BÃ¡rbara Herrera

List of Publications by Year
in descending order

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43	889	516215 16	476904 29
papers	citations	h-index	g-index

43	43	43	573
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Theoretical study of the substituent effect on the Oâ€“H insertion reaction of copper carbenoids. Theoretical Chemistry Accounts, 2022, 141, 1.	0.5	1
2	Theoretical Study of the Mechanism of Catalytic Enanteoselective Nâ€“H and Oâ€“H Insertion Reactions. Journal of Physical Chemistry A, 2020, 124, 2-11.	1.1	8
3	Mechanistic Insight toward Understanding the Role of Charge in Thiourea Organocatalysis. Journal of Organic Chemistry, 2020, 85, 585-593.	1.7	11
4	On the nature of the interaction of copper hydride and halide with substituted ethylene and acetylene. Journal of Molecular Modeling, 2020, 26, 61.	0.8	2
5	Reaction Mechanism of Li and Mg Carbenoid Cyclopropanations: Metal-Ï€ and Ïƒ Interactions. ACS Omega, 2019, 4, 19452-19461.	1.6	5
6	Theoretical study of C-arylations with aryl halides to determine the reaction mechanism, the effect of substituents and heteroatoms. Physical Chemistry Chemical Physics, 2019, 21, 10163-10170.	1.3	6
7	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
8	An extension of the Marcus equation: the Marcus potential energy function. Journal of Molecular Modeling, 2018, 24, 104.	0.8	10
9	Study of antiradical mechanisms with dihydroxybenzenes using reaction force and reaction electronic flux. Physical Chemistry Chemical Physics, 2017, 19, 14512-14519.	1.3	11
10	Elucidating the Catalytic Role of Mg(II) in the Intramolecular Proton Transfer Reaction in Thymine. Journal of the Mexican Chemical Society, 2017, 56, .	0.2	0
11	Reaction electronic flux and its role in DNA intramolecular proton transfers. Journal of Molecular Modeling, 2016, 22, 145.	0.8	8
12	Effect of beryllium bonds on the ketoâ€“enol tautomerism of formamide derivatives: a subtle basicityâ€“acidity balance. Theoretical Chemistry Accounts, 2016, 135, 1.	0.5	5
13	Role of water in intramolecular proton transfer reactions of formamide and thioformamide. Theoretical Chemistry Accounts, 2016, 135, 1.	0.5	17
14	Extending the halogen-bonded supramolecular synthon concept to 1,3,4-oxadiazole derivatives. CrystEngComm, 2016, 18, 42-47.	1.3	11
15	Formation of Nanoparticles and Decoration of Organic Crystals. , 2016, , 549-564.		0
16	Atomic decomposition of conceptual DFT descriptors: application to proton transfer reactions. Physical Chemistry Chemical Physics, 2015, 17, 17797-17808.	1.3	37
17	Insights into the chemical meanings of the reaction electronic flux. Theoretical Chemistry Accounts, 2015, 134, 1.	0.5	20
18	Formation of Nanoparticles and Decoration of Organic Crystals. , 2015, , 1-14.		1

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19	New insights into the gas-phase unimolecular fragmentations of [Cysteineâ€“Ca]2+ complexes. Computational and Theoretical Chemistry, 2014, 1047, 38-46.	1.1	2
20	The mechanism of Menshutkin reaction in gas and solvent phases from the perspective of reaction electronic flux. Journal of Molecular Modeling, 2014, 20, 2353.	0.8	24
21	The mechanism of chemisorption of hydrogen atom on graphene: Insights from the reaction force and reaction electronic flux. Journal of Chemical Physics, 2014, 141, 134701.	1.2	27
22	Using the reaction force and the reaction electronic flux on the proton transfer of formamide derived systems. Physical Chemistry Chemical Physics, 2014, 16, 14489.	1.3	29
23	Influence of the monoclinic and tetragonal zirconia phases on the water gas shift reaction. A theoretical study. Journal of Molecular Modeling, 2013, 19, 2885-2891.	0.8	7
24	A Relation between Different Scales of Electrophilicity: Are the Scales Consistent Along a Chemical Reaction?. Journal of Physical Chemistry A, 2012, 116, 7074-7081.	1.1	9
25	Applying Sanderson rules to the formation reaction of hydrogen-bonded dimers. Computational and Theoretical Chemistry, 2012, 990, 222-226.	1.1	4
26	Study of ring influence and electronic response to proton transfer reactions. Reaction electronic flux analysis. Journal of Molecular Modeling, 2011, 17, 1051-1060.	0.8	3
27	The mechanism of methanol decomposition by CuO. A theoretical study based on the reaction force and reaction electronic flux analysis. Journal of Molecular Modeling, 2011, 17, 1625-1633.	0.8	19
28	The reaction electronic flux in chemical reactions. Science China Chemistry, 2011, 54, 1982-1988.	4.2	52
29	Formation of Copper Nanoparticles Supported onto Inclusion Compounds of Î±-cyclodextrin: A New Route to Obtain Copper Nanoparticles. Molecular Crystals and Liquid Crystals, 2010, 521, 246-252.	0.4	8
30	The impact of Cu atoms on the reactivity of ZrO2 oligomers. Journal of Molecular Modeling, 2009, 15, 405-410.	0.8	4
31	INCLUSION COMPOUNDS OF Î±-CYCLODEXTRIN WITH ALKYLTHIOLS. Journal of the Chilean Chemical Society, 2008, 53, .	0.5	19
32	The Electronic Flux in Chemical Reactions. Insights on the Mechanism of the Maillard Reaction. AIP Conference Proceedings, 2007, , .	0.3	2
33	The Role of Reaction Force and Chemical Potential in Characterizing the Mechanism of Double Proton Transfer in the Adenineâ‹¯Uracil Complex. Journal of Physical Chemistry A, 2007, 111, 5921-5926.	1.1	131
34	Phenolysis and benzenethiolysis reactions of carbonyl and thiocarbonyl compounds from the perspective of the HSAB principle. Computational and Theoretical Chemistry, 2007, 811, 91-96.	1.5	3
35	Characterization of the reactive conformations of protonated histamine through the reaction force analysis and the dual descriptor of chemical reactivity. Computational and Theoretical Chemistry, 2007, 817, 111-118.	1.5	13
36	Structure and Medium Effects on the Photochemical Behavior of Nonfluorinated Quinolone Antibioticsâ€. Photochemistry and Photobiology, 2007, 83, 511-519.	1.3	7

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37	Cubane oligomers: A density functional theory study. Computational and Theoretical Chemistry, 2006, 769, 183-187.	1.5	16
38	The reaction force: Three key points along an intrinsic reaction coordinate. Journal of Chemical Sciences, 2005, 117, 467-472.	0.7	122
39	On the Mechanism of Hydrogen Transfer in the HSCH(O) â‡Œ (S)CHOH and HSNO â‡Œ SNOH Reactions. Journal of Physical Chemistry A, 2005, 109, 1748-1751.	1.1	93
40	The role of the reaction force to characterize local specific interactions that activate the intramolecular proton transfers in DNA basis. Journal of Chemical Physics, 2004, 121, 7096-7102.	1.2	74
41	Theoretical Study of the HXNY â†' XNYH (X,Y = O,S) Intramolecular Proton Transfer Reactions. Journal of Physical Chemistry A, 2004, 108, 1830-1836.	1.1	21
42	Conformational Effects on Glycine Ionization Energies and Dyson Orbitals. Journal of Physical Chemistry A, 2004, 108, 11703-11708.	1.1	28
43	Theoretical study of the internal rotation of cubylcubane and cubylcubane difluoride. Chemical Physics Letters, 2001, 344, 193-199.	1.2	8