

# How to Conceptualize Catalytic Cycles? The Energetic S

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Citation Report

#	ARTICLE	IF	CITATIONS
15	How Racemic Secondary Alkyl Electrophiles Proceed to Enantioselective Products in Negishi Cross-Coupling Reactions. <i>Organometallics</i> , 2011, 30, 3284-3292.	1.1	60
16	Selective Homogeneous Hydrogenation of Biogenic Carboxylic Acids with [Ru(TriPhos)H] <sub>2</sub> : A Mechanistic Study. <i>Journal of the American Chemical Society</i> , 2011, 133, 14349-14358.	6.6	233
17	Theoretical Investigation for the Cycle Reaction of N <sub>2</sub> O (x <sup>1</sup> â <sup>+</sup> ) with CO (x <sup>1</sup> â <sup>+</sup> ) Catalyzed by IrO <sub>2</sub> (x <sup>1</sup> â <sup>+</sup> ) (x <sup>1</sup> â <sup>+</sup> = 1,) <i>Tj ETQq0 0 0 rgBT /Overlo</i> A, 2011, 115, 11023-11032.	1.1	18
18	Nickel-catalyzed amination of aryl carbamates and sequential site-selective cross-couplings. <i>Chemical Science</i> , 2011, 2, 1766.	3.7	148
19	Theoretical views on the cycle reaction of N <sub>2</sub> O (1 <sup>+</sup> )+NH <sub>3</sub> (1A <sub>1</sub> )+O <sub>2</sub> catalyzed by Fe <sup>+</sup> and utilizing the energy span model to study its kinetic information. <i>Computational and Theoretical Chemistry</i> , 2011, 974, 143-150.	1.1	3
20	What makes for a good catalytic cycle? A theoretical study of the SPhos ligand in the Suzuki-Miyaura reaction. <i>Chemical Communications</i> , 2011, 47, 4935.	2.2	42
21	Finding the key transition states and intermediates controlling net reaction rates and selectivity. <i>Nature Precedings</i> , 2011, , .	0.1	0
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23	NHC catalyzed CO <sub>2</sub> fixation with epoxides: Probable mechanisms reveal ter molecular pathway. <i>Tetrahedron Letters</i> , 2011, 52, 5403-5406.	0.7	49
24	Indenyl effect in dissociative reactions. Nucleophilic substitution in iron carbonyl complexes: a case study. <i>Dalton Transactions</i> , 2011, 40, 11138.	1.6	18
25	A Theoretical Study of Hydrogen Transfer Catalyzed by an Ir <sup>III</sup> PC(sp <sup>3</sup> ) <sub>3</sub> P Pincer Complex. <i>ChemCatChem</i> , 2011, 3, 1348-1353.	1.8	7
26	The Rate-Determining Step is Dead. Long Live the Rate-Determining State!. <i>ChemPhysChem</i> , 2011, 12, 1413-1418.	1.0	129
27	Origin of Asymmetric Induction in Bicyclic Guanidine-Catalyzed Thio-Michael Reaction: A Bifunctional Mode of Lewis Acid-Brønsted Acid Activation. <i>Journal of Organic Chemistry</i> , 2012, 77, 6553-6562.	1.7	38
28	Turning Over-Definitions in Catalytic Cycles. <i>ACS Catalysis</i> , 2012, 2, 2787-2794.	5.5	431
29	Mechanistic Investigation of the Ruthenium-N-Heterocyclic-Carbene-Catalyzed Amidation of Amines with Alcohols. <i>Chemistry - A European Journal</i> , 2012, 18, 15683-15692.	1.7	66
30	Mechanism of the Gold(I)-Catalyzed Rearrangement of Alkynyl Sulfoxides: A DFT Study. <i>Organometallics</i> , 2012, 31, 3043-3055.	1.1	41
31	A Theoretical Study of Metal-Metal Cooperativity in the Homogeneous Water Gas Shift Reaction. <i>Inorganic Chemistry</i> , 2012, 51, 377-385.	1.9	25
32	DFT study on the mechanism of water-assisted dihydrogen elimination in group 6 octahedral metal hydride complexes. <i>Dalton Transactions</i> , 2012, 41, 11018.	1.6	12

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41	Role of Explicit Solvents in Palladium(II)-Catalyzed Alkoxylation of Arenes: An Interesting Paradigm for Preferred Outer-Sphere Reductive Elimination over Inner-Sphere Pathway. <i>Organometallics</i> , 2012, 31, 6466-6481.	1.1	42
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43	Rollover Cyclometalation Pathway in Rhodium Catalysis: Dramatic NHC Effects in the C-H Bond Functionalization. <i>Journal of the American Chemical Society</i> , 2012, 134, 17778-17788.	6.6	157
44	Theoretical study on the mechanism and stereochemistry of salicylaldehyde-Al(III)-catalyzed hydrophosphonylation of benzaldehyde. <i>Computational and Theoretical Chemistry</i> , 2012, 989, 44-50.	1.1	7
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81	Isolated catalyst sites on amorphous supports: A systematic algorithm for understanding heterogeneities in structure and reactivity. <i>Journal of Chemical Physics</i> , 2013, 138, 204105.	1.2	41
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87	In Silico Design of Heteroaromatic Half-Sandwich Rh <sup>I</sup> Catalysts for Acetylene [2+2+2] Cyclotrimerization: Evidence of a Reverse Indenyl Effect. <i>Chemistry - A European Journal</i> , 2013, 19, 13337-13347.	1.7	27
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98	On the Mechanism of the Dehydroaromatization of Hexane to Benzene by an Iridium Pincer Catalyst. <i>Chemistry - A European Journal</i> , 2013, 19, 4069-4077.	1.7	20
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105	Reactivity and Regioselectivity of Methylacetylene Cyclotrimerization over the Phillips Cr/Silica Catalyst: A DFT Study. <i>ACS Catalysis</i> , 2013, 3, 1172-1183.	5.5	22
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107	Mechanistic Study of Borylation of Nitriles Catalyzed by Rh <sup>+</sup> B and Ir <sup>+</sup> B Complexes via C <sup>+</sup> CN Bond Activation. <i>Organometallics</i> , 2013, 32, 926-936.	1.1	48
108	Computational mechanistic study on oxidative esterification of alcohols to esters catalyzed by palladium complex. <i>Journal of Organometallic Chemistry</i> , 2013, 740, 10-16.	0.8	2
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128	$\pi$ -Complexation in Nickel-Catalyzed Cross-Coupling Reactions. <i>Journal of Organic Chemistry</i> , 2014, 79, 1836-1841.	1.7	33

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