

Renato Contreras

List of Publications by Year in descending order

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148
papers

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109137

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docs citations

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times ranked

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#	ARTICLE	IF	CITATIONS
1	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
2	A direct evaluation of regional Fukui functions in molecules. <i>Chemical Physics Letters</i> , 1999, 304, 405-413.	1.2	420
3	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
4	On the condensed Fukui function. <i>Journal of Chemical Physics</i> , 2000, 113, 2544-2551.	1.2	345
5	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
6	Quantum Mechanical Continuum Solvation Models for Ionic Liquids. <i>Journal of Physical Chemistry B</i> , 2012, 116, 9122-9129.	1.2	225
7	Sigma-pi separation of the electron localization function and aromaticity. <i>Journal of Chemical Physics</i> , 2004, 120, 1670-1673.	1.2	210
8	Self consistent field theory of solvent effects representation by continuum models: Introduction of desolvation contribution. <i>Theoretica Chimica Acta</i> , 1984, 65, 1-11.	0.9	166
9	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
10	Comparison between Experimental and Theoretical Scales of Electrophilicity in Benzhydryl Cations. <i>Journal of Organic Chemistry</i> , 2002, 67, 4747-4752.	1.7	133
11	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
12	Definition of a Nucleophilicity Scale. <i>Journal of Physical Chemistry A</i> , 2006, 110, 8181-8187.	1.1	116
13	A Theoretical Study on the Relationship between Nucleophilicity and Ionization Potentials in Solution Phase. <i>Journal of Physical Chemistry A</i> , 2003, 107, 5588-5593.	1.1	100
14	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
15	Woodward-Hoffmann Rule in the Light of the Principles of Maximum Hardness and Minimum Polarizability: A DFT and Ab Initio SCF Studies. <i>Journal of the American Chemical Society</i> , 2000, 122, 348-351.	6.6	90
16	Reactivity of the carbon-carbon double bond towards nucleophilic additions. A DFT analysis. <i>Tetrahedron</i> , 2004, 60, 6585-6591.	1.0	84
17	Electronic Contributions to the ρ Parameter of the Hammett Equation. <i>Journal of Organic Chemistry</i> , 2003, 68, 6060-6062.	1.7	80
18	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

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19	A proposal for a new local hardness as selectivity index. <i>Chemical Physics Letters</i> , 2004, 383, 181-187.	1.2	77
20	Solvent Effects on Electrophilicity. <i>Journal of the American Chemical Society</i> , 2001, 123, 5527-5531.	6.6	73
21	Structure-genotoxic activity relationships of pesticides: comparison of the results from several short-term assays. <i>Mutation Research - Environmental Mutagenesis and Related Subjects Including Methodology</i> , 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. <i>Journal of Organic Chemistry</i> , 2009, 74, 9173-9179.	1.7	69
23	Comparison among Four Different Ways to Condense the Fukui Function. <i>Journal of Physical Chemistry A</i> , 2005, 109, 3220-3224.	1.1	67
24	On the SCF theory of continuum solvent effects representation: Introduction of local dielectric effects. <i>International Journal of Quantum Chemistry</i> , 1985, 27, 293-301.	1.0	61
25	Nucleophilicity Index from Perturbed Electrostatic Potentials. <i>Journal of Physical Chemistry A</i> , 2007, 111, 2442-2447.	1.1	59
26	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
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. <i>Biophysical Journal</i> , 2007, 92, 430-439.	0.2	49
28	Mechanistic pathways of aromatic nucleophilic substitution in conventional solvents and ionic liquids. <i>New Journal of Chemistry</i> , 2014, 38, 2611-2618.	1.4	48
29	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
30	Relationships between the Electrophilicity Index and Experimental Rate Coefficients for the Aminolysis of Thiocarbonates and Dithiocarbonates. <i>Journal of Organic Chemistry</i> , 2005, 70, 1754-1760.	1.7	44
31	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
32	Gutmann's Donor Numbers Correctly Assess the Effect of the Solvent on the Kinetics of S_NAr Reactions in Ionic Liquids. <i>Chemistry - A European Journal</i> , 2016, 22, 13347-13351.	1.7	41
33	N-borane adducts of oxazolidines derived from ephedrine and pseudo-ephedrine. Study of stereochemistry by nuclear magnetic resonance. <i>Tetrahedron</i> , 1984, 40, 3829-3838.	1.0	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. <i>Journal of Physical Chemistry A</i> , 2002, 106, 11227-11233.	1.1	40
35	N-Heterocyclic carbene copper(σ) complex-catalyzed synthesis of 2-aryl benzoxazoles and benzothiazoles. <i>RSC Advances</i> , 2016, 6, 82401-82408.	1.7	40
36	Group electrophilicity as a model of nucleofugality in nucleophilic substitution reactions. <i>Chemical Physics Letters</i> , 2006, 422, 340-344.	1.2	37

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37	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
38	Specific nucleophile-electrophile interactions in nucleophilic aromatic substitutions. <i>Organic and Biomolecular Chemistry</i> , 2013, 11, 2302.	1.5	35
39	Some relationships within the nonlocal (pair-site) chemical reactivity formalism of density functional theory. <i>Journal of Chemical Physics</i> , 2000, 113, 10861-10866.	1.2	33
40	Effect of electron-withdrawing substituents on the electrophilicity of carbonyl carbons. <i>Tetrahedron</i> , 2005, 61, 417-422.	1.0	33
41	The Chromophore Structure of the Cyanobacterial Phytochrome Cph1 As Predicted by Time-Dependent Density Functional Theory. <i>Journal of Physical Chemistry B</i> , 2008, 112, 16253-16256.	1.2	33
42	Relationship between nucleophilicity/electrophilicity indices and reaction mechanisms for the nucleophilic substitution reactions of carbonyl compounds. <i>Journal of Physical Organic Chemistry</i> , 2004, 17, 273-281.	0.9	32
43	Proton transfer in water polymers as a model for intimate and solvent-separated ion pairs. <i>The Journal of Physical Chemistry</i> , 1984, 88, 1905-1908.	2.9	31
44	The Markovnikov Regioselectivity Rule in the Light of Site Activation Models. <i>Journal of Physical Chemistry A</i> , 2002, 106, 7844-7849.	1.1	31
45	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
46	Chemical Reactivity in the $\{N, NS, v(r)\}$ Space. <i>Journal of Physical Chemistry A</i> , 2003, 107, 3831-3835.	1.1	29
47	Time-Dependent DFT on Phytochrome Chromophores: A Way to the Right Conformer. <i>Journal of Physical Chemistry Letters</i> , 2010, 1, 796-801.	2.1	29
48	π -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
49	The maximum hardness and minimum polarizability principles as the basis for the study of reaction profiles. <i>Theoretical Chemistry Accounts</i> , 2003, 110, 421-427.	0.5	26
50	Relationship between local electrophilicity and rate coefficients for the hydrolysis of carbenium ions. <i>Tetrahedron</i> , 2005, 61, 889-895.	1.0	26
51	On the variations of electronic chemical potential and chemical hardness induced by solvent effects. <i>Chemical Physics Letters</i> , 2006, 433, 54-57.	1.2	26
52	Empirical scale of nucleophilicity for substituted pyridines. <i>Chemical Physics Letters</i> , 2006, 422, 204-209.	1.2	25
53	Nucleofugality index in $\hat{\pi}$ -elimination reactions. <i>Chemical Physics Letters</i> , 2007, 439, 177-182.	1.2	25
54	Electrofugality index for benzhydryl derivatives. <i>Chemical Physics Letters</i> , 2007, 447, 375-378.	1.2	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.	1.2	25
56	Relationship between the electronic chemical potential and proton transfer barriers. Chemical Physics Letters, 1997, 269, 419-427.	1.2	24
57	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
58	Global and Local Analysis of the Gas-Phase Acidity of Haloacetic Acids. Journal of Physical Chemistry A, 2000, 104, 5882-5887.	1.1	24
59	An unusual halogenated meroditerpenoid from <i>Styopodium flabelliforme</i> : Studies by NMR spectroscopic and computational methods. Phytochemistry, 2009, 70, 1315-1320.	1.4	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.	1.7	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.	1.2	23
62	Experimental and theoretical study on the oxidation mechanism of dopamine in n-octyl pyridinium based ionic liquids-carbon paste modified electrodes. Electrochimica Acta, 2013, 111, 846-854.	2.6	23
63	Lewis Molecular Acidity of Ionic Liquids from Empirical Energy-Density Models. Journal of Physical Chemistry B, 2013, 117, 1911-1920.	1.2	23
64	On the mechanism of CO ₂ electro-cycloaddition to propylene oxides. Journal of CO ₂ Utilization, 2016, 16, 114-120.	3.3	23
65	Solvation energies from the linear response function of density functional theory. Chemical Physics Letters, 1996, 260, 236-242.	1.2	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.	1.1	22
67	Relationship between the electrophilicity of substituting agents and substrate selectivity in Friedel-Crafts reactions. Tetrahedron, 2005, 61, 831-836.	1.0	22
68	Local hardness: An application to electrophilic additions. Chemical Physics Letters, 2007, 446, 170-175.	1.2	22
69	Changes in the S_NAr reaction mechanism brought about by preferential solvation. RSC Advances, 2015, 5, 99322-99328.	1.7	22
70	Electrophilicity of quinones and its relationship with hydride affinity. Chemical Physics Letters, 2009, 471, 168-173.	1.2	21
71	Quantitative characterization of group electrophilicity and nucleophilicity for intramolecular Diels-Alder reactions. Organic and Biomolecular Chemistry, 2010, 8, 3678.	1.5	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.	2.0	20

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73	Local reactivity index defined through the density of states describes the basicity of alkaline-exchanged zeolites. <i>Journal of Chemical Physics</i> , 2002, 116, 4311-4316.	1.2	19
74	Solvent effects in ionic liquids: empirical linear energy-density relationships. <i>Physical Chemistry Chemical Physics</i> , 2012, 14, 10041.	1.3	18
75	Theoretical insights into the E1cB/E2 mechanistic dichotomy of elimination reactions. <i>Organic and Biomolecular Chemistry</i> , 2019, 17, 9874-9882.	1.5	18
76	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
77	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
78	On the Catalytic Effect of Water in the Intramolecular Diels-Alder Reaction of Quinone Systems: A Theoretical Study. <i>Molecules</i> , 2012, 17, 13687-13703.	1.7	17
79	Global and Local Reactivity and Activation Patterns of HOOX (X = H, NO ₂ , CO ₂ ⁻ , SO ₃ ⁻) Peroxides with Solvent Effects. <i>Journal of Physical Chemistry A</i> , 2003, 107, 10098-10104.	1.1	16
80	A computational ONIOM model for the description of the H-bond interactions between NU2058 analogues and CDK2 active site. <i>Chemical Physics Letters</i> , 2009, 479, 149-155.	1.2	16
81	Phenomenological chemical reactivity theory for mobile electrons. <i>Theoretical Chemistry Accounts</i> , 2010, 126, 45-54.	0.5	16
82	Are Electrophilicity and Electrofugality Related Concepts? A Density Functional Theory Study. <i>Organic Letters</i> , 2011, 13, 822-824.	2.4	16
83	Effect of the nature of the nucleophile and solvent on an S _N Ar reaction. <i>New Journal of Chemistry</i> , 2018, 42, 260-264.	1.4	16
84	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
85	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
86	Homofugality: A new reactivity index describing the leaving group ability in homolytic substitution reactions. <i>Chemical Physics Letters</i> , 2006, 424, 437-442.	1.2	15
87	Site activation effects promoted by intramolecular hydrogen bond interactions in S _N Ar reactions. <i>RSC Advances</i> , 2014, 4, 30638-30643.	1.7	15
88	Theoretical study of lithium-fluoride and lithium-chloride ion pairs in aqueous solution. An SCF-CNDO/2 approach including continuum solvent effects. <i>International Journal of Quantum Chemistry</i> , 1986, 30, 581-590.	1.0	14
89	Molecular modelling of lithium intercalation in. <i>Journal of Physics Condensed Matter</i> , 1997, 9, 3011-3021.	0.7	14
90	Two state reactivity mechanism for the rearrangement of hydrogen peroxy nitrite to nitric acid. <i>Chemical Physics Letters</i> , 2008, 457, 216-221.	1.2	14

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91	Structure-reactivity relationships for electrophilic sugars in interaction with nucleophilic biological targets. <i>Bioorganic and Medicinal Chemistry</i> , 2008, 16, 3184-3190.	1.4	14
92	Reactivity of benzohydrazide derivatives towards acetylation reaction. Experimental and theoretical studies. <i>Chemical Physics Letters</i> , 2010, 488, 86-89.	1.2	14
93	Bond Fukui Functions As Descriptor of the Electron Density Reorganization in π Conjugated Systems. <i>Journal of Organic Chemistry</i> , 2012, 77, 90-95.	1.7	14
94	Regional Electrophilic and Nucleophilic Fukui Functions Efficiently Highlight the Lewis Acidic/Basic Regions in Ionic Liquids. <i>Journal of Physical Chemistry B</i> , 2014, 118, 3696-3701.	1.2	14
95	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
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 lumiflavine-1-methylnicotinamide model system using group softness. <i>Tetrahedron</i> , 2004, 60, 4189-4196.	1.0	12
98	Theoretical Study on CDK2 Inhibitors Using a Global Softness Obtained from the Density of States. <i>Journal of Physical Chemistry B</i> , 2007, 111, 3293-3297.	1.2	12
99	Higher order derivatives for nuclear indexes in the framework of density functional theory. <i>Journal of Chemical Physics</i> , 2001, 115, 6822-6826.	1.2	11
100	Local reactivity index as descriptor of benzene adsorption in cluster models of exchanged zeolite-Y. <i>Chemical Physics Letters</i> , 2004, 383, 612-616.	1.2	11
101	Non-electrostatic components of short and strong hydrogen bonds induced by compression inside fullerenes. <i>Chemical Physics Letters</i> , 2010, 486, 119-122.	1.2	11
102	Permanent group effect on nucleofugality in aryl benzoates. <i>Chemical Physics Letters</i> , 2010, 498, 221-225.	1.2	11
103	Activation of Electrophile/Nucleophile Pair by a Nucleophilic and Electrophilic Solvation in a S _N Ar Reaction. <i>Frontiers in Chemistry</i> , 2018, 6, 509.	1.8	11
104	Energy-density relationships for the treatment of ion solvation within density-functional theory. <i>Physical Review A</i> , 1994, 49, 3439-3444.	1.0	10
105	Analysis of gas phase proton transfer using density functional theory. The H ₂ O + HX (X = F, Cl and OH) system. <i>Chemical Physics Letters</i> , 1996, 256, 15-20.	1.2	10
106	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
107	Understanding the influence of Lewis acids in the regioselectivity of the Diels-Alder reactions of 2-methoxy-5-methyl-1,4-benzoquinone: A DFT study. <i>Computational and Theoretical Chemistry</i> , 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. <i>Chemical Physics Letters</i> , 1986, 127, 169-171.	1.2	9

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109	A model for the charge capacity of 1T-TiS ₂ intercalated with Li. <i>International Journal of Quantum Chemistry</i> , 1995, 56, 819-823.	1.0	9
110	Relationship between solvation energy, chemical potential and hardness variations. <i>Computational and Theoretical Chemistry</i> , 1997, 390, 169-175.	1.5	9
111	Î ² -Scission of thioimidoyl radicals (R1-N=C-S-R2): A theoretical scale of radical leaving group ability. <i>Chemical Physics Letters</i> , 2007, 443, 383-388.	1.2	9
112	On the Role of Short and Strong Hydrogen Bonds on the Mechanism of Action of a Model Chymotrypsin Active Site. <i>Journal of Physical Chemistry A</i> , 2009, 113, 5769-5772.	1.1	9
113	Lewis Acidity/Basicity Changes in Imidazolium Based Ionic Liquids Brought About by Impurities. <i>Journal of Physical Chemistry B</i> , 2015, 119, 13160-13166.	1.2	9
114	Methodological Issues in First-Principle Calculations of CH ₃ NH ₃ PbI ₃ Perovskite Surfaces: Quantum Confinement and Thermal Motion. <i>ACS Omega</i> , 2020, 5, 29477-29491.	1.6	9
115	Understanding the stereo- and regioselectivities of the polar Diels-Alder reactions between 2-acetyl-4-benzoquinone and methyl substituted 1,3-butadienes: a DFT study. <i>Journal of Physical Organic Chemistry</i> , 2009, 22, 578-584.		8
116	Kinetic and theoretical study on nucleofugality in the phenolysis of 3-nitrophenyl and 4-nitrophenyl 4-cyanophenyl thionocarbonates. <i>Chemical Physics Letters</i> , 2013, 572, 130-135.	1.2	8
117	Philicity and Fugality Scales for Organic Reactions. <i>Advances in Chemistry</i> , 2014, 2014, 1-13.	1.1	8
118	Mechanistic insights into the ANRORC-like rearrangement between methylhydrazine and 1,2,4-oxadiazole derivatives. <i>Organic and Biomolecular Chemistry</i> , 2015, 13, 9439-9444.	1.5	8
119	Solvent effect on a model S _N Ar reaction in ionic liquid/water mixtures at different compositions. <i>New Journal of Chemistry</i> , 2018, 42, 9645-9650.	1.4	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. <i>International Journal of Quantum Chemistry</i> , 1988, 33, 41-52.	1.0	7
121	Wave function instabilities in the cis-trans isomerization and singlet-triplet energy gaps in a push-pull compound. <i>Journal of Chemical Physics</i> , 2003, 119, 4112-4116.	1.2	7
122	Invariance of electrophilicity of independent fragments. Application to intramolecular Diels-Alder reactions. <i>Chemical Physics Letters</i> , 2010, 499, 272-277.	1.2	7
123	How Meaningful Is the Halogen Bonding in 1-Ethyl-3-methyl Imidazolium-Based Ionic Liquids for CO ₂ Capture?. <i>Journal of Physical Chemistry B</i> , 2018, 122, 7907-7914.	1.2	7
124	Quantum mechanical calculation of thermodynamic functions of solvation of ammonium ions in water. <i>Canadian Journal of Chemistry</i> , 1985, 63, 1746-1749.	0.6	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 urea-betaine system. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 1994-2004.	1.3	6
126	On the SCF theory of continuum solvent effects representation II. Quantum chemical calculation of thermodynamic properties of some acid-base equilibria in solution. <i>International Journal of Quantum Chemistry</i> , 1986, 30, 573-584.	1.0	5

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127	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
128	Basicity and solvent effects on hydrogen bonding in NR ₃ i _{1/2} i _{1/2} i _{1/2} HCOOH (R=H, CH ₃) model systems. <i>International Journal of Quantum Chemistry</i> , 1999, 74, 387-394.	1.0	4
129	Proton transport catalysis in intramolecular rearrangements: A density functional theory study. <i>Chemical Physics Letters</i> , 2008, 464, 271-275.	1.2	4
130	On the Principle of Spin Potential Equalization. <i>Journal of Physical Chemistry A</i> , 2009, 113, 1390-1396.	1.1	4
131	On the Gas-Phase Electronic Chemical Potential of Anions. <i>Journal of Chemical Theory and Computation</i> , 2009, 5, 2944-2949.	2.3	4
132	Endohedral Cluster of Li ₁₀ O with T _d Symmetry. <i>Journal of Physical Chemistry A</i> , 2009, 113, 13451-13456.	1.1	3
133	Predicting the reaction mechanism of nucleophilic substitutions at carbonyl and thiocarbonyl centres of esters and thioesters. <i>Journal of Physical Organic Chemistry</i> , 2012, 25, 1359-1364.	0.9	3
134	Quantitative characterization of the global philicity patterns of common diene/dienophile pairs in cycloaddition reactions II: the interacting pair model. <i>Tetrahedron Letters</i> , 2015, 56, 1767-1770.	0.7	3
135	Gutmann's Donor and Acceptor Numbers for Ionic Liquids and Deep Eutectic Solvents. <i>Frontiers in Chemistry</i> , 2022, 10, 861379.	1.8	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.	0.8	2
137	The electronic chemical potential as a basis for a cluster model approximation for intercalation of Li in 1T - TiS ₂ . <i>Computational and Theoretical Chemistry</i> , 1995, 335, 161-166.	1.5	2
138	Hydrogen bonding and dissociation effects on the gas phase proton transfer reactions of ozone. <i>Theoretical Chemistry Accounts</i> , 1998, 99, 60-63.	0.5	2
139	Origins of the ANRORC reactivity in nitroimidazole derivatives. <i>RSC Advances</i> , 2016, 6, 25215-25221.	1.7	2
140	Inertia defects of urea. <i>Journal of Molecular Structure</i> , 1986, 142, 91-92.	1.8	1
141	Desolvation effects on the dissociation energy of diatomic molecules: Ab initio study of the dissociation of Li-F in polar media. <i>Theoretica Chimica Acta</i> , 1993, 86, 211-217.	0.9	1
142	Molecular modelling of the photoconduction mechanism by charged solitons intrans-polyacetylene: I. <i>Molecular Engineering</i> , 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. <i>Letters in Organic Chemistry</i> , 2011, 8, 125-131.	0.2	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, .	0.2	1
146	Origin of the Synchronicity on the Transition Structures of Polar Diels-Alder Reactions. Are these Reactions [4 + 2] Processes?. ChemInform, 2003, 34, no.	0.1	0
147	Microbial Transformation of Marine Halogenated Sesquiterpenes. Natural Product Communications, 2010, 5, 1934578X1000501.	0.2	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.	3.2	0