solvation effects by neoteric solvents. Current Opinion in Green and Sustainable Chemistry, 2020, 26, 100395.	5.9	0