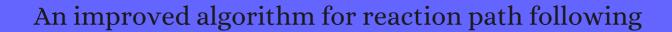
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627	Self-catalytic mechanism of prebiotic reactions: II. From urea and glycinamide to hypoxanthine. <b>2021</b> , 121, e26508	
626	Negative-mode mass spectrometric study on dc corona, ac corona and dielectric barrier discharge ionization in ambient air containing H2O2, 2,4,6-trinitrotoluene (TNT), and 1,3,5-trinitroperhydro-1,3,5-triazine (RDX). <b>2021</b> , 459, 116440	5
625	Regio- and stereochemistry in the intramolecular $[4 + 2]$ and intermolecular $[3 + 2]$ cycloaddition reactions in the synthesis of epoxypyrrolo[3,4-g]indazoles: a density functional theory study. <b>2021</b> , 75, 951-965	2
624	Deep Eutectic Solvent Choline Chloride/-toluenesulfonic Acid and Water Favor the Enthalpy-Driven Binding of Arylamines to Maleimide in Aza-Michael Addition. <b>2021</b> , 86, 223-234	1
623	Quantum chemical study on the formation of isopropyl cyanide and its linear isomer in the interstellar medium. <b>2021</b> , 20, 62-72	0
622	DFT study on the [4+4] domino cycloaddition of ynones with benzylidenepyrazolones to access eight-membered cyclic ethers: effects of DBU vs. Et3N. <b>2021</b> , 45, 131-140	2
621	Quantum chemical study on the ozonolysis mechanism of guaiacol and the structure-reactivity relationship of phenols with hydroxyl, methoxy, and methyl substituents. <b>2021</b> , 420, 127629	3
620	Mechanistic Investigation on Chemiluminescent Formaldehyde Probes. <b>2021</b> , 27, 5712-5720	6
619	Computational prediction on the catalytic activity of heterobimetallic complex featuring M?M' triple bond in acetylene cyclotrimerization: Mechanistic study. <b>2021</b> , 42, 484-491	2
618	The density functional theory study of 2D nonmetallic catalyst defective graphene for acetylene hydration. <b>2021</b> , 121, e26561	
617	Theoretical study on the atmospheric degradation mechanism and subsequent products of E,E-2,4-hexadienal with hydroxyl radical. <b>2021</b> , 121, e26563	2
616	Cleavage of C-O and C-H bonds in ethers by a genuine Si[double bond, length as m-dash]O bond. <b>2021</b> , 50, 1413-1421	1

615	Flow Synthesis of 2-[Methyl(pyridin-2-yl)amino]ethanol: An Experimental and Computational Study. <b>2021</b> , 44, 283-290	1
614	ECatalysis in Carbon Flatland-Flipping [8]Annulene on Graphene. 2021, 27, 3420-3426	3
613	Sulfur-assisted large-scale synthesis of graphene microspheres for superior potassium-ion batteries. <b>2021</b> , 14, 965-974	106
612	The kinetic mechanism of acetylene hydrogenation to prepare ethane over FexOy clusters: A DFT study. <b>2021</b> , 230, 116170	5
611	Experimental and computational studies of the mechanism of base-catalyzed ring opening of 2-(chloromethyl)oxirane by benzoic acid. <b>2021</b> , 53, 356-368	
610	Reaction kinetics of a series of alkanes with ClO and BrO radicals: A theoretical study. <b>2021</b> , 53, 189-206	О
609	Rapid computational evaluation of small-molecule hydrolase mimics for preorganized H-bond networks. <b>2021</b> , 121, e26423	0
608	Mechanistic examination of C -C tyrosyl bond cleavage: Spectroscopic investigation of the generation of ⊞-glycyl radical cations from tyrosyl (glycyl/alanyl)tryptophan. <b>2020</b> , 56, e4630	1
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606	Mechanisms of Csp3-H or Nsp2-H functionalization of 2,3-diaminoindoles with triplet O2: A density functional theory investigation. <b>2021</b> , 34, e4134	
605	Mechanistic and kinetic study on the reaction of the Cl-initiated atmospheric degradation of CFCl2O2. <b>2021</b> , 34, e4130	
604	Influence of H2O and NH3 on the reaction of HO2 with NO in troposphere: Theoretical investigation of HNO3 formation pathways. <b>2021</b> , 121, e26432	O
603	Mechanistic insights into the insertion and addition reactions of group 13 analogues of the six-membered N-heterocyclic carbenes: interplay of electrophilicity, basicity, and aromaticity governing the reactivity <b>2021</b> , 11, 20070-20080	
602	Competition and conversion between pnicogen bonds and hydrogen bonds involving prototype organophosphorus compounds. <b>2021</b> , 23, 18794-18805	1
601	The favorable routes for the hydrolysis of CHOO with (HO) ( $n = 1-4$ ) investigated by global minimum searching combined with quantum chemical methods. <b>2021</b> , 23, 12749-12760	0
600	Mechanistic Studies of Reduction and Initiation over the Vanadium-Oxide Polyethylene Catalyst. <b>2021</b> , 125, 2393-2402	1
599	A Computational Study on the Attack of Nitrogen and Oxygen Atoms to Toluene. <b>2021</b> , 620-631	3
598	Theoretical insight into the origins of chemo- and diastereo-selectivity in the palladium-catalysed (3 + 2) cyclisation of 5-alkenyl thiazolones.	2

597	Exploring water adsorption and reactivity in a series of doped aluminum cluster anions. 2021, 23, 23896-2	3908
596	Conversion of carbon dioxide to a novel molecule NCNBO mediated by NbBN anions at room temperature. <b>2021</b> , 23, 22613-22619	2
595	Influence of Water on the Gas-Phase Reaction of Dimethyl Sulfide with BrO in the Marine Boundary Layer. <b>2021</b> , 6, 2410-2419	4
594	Non-peripherally substituted metallophthalocyanines catalyzed diastereoselective carbonyl-ylide reactions: Synthesis and DFT calculations. <b>2021</b> , 80, 131892	
593	External electric field: a new catalytic strategy for the anti-Markovnikov hydrohydrazination of parent hydrazine <b>2021</b> , 11, 11595-11605	1
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590	Perylene bisimide cyclophanes as receptors for planar transition structures leatalysis of stereoinversions by shape-complementarity and noncovalent Interactions. <b>2021</b> , 8, 4408-4418	2
589	Mechanistic understanding of methane-to-methanol conversion on graphene-stabilized single-atom iron centers.	1
588	DFT insights into the Ni-catalyzed regioselective hydrocarboxylation of unsaturated alkenes with CO. <b>2021</b> , 50, 15084-15093	O
587	Self-catalytic mechanism of prebiotic reactions: from formamide to pterins and guanine. <b>2021</b> , 23, 19043-	19053
586	Computational and Experimental Insights into Asymmetric Rh-Catalyzed Hydrocarboxylation with CO2. <b>2021</b> , 2021, 663-670	1
585	Computational Investigation of Substituent Effect on the Thermodynamics and Kinetics of Hydrocarbyl Elimination from a Rhodium(I) Iminyl Complex. <b>2021</b> , 95, 163-171	
584	Study on the Reaction of Nanosized Yttrium Oxide Cluster Anions with n-Butane in the Gas Phase. <b>2021</b> , 79, 490	O
583	Silica-supported Nb(III)IIH3 species can act as an efficient catalyst for the non-oxidative coupling of methane. <b>2021</b> , 45, 12260-12270	О
582	Nucleophilic catalysis of p-substituted aniline derivatives in acylhydrazone formation and exchange. <b>2021</b> , 19, 7202-7210	1
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580	Hydrogenation of CO2 to methanol by the diphosphinefluthenium(II) cationic complex: a DFT investigation to shed light on the decisive role of carboxylic acids as promoters. <b>2021</b> , 11, 3556-3567	0

579	A computational approach to understand the role of metals and axial ligands in artificial heme enzyme catalyzed C-H insertion. <b>2021</b> , 23, 9500-9511	5
578	Probing the anomeric effect and mechanism of isomerization of oxazinane rings by DFT methods. <b>2021</b> , 19, 1066-1082	Ο
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576	Catalytic conversion of NO and CO into N2 and CO2 by rhodiumBluminum oxides in the gas phase.	Ο
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571	C3N Non-metallic Catalyst for Propane Dehydrogenation: A Density Functional Theory Study. <b>2021</b> , 151, 3154-3164	
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566	An experimental and mechanism study on the regioselective click reaction toward the synthesis of thiazolidinone-triazole. <b>2021</b> , 7, e06113	5
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564	CO Activation and Hydrogenation by Palladium Hydride Cluster Anions. <b>2021</b> , 125, 1747-1753	2
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562	The sequential activation of H and N mediated by the gas-phase ScN clusters: Formation of amido unit. <i>Journal of Chemical Physics</i> , <b>2021</b> , 154, 054307	6

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557	Guanidine-Amide-Catalyzed Aza-Henry Reaction of Isatin-Derived Ketimines: Origin of Selectivity and New Catalyst Design. <b>2021</b> , 26,	
556	Thermal curing mechanism of acetylene-terminated polyimides: A combination of density functional theory computation and microkinetic analysis. <b>2021</b> , 218, 123529	2
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549	Mechanistic insight on the inhibition of D, D-carboxypeptidase from by -lactam antibiotics: an ONIOM acylation study. <b>2021</b> , 1-11	
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547	The key role of adsorbate-catalyst interactions into catalytic activity of [CTA+]-Si-MCM-41 from electron density analysis. <b>2021</b> , 504, 111472	1
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544	Tuning catalytic activity of dimolybdenum paddlewheel complexes by ligands: mechanism study on the radical addition reaction of CCl4 to 1-hexene. 1	

543	Theoretical study of the reactions of hydrogen atom with methyl and ethyl hydroperoxides. e1919324	О
542	Impact of the Water Molecule on the Gas-Phase Reaction between Acetone and Cl Atoms. <b>2021</b> , 5, 920-930	1
541	Theoretical insights into the degradation of tyrosol stimulated by hydroxyl and sulfate radicals in wastewater and ecotoxicity evaluation. <b>2021</b> , 293, 126161	3
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539	Atmospheric insight into the reaction mechanism and kinetics of isopropenyl methyl ether (i-PME) initiated by OH radicals and subsequent oxidation of product radicals. <b>2021</b> , 28, 45646-45662	1
538	Thermo-kinetic theoretical studies on pyrolysis of dimethoxymethane fuel additive. <b>2021</b> , 290, 119970	8
537	Mechanistic insights into the autocatalyzed rearrangement of 2-bromooxazolines to 2-bromoisocyanates by means of high-level quantum chemical methods. <b>2021</b> , 34, e4214	
536	Activation of Carbon Dioxide by CoCD ( = 0-4) Anions. <b>2021</b> , 125, 3710-3717	2
535	Metal-free visible-light-catalyzed synthesis of 3-methyl-3,4-dihydroisoquinolin-1(2H)-one: mechanism, DFT calculation and optical properties. <b>2021</b> , 75, 4069-4074	
534	Interaction of ethane with singlet oxygen: A theoretical study of potential energy surfaces. <b>2021</b> , 1891, 012020	1
533	Structures of a non-ribosomal peptide synthetase condensation domain suggest the basis of substrate selectivity. <b>2021</b> , 12, 2511	9
532	New Mechanistic Insights into Atmospheric Oxidation of Aniline Initiated by OH Radicals. <b>2021</b> , 55, 7858-7868	3
531	Geometric Isomerism and DFT Theoretical Explanation of the Unexpected Formation of N, N-disubstituted Formamidines from 2-amino-3-cyano-4.6- diarylpyridines. <b>2021</b> , 1, 21-29	
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529	Theoretical insights into the dimerization mechanism of aluminum species at two different pH conditions. <b>2021</b> , 520, 120311	1
528	A density functional theory investigation on bis(diethylamino)cyclopropenylidene catalyzed synthesis of 1,4-bifunctional compounds. <b>2021</b> , 34, e4219	1
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525	Solvent and temperature effects on the tautomerization of a carbonitrile molecule: A conductor-like polarizable continuum model (CPCM) study. <b>2021</b> , 20, 59-68	1
524	Molecular-Scale Mechanism of Sequential Reaction of Oxalic Acid with SO: Potential Participator in Atmospheric Aerosol Nucleation. <b>2021</b> , 125, 4200-4208	2
523	Exploring paths of chemical transformations in molecular and periodic systems: An approach utilizing force. <b>2021</b> , 11, e1538	15
522	A theoretical study on screening ionic liquids for SO2 capture under low SO2 partial pressure and high temperature. <b>2021</b> , 98, 161-167	2
521	Non-noble metal single atom catalysts with S, N co-doped defective graphene support: A theoretical study of highly efficient acetylene hydration. <b>2021</b> , 27, 102216	2
520	Mechanisms of Diels-Alder reactions between pyridines and dienophiles: A DFT investigation. <b>2021</b> , 34, e4254	O
519	Cations Derived from Fentanyls Generated by Atmospheric Pressure Photoionization in the Presence of Ammonia: An IMS-MS Study. <b>2021</b> , 32, 1700-1706	
518	Chemical insights into the atmospheric oxidation of thiophene by hydroperoxyl radical. <b>2021</b> , 11, 13049	1
517	Asymmetric [2´+´2] cycloaddition of isatin with ketene catalyzed by N, N'-dioxide-Sc(III) complex: Mechanism and selectivity. <b>2021</b> , 510, 111657	
516	Generation, Characterization, and Dissociation of Radical Cations Derived from Prolyl-glycyl-glycine. <b>2021</b> , 125, 6121-6129	Ο
515	Reinvestigation of tandem dimerization and 1,3-alkyl shift in 3-benzylbenzothiazolylidene carbene: Experimental and theoretical results. <b>2021</b> , 1233, 130103	
514	Theoretical study of hydrogen abstraction from quadricyclane by small radicals. <b>2021</b> , 1200, 113232	O
513	A tautomeric ligand enables directed C-H hydroxylation with molecular oxygen. <b>2021</b> , 372, 1452-1457	25
512	Theoretical study on CO2 hydrogenation mediated by Ru-PNP pincer complexes: An implication towards rational catalyst design. <b>2021</b> , 943, 121842	
511	Effect of the Nucleophile's Nature on Chloroacetanilide Herbicides Cleavage Reaction Mechanism. A DFT Study. <b>2021</b> , 22,	0
510	Theoretical study of the reactions of propargyl radical with methanol and ethanol. <b>2021</b> , 119,	
509	Thermal Decomposition of 2-Methyltetrahydrofuran behind Reflected Shock Waves over the Temperature Range of 1179-1361 K. <b>2021</b> , 125, 5406-5422	1
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506	Investigation of the thermal stability of the antihypertensive drug nebivolol under different conditions: Experimental and computational analysis. 1	O
505	A Density Functional Theory Study on Et-BAC-Catalyzed 1,6-Conjugate Addition of -Chlorobenzaldehyde to -Quinone Methide for the Synthesis of ⊞,⊞-Diarylated Ketones. <b>2021</b> , 86, 9040-9054	2
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503	Degradation mechanism of tris(2-chloroethyl) phosphate (TCEP) as an emerging contaminant in advanced oxidation processes: A DFT modelling approach. <b>2021</b> , 273, 129674	4
502	First-principle kinetic studies of unimolecular pyrolysis of isopropyl esters as biodiesel surrogates. <b>2021</b> , 140, 1	2
501	Theoretical investigations on mechanisms and kinetics of methylketene with O(P) reaction in the atmosphere. <b>2021</b> , 27, 228	
500	Combined crossed molecular beams and computational study on the $N(2D) + HCCCN(X1H)$ reaction and implications for extra-terrestrial environments. e1948126	3
499	How Does Ti-Doping Affect Hydrogen Storage Properties of MgH2 at Nanosize?. <b>2021</b> , 95, 1424-1431	O
498	Simultaneous construction of axial and planar chirality by gold/TY-Phos-catalyzed asymmetric hydroarylation. <b>2021</b> , 12, 4609	8
497	Mechanism and regioselectivity of [Cu-Fe] heterobimetallic-catalyzed hydroboration of pyridines: DFT investigation. <b>2021</b> , 511, 111722	1
496	Mechanism and kinetic study for the reaction of allyl cyanide with Cl atom in the presence of O2. <b>2021</b> , 1201, 113286	1
495	Theoretical study of the DielsAlder reaction of 3-bromo-1-phenylprop-2-ynone with furan and 2-methylfuran. <b>2021</b> , 140, 1	2
494	Experimental and Computational Evaluation of Tantalocene Hydrides for CH Activation of Arenes. <b>2021</b> , 40, 2666-2677	1
493	Theoretical Investigation of HER Mechanism Using Density Functional and Ab Initio Calculations. <b>2021</b> , 42, 1289	
492	Study of the Reaction of Hydroxylamine with Iridium Atomic and Cluster Anions ( = 1-5). <b>2021</b> , 125, 5922-5932	4
491	Metal-free and iron(II)-assisted oxidation of cyclohexane to adipic acid with ozone: A theoretical mechanistic study. <b>2021</b> , 399, 52-66	5
490	Computational Investigation on the Formation and Decomposition Reactions of the CHO Compound. <b>2021</b> , 6, 17965-17976	2

489	Mechanistic Insights into the Dual Directing Group-Mediated C-H Functionalization/Annulation a Hydroxyl Group-Assisted M-M-M Pathway. <b>2021</b> , 6, 17642-17650	3
488	Atmospheric fate of formyl chloride and mechanisms of the gas-phase reactions with OH radicals and Cl atoms. <b>2021</b> , 777, 138709	1
487	Formation mechanism of chloropicrin from amines and free amino acids during chlorination: A combined computational and experimental study. <b>2021</b> , 416, 125819	O
486	Theoretical study on the flash vacuum gas-phase pyrolysis reaction mechanism of 2-(2-benzylidenehydrazinyl)pyridine and analogous. <b>2021</b> , 1202, 113297	
485	Accurate reaction barriers and rate constants of H-abstraction from primary, secondary, and tertiary amines by H atom determined with the isodesmic reaction method. <b>2021</b> , 776, 138708	
484	Photolysis of 3-Azido-3-phenyl-3H-isobenzofuran-1-one at Ambient and Cryogenic Temperatures. <b>2021</b> ,	
483	thlorovinylaldehydes as intermediates in the synthesis of new substituted ¶uoroalkoxyvinyl aldehydes and corresponding alcohols. <b>2021</b> , 248, 109837	2
482	Insights into the Factors Controlling the Origin of Activation Barriers in Group 13 Analogues of the Four-Membered N-Heterocyclic Carbenes. <b>2021</b> , 6, 22272-22283	
481	Combined Experimental and Computational Mechanistic Investigation of the Palladium-Catalyzed Decarboxylative Cross-Coupling of Sodium Benzoates with Chloroarenes. <b>2021</b> , 86, 11419-11433	O
480	Enhanced catalytic performance of oxidized Ru supported on N-doped mesoporous carbon for acetylene hydrochlorination. <b>2021</b> , 623, 118236	3
479	A theoretical study on gas-phase reaction of methylketene with OH: mechanism, kinetics, and insights. 1	1
478	Quantum Mechanical Investigation of the Oxidative Cleavage of the C-C Backbone Bonds in Polyethylene Model Molecules. <b>2021</b> , 13,	3
477	Computational Study of the Effect of Doping with Ti on NaAlH4 Nanocluster Dehydrogenation. <b>2021</b> , 95, 1646-1654	
476	Theoretical investigations on mechanisms and kinetics of methylketene with H reaction in the atmosphere. e4274	
475	Catalytic performance of Pt3Ni cluster toward ethane activation. <b>2021</b> , 548, 111204	0
474	Mechanism and Selectivity of Cyclopropanation of 3-Alkenyl-oxindoles with Sulfoxonium Ylides Catalyzed by a Chiral ,'-Dioxide-Mg(II) Complex. <b>2021</b> , 86, 11683-11697	4
473	Network structure and properties of crosslinked bio-based epoxy resin composite: An in-silico multiscale strategy with dynamic curing reaction process. <b>2021</b> , 7, 100063	O
472	Mechanistic study of vanadium-modified and sulfation-modified Phillips catalyst. <b>2021</b> , 513, 111777	

471	Kinetics study on the reactions of dimethyl ether with triplet oxygen and hydrogen atoms. <b>2021</b> , 779, 138855	3
470	Theoretical insight into the mechanisms of the gas-phase decomposition of azidoacetone. <b>2021</b> , 778, 138833	
469	Computational Mechanistic Study of Fused Phenol Formations from 1,6-Heptadiyne Involving Carbyne Complexes.	0
468	Enantioselective synthesis of D-lactic acid via chemocatalysis using MgO: Experimental and molecular-based rationalization of the triose's reactivity and preliminary insights with raw biomass. <b>2021</b> , 292, 120145	15
467	Reaction of CO3IIwith trinitrotoluene (TNT) in CO2 plasma: Experimental and theoretical study on the formation of [TNT´+ O]IIIand its fragmentation pathways. <b>2021</b> , 467, 116622	1
466	Theoretical insights into the enhancement of 1-Methyl-2,4,5-trinitroimidazole yield by exchanging of group introduction order. <b>2021</b> , 779, 138834	O
465	Potential environmental fate and risk based on the hydroxyl radical-initiated transformation of atmospheric 1,2-dibromo-4-(1,2dibromoethyl)cyclohexane stereoisomers. <b>2021</b> , 417, 126031	О
464	High-Pressure-Limit and Pressure-Dependent Rate Rules for Unimolecular Reactions Related to Hydroperoxy Alkyl Radicals in Normal Alkyl Cyclohexane Combustion. 1. Concerted HO Elimination Reaction Class. 2021, 125, 8942-8958	2
463	A theoretical study of mydroxybutenyl with O2 on the HOC4H6OO potential energy surface. <b>2021</b> , 140, 1	
462	Dramatic catalytic activation of kinetically inert disilane hydrolysis in metallic iron particulate via barrierless chemical dissociation: First-principles study. <b>2021</b> , 560, 149988	3
461	Theoretical study of the reactions of triplet Oxygen atom with methyl and ethyl hydroperoxides.	
460	Protein-Ligand Binding Molecular Details Revealed by Terahertz Optical Kerr Spectroscopy: A Simulation Study. <b>2021</b> , 1, 1788-1797	1
459	Aminolysis and hydrolysis of an organophosphorus pesticide: A theoretical insight into the reaction mechanism for thio methyl parathion. <b>2021</b> , 1203, 113348	1
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181	Organocatalytic Synthesis of Chiral Allene Catalyzed by Chiral Phosphoric Acid Via Asymmetric 1,8-Addition of Indole Imine Methide: Mechanism and Origin of Enantioselectivity.	
180	Multiple CO2 reduction mediated by heteronuclear metal carbide cluster anions RhTaC2[]	1
179	Controlled masking and targeted release of redox-cycling ortho-quinones via a CII bond-cleaving 1,6-elimination. <b>2022</b> , 14, 754-765	1
178	Eco-Friendly Synthesis of 5-Hydroxymethylfurfural and Its Applications as a Starting Material to Synthesize Valuable Heterocyclic Compounds. <b>2022</b> , 10, 8673-8684	2
177	What Determines the Drastic Reactivity of Nbn+ Clusters with Nitric Oxide under Thermalized Conditions?.	1
176	Mechanistic insights into the active intermediates of 2,6-diaminopyridine dinitration. 2022,	
175	Single Ti3+ Ion Catalyzes NO Reduction on Stoichiometric Titanium Oxide Cluster Anions (TiO2)n□ (n = 1៧1). 8768-8775	0
174	Photocatalyst-free light driven dehydrogenation of alcohols into carbonyl compounds under mild conditions.	
173	Oxo-Rhenium-Mediated Allylation of Furanoside Derivatives: A Computational Study on the Mechanism and the Stereoselectivity.	0
172	Solvent promoted tautomerism in thione-containing tetraazatricyclics: evidence from 1H NMR spectroscopy and transition state studies. <b>2022</b> , 28,	Ο
171	Competing mechanisms of CO hydrogenation to ethanol over TM/Mo6S8 catalysts. 2022, 224, 116031	
170	Regulating the competitive reaction pathway in glycerol conversion to lactic acid/glycolic acid selectively. <b>2022</b> , 413, 407-416	O
169	Mechanism and safety analysis of acetylene decomposition explosion: A combined ReaxFF MD with DFT study. <b>2022</b> , 327, 124996	0
168	Mechanism of the Phosphine-Catalyzed $[3 + 3]$ Annulation with MBH Carbonates as the Potential Dipoles.	
167	DFT investigates the mechanisms of cross-dehydrogenative coupling between heterocycles and acetonitrile.	
166	Ru-Catalyzed Hydroboration of Ynones Leads to a Nontraditional Mode of Reactivity. <b>2022</b> , 144, 14846-1485	55 1

165	Roles of CO2 in Controlling the Chemoselectivity of [LCu-Fp] Heterobimetallic-Catalyzed CO2 Hydroboration Reduction: A Computational Study. <b>2022</b> , 41, 1922-1930	
164	Theoretical Investigations of the OH-Initialized Oxidation of 4-Methyl-3-Penten-2-One in the Atmosphere.	O
163	Waterlas Shift Catalyzed by Iridiumlanadium Oxide Clusters IrVO2lwith Iridium in a Rare Oxidation State of II. <b>2022</b> , 126, 5294-5301	0
162	Combustion Characteristic of 2,3,3,3-tetrafluroropropene (R1234yf). <b>2022</b> ,	
161	Investigation of the Gas-Phase Reaction of Nopinone with OH Radicals: Experimental and Theoretical Study. <b>2022</b> , 13, 1247	
160	Ir and NHC Dual Chiral Synergetic Catalysis: Mechanism and Stereoselectivity in Butyrolactone Formation.	2
159	Distinctive Mechanistic Scenarios and Substituent Effects of Gold(I) versus Copper(I) Catalysis for Hydroacylation of Terminal Alkynes with Glyoxal Derivatives.	
158	Intramolecular Diels∆lder Reactions of ∃-Bromostyrene-Functionalized Unsaturated Carboxamides. <b>2022</b> , 87, 11148-11164	1
157	Mechanistic Study of Asymmetric Alkynylation of Isatin-Derived Ketimine Mediated by a Copper/Guanidine Catalyst.	
156	Racemization Pathway for MoO2(acac)2 Favored over RayDutt, Bailar, and ConteHippler Twists.	Ο
155	Mechanistic aspects of the Pd(OAc) n ( $n=1B$ ) catalyzed ethylene acetoxylation: A density functional theory study.	
154	NHC-catalyzed [3´+´4] annulation between 2-dromoenal and aryl 1,2-diamine: Insights into mechanisms, chemo and stereoselectivities. <b>2022</b> , 530, 112604	
153	First-principles investigation of interaction between the atomic oxygen species and carbon nanostructures. <b>2022</b> , 9, 100201	0
152	Solvent-mediated selectivity control of furfural hydrogenation over a N-doped carbon-nanotube-supported Co/CoOx catalyst. <b>2022</b> , 318, 121838	O
151	Ortho-Phosphinoarenesulfonamide-Mediated Staudinger Reduction of Aryl and Alkyl Azides. <b>2022</b> , 27, 5707	0
150	Experimental and theoretical insight into the transformation behaviors and risk assessment of Flutamide in UV/O3/PMS system. <b>2022</b> , 375, 134167	O
149	Understanding the effect of the divalent cations (Ni, Cu, and Zn) exchanged FAU zeolite on the kinetic of CO2 cycloaddition with ethylene oxide: A DFT study. <b>2022</b> , 117, 108321	0
148	Ultraviolet dechlorination of tetrachloro-p-benzoquinone by hydrogen sulfide: Theoretical confirmation of the significance of hydrosulfide radical. <b>2022</b> , 308, 136372	Ο

147	Dft Study on Aerial Degradation of Product Radicals Derived from the Reaction of 1h-Heptafluorocyclopentene (Cyc-Cf2cf2cf2cf=Ch] with Oh Radical.	O
146	Suppression of Reversible Photocyclization Reaction Induced Fluorescence Enhancement: A Theoretical Study.	O
145	Ultraviolet Dechlorination of Tetrachloro-P-Benzoquinone by Hydrogen Sulfide: Theoretical Confirmation of the Significance of Hydrosulfide Radical.	O
144	Effect of (H2O)n (n = 0B, 13) on the NH3 + OH reaction in the gas and liquid phases. <b>2022</b> , 12, 28010-28019	O
143	Theoretical Study of the Reaction O(3P) + 1,2-Butadiene. <b>2022</b> , 249-263	O
142	The S\$\$^+\$\$(\$\$^4\$\$S)+SiH\$\$_{2}\$\$(\$\$^1\$\$A\$\$_1\$\$) Reaction: Toward the Synthesis of Interstellar SiS. <b>2022</b> , 233-245	O
141	Theoretical insights into the mechanism and origin of chemoselectivity in the catalyst- and directing group-dependent oxidative cyclization of diynes with pyridine N-oxides. <b>2022</b> , 9, 5168-5177	O
140	Identification of chlorinated products from tyrosine and tyrosyl dipeptides during chlorination: a computational study.	O
139	Computational exploration for possible reaction pathways, regioselectivity, and influence of substrate in gold-catalyzed cycloaddition of cyanamides with enynamides. <b>2022</b> , 12, 22939-22945	0
138	First-principles calculations for determining the mechanism of the photocatalytic selective oxidation of toluene to benzaldehyde on the g-C3N4 catalyst. <b>2022</b> , 46, 16922-16931	O
137	Formation Routes of CO from O(1D)+Toluene: A Computational Study. <b>2022</b> , 260-269	O
136	A Theoretical Investigation of the Reactions of N(\$\$^2\$\$D) and CN with Acrylonitrile and Implications for the Prebiotic Chemistry of Titan. <b>2022</b> , 246-259	O
135	Unraveling origin of chemoselectivity and regioselectivity of iridium-catalyzed B(4)⊞ functionalization of o -carborane by alkyne.	0
134	Density Functional Theory Study of Low-Dimensional (2D, 1D, 0D) Boron Nitride Nanomaterials Catalyzing Acetylene Acetate Reaction. <b>2022</b> , 23, 9997	O
133	Reaction N(2D) + CH2CCH2 (Allene): An Experimental and Theoretical Investigation and Implications for the Photochemical Models of Titan.	O
132	Metal free activation of water and ammonia by neutral tricoordinate pyramidal boron: a computational study.	O
131	Temperature and Pressure-Dependent Rate Constants for the Reaction of the Propargyl Radical with Molecular Oxygen. <b>2022</b> , 7, 33470-33481	0
130	The N(2D) + CH2CHCN (Vinyl Cyanide) Reaction: A Combined Crossed Molecular Beam and Theoretical Study and Implications for the Atmosphere of Titan. <b>2022</b> , 126, 6110-6123	O

129	Thorough Understanding of Bioluminophore Production in Bacterial Bioluminescence. <b>2022</b> , 126, 6604-6616	О
128	Analysis of the Fragmentation Pathways for the Collision-Induced Dissociation of Protonated Cyclophosphamide: A Mass Spectrometry and Quantum Mechanical Study. <b>2022</b> , 62, 4411-4419	O
127	CH4 activation by PtX+ (X = F, Cl, Br, I). 10,	O
126	A Quantum Chemical Investigation into the Molecular Mechanism of the Atmospheric Reactions of Chemi-Ions with Nitrogen and Nitrogen Oxides. <b>2022</b> , 24, 1257	О
125	Methane Activation by Vanadium Oxide Cluster Anions (V2O5)NO[[N = 1f]8].	О
124	Organocatalytic synthesis of chiral allene catalyzed by chiral phosphoric acid via asymmetric 1,8-addition of indole imine methide: Mechanism and origin of enantioselectivity. <b>2022</b> , 530, 112648	O
123	Role of monomolecular water and bimolecular water in IO + CH2O reaction. <b>2022</b> , 28,	O
122	Advances on Understanding Coke Gasification Process with CO 2 : A Report from Density Functional Theory. <b>2022</b> , 7,	Ο
121	Revisiting the burden borne by fumarase: enzymatic hydration of an olefin.	О
120	Graph-Driven Reaction Discovery: Progress, Challenges, and Future Opportunities.	1
119	High-temperature mid-IR absorption spectra and reaction kinetics of 1,3-dioxolane. 2022,	О
118	Reactive orbital energy theory serving a theoretical foundation for the electronic theory of organic chemistry.	O
117	Experimental and Theoretical Study of Oxolan-3-one Thermal Decomposition.	O
116	Mapping out the reaction network of humin formation at the initial stage of fructose dehydration in water. <b>2022</b> ,	O
115	Theoretical investigation for the reactions of hydrogen atom with dimethyl sulfide, ethyl methyl sulfide: Mechanism and kinetics properties. <b>2022</b> , 1217, 113893	0
114	Mechanism of [3+2] Annulations between Indole-2-formaldehydes and Isatins Mediated by N-Heterocyclic Carbene: A DFT Study.	Ο
113	Theoretical insights into the gaseous and heterogeneous reactions of halogenated phenols with DH radicals: mechanism, kinetics and role of (TiO2)n clusters in degradation processes.	0
112	Catalytic NO Reduction by NO Pre-Adsorbed RhCeO2NO- Clusters.	O

111	An Ab Initio Investigation on Relevant Oligomerization Reactions of Toluene Diisocyanate (TDI). <b>2022</b> , 14, 4183	О
110	Hydrolysis of an organophosphorus pesticide: a computational reaction study on triazophos. <b>2022</b> , 141,	О
109	Mechanistic Insights into Cobalt-Catalyzed Regioselective C4-Alkenylation of 3-Acetylindole: A Detailed Theoretical Study.	0
108	Toward efficient functionalization of polystyrene backbone through ketene chemistry: Synthesis, characterization, and DFT study.	O
107	Experimental and Theoretical Evidence for Relativistic Catalytic Activity in CIII Activation of N-Phenylbenzamide Using a Cationic Iridium Complex. <b>2022</b> , 126, 7627-7638	1
106	Decomposition mechanism of hydrofluorocarbon (HFC-245fa) in supercritical water: A ReaxFF-MD and DFT study. <b>2022</b> ,	О
105	Theoretical study of the mechanism and kinetics of the atmospheric reaction of acrylic acid with NO 3 radical.	О
104	Unexpected Gas-Phase Nitrogen Dxygen Smiles Rearrangement: Collision-Induced Dissociation of Deprotonated 2-(N-Methylanilino)ethanol and Morpholinylbenzoic Acid Derivatives. <b>2022</b> , 33, 2120-2128	O
103	Combining density functional theory and CFD-PBM model to predict TiO2 nanoparticle evolution during chemical vapor deposition. <b>2022</b> , 140174	1
102	DFT study on aerial degradation of product radicals derived from the reaction of 1HHeptafluorocyclopentene (cyc-CF2CF2CF2CF2CF2CF) with OH radical. <b>2022</b> , 1217, 113915	O
101	A Computational Study of the MoO2(acac)2 Catalyzed Epoxidation of Ethylene with Hydrogen Peroxide and t-Butyl Hydroperoxid.	0
100	Computational studies on thermo-kinetics aspects of pyrolysis of isopropyl acetate and its methyl, bromide and hydroxyl derivatives. <b>2022</b> , 8, e11274	O
99	Thermal hazard characteristics and essential mechanism study of 1-hydroxybenzotriazole: Thermodynamic study combined DFT simulation. <b>2022</b> , 168, 713-722	0
98	Resource utilization of waste HFC-134a refrigerant by supercritical gasification method: A reactive molecular dynamic study. <b>2022</b> , 168, 399-409	1
97	Mechanistic insights into the self-esterification of lactic acid under neutral and acidic conditions. <b>2023</b> , 1273, 134336	0
96	Stereochemical inversion of pillar[5]arene. NMR and DFT studies. <b>2023</b> , 1274, 134403	O
95	Facile C?O Bond Cleavage on Polynuclear Vanadium Nitride Clusters V4N5	0
94	Direct Conversion of N2 and O2 to Nitric Oxide at Room Temperature Initiated by Double Aromaticity in the Y2BO+ Cation. 10697-10704	1

93	Low-Temperature Production of Glyceric Acid from Biomass-Based Sugar via the Cooperative Roles of MgO and NaBF4. <b>2022</b> , 61, 16689-16701	O
92	Computational investigation on mechanisms and kinetics of gas-phase reactions of 4-hydroxy-2-pentanone (4H2P) with hydroxyl radicals and subsequent reactions of CH3C(O)CH2C•(OH)CH3 radical. <b>2022</b> , 141,	O
91	Impact of a single water molecule on the atmospheric oxidation of thiophene by hydroperoxyl radical. <b>2022</b> , 12,	Ο
90	Inorganic Bergman Cyclization: An Appeal From Theory.	O
89	Temperature and pressure dependent rate constants of the reactions of $\mathbb{D}H$ with cyclopentene from Variational TST and SS-QRRK methods.	O
88	Femtosecond intramolecular rearrangement of the CH3NCS radical cation.	O
87	Theoretical investigations on the reaction of ethenol with triplet oxygen atom.	O
86	Quantum Chemical Investigation on Hydrolysis of Orally Active Organometallic Ruthenium(II) and Osmium(II) Anticancer Drugs and Their Interaction with Histidine.	0
85	The influence of (H2O)1 in the HOBr + HO2 gas-phase reaction. 2022, 12, 36028-36037	O
84	A Receding Horizon Trajectory Tracking Strategy for Input-Constrained Differential-Drive Robots via Feedback Linearization. <b>2022</b> , 1-8	O
83	Theoretical Investigations on the Reactivity Influence Factors of 4Mn(CO)5 Catalyzed Alkynes Hydrosilylation and Hydrogermylation.	O
82	The scavenging mechanism of aminopyrines towards hydroxyl radical: A computational mechanistic and kinetics investigation. <b>2023</b> , 1219, 113973	O
81	OH/O3-initiated transformation of primidone in AOPs based on the theoretical calculations: Mechanisms, kinetics, and eco-toxicity assessments. <b>2023</b> , 11, 109167	O
80	Combustion inhibition of cup-burner flame with C2HF3Cl2 and its kinetics mechanism investigation. <b>2023</b> , 813, 140275	O
79	Electronic and Steric Control of Rates and Selectivities in Rhodium-Catalyzed [2+2+2] Cycloadditions for Constructing Fused Tricyclic Hydronaphthofurans: A Density Functional Theory Study. <b>2022</b> , 87, 16328-16342	0
78	Stepwise Polymetalation around an sp3 Benzyl Carbon Atom. <b>2022</b> , 41, 3493-3498	O
77	Influence of H2SO4 <sup>444</sup> H2O and (H2SO4)2 on the Hydrolysis of Formaldehyde: A Potential Source of Methanediol in the Troposphere. <b>2022</b> , 6, 2779-2789	1
76	Valorisation of Corncob Residue towards the Sustainable Production of Glucuronic Acid. <b>2022</b> , 12, 1603	O

75	Atmospheric degradation mechanisms and kinetics for OH-initiated oxidation of trans-⊕cimene.	O
74	A DFT Study on the Mechanism of Active Species in Selective Photocatalytic Oxidation of Toluene into Benzaldehyde on (WO 3) 3 Clusters. <b>2022</b> , 7,	О
73	Expansion of nanotube cap due to migration of sp atoms from lateral surface. 2022, 115624	O
72	Structure and Spectroscopic Signatures of Interstellar Sodium Isocyanate Isomers. <b>2022</b> , 941, 40	o
71	A Computational Perspective on the Chemical Reaction of HFO-1234zc with the OH Radical in the Gas Phase and in the Presence of Mineral Dust.	0
70	Visible Light-Induced Coupling Cyclization Reaction of ∃-Diazosulfonium Triflates with ∃-Oxocarboxylic Acids or Alkynes. <b>2022</b> , 87, 16604-16616	0
69	A Molecular Level Interpretation of the Underlying Chemical Phenomenon of Semi-coke and Coke Formation: A Treatise from Ab Initio Calculations. <b>2022</b> , 7,	0
68	Gas-phase reactions driven by polarized metal-metal bonding in atomic clusters.	О
67	Mechanistic insights into the challenges of organocatalytic Beckmann rearrangement reactions.	O
66	Revisiting the Burden Borne by Fumarase: Enzymatic Hydration of an Olefin. <b>2023</b> , 62, 476-493	o
65	Research on oxidation decomposition mechanism of fluoroethane. 2023,	O
64	Reactions O(3P, 1D) + HCCCN(X1 $\mathbb H$ ) (Cyanoacetylene): Crossed-Beam and Theoretical Studies and Implications for the Chemistry of Extraterrestrial Environments.	o
63	Cooperative Asymmetric Dual Catalysis Involving a Chiral N-Heterocyclic Carbene Organocatalyst and Palladium in an Annulation Reaction: Mechanism and Origin of Stereoselectivity. 1133-1148	0
62	Tropospheric Oxidation of 1,1,2,3-Tetrafluoropropene (CF2=CFIH2F) Initiated by OH Radical and Aerial Degradation of Its Product Radicals.	0
61	Unsupervised Reaction Pathways Search for the Oxidation of Hypergolic Ionic Liquids: 1-Ethyl-3-methylimidazolium Cyanoborohydride (EMIM+/CBHDas a Case Study.	1
60	Computational study of the alcoholysis for organophosphorus pesticides: The reaction of phoxim with methanol.	o
59	Comparison of nitrate formation mechanisms from free amino acids and amines during ozonation: a computational study.	0
58	A study of the thermodynamics and mechanisms of the atmospherically relevant reaction dimethyl sulphide (DMS) with atomic chlorine (Cl) in the absence and presence of water, using electronic structure methods. <b>2023</b> , 25, 4780-4793	O

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57	Influence of the Element and Substituent Effects on the Reactivity of Catching Reactions of Difluorocarbene by Benzene-Bridged and Group-13/Group-15-Based Frustrated Lewis Pairs. <b>2023</b> , 62, 1018-1031	0
56	Mechanisms and Energetics for Hydrogen Abstraction of Thymine Photosensitized by Benzophenone from Theoretical Principle.	O
55	Role of Noncovalent Interactions in Inducing High Enantioselectivity in an Alcohol Reductive Deoxygenation Reaction Involving a Planar Carbocationic Intermediate. <b>2023</b> , 145, 2884-2900	O
54	Theoretical Study on the Formation of 2-Pyrone Derivatives from the Reaction of Alkynes with Carbon Dioxide in the Presence of Nickel Catalyst.	O
53	Intramolecular cyclization reactions of arylpropargyl amides of electron-deficient 日,相kenyl carboxylates and related compounds. <b>2023</b> , 21, 2172-2187	0
52	Insights into the ruthenium-catalysed selective reduction of cardanol derivatives via transfer hydrogenation: a density functional theory study.	O
51	Silacyclopropenylsilylene-NHC Complex: Synthesis by (1+2) Retro-cycloaddition, Dynamic Behavior in Solution, and Ring-expansion Reaction. <b>2023</b> , 52, 124-127	О
50	Kinetics, Products, and Mechanisms Study of the Atmospheric Degradation of (E)-4-Methoxy-3-buten-2-one with Hydroxyl Radicals.	O
49	Electrostatic interactions, binding energies and structures of the Be+2•. 2023, 1222, 114070	O
48	Theoretical prediction of the catalytic efficiency of non-metalated pincer-like phosphorus compounds for the hydrogenation of carbon-monoxide with ammonia-borane. <b>2023</b> , 817, 140405	O
47	Theoretical Investigation on Hydrogen Abstraction Reactions of Sulfur Compounds $HSX(O)H$ and $CH3SX(O)H$ (X = C, S) by OH Radicals.	O
46	Chemo- and regioselectivities of the TBAF-catalyzed C F bond allylation of trifluoromethylalkenes: A theoretical view. <b>2023</b> , 542, 113111	O
45	Reaction mechanism and kinetics of H and Cl atom abstraction in Dichloromethane with OH radical. <b>2023</b> , 1223, 114082	О
44	Mechanisms and origins of stereoselectivity involved in NHC-catalyzed [3 $^{\prime}$ + $^{\prime}$ 3] Annulation of 2-bromoenals and 軟etothioamides: A DFT study. <b>2023</b> , 542, 113135	O
43	Theoretical investigation into activation of hydroperoxides by excited quinones under ultraviolet irradiation. <b>2023</b> , 463, 142423	0
42	In-depth DFT insights into the crucial role of hydrogen bonding network in CO2 fixation into propylene oxide promoted by Biomass-Derived deep eutectic solvents. <b>2023</b> , 380, 121737	O
41	New insights into the reactivity of the triscyclopentadienyl monothiolate uranium(IV) complexes: CS2 and CO2 insertion and redox properties. A DFT theoretical approach. <b>2023</b> , 992, 122692	О
40	High-density pyridine-FeN4 active sites for acetylene hydrochlorination. 2023,	O

39	Pyrolytic elimination of ethylene from ethoxyquinolines and ethoxyisoquinolines: a computational study. <b>2023</b> , 13,	0
38	CH Activation by Iron-Vanadium Bimetallic Oxide Cluster Anions FeV 3 O 10 Land FeV 5 O 15 🛭 A Comparison with Scandium-Vanadium Oxide Clusters.	O
37	High-temperature mid-IR absorption and reaction kinetics of 2-methyl-1,3-dioxolane: An experimental and theoretical study. <b>2023</b> , 13, 100165	0
36	Visible Light-Induced Synthesis of 2-Oxazolidinones through One-Pot Coupling of Benzylamines, Epoxides and CO 2. <b>2023</b> , 26,	O
35	Mechanistic insight into the degradation of 1H-benzotriazole and 4-methyl-1H-benzotriazole by DH-based advanced oxidation process and toxicity assessment. <b>2023</b> , 30, 49150-49161	О
34	Synthesis of Disubstituted Carboxonium Derivatives of Closo-Decaborate Anion [2,6-B10H8O2CC6H5][ITheoretical and Experimental Study. <b>2023</b> , 28, 1757	O
33	Lipophilic Guanidine with Enhanced Stability for Use in Cesium Separation from Legacy High-Level Nuclear Waste. <b>2023</b> , 62, 3684-3694	О
32	Tailoring the mechanistic pathways and kinetics of OH-addition reaction of sulfoxaflor and its ecotoxicity assessment. <b>2023</b> , 30, 50209-50224	O
31	Kinetic Properties Study of H Atom Abstraction by CH3½ Radicals from Fuel Molecules with Different Functional Groups. <b>2023</b> , 127, 1960-1974	O
30	Dissociative photoionization of m-xylene. <b>2023</b> , 36, 41-49	O
30 29	Dissociative photoionization of m-xylene. <b>2023</b> , 36, 41-49  Time-resolved, Gas-phase Kinetic and Quantum Chemical Studies of the Reaction of Germylene with Hydrogen Chloride.	0
	Time-resolved, Gas-phase Kinetic and Quantum Chemical Studies of the Reaction of Germylene	
29	Time-resolved, Gas-phase Kinetic and Quantum Chemical Studies of the Reaction of Germylene with Hydrogen Chloride.	0
29	Time-resolved, Gas-phase Kinetic and Quantum Chemical Studies of the Reaction of Germylene with Hydrogen Chloride.  C(sp3)  Oxidative Addition at Tantalocene Hydrides.  Coordination of sorbitol to Ga(OTf)3 in the liquid phase: an experimental and theoretical study.	0
29 28 27	Time-resolved, Gas-phase Kinetic and Quantum Chemical Studies of the Reaction of Germylene with Hydrogen Chloride.  C(sp3) M Oxidative Addition at Tantalocene Hydrides.  Coordination of sorbitol to Ga(OTf)3 in the liquid phase: an experimental and theoretical study. 2023, 25, 8507-8514  Metal-free catalysis on the reactions of nitric acid with aliphatic aldehydes: A new potential source	0 0
29 28 27 26	Time-resolved, Gas-phase Kinetic and Quantum Chemical Studies of the Reaction of Germylene with Hydrogen Chloride.  C(sp3)  Oxidative Addition at Tantalocene Hydrides.  Coordination of sorbitol to Ga(OTf)3 in the liquid phase: an experimental and theoretical study. 2023, 25, 8507-8514  Metal-free catalysis on the reactions of nitric acid with aliphatic aldehydes: A new potential source of organic nitrates. 2023, 299, 119673  Unveiling the theoretical aspects of superelectrophilic activation in an inverse demand Diels-Alder	0 0
29 28 27 26 25	Time-resolved, Gas-phase Kinetic and Quantum Chemical Studies of the Reaction of Germylene with Hydrogen Chloride.  C(sp3) M Oxidative Addition at Tantalocene Hydrides.  Coordination of sorbitol to Ga(OTf)3 in the liquid phase: an experimental and theoretical study. 2023, 25, 8507-8514  Metal-free catalysis on the reactions of nitric acid with aliphatic aldehydes: A new potential source of organic nitrates. 2023, 299, 119673  Unveiling the theoretical aspects of superelectrophilic activation in an inverse demand Diels-Alder reaction. 2023, 29,  Crosslinking Rapidly Cured Epoxy Resin Thermosets: Experimental and Computational Modeling	0 0 0

21	Reciprocity of C?O?IInteractions with the dominant anionIbn fullerene (C60)Ibmine-based organocatalysts: a mechanistic elucidation for addition vs. decarboxylation reaction. <b>2023</b> , 25, 10647-10660	O
20	Comprehensive computational study on reaction mechanism of N-Nitroso dimethyl amine formation from substituted hydrazine derivatives during ozonation. <b>2023</b> , 9, e14511	O
19	Excited-State Intramolecular Proton Transfer in Salicylidene-H-Hydroxy Carboxylate Derivatives: Direct Detection of the Triplet Excited State of the cis-Keto Tautomer. <b>2023</b> , 127, 2765-2778	O
18	Visible light-catalyzed intermolecular [2+2] cycloaddition of 1,2-dihydropyridines: A combined experimental and DFT study. <b>2023</b> , 136, 133357	O
17	Stereoretentive Formation of Cyclobutanes from Pyrrolidines: Lessons Learned from DFT Studies of the Reaction Mechanism. <b>2023</b> , 88, 4619-4626	О
16	Unraveling the role of absorbed O/OH on methane total oxidation on Cu surface. 2023, 819, 140444	Ο
15	Ligand Control in Co-Catalyzed Regio- and Enantioselective Hydroboration: Homoallyl Secondary Boronates via Uncommon 4,3-Hydroboration of 1,3-Dienes. <b>2023</b> , 145, 7462-7481	О
14	The molecular level study of the fate of the CH3CH2C(O)OCH(O)CH3 radical derived from ethyl propionate. <b>2023</b> , 49, 711-719	O
13	A DFT study of the catalytic ODH of n-hexane over a cluster model of vanadium oxide. <b>2023</b> , 541, 113078	О
12	Photodissociation dynamics of acetaldehyde at 267 nm: A computational study of the CO -forming channels.	O
11	A metal Lewis base activation model for Pd-catalyzed hydroamination of amines and 1,3-dienes.	О
10	Two Carbon Dioxide Molecules Consecutively Reduced by Metal-Free B2O2[Anions. <b>2023</b> , 127, 3082-3087	O
9	Theoretical Study of the Mechanism of Palladium-Catalyzed Arylation of Alkenyl Carboxylates. <b>2023</b> , 17, 68-95	О
8	Rapidly Cured Multifunctional Epoxy Resins with Switchable Curing Temperature and Exceptional Electrical Properties.	Ο
7	Conversion of Dinitrogen and Oxygen to Nitric Oxide Mediated by Triatomic Yttrium Cations: Reversible NI Bond Switching. <b>2023</b> , 62, 6102-6108	О
6	Thermal hazard and pyrolysis mechanism investigation using thermal analysis coupled with quantum-chemical DFT simulation for 1-hydroxy-7-azabenzotriazole.	O
5	Understanding the insight into the mechanisms and dynamics of the OH-initiated oxidation of CHF2CF2OCHF2 and the subsequent reactions in the presence of NO and O2. <b>2023</b> , 122, 108489	О
4	Filtration of the preferred catalyst for reverse water-gas shift among the Rhn- (n = 3-11) clusters by mass spectrometry under variable temperatures.	O

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