

# Formulation of the reaction coordinate

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Citation Report

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17	An Orbital Interaction Rationale for Organic Molecules and Reactions. Israel Journal of Chemistry, 1975, 14, 1-10.	1.0	0
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22	The potential energy surfaces of polyatomic molecules. Structure and Bonding, 1977, , 93-146.	1.0	28
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37	Reaction Paths on Multidimensional Energy Hypersurfaces. <i>Angewandte Chemie International Edition in English</i> , 1980, 19, 1-13.	4.4	211
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1738	The Beckmann rearrangement in the framework of reaction electronic flux. <i>Theoretical Chemistry Accounts</i> , 2017, 136, 1.	0.5	7
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1744	Context-Driven Exploration of Complex Chemical Reaction Networks. <i>Journal of Chemical Theory and Computation</i> , 2017, 13, 6108-6119.	2.3	87
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1750	Radical Behavior of CO <sub>2</sub> versus its Deoxygenation Promoted by Vanadium Aryloxide Complexes: How the Geometry of Intermediate CO <sub>2</sub> Adducts Determines the Reactivity.. <i>Chemistry - A European Journal</i> , 2017, 23, 17269-17278.	1.7	13
1751	Selective Alkene Insertion into Inert Hydrogenâ€“Metal Bonds Catalyzed by Mono(phosphorus) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50 66 Cluster transformation of	1.1	4
1752	[Cu <sub>3</sub> ( $\mu_3$ -H)( $\mu_2$ -BH <sub>4</sub> )(PPh <sub>2</sub> ) <sub>2</sub> (NH <sub>3</sub> ) <sub>3</sub> ](BF <sub>4</sub> ) <sub>3</sub> to [Cu <sub>3</sub> ( $\mu_3$ -H)( $\mu_2$ -S <sub>2</sub> CH)(PPh <sub>2</sub> ) <sub>2</sub> (NH <sub>3</sub> ) <sub>3</sub> ] via reaction with CS <sub>2</sub> . X-ray structural characterisation and reactivity of cationic clusters explored by multistage mass spectrometry and computational studies. <i>Dalton Transactions</i> ,	1.1	6
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1763	A molecular electron density theory study of [3+2] cycloaddition reactions of chiral azomethine ylides with $\beta$ -nitrostyrene. <i>Theoretical Chemistry Accounts</i> , 2017, 136, 1.	0.5	21
1764	Oxidative Heck Reaction as a Tool for Para-selective Olefination of Aniline: A DFT Supported Mechanism. <i>Journal of Organic Chemistry</i> , 2017, 82, 10635-10640.	1.7	26
1765	Gold-catalyzed domino cyclizationâ€“alkynylation reactions with EBX reagents: new insights into the reaction mechanism. <i>Dalton Transactions</i> , 2017, 46, 12257-12262.	1.6	25
1766	Mechanistic Study on Platinum-Catalyzed Domino Reaction of Benziodoxole and Pyrrole Homopropargylic Ethers for Indole Synthesis. <i>Organometallics</i> , 2017, 36, 2843-2852.	1.1	15

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1897	An ab initio study and the corresponded instructing improvement of the multicomponent reaction consisted of acetone, aniline and 4-hydrocoumarine. <i>Computational and Theoretical Chemistry</i> , 2018, 1145, 22-27.	1.1	1
1898	Data-driven computation of molecular reaction coordinates. <i>Journal of Chemical Physics</i> , 2018, 149, 154103.	1.2	18
1899	Computational investigation of the control of the thermodynamics and microkinetics of the reductive amination reaction by solvent coordination and a co-catalyst. <i>RSC Advances</i> , 2018, 8, 36662-36674.	1.7	8
1900	Ab initio study of mechanism of forming a Si-heterocyclic spiro-Sn-heterocyclic ring compound by cycloaddition reaction of H <sub>2</sub> Si=S=Sn: and ethylene. <i>Main Group Chemistry</i> , 2018, 17, 285-292.	0.4	1
1901	Theoretical Study on the Mechanism of Rearrangement Reactions of Bicyclic Derivatives of Cyclopropane to Monocyclic Derivatives under the Catalysis of Pt-Salt. <i>ACS Omega</i> , 2018, 3, 16165-16174.	1.6	3
1902	A quantum-chemical insight on chemical fixation carbon dioxide with epoxides co-catalyzed by MIL-101 and tetrabutylammonium bromide. <i>Journal of CO<sub>2</sub> Utilization</i> , 2018, 28, 200-206.	3.3	35
1903	Mechanistic studies: enantioselective palladium( <i>ii</i> )-catalyzed intramolecular aminoarylation of alkenes by dual N-H and aryl C-H bond cleavage. <i>Organic Chemistry Frontiers</i> , 2018, 5, 3256-3262.	2.3	4
1904	Computational study of Rh(I)-Catalyzed Cycloaddition-Fragmentation of N-cyclopropylacrylamides. <i>Tetrahedron</i> , 2018, 74, 6475-6483.	1.0	2
1905	Non-innocent PNN ligand is important for CO oxidation by N <sub>2</sub> O catalyzed by a (PNN)Ru-H pincer complex: insights from DFT calculations. <i>Dalton Transactions</i> , 2018, 47, 15324-15330.	1.6	6
1906	Theoretical Study on the Kinetics for the Reactions of Heptyl Radicals with Methanol. <i>Chemical Research in Chinese Universities</i> , 2018, 34, 786-791.	1.3	0
1907	Copper-Catalyzed Intramolecular Annulation of Conjugated Enynones to Substituted 1 <i>H</i> -Indenes and Mechanistic Studies. <i>Journal of Organic Chemistry</i> , 2018, 83, 13243-13255.	1.7	26
1908	Mechanistic insight into the Rh-catalyzed mono- and double-decarbonylation of 1,4-diphenylbut-3-yne-1,2-dione: A computational study. <i>Journal of Organometallic Chemistry</i> , 2018, 877, 32-36.	0.8	2
1909	Mechanistic Insights into Cyclopropenes-Involved Carbonylative Carbocyclization Catalyzed by Rh(I) Catalyst: A DFT Study. <i>Journal of Organic Chemistry</i> , 2018, 83, 12734-12743.	1.7	13
1910	Pyrolysis of (thio)carbonates via computation analysis. <i>Journal of Theoretical and Computational Chemistry</i> , 2018, 17, 1850041.	1.8	0

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1911	Synthesis, structure, and condensed-phase reactivity of $[\text{Ag}(\text{P}(\text{C}_6\text{H}_5)_3)_3(\text{P}(\text{C}_6\text{H}_5)_3)_4\text{L}(\text{P}(\text{C}_6\text{H}_5)_3)_3\text{BF}_4]$ ( $\text{L}(\text{P}(\text{C}_6\text{H}_5)_3)_3 = \text{bis}(\text{diphenylphosphino})\text{amine}$ ) with $\text{CS}_2$ . Dalton Transactions, 2018, 47, 14713-14725.	1.6	10
1912	Reaction mechanisms and kinetics of the $\beta$ -elimination processes of compounds $\text{CHF}_2\text{CH}_2\text{SiF}_3$ (“ $\beta$ ”: DFT and CBS-QB3 methods using Rice-Ramsperger-Kassel-Marcus and transition state theories). Journal of Fluorine Chemistry, 2018, 216, 71-80.	0.9	6
1913	The mechanism and origin of the regioselectivity of cobalt-catalyzed annulation of allenes with benzamide: a computational study. Dalton Transactions, 2018, 47, 13592-13601.	1.6	2
1914	Stochastic Formalism for Thermally Driven Distribution Frontier: A Nonempirical Approach to the Potential Escape Problem. Journal of the Physical Society of Japan, 2018, 87, 063801.	0.7	3
1915	Alkylation versus trans-silylation of N-methyl-N-trimethylsilylacetamide with ambident electrophiles (chloromethyl)fluorosilanes. Journal of Organometallic Chemistry, 2018, 876, 66-77.	0.8	7
1916	Mechanistic insight into the Rh(III)-catalyzed cascade annulation of $\beta$ -ethynylanilines with diazo compounds towards Benzo[a]carbazoles. Journal of Organometallic Chemistry, 2018, 876, 17-25.	0.8	2
1917	Theoretical investigation of gold(I)-catalyzed intramolecular SEAr in isoxazole derivatives: Mechanisms, origin of regioselectivity, and role of hydrogen acceptor. Molecular Catalysis, 2018, 460, 27-35.	1.0	11
1918	A Reaction Mechanism for Gold-Catalyzed Hydroamination/Cyclization of <i>o</i> -Phenylendiamine and Propargylic Alcohols. A DFT Study. Organometallics, 2018, 37, 3035-3044.	1.1	8
1919	Mechanistic Insights into the Nickel-Catalyzed Cross-Coupling Reaction of Benzaldehyde with Benzyl Alcohol via $\text{C}^{\alpha}\text{H}$ Activation: A Theoretical Investigation. Journal of Organic Chemistry, 2018, 83, 11905-11916.	1.7	7
1920	Designed model for the Morita-Baylis-Hillman reaction mechanism in the presence of CaO and CaO modified with ionic liquid as a solid base catalyst: a DFT and MP2 investigation. Theoretical Chemistry Accounts, 2018, 137, 1.	0.5	0
1921	Copolymerization of ethylene with styrene catalyzed by a scandium catalyst. Polymer Chemistry, 2018, 9, 4757-4763.	1.9	12
1922	Mechanism of Photocatalytic Cyclization of Bromoalkenes with a Dimeric Gold Complex. Organometallics, 2018, 37, 1725-1733.	1.1	9
1923	Mechanistic Insights into the Ni-Catalyzed Reductive Carboxylation of $\text{C}^{\alpha}\text{O}$ Bonds in Aromatic Esters with $\text{CO}_2$ : Understanding Remarkable Ligand and Traceless Directing Group Effects. Chemistry - an Asian Journal, 2018, 13, 1570-1581.	1.7	5
1924	$\text{C}_2\text{N}$ -supported single metal ion catalysts for HCOOH dehydrogenation. Journal of Materials Chemistry A, 2018, 6, 11105-11112.	5.2	40
1925	Solvent effect on isomerization reaction of $[(\text{C}_5\text{H}_5)(\text{CO})_2\text{Re}(\text{C}_2\text{H}_5)(\text{C}_6\text{H}_5)]$ carbene complex to $[(\text{C}_5\text{H}_5)(\text{CO})(\text{COC}_2\text{H}_5)\text{Re}(\text{C}_6\text{H}_5)]$ carbyne complex: A computational investigation. Journal of Molecular Liquids, 2018, 265, 164-171.	2.3	14
1926	Boron Ester-Catalyzed Amidation of Carboxylic Acids with Amines: Mechanistic Rationale by Computational Study. Chemistry - an Asian Journal, 2018, 13, 2685-2690.	1.7	10
1927	The Effect of Polymer Structures on Complete Degradation: A First-Principles Study. ChemistryOpen, 2018, 7, 463-466.	0.9	5
1928	Theoretical investigation of Banert cascade reaction. Royal Society Open Science, 2018, 5, 171075.	1.1	7

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1930	Mechanistic investigation in the [1,4] and [1,2] Wittig rearrangement reactions: a DFT study. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 21457-21473.	1.3	3
1931	Computational study of the mechanism of amide bond formation <i>via</i> CS <sub>2</sub> -releasing 1,3-acyl transfer. <i>Organic and Biomolecular Chemistry</i> , 2018, 16, 5808-5815.	1.5	10
1932	Hydrolysis of an organophosphorus pesticide: a theoretical investigation of the reaction mechanism for acephate. <i>Theoretical Chemistry Accounts</i> , 2018, 137, 1.	0.5	4
1933	Revealing carbocations in highly asynchronous concerted reactions: The ene-type reaction between dithiocarboxylic acids and alkenes. <i>Tetrahedron</i> , 2018, 74, 5627-5634.	1.0	13
1934	Mechanism of Direct C-H Arylation of Pyridine via a Transient Activator Strategy: A Combined Computational and Experimental Study. <i>Journal of Organic Chemistry</i> , 2018, 83, 10389-10397.	1.7	14
1935	Mechanisms of the synthesis of trialkylsubstituted alkenylboronates from unactivated internal alkynes catalyzed by copper: A theoretical study. <i>Journal of Organometallic Chemistry</i> , 2018, 864, 154-159.	0.8	10
1936	The Dual Role of Gold(I) Complexes in Photosensitizer-Free Visible-Light-Mediated Gold-Catalyzed 1,2-Difunctionalization of Alkynes: A DFT Study. <i>Chemistry - A European Journal</i> , 2018, 24, 14119-14126.	1.7	29
1937	Solvent effects on the coupling reaction of CO <sub>2</sub> with PO catalyzed by hydroxyl imidazolium ionic liquid: Comparison of different models. <i>Journal of CO<sub>2</sub> Utilization</i> , 2018, 27, 99-106.	3.3	17
1938	A Molecular Electron Density Theory Study of the Role of the Copper Metalation of Azomethine Ylides in [3 + 2] Cycloaddition Reactions. <i>Journal of Organic Chemistry</i> , 2018, 83, 10959-10973.	1.7	41
1939	Visualization of the Intrinsic Reaction Coordinate and Global Reaction Route Map by Classical Multidimensional Scaling. <i>Journal of Chemical Theory and Computation</i> , 2018, 14, 4263-4270.	2.3	39
1940	Theoretical study on the vibrationally resolved spectra and quantum yield of blue phosphorescent iridium(III) complexes with 2-(4-fluoro-3-(trifluoromethyl)-phenyl)pyridine as the cyclometalated ligand. <i>Organic Electronics</i> , 2018, 61, 125-133.	1.4	9
1941	Mechanisms of Rhodium(III)-Catalyzed C-H Functionalizations of Benzamides with $\hat{I}$ , $\hat{I}$ -Difluoromethylene Alkynes. <i>Journal of Organic Chemistry</i> , 2018, 83, 9220-9230.	1.7	34
1942	Mechanism of Palladium-Catalyzed Alkylation of Aryl Halides with Alkyl Halides through C-H Activation: A Computational Study. <i>Organometallics</i> , 2018, 37, 2222-2231.	1.1	19
1943	Mechanism of CO <sub>2</sub> capture in nanostructured sodium amide encapsulated in porous silica. <i>Surface and Coatings Technology</i> , 2018, 350, 227-233.	2.2	7
1944	An investigation of molecular mechanism and the role of Te-bridged-atom in the formation of polysubstituted pyridines via Hetero-Diels-Alder reaction of isotellurazole with acetylenic dienophile: a molecular electron density study. <i>Journal of Chemical Sciences</i> , 2018, 130, 1.	0.7	7
1945	Syntheses of Substituted 1,4-Disila-2,5-cyclohexadienes from Cyclic Hexasilane Si <sub>6</sub> Me <sub>12</sub> and Alkynes via Successive Si-Si Bond Activation by Pd/Isocyanide Catalysts. <i>Organometallics</i> , 2018, 37, 2531-2543.	1.1	11
1946	Theoretical Mechanistic Study of Nickel(0)/Lewis Acid Catalyzed Polyfluoroarylcyanation of Alkynes: Origin of Selectivity for C-CN Bond Activation. <i>Organometallics</i> , 2018, 37, 2594-2601.	1.1	12

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1948	Variation of the Intersection Point of the Potential Surface Crossing Induced by the Laser Phase Along the Reaction Path in Ion-Molecule Reactions: Application To Li+ + CH4. <i>Journal of Structural Chemistry</i> , 2018, 59, 20-27.	0.3	0
1949	Rhodium Complexes of a New Generation Sapphyrin: Unique Structures, Axial Chirality, and Catalysis. <i>Chemistry - A European Journal</i> , 2018, 24, 17255-17261.	1.7	13
1950	Computational study on the mechanisms of [2+3] and [2+2] cycloisomerization reaction catalyzed by gold complex. <i>Journal of Organometallic Chemistry</i> , 2018, 874, 63-69.	0.8	8
1951	Theoretical Insight into Ligand- and Counterion-Controlled Regiodivergent Reactivity in Synthesis of Borylated Furans: 1,2-H vs 1,2-B Migration. <i>ACS Catalysis</i> , 2018, 8, 9252-9261.	5.5	22
1952	Mechanistic exploration of CpRe(CO)3-catalyzed coupling of chloromethyloxirane with CO2: Unexpected potentials of CO ligands. <i>Molecular Catalysis</i> , 2018, 458, 25-32.	1.0	2
1953	The tautomerization and ring closure in the Claisen rearrangement: A DFT study. <i>International Journal of Quantum Chemistry</i> , 2018, 118, e25677.	1.0	2
1954	Intramolecular [3 + 2] Cycloaddition Reactions of Unsaturated Nitrile Oxides. A Study from the Perspective of Bond Evolution Theory (BET). <i>Journal of Physical Chemistry A</i> , 2018, 122, 7472-7481.	1.1	17
1955	DFT Studies on Ni-Mediated C-F Cleavage for the Synthesis of Cyclopentadiene Derivatives. <i>Frontiers in Chemistry</i> , 2018, 6, 319.	1.8	8
1956	A molecular electron density theory study of the asymmetric hetero-Diels-Alder cycloaddition reaction between ferrocenyl-substituted thiabutadiene and methyl propiolate. <i>Computational and Theoretical Chemistry</i> , 2018, 1140, 117-124.	1.1	9
1957	A Molecular Electron Density Theory Study of the Competitiveness of Polar Diels-Alder and Polar Alder-ene Reactions. <i>Molecules</i> , 2018, 23, 1913.	1.7	13
1958	A molecular electron density theory study on the [3+2] cycloaddition reaction of thiocarbonyl ylides with hetaryl thioketones. <i>New Journal of Chemistry</i> , 2018, 42, 11819-11830.	1.4	7
1959	The reactivity of coordinatively unsaturated iridium methylene complex Ir CH2[N(SiMe2CH2PPh2)2]: A quantum chemistry study. <i>Computational and Theoretical Chemistry</i> , 2018, 1138, 91-98.	1.1	4
1960	Computational Study on Gold-Catalyzed Cascade Reactions of 1,4-Diynes and Pyrroles: Mechanism, Regioselectivity, Role of Catalyst, and Effects of Substituent and Solvent. <i>Organometallics</i> , 2018, 37, 1927-1936.	1.1	15
1961	Sequential Intramolecular Diels-Alder Reaction of 3-Heteroaryl-2-propenylamides of Ethenetricarboxylate. <i>Journal of Heterocyclic Chemistry</i> , 2019, 56, 2592-2603.	1.4	2
1962	An investigation of the molecular mechanism, chemoselectivity and regioselectivity of cycloaddition reaction between acetonitrile N-Oxide and 2,5-dimethyl-2H-[1,2,3]diazaphosphole: a MEDT study. <i>Journal of Chemical Sciences</i> , 2019, 131, 1.	0.7	15
1963	The separation of the reaction coordinate in transition state theory: Regularity and dimensionality reduction resulting from local symmetry. <i>Journal of Chemical Physics</i> , 2019, 150, 164310.	1.2	2
1964	Mechanistic Insight into Propylene Epoxidation with H <sub>2</sub> O <sub>2</sub> over Titanium Silicalite-1: Effects of Zeolite Confinement and Solvent. <i>Journal of Physical Chemistry B</i> , 2019, 123, 7410-7423.	1.2	21

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1965	Reaction Mechanisms on Unusual 1,2-Migrations of N-Heterocyclic Carbene-Ligated Transition Metal Complexes. <i>Chemistry - an Asian Journal</i> , 2019, 14, 3313-3319.	1.7	7
1966	Are one-step aromatic nucleophilic substitutions of non-activated benzenes concerted processes?. <i>Organic and Biomolecular Chemistry</i> , 2019, 17, 8185-8193.	1.5	11
1967	Cis-Trans Interconversion in Ruthenium(II) Bipyridine Complexes. <i>Inorganic Chemistry</i> , 2019, 58, 11606-11613.	1.9	13
1968	Direct Air Capture of CO <sub>2</sub> with an Amine Resin: A Molecular Modeling Study of the Deactivation Mechanism by CO <sub>2</sub> . <i>Industrial &amp; Engineering Chemistry Research</i> , 2019, 58, 14705-14708.	1.8	10
1969	Mechanistic Features in Al(I)-Mediated Oxidative Addition of Aryl C-F Bonds: Insights From Density Functional Theory Calculations. <i>Frontiers in Chemistry</i> , 2019, 7, 596.	1.8	11
1970	On the catalytic transfer hydrogenation of nitroarenes by a cubane-type Mo <sub>3</sub> S <sub>4</sub> cluster hydride: disentangling the nature of the reaction mechanism. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 17221-17231.	1.3	6
1971	Transient and intermediate carbocations in ruthenium tetroxide oxidation of saturated rings. <i>Beilstein Journal of Organic Chemistry</i> , 2019, 15, 1552-1562.	1.3	4
1972	Methane Activation by (n=0, 1, 2; m= 1, 2): Reactivity Parameters, Electronic Properties and Binding Energy Analysis. <i>ChemistrySelect</i> , 2019, 4, 7912-7921.	0.7	0
1973	Theoretical and Experimental Reactivity Predictors for the Electrocatalytic Activity of Copper Phenanthroline Derivatives for the Reduction of Dioxygen. <i>Journal of Physical Chemistry C</i> , 2019, 123, 19468-19478.	1.5	18
1974	Blind Search for Complex Chemical Pathways Using Harmonic Linear Discriminant Analysis. <i>Journal of Chemical Theory and Computation</i> , 2019, 15, 4507-4515.	2.3	19
1975	First-principles microkinetic study of methane and hydrogen sulfide catalytic conversion to methanethiol/dimethyl sulfide on Mo <sub>6</sub> S <sub>8</sub> clusters: activity/selectivity of different promoters. <i>Catalysis Science and Technology</i> , 2019, 9, 4573-4580.	2.1	5
1976	Elucidation of key factors in nickel-diphosphines catalyzed isomerization of 2-methyl-3-butenenitrile. <i>Journal of Catalysis</i> , 2019, 377, 13-19.	3.1	6
1977	A Modified Cationic Mechanism for PdCl <sub>2</sub> -Catalyzed Transformation of a Homoallylic Alcohol to an Allyl Ether. <i>Organometallics</i> , 2019, 38, 2953-2962.	1.1	10
1978	Comparative DFT study on the platinum catalyzed [3+2] and [2+2] cycloaddition reactions between the derivatives of allene and alkene. <i>Computational and Theoretical Chemistry</i> , 2019, 1163, 112507.	1.1	2
1979	Gold(I)-catalyzed [4+1]/[4+3] annulations of diazo esters with hexahydro-1,3,5-triazines: Theoretical study of mechanism and regioselectivity. <i>Journal of Organometallic Chemistry</i> , 2019, 897, 70-79.	0.8	5
1980	Enhance the efficiency of 5-fluorouracil targeted delivery by using a prodrug approach as a novel strategy for prolonged circulation time and improved permeation. <i>International Journal of Pharmaceutics</i> , 2019, 568, 118491.	2.6	15
1981	Theoretical Study of the Potential Energy Profile of the HBr <sup>+</sup> + CO <sub>2</sub> → HOCO <sup>+</sup> + Br <sup>-</sup> Reaction. <i>Journal of Physical Chemistry A</i> , 2019, 123, 9791-9799.	1.1	4
1982	Effectiveness of the bimetallic catalytic center over the monometallic one for catalyzing the rearrangement of cyclopropanated bicyclic derivatives. <i>Journal of Organometallic Chemistry</i> , 2019, 899, 120907.	0.8	1

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1984	The transition state and cognate concepts. <i>Advances in Physical Organic Chemistry</i> , 2019, 53, 29-68.	0.5	8
1985	Mechanism and stereospecificity of Z-enamide synthesis from salicylaldehydes with isoxazoles using DFT calculations. <i>Journal of Organometallic Chemistry</i> , 2019, 903, 120981.	0.8	0
1986	Direct Air Capture of CO <sub>2</sub> with an Amine Resin: A Molecular Modeling Study of the Oxidative Deactivation Mechanism with O <sub>2</sub> . <i>Industrial &amp; Engineering Chemistry Research</i> , 2019, 58, 17760-17767.	1.8	13
1987	Stereoselective cyclopropanation of olefins through ammonium ylides: A molecular electron density theory study. <i>Journal of Physical Organic Chemistry</i> , 2019, 32, e4008.	0.9	3
1988	C-H Activation versus Ring Opening and Inner- versus Outer-Sphere Concerted Metalation-Deprotonation in Rh(III)-Catalyzed Oxidative Coupling of Oxime Ether and Cyclopropanol: A Density Functional Theory Study. <i>Journal of Organic Chemistry</i> , 2019, 84, 11150-11160.	1.7	17
1989	Ab initio study of mechanism of forming a Si-heterocyclic spiro-Sn-heterocyclic ring compound by cycloaddition reaction of Me <sub>2</sub> Si=Sn and ethene. <i>Progress in Reaction Kinetics and Mechanism</i> , 2019, 44, 114-121.	1.1	0
1990	DFT Studies on Metal-Controlled Regioselective Amination of <i>N</i> -Acylpyrazoles with Azodicarboxylates. <i>Journal of Organic Chemistry</i> , 2019, 84, 12399-12407.	1.7	5
1991	A molecular electron density theory study of the mechanism, chemo- and stereoselectivity of the epoxidation reaction of <i>R</i> -carvone with peracetic acid. <i>RSC Advances</i> , 2019, 9, 28500-28509.	1.7	15
1992	Mechanistic Study on the Decarboxylative <i>sp</i> <sup>3</sup> C-N Cross-Coupling between Alkyl Carboxylic Acids and Nitrogen Nucleophiles via Dual Copper and Photoredox Catalysis. <i>Inorganic Chemistry</i> , 2019, 58, 12669-12677.	1.9	14
1993	Metallalkenyl, Metallacyclopropene, or Metallallylcarbenoid? Ru-Catalyzed Annulation between Benzoic Acid and Alkyne. <i>ACS Catalysis</i> , 2019, 9, 9387-9392.	5.5	19
1994	Mechanisms and kinetic studies of OH-initiated atmospheric oxidation of methoxyphenols in the presence of O <sub>2</sub> and NO <sub>x</sub> . <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 21856-21866.	1.3	19
1995	Hydroxyl-functionalized pyrazolium ionic liquids to catalyze chemical fixation of CO <sub>2</sub> : Further benign reaction condition for the single-component catalyst. <i>Journal of Molecular Liquids</i> , 2019, 293, 111479.	2.3	18
1996	Computational Mechanistic Insights on the NO Oxidation Reaction Catalyzed by Non-Heme Biomimetic Cr-N-Tetramethylated Cyclam Complexes. <i>International Journal of Molecular Sciences</i> , 2019, 20, 3955.	1.8	2
1997	Mechanistic Insight into the Ring-Opening Polymerization of $\epsilon$ -Caprolactone and L-Lactide Using Ketimine-Ligated Aluminum Catalysts. <i>Polymers</i> , 2019, 11, 1530.	2.0	7
1998	Competition of Secondary versus Tertiary Carbenium Routes for the Type B Isomerization of Alkenes over Acid Zeolites Quantified by Ab Initio Molecular Dynamics Simulations. <i>ACS Catalysis</i> , 2019, 9, 9813-9828.	5.5	35
1999	Ion reactions in atmospherically-relevant clusters: mechanisms, dynamics and spectroscopic signatures. <i>Faraday Discussions</i> , 2019, 217, 342-360.	1.6	3
2000	Site-selectivity control in hetero-Diels-Alder reactions of methylenedioxy derivatives of lawsone through modification of the reactive carbonyl group: an experimental and theoretical study. <i>Organic and Biomolecular Chemistry</i> , 2019, 17, 692-702.	1.5	4

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2002	Theoretical studies on Rh(III)-catalyzed regioselective C-H bond cyanation of indole and indoline. <i>Dalton Transactions</i> , 2019, 48, 168-175.	1.6	9
2003	Binding affinity of pyridines with Am <sup>III</sup> /Cm <sup>III</sup> elucidated by density functional theory calculations. <i>Dalton Transactions</i> , 2019, 48, 1613-1623.	1.6	5
2004	Unveiling the high reactivity of cyclohexynes in [3 + 2] cycloaddition reactions through the molecular electron density theory. <i>Organic and Biomolecular Chemistry</i> , 2019, 17, 498-508.	1.5	11
2005	Location of the Active Sites for Ethylcyclohexane Hydroisomerization by Ring Contraction and Expansion in the EUO Zeolitic Framework. <i>ACS Catalysis</i> , 2019, 9, 1692-1704.	5.5	14
2006	Does the Neophyl-like Rearrangement Play a Decisive Role in Intramolecular Cyclization of Iminyl Radicals? A Combined Quantum Chemistry and Numerical Simulation Investigation of the Cyclization Mechanism and Product Distributions of Bicyclic 2-Allyl-2-methyl-2,3-dihydro-1H-inden-1-iminyl Radical and Several Iminyl Model Compounds. <i>Journal of Organic Chemistry</i> , 2019, 84, 2721-2731.	1.7	4
2007	Mechanism and Origins of Enantioselectivity of Iridium-Catalyzed Intramolecular Silylation of Unactivated C(sp <sup>3</sup> )-H Bonds. <i>Journal of Organic Chemistry</i> , 2019, 84, 2372-2376.	1.7	18
2008	The plutonium chemistry of Pu+O <sub>2</sub> system: the theoretical investigation of the plutonium-oxygen interaction. <i>Journal of the Iranian Chemical Society</i> , 2019, 16, 1157-1162.	1.2	4
2009	Substituent Effects on Reactions of [RhCl(COD)] <sub>2</sub> with Diazoalkanes. <i>Organometallics</i> , 2019, 38, 905-915.	1.1	8
2010	Mechanistic Insight into Palladium-Catalyzed Carbocyclization-Functionalization of Bisallene: A Computational Study. <i>ChemCatChem</i> , 2019, 11, 1228-1237.	1.8	20
2011	Advances in designs and mechanisms of semiconducting metal oxide nanostructures for high-precision gas sensors operated at room temperature. <i>Materials Horizons</i> , 2019, 6, 470-506.	6.4	493
2012	A mechanistic investigation into N-heterocyclic carbene (NHC) catalyzed umpolung of ketones and benzonitriles: is the cyano group better than the classical carbonyl group for the addition of NHC?. <i>Organic Chemistry Frontiers</i> , 2019, 6, 523-531.	2.3	4
2013	Theoretical studies on the mechanism of Ru(II)-catalyzed regioselective C-H allylation of indoles with allyl alcohols. <i>Dalton Transactions</i> , 2019, 48, 9181-9186.	1.6	3
2014	An effective method to make polymers degrade readily: spatial isomerization. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 16905-16909.	1.3	4
2015	A molecular electron density theory study of the insertion of CO into frustrated Lewis pair boron-amidines: a [4 + 1] cycloaddition reaction. <i>Dalton Transactions</i> , 2019, 48, 9214-9224.	1.6	4
2016	Reassessment of the Mechanisms of Thermal C-H Bond Activation of Methane by Cationic Magnesium Oxides: A Critical Evaluation of the Suitability of Different Density Functionals. <i>ChemPhysChem</i> , 2019, 20, 1812-1821.	1.0	5
2017	Mechanistic insight into Ni-catalyzed cyclooligomerization of enones with methylene equivalents: The control of ring-size selectivity. <i>Journal of Catalysis</i> , 2019, 375, 213-223.	3.1	4
2018	Synthesis and Catalytic Reactivity of Bis(molybdenum-trihalide) Complexes Bridged by Ferrocene Skeleton toward Catalytic Nitrogen Fixation. <i>Organometallics</i> , 2019, 38, 2863-2872.	1.1	13

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2020	Theoretical Insight into the Mechanism and Origin of Divergent Reactivity in the Synthesis of Benzo-Heterocycles from <i>o</i> -Alkynylbenzamides Catalyzed by Gold and Platinum Complexes. <i>Journal of Organic Chemistry</i> , 2019, 84, 9705-9713.	1.7	17
2021	Is the pericyclic transition structure of aza-Diels-Alder reaction aromatic?. <i>Journal of Molecular Graphics and Modelling</i> , 2019, 91, 119-129.	1.3	4
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2024	Theoretical Study on the Conversion Mechanism of Biobased 2,5-Dimethylfuran and Acrylic Acid into Aromatics Catalyzed by Brønsted Acid Ionic Liquids. <i>Industrial &amp; Engineering Chemistry Research</i> , 2019, 58, 11111-11120.	1.8	12
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2027	Tautomerism and stereodynamics in Schiff bases from gossypol and hemigossypol with <i>N</i> -aminoheterocycles. <i>Organic and Biomolecular Chemistry</i> , 2019, 17, 6229-6250.	1.5	13
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2038	DFT Study on the Mechanism of Palladium(0)-Catalyzed Reaction of Aryl Iodides, Norbornene, and Di-tert-butyl diaziridinone. <i>Organometallics</i> , 2019, 38, 2189-2198.	1.1	14
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2043	On the origin of the difference between type A and type B skeletal isomerization of alkenes catalyzed by zeolites: The crucial input of ab initio molecular dynamics. <i>Journal of Catalysis</i> , 2019, 373, 361-373.	3.1	38
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2052	Solvent effect on Hetero-Diels-Alder reaction of isoselenazole with symmetrical acetylenic dienophiles: A MEDT study. <i>Computational and Theoretical Chemistry</i> , 2019, 1154, 17-25.	1.1	8
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2057	Intramolecular Imino-ene Reaction of Azirines: Regioselectivity, Diastereoselectivity, and Computational Insights. <i>Journal of Organic Chemistry</i> , 2019, 84, 4095-4103.	1.7	4
2058	A Highly Active Catalyst System for Suzuki-Miyaura Coupling of Aryl Chlorides. <i>Organometallics</i> , 2019, 38, 1459-1467.	1.1	25
2059	DFT study of fructose dehydration to 5-hydroxymethylfurfural catalyzed by imidazolium-based ionic liquid. <i>Chemical Physics Letters</i> , 2019, 723, 175-181.	1.2	19
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2061	Novel aluminum complexes bearing 2-(aminomethylene)malonate ligands with high efficiency and controllability in ring-opening polymerization of $\epsilon$ -caprolactone. <i>European Polymer Journal</i> , 2019, 115, 399-408.	2.6	11
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2064	DFT mechanistic investigation into phenol dearomatization mediated by an iodine reagent. <i>Organic and Biomolecular Chemistry</i> , 2019, 17, 3521-3528.	1.5	29
2065	Key Mechanistic Features in Palladium-Catalyzed Methylcyclopropanation of Norbornenes With Vinyl Bromides: Insights From DFT Calculations. <i>Frontiers in Chemistry</i> , 2019, 7, 169.	1.8	6
2066	Theoretical Investigation of Regioselectivity in the Rh-Catalyzed Coupling Reaction of 3-Phenylthiophene with Styrene. <i>European Journal of Organic Chemistry</i> , 2019, 2998-3004.	1.2	3
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2070	CO substitution vs C Si cleavage in the reactions of $[(\eta^5-Cp)M_3(CO)_9(CCSiR_3)]$ ( $M = Ru, Me, Ph$ ; $M = Os$ ) <i>Tetrahedron</i> , 2019, 75, 492, 8-17.	1.2	3
2071	Highly regioselective synthesis of 7-oxo-7H-[1,3,4]thiadiazolo[3,2- <i>a</i> ]pyrimidine-5-carboxylate derivatives under mild conditions. <i>Tetrahedron Letters</i> , 2019, 60, 1399-1403.	0.7	7
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2074	Oxidation reaction mechanism and kinetics between OH radicals and alkyl-substituted aliphatic thiols: OH-addition pathways. <i>Progress in Reaction Kinetics and Mechanism</i> , 2019, 44, 157-174.	1.1	1
2075	Effect of ionic liquids clusters microenvironment on cycloaddition reaction of carbon dioxide. <i>Journal of Molecular Liquids</i> , 2019, 284, 68-74.	2.3	11
2076	Aromaticity-promoted C <sup>+</sup> F Bond Activation in Rhodium Complex: A Facile Tautomerization. <i>Chemistry - an Asian Journal</i> , 2019, 14, 1937-1940.	1.7	20
2077	Atmospheric oxidation reactions of imidazole initiated by hydroxyl radicals: kinetics and mechanism of reactions and atmospheric implications. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 8445-8456.	1.3	31
2078	Substitution effects on olefin epoxidation catalyzed by Oxoiron(IV) porphyrin $\pi$ -cation radical complexes: A dft study. <i>Journal of Computational Chemistry</i> , 2019, 40, 1780-1788.	1.5	12
2079	Copper( <sup>i</sup> / <sub>sc</sub> ) <sup>&lt;sc&gt;i&lt;/sc&gt;</sup> -catalyzed asymmetric aza Diels-Alder reactions of azoalkenes toward fulvenes: a molecular electron density theory study. <i>New Journal of Chemistry</i> , 2019, 43, 4765-4776.	1.4	21
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2087	Formation and reactions of the 1, 8-naphthyridine (napy) ligated geminally dimetallated phenyl complexes [(napy)Cu <sub>2</sub> (Ph)] <sup>+</sup> , [(napy)Ag <sub>2</sub> (Ph)] <sup>+</sup> and [(napy)CuAg(Ph)] <sup>+</sup> . <i>European Journal of Mass Spectrometry</i> , 2019, 25, 30-43.	0.5	1
2088	A Molecular Electron Density Theory Study of the Chemoselectivity, Regioselectivity, and Diastereofacial Selectivity in the Synthesis of an Anticancer Spiroisoxazoline derived from $\hat{\pm}$ -Santonin. <i>Molecules</i> , 2019, 24, 832.	1.7	39
2089	Proton supplier role of binuclear gold complexes in promoting hydrofunctionalisation of nonactivated alkenes. <i>Catalysis Science and Technology</i> , 2019, 9, 1420-1426.	2.1	11
2090	The role of the halogen bond in iodothyronine deiodinase: Dependence on chalcogen substitution in naphthyl-based mimetics. <i>Journal of Computational Chemistry</i> , 2019, 40, 944-951.	1.5	14

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2093	Optical properties and response mechanism analysis of multi-branched fluorescent probes based on intramolecular charge transfer. <i>Chinese Journal of Chemical Physics</i> , 2019, 32, 467-473.	0.6	1
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2095	Catalyst-Dependent Chemoselectivity in the Dirhodium-Catalyzed Cyclization Reactions Between Enodiazacetamide and Nitrosoarene: A Theoretical Study. <i>Frontiers in Chemistry</i> , 2019, 7, 586.	1.8	6
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2098	Bonding rearrangements in organometallic reactions: from orbitals to curly arrows. <i>Dalton Transactions</i> , 2019, 48, 15740-15752.	1.6	14
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2101	Features of Mechanism of Cycloaddition Reaction between $\text{H}_2\text{Sn}=\text{Sn}$ : and Ethylene. <i>Russian Journal of Physical Chemistry A</i> , 2019, 93, 2182-2186.	0.1	0
2102	Can Alkaline Hydrolysis of $^3\text{H}$ -HCH Serve as a Model Reaction to Study Its Aerobic Enzymatic Dehydrochlorination by LinA?. <i>International Journal of Molecular Sciences</i> , 2019, 20, 5955.	1.8	7
2103	Theoretical calculation studies on the rearrangement mechanisms of arenesulfenilides to generate <i>o</i> - and <i>p</i> -aminodiphenyl sulfides. <i>Organic and Biomolecular Chemistry</i> , 2019, 17, 10088-10096.	1.5	8
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2114	Origins of chemoselectivity of Rh(III)-Catalyzed C-H activation of N-(pivaloyloxy)benzamide: Insights from density functional theory calculations. <i>Journal of Organometallic Chemistry</i> , 2019, 880, 163-169.	0.8	4
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2121	Intramolecular Cyclization of 3,3-Diarylpropenylamides of Electron-Deficient Alkenes: Stereoselective Synthesis of Functionalized Hexahydrobenzo[ <i>f</i> ]isoindoles. <i>European Journal of Organic Chemistry</i> , 2019, 2019, 204-220.	1.2	2
2122	Participation of furoxan carbonitrile oxide in [3+2] cycloaddition reaction toward C≡N triple bond: a Molecular Electron Density Theory study of regioselectivity and mechanistic aspect. <i>Structural Chemistry</i> , 2019, 30, 317-326.	1.0	7
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2124	Ion Permeation through a Phospholipid Membrane: Transition State, Path Splitting, and Calculation of Permeability. <i>Journal of Chemical Theory and Computation</i> , 2019, 15, 720-730.	2.3	24
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2126	Prebiotic chemistry and origins of life research with atomistic computer simulations. <i>Physics of Life Reviews</i> , 2020, 34-35, 105-135.	1.5	25

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2128	Kinetics and oxidation mechanism of pyrene initiated by hydroxyl radical. A theoretical investigation. <i>Chemical Physics</i> , 2020, 528, 110522.	0.9	20
2129	Mechanistic insights into the origin of substituent-directed product Z/E selectivity for gold-catalyzed [4+1]-annulations of 1,4-diyne-3-ols with isoxazoles: A DFT study. <i>Molecular Catalysis</i> , 2020, 480, 110647.	1.0	5
2130	Mechanism and Stereoselectivity of the Elementometalation Process of Activated Alkyne $R_1C\equiv\frac{1}{2}CR(R_2\frac{3}{4}CO_2)$ $Tj_{1.5}^{ETOq1}$ 1 0,784314	1.5	7
2131	Performance studies of CO <sub>2</sub> transformation to methanol by zwitterionic indenylammonium derivatives as a new class of carbon-centered organocatalysts. <i>Structural Chemistry</i> , 2020, 31, 585-598.	1.0	3
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2249	Theoretical Insight into Palladium(II)-Counterion-Ligand Cooperative Regiodivergent Syntheses of Indolo[3,2- <i>c</i> ]coumarins and Benzofuro[3,2- <i>c</i> ]quinolinones from Diphenylethyne Derivatives. <i>Inorganic Chemistry</i> , 2020, 59, 4741-4752.	1.9	6
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