

# 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.	2.3	60
16	Selective Homogeneous Hydrogenation of Biogenic Carboxylic Acids with [Ru(TriPhos)H] <sup>+</sup> : A Mechanistic Study. <i>Journal of the American Chemical Society</i> , 2011, 133, 14349-14358.	13.7	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,) Tj ETQg 0 0 0 reg BT /Overlo A, 2011, 115, 11023-11032.	2.3	13
18	Nickel-catalyzed amination of aryl carbamates and sequential site-selective cross-couplings. <i>Chemical Science</i> , 2011, 2, 1766.	7.4	148
19	Theoretical views on the cycle reaction of N <sub>2</sub> O (1 <sup>1</sup> â <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.	2.5	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.	4.1	42
21	Finding the key transition states and intermediates controlling net reaction rates and selectivity. <i>Nature Precedings</i> , 2011, , .	0.1	0
22	Finding the key transition states and intermediates controlling net reaction rates and selectivity. <i>Nature Precedings</i> , 2011, , .	0.1	1
23	NHC catalyzed CO <sub>2</sub> fixation with epoxides: Probable mechanisms reveal ter molecular pathway. <i>Tetrahedron Letters</i> , 2011, 52, 5403-5406.	1.4	49
24	Indenyl effect in dissociative reactions. Nucleophilic substitution in iron carbonyl complexes: a case study. <i>Dalton Transactions</i> , 2011, 40, 11138.	3.3	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.	3.7	7
26	The Rate-Determining Step is Dead. Long Live the Rate-Determining State!. <i>ChemPhysChem</i> , 2011, 12, 1413-1418.	2.1	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.	3.2	38
28	Turning Over-Definitions in Catalytic Cycles. <i>ACS Catalysis</i> , 2012, 2, 2787-2794.	11.2	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.	3.3	66
30	Mechanism of the Gold(I)-Catalyzed Rearrangement of Alkynyl Sulfoxides: A DFT Study. <i>Organometallics</i> , 2012, 31, 3043-3055.	2.3	41
31	A Theoretical Study of Metal-Metal Cooperativity in the Homogeneous Water Gas Shift Reaction. <i>Inorganic Chemistry</i> , 2012, 51, 377-385.	4.0	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.	3.3	12

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33	Theoretical study on the mechanism of Ag-catalyzed synthesis of 3-alkylideneoxindoles from N-aryl-1,2-diazoamides: a Lewis acid or Ag-carbene pathway?. <i>Organic and Biomolecular Chemistry</i> , 2012, 10, 6294.	2.8	15
34	Theoretical Insight into PtCl <sub>2</sub> -Catalyzed Isomerization of Cyclopropenes to Allenes. <i>Organometallics</i> , 2012, 31, 4769-4778.	2.3	13
35	Theoretical Investigation on the Chiral Diamine-Catalyzed Epoxidation of Cyclic Enones: Mechanism and Effects of Cocatalyst. <i>Journal of Physical Chemistry A</i> , 2012, 116, 1251-1260.	2.5	14
36	Toward Predicting Full Catalytic Cycle Using Automatic Reaction Path Search Method: A Case Study on HCo(CO) <sub>3</sub> -Catalyzed Hydroformylation. <i>Journal of Chemical Theory and Computation</i> , 2012, 8, 380-385.	5.3	61
37	DFT and Experimental Studies on the PtX <sub>2</sub> /X-Catalyzed Olefin Hydroamination: Effect of Halogen, Amine Basicity, and Olefin on Activity, Regioselectivity, and Catalyst Deactivation. <i>Organometallics</i> , 2012, 31, 294-305.	2.3	22
38	Mechanistic and Stereochemical Insights on the Pt-Catalyzed Rearrangement of Oxiranylpropargylic Esters to Cyclopentenones. <i>Journal of Organic Chemistry</i> , 2012, 77, 8733-8743.	3.2	17
39	Hydrofluoroarylation of Alkynes with Ni Catalysts. C-H Activation via Ligand-to-Ligand Hydrogen Transfer, an Alternative to Oxidative Addition. <i>Organometallics</i> , 2012, 31, 1300-1314.	2.3	161
40	Mechanistic Studies of the CuH-Catalyzed Synthesis of 1-Hydroxyallenes. <i>Organometallics</i> , 2012, 31, 8024-8030.	2.3	11
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.	2.3	42
42	The Importance of Hydrogen Bonding to Stereoselectivity and Catalyst Turnover in Gold-Catalyzed Cyclization of Monoallylic Diols. <i>Journal of the American Chemical Society</i> , 2012, 134, 16307-16318.	13.7	67
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.	13.7	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.	2.5	7
45	New insights into the two catalyst cycles of the Pt-catalyzed oxidation of methane by oxygen: Spin-orbit coupling, spin-inversion probabilities, and kinetic information. <i>Computational and Theoretical Chemistry</i> , 2012, 989, 75-85.	2.5	9
46	Theoretical studies on the reaction of NO <sub>2</sub> with CO catalyzed by bare Os <sup>+</sup> cations and its kinetic information. <i>Computational and Theoretical Chemistry</i> , 2012, 993, 1-6.	2.5	2
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51	Theoretical investigations of spin-orbit coupling and kinetics in reaction NO <sub>2</sub> with CO catalyzed by gas phase bare Ir <sup>+</sup> . Computational and Theoretical Chemistry, 2012, 1001, 15-19.	2.5	2
52	Theoretical studies on the mechanism of oxazole with CO <sub>2</sub> catalyzed by gold(I) complexes. Journal of Molecular Catalysis A, 2012, 363-364, 31-40.	4.8	14
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54	Mild and Efficient Nickel-Catalyzed Heck Reactions with Electron-Rich Olefins. Journal of the American Chemical Society, 2012, 134, 443-452.	13.7	138
55	Mechanistic Investigation on Scandium-Catalyzed C-H Addition of Pyridines to Olefins. Organometallics, 2012, 31, 3930-3937.	2.3	66
56	A density functional theory study of hydrogen dissociation and diffusion at the perimeter sites of Au/TiO <sub>2</sub> . Physical Chemistry Chemical Physics, 2012, 14, 3741.	2.8	52
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59	Transition metal catalysis by density functional theory and density functional theory/molecular mechanics. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2012, 2, 375-385.	14.6	91
60	A refinement of everyday thinking: the energetic span model for kinetic assessment of catalytic cycles. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2012, 2, 795-815.	14.6	175
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62	On the Mechanism of the [Cp <sub>2</sub> Mo(OH)(OH <sub>2</sub> )] <sup>+</sup> -Catalyzed Nitrile Hydration to Amides: A Theoretical Study. Organometallics, 2012, 31, 1618-1626.	2.3	22
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65	Mechanistic Origin of Regioselectivity in Nickel-Catalyzed Olefin Hydroheteroarylation through C-H Activation. Organometallics, 2012, 31, 4356-4366.	2.3	56
67	On the Interpretation of Deuterium Kinetic Isotope Effects in C-H Bond Functionalizations by Transition-Metal Complexes. Angewandte Chemie - International Edition, 2012, 51, 3066-3072.	13.8	1,673
68	Bifunctional Rhenium Complexes for the Catalytic Transfer-Hydrogenation Reactions of Ketones and Imines. Chemistry - A European Journal, 2012, 18, 5701-5714.	3.3	40
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74	Carboxylation of Arene C-H Bonds with CO <sub>2</sub> : A DFT-Based Approach to Catalyst Design. <i>Chemistry - A European Journal</i> , 2012, 18, 170-177.	3.3	60
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77	Theoretical Toolkits for Inorganic and Bioinorganic Complexes: Their Applications and Insights. , 2013, , 1-57.		1
78	Enantioselective Synthesis. , 2013, , 807-831.		2
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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.	3.0	41
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86	Kinetic study on effect of novel cationic dimeric surfactants for the cleavage of carboxylate ester. <i>Journal of Physical Organic Chemistry</i> , 2013, 26, 626-631.	1.9	16
87	In Silico Design of Heteroaromatic Halfâ€“Sandwich Rh <sup>I</sup> Catalysts for Acetylene [2+2+2] Cyclotrimerization: Evidence of a Reverse Indenylâ€“Effect. <i>Chemistry - A European Journal</i> , 2013, 19, 13337-13347.	3.3	27
88	Dinuclear complexes of copper and zinc with m-xylene/cyclohexane-linked bis-aspartic acids: Synthesis, characterization, dioxygen activation, and catalytic oxidation of nitrobenzene in pure aqueous solution. <i>Dalton Transactions</i> , 2013, 42, 10898.	3.3	6

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89	Ruthenium-Mediated C-H Functionalization of Pyridine: The Role of Vinylidene and Pyridylidene Ligands. <i>Journal of the American Chemical Society</i> , 2013, 135, 2222-2234.	13.7	79
90	Quantum Chemical Calculations with the Inclusion of Nonspecific and Specific Solvation: Asymmetric Transfer Hydrogenation with Bifunctional Ruthenium Catalysts. <i>Journal of the American Chemical Society</i> , 2013, 135, 2604-2619.	13.7	151
91	Reply to Comment on "Turning Over" Definitions in Catalytic Cycles. <i>ACS Catalysis</i> , 2013, 3, 380-380.	11.2	18
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93	Mechanism of Ketone Allylation with Allylboronates as Catalyzed by Zinc Compounds: A DFT Study. <i>Chemistry - A European Journal</i> , 2013, 19, 124-134.	3.3	12
94	Rhodium catalyzed hydroamination of C <sub>2</sub> H <sub>4</sub> with NH <sub>3</sub> with pincer derived PE(CH <sub>2</sub> CH <sub>2</sub> X)P ligands "Fighting the energy span. <i>Journal of Organometallic Chemistry</i> , 2013, 748, 13-20.	1.8	10
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96	Role of base assisted proton transfer in N-heterocyclic carbene-catalyzed intermolecular Stetter reaction. <i>Tetrahedron Letters</i> , 2013, 54, 7144-7146.	1.4	15
97	On the gas-phase (n=1, 2) catalyzed reduction of N <sub>2</sub> O by H <sub>2</sub> : A density functional study. <i>Computational and Theoretical Chemistry</i> , 2013, 1013, 78-84.	2.5	2
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.	3.3	20
99	Resonance theory of catalytic action of transition-metal complexes: Isomerization of quadricyclane to norbornadiene catalyzed by metal porphyrins. <i>International Journal of Quantum Chemistry</i> , 2013, 113, 1833-1846.	2.0	9
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102	Computational Study of Gold-Catalyzed Homo- and Cross-Coupling Reactions. <i>Journal of Organic Chemistry</i> , 2013, 78, 4929-4939.	3.2	29
103	Mechanistic Study of a Ru-Xantphos Catalyst for Tandem Alcohol Dehydrogenation and Reductive Aryl-Ether Cleavage. <i>ACS Catalysis</i> , 2013, 3, 963-974.	11.2	42
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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.	11.2	22
106	Unraveling the Reaction Mechanism on Nitrile Hydration Catalyzed by [Pd(OH <sub>2</sub> ) <sub>4</sub> ] <sup>2+</sup> : Insights from Theory. <i>Inorganic Chemistry</i> , 2013, 52, 7541-7549.	4.0	16

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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.	2.3	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.	1.8	2
109	Catalysts or Initiators? Beckmann Rearrangement Revisited. <i>Journal of Organic Chemistry</i> , 2013, 78, 6782-6785.	3.2	32
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111	Catalytic Phenol Hydroxylation with Dioxigen: Extension of the Tyrosinase Mechanism beyond the Protein Matrix. <i>Angewandte Chemie - International Edition</i> , 2013, 52, 5398-5401.	13.8	122
112	Mechanisms of the Water-Gas Shift Reaction Catalyzed by Ruthenium Pentacarbonyl: A Density Functional Theory Study. <i>Inorganic Chemistry</i> , 2013, 52, 4786-4794.	4.0	23
113	Methane CH Activation by Palladium Complexes with Chelating Bis(NHC) Ligands: A DFT Study. <i>Organometallics</i> , 2013, 32, 3469-3480.	2.3	66
114	Reduction of N <sub>2</sub> O by CO over Fe- and Cu-BEA zeolites: An experimental and computational study of the mechanism. <i>Microporous and Mesoporous Materials</i> , 2013, 167, 254-266.	4.4	23
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121	d <sup>10</sup> -ML <sub>2</sub> Complexes: Structure, Bonding, and Catalytic Activity. <i>Structure and Bonding</i> , 2014, , 139-161.	1.0	1
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128	$\pi$ -Complexation in Nickel-Catalyzed Cross-Coupling Reactions. <i>Journal of Organic Chemistry</i> , 2014, 79, 1836-1841.	3.2	33



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131	Chromium Catalysts for Ethylene Polymerization and Oligomerization. <i>Advances in Chemical Engineering</i> , 2014, , 127-191.	0.9	13
132	Stereoselective Rhodium-Catalysed [2+2+2] Cycloaddition of Linear Allene-Ene/Alkene Substrates: Reactivity and Theoretical Mechanistic Studies. <i>Chemistry - A European Journal</i> , 2014, 20, 5034-5045.	3.3	37
133	Direct Allylic Functionalization Through Pd-Catalyzed C-H Activation. <i>European Journal of Organic Chemistry</i> , 2014, 2014, 5863-5883.	2.4	132
134	Mechanistic Study on Rh-Catalyzed Stereoselective C-C/C-H Activation of <i>tert</i> -Cyclobutanol. <i>Chemistry - A European Journal</i> , 2014, 20, 3839-3848.	3.3	29
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142	Physicochemical Mechanism of Light-Driven DNA Repair by (6-4) Photolyases. <i>Annual Review of Physical Chemistry</i> , 2014, 65, 275-292.	10.8	42
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144	Role of the Base in Buchwald-Hartwig Amination. <i>Journal of Organic Chemistry</i> , 2014, 79, 11961-11969.	3.2	74
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147	Indenyl Effect Due to Metal Slippage? Computational Exploration of Rhodium-Catalyzed Acetylene [2+2+2] Cyclotrimerization. <i>ChemPhysChem</i> , 2014, 15, 219-228.	2.1	32
148	Importance of Ligand Exchanges in Pd(II)-Brønsted Acid Cooperative Catalytic Approach to Spirocyclic Rings. <i>Journal of the American Chemical Society</i> , 2014, 136, 15998-16008.	13.7	61



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150	DFT Virtual Screening Identifies Rhodium- $\alpha$ -Amidinate Complexes As Potential Homogeneous Catalysts for Methane-to-Methanol Oxidation. <i>ACS Catalysis</i> , 2014, 4, 4455-4465.	11.2	24
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#	ARTICLE	IF	CITATIONS
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#	ARTICLE	IF	CITATIONS
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#	ARTICLE	IF	CITATIONS
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