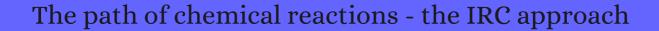
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481	Roads Not Taken: Mechanism and Origins of Regio- and Chemoselectivity of Directed Colli-Catalyzed Alkenylation of N-Pyridyl 2-Pyridone.	О
480	DFT Mechanistic Study of the Cyclopropanation of Styrene and Aryldiazodiacetate Catalyzed by Tris(pentafluorophenyl)borane <b>2022</b> , 7, 12900-12909	

479	BF3IIatalyzed DielsIAlder Reaction between Butadiene and Methyl Acrylate in Aqueous SolutionIAn URVA and Local Vibrational Mode Study. <b>2022</b> , 12, 415		0
478	Bis(imino)acenaphthene (BIAN)-Supported N-Heterocyclic Carbene Palladium Complexes with Ancillary Ligands: Readily Activated Precatalysts for Direct CH Arylation of Thiophenes.		Ο
477	CO 2 trapping of selected N -heterocyclic vinylidenes with an NBO mechanistic scrutiny by DFT.		
476	Quantum Tunnelling Driven H Formation on Graphene 2022, 3173-3181		2
475	New Insights and Predictions into Complex Homogeneous Reactions Enabled by Computational Chemistry in Synergy with Experiments: Isotopes and Mechanisms <i>Accounts of Chemical Research</i> , <b>2022</b> ,	24.3	5
474	H2 generation from catalytic water dissociation on doped nanocluster Pt6X (X=C, Si, and Ge). <b>2022</b> , 432, 127990		
473	Theoretical insights into the transformation mechanism and eco-toxicity effects of 5-Fluorouracil by O3 and 4OH in waters. <b>2022</b> , 160, 541-550		1
472	Theoretical study on the mechanism of NiAl bimetallic catalyzed dual CH cyclization of amides and alkynes. <b>2022</b> , 522, 112230		Ο
471	Mechanistic study on oxidative degradation and deposition of exo-tetrahydrodicyclopentadiene. <b>2022</b> , 317, 123533		0
470	Ni-Catalyzed Dearomative Cycloaddition of Alkynes to 10 Aromatic Benzothiophenes: Elucidation of Reaction Mechanism. <b>2021</b> , 94, 2727-2738		
469	Catalyst-Controlled Stereoselective Construction of Indole-Fused Heterocycles through Cycloadditions of Indolyl-Allenes: A Theoretical Investigation. <b>2021</b> , 95, 2567-2572		
468	Mechanistic study of cobalt(I)-catalyzed asymmetric coupling of ethylene and enynes to functionalized cyclobutanes <b>2021</b> ,		
467	Ethylene-Triggered Regioselectivity Switch of Dimethylbutadiene in Their Copolymerization: Formation of Plastic Rubber and Mechanism. 2022, 12, 953-962		1
466	The Oxidation Cascade of a Rare Multifunctional P450 Enzyme Involved in Asperterpenoid A Biosynthesis <b>2021</b> , 9, 785431		1
465	The mechanism of sugar produced from simple glycolaldehyde derivative at ambient conditions. <b>2022</b> , 122,		
464	Synthesis and Application of Constrained Amidoboronic Acids Using Amphoteric Boron-Containing Building Blocks <b>2021</b> ,		O
463	Hydroboration and Hydrosilylation of a Molybdenum litride Complex Bearing a PNP-Type Pincer Ligand. <b>2022</b> , 41, 366-373		2
462	Boosting Palladium-Catalyzed Aryl-Nitro Bond Activation Reaction by Understanding the Electronic, Electrostatic, and Polarization Effect: A Computational Study from a Basic Understanding to Ligand Design <b>2021</b> ,		1

461	BF -Catalyzed Mukaiyama aldol reaction of acetaldehyde with 2-siloxy-1-propene 2021,	O
460	Exploring the reaction pathway involved in the dibenzo-18-crown-6 synthesis from catechol and bis(2-chloroethyl) ether in presence of base. <b>2022</b> , 35,	O
459	Model Setup and Procedures for Prediction of Enzyme Reaction Kinetics with QM-Only and QM:MM Approaches. <b>2022</b> , 2385, 175-236	О
458	Generation of Phenol and Molecular Hydrogen through Catalyst-Free C-H Activation of Benzene by Water Radical Cations <b>2021</b> ,	1
457	Rapid Water Diffusion at Cryogenic Temperatures through an Inchworm-like Mechanism 2021,	1
456	Towards low-energy-light-driven bistable photoswitches: ortho-fluoroaminoazobenzenes. <b>2021</b> , 21, 159	3
455	Oxidation of Triorganosilanes and Related Compounds by Chlorine Dioxide. <b>2021</b> , 91, 2391-2402	О
454	Effects of Axial Solvent Coordination to Dirhodium Complexes on the Reactivity and Selectivity in CH Insertion Reactions: A Computational Study. <b>2021</b> , 40, 4120-4132	1
453	Exploring the reactivity of homoleptic organozincs towards SO: synthesis and structure of a homologous series of organozinc sulfinates <b>2022</b> ,	0
452	The critical role of Asp206 stabilizing residues on the catalytic mechanism of the Ideonella sakaiensis PETase.	О
451	Density Functional Theory Study on the Mechanism of Organophosphine-Catalyzed [4+2] Cycloaddition Reaction. <b>2022</b> , 42, 830	O
450	Synthesis of an advanced metal-guided photochromic system for molecular keypad lock: detailed experimental findings and theoretical understanding.	O
449	How Ionization Catalyzes Diels-Alder Reactions 2022,	0
448	Selectivity: An Electron Density Perspective. <b>2022</b> , 187-208	
447	From Molecules with a Planar Tetracoordinate Carbon to an Astronomically Known CH Carbene <b>2022</b> ,	O
446	Computational study on the mechanism of metal-free photochemical borylation of aryl halides.	O
445	On the Mechanisms of Chemical Reactions. <b>2022</b> , 463-479	0
444	Reaction Electronic Flux. <b>2022</b> , 229-244	

443	Study of the Addition Mechanism of 1-Indazole and Its 4-, 5-, 6-, and 7-Nitro Derivatives to Formaldehyde in Aqueous Hydrochloric Acid Solutions <b>2022</b> ,	О
442	Rhodium-based bidentate phosphorus ligand catalyst for direct synthesis of ethylene glycol. <b>2022</b> , 524, 112288	
441	Theoretical investigation on the mechanism and kinetics of the OH-initiated atmospheric degradation of p-chloroaniline via OH-addition and hydrogen abstraction pathways <b>2022</b> , 114, 108198	
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431	Theoretical Study on Reaction Mechanisms of Dinitrogen Activation and Coupling by Carbene-Stabilized Borylenes in Comparison with Intramolecular C-H Bond Activation <b>2022</b> ,	0
430	Cytotoxicity of Alizarine versus Tetrabromocathecol Cyclometalated Pt(II) Theranostic Agents: A Combined Experimental and Computational Investigation <b>2022</b> ,	O
429	DFT Study on the Biosynthesis of Asperterpenol and Preasperterpenoid Sesterterpenoids: Exclusion of Secondary Carbocation Intermediates and Origin of Structural Diversification <b>2022</b> ,	1
428	Potential Catalytic Role of Small Heterocycles in Interstellar H Formation: A Laboratory Astrochemistry Study on Furan and Its Hydrogenated Forms <b>2022</b> ,	2
427	Computational Evidence for Tunneling and a in the Biosynthesis of Tetrahydrocannabinol 2022,	1
426	Combustion Kinetics of N-Propylamine: Theoretical Calculations and Ignition Delay Time Measurements.	

425	Investigating the competing E2 and S2 mechanisms for the microsolvated HO(HO) + CHCHX ( $X = Cl$ , Br, I) reactions <b>2022</b> ,	1
424	Theoretical Study on Asymmetric Ketone Hydrogenation Catalyzed by Mn Complexes: From the Catalytic Mechanism to the Catalyst Design.	Ο
423	Structural Estimation and Hazard Evaluation of Potentially Explosive Residual Silanes Generated in Semiconductor Manufacturing Processes.	
422	Antioxidant activity of eugenol and its acetyl and nitroderivatives: the role of quinone intermediates-a DFT approach of DPPH test <b>2022</b> , 28, 133	O
421	Investigation of water substitution at Ru complexes by conceptual density function theory approach <b>2022</b> ,	0
420	Anticancer Agents Derived from Cyclic Thiosulfonates: Structure-Reactivity and Structure-Activity Relationships <b>2022</b> ,	
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418	Revisiting Nickel-Catalyzed Carbonylations: (Unexpected) Observation of Substrate-Dependent Mechanistic Differences.	
417	Water coordinated on Cu(I)-based catalysts is the oxygen source in CO reduction to CO <b>2022</b> , 13, 2577	
416	Kinetic and Mechanistic Investigations of OH-Initiated Atmospheric Degradation of Methyl Butyl Ketone <b>2022</b> ,	O
415	Transmembrane Protease Serine 2 Proteolytic Cleavage of the SARS-CoV-2 Spike Protein: A Mechanistic Quantum Mechanics/Molecular Mechanics Study to Inspire the Design of New Drugs To Fight the COVID-19 Pandemic <b>2022</b> ,	1
414	Dynamic Metal-Iodide Bonds in a Tetracoordinated Cadmium-Based Metal-Organic Framework Boosting Efficient CO Cycloaddition under Solvent- and Cocatalyst-Free Conditions <b>2022</b> ,	1
413	A Computational Study on the Photochemical O-H Functionalization of Alcohols with Diazoacetates <b>2022</b> , 87, 6832-6837	2
412	Unveiling the mechanism of the triethyl phosphate hydrolysis reaction in the synthesis of the sol-gel-derived 58S bioactive glass. <b>2022</b> , 24, 100929	
411	DFT studies on the mechanisms of nickel-catalyzed reductive-coupling cyanation of aryl bromide. <b>2022</b> , 970-971, 122368	0
410	Bridging heterogeneous and homogeneous catalysts by ultrathin metal-polyphthalocyanine-based nanosheets from electron-coupled transalkylation delamination. <b>2022</b> , 98, 107297	O
409	Photochemical degradation pathways of cell-free antibiotic resistance genes in water under simulated sunlight irradiation: Experimental and quantum chemical studies <b>2022</b> , 302, 134879	
408	Design and self-catalytic mechanism of aluminum precursors bearing amino ligands for Al2S3 atomic layer deposition. <b>2022</b> , 595, 153516	O

407	Automated reaction mechanisms and kinetics with the nudged elastic band method-based AMK_Mountain and its description of the preliminary alkaline hydrolysis of nitrocellulose monomer <b>2022</b> ,	1
406	UNRAVELLING THE MECHANISM OF COBALT (II) CATALYZED O-ARYLATION REACTION BETWEEN ARYL HALIDES AND PHENOLS: A DFT STUDY. <b>2022</b> , 122385	O
405	Kinetics and Mechanism of the Barton-Kellogg Oleflation: A Computational DFT Study Using CTST Theory and Topological Approaches.	
404	Stabilization of Energetic Compounds into the Nanoscale Carbon Materials: Insights from Computational Simulations. <b>2022</b> , 53-68	
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402	A Deeper Analysis of the Role of Synchronicity on the Bell-Evans-Polanyi Plot in Multibond Chemical Reactions: A Path-Dependent Reaction Force Constant.	2
401	Computational Mechanism Investigation of Bismuth(BiIII/BiV) Redox-catalyzed Fluorination of Arylboronic Esters.	O
400	Plasma-promoted reactions of the heterobimetallic anions CuNb®with dinitrogen and subsequent reactions with carbon dioxide: formation of CN bonds.	1
399	Glossary of terms used in physical organic chemistry (IUPAC Recommendations 2021). <b>2022</b> , 94, 353-534	4
398	Effect of Water Molecule on the Complete Series Reactions of Chlorothiobenzenes with H/•OH: A Theoretical Study. <b>2022</b> , 13, 849	
397	Copper Nanoclusters for Catalytic Carbon <b>©</b> arbon and Carbon <b>N</b> itrogen Bond Formations.	O
396	Dearomative Cycloaddition of an Isolable Dialkylsilylene with Diaryl Ketones.	O
395	Activated carbon supported nitrogen-containing diheterocycle mercury-free catalyst for acetylene hydrochlorination. <b>2022</b> , 525, 112366	O
394	Computational insights into hydroboration with acyclic <code>\B-Borylamido-germylene</code> and stannylene catalysts: Cooperative dual catalysis the key to system efficiency. <b>2022</b> , 222, 115907	
393	Theoretical investigation on degradation of DEET by <b>DH</b> in aqueous solution: Mechanism, kinetics, process optimization and toxicity evaluation. <b>2022</b> , 362, 132260	O
392	Theoretical Study on the Mechanism of the Carbonylation Cyclization of 1,5-Diynes with Hydrosilanes.	
391	Modelling the Radical Chemistry on Ice Surfaces: An Integrated Quantum Chemical and Experimental Approach. <b>2022</b> , 9,	
390	Theoretical Study of N⊞ ⊞ond Activation by Nickel(0) Complex: Reaction Mechanism, Electronic Processes, and Prediction of Better Ligand.	O

389	Studies on Synthesis of Sub-Nanometre Size Pt Particles Stabilized on ZrO 2 Matrix for Formic Acid Mediated Synthesis of Evalerolactone. <b>2022</b> , 7,	O
388	The Homogeneous Gas-Phase Formation Mechanism of PCNs from Cross-Condensation of Phenoxy Radical with 2-CPR and 3-CPR: A Theoretical Mechanistic and Kinetic Study. <b>2022</b> , 23, 5866	
387	Hidden[Nanoscale Catalysis in Alkyne Hydrogenation with Well-Defined Molecular Pd/NHC Complexes. 6980-6996	1
386	Does an Enol Pathway Preclude High Stereoselectivity in Iron-Catalyzed Indole CH Functionalization via Carbene Insertion?.	2
385	CO Oxidation over HKUST-1 Catalysts: The Role of Defective Sites.	
384	Mechanisms of complete dissociation of CO2 on iron clusters.	
383	Predicting Dinitrogen Activation by Carborane-Based Frustrated Lewis Pairs.	O
382	Unraveling the reaction mechanism on pyrolysis of 1,3,5-trinitro-1,3,5-triazinane (RDX). <b>2022</b> , 242, 112220	O
381	Reaction between propionaldehyde and hydroxyperoxy radical in the atmosphere: A reaction route for the sink of propionaldehyde and the formation of formic acid. <b>2022</b> , 284, 119202	O
380	A DFT study of the active role of the phosphate group of an internal aldimine in a transamination reaction.	
379	Theoretical Study of The Role of the Non-innocent Phenolate Ligand of a Nickel Complex in Water Oxidation.	
378	Harvesting the fragment-based nature of bifunctional organocatalysts to enhance their activity.	O
377	Theoretical study on the mechanism, chemo- and enantioselectivity of the Ag- vs. Rh-catalyzed intramolecular carbene transfer reaction of diazoacetamides. <b>2022</b> , 12, 18197-18208	O
376	Quantum chemical study of the hydrolysis of oxidized endogenous psychedelic N,N-dimethyltryptamine. <b>2022</b> , 113789	
375	How Does Electronic Activity Drive Chemical Reactions? Insights from the Reaction Electronic Flux for the Conversion of Dopamine into Norepinephrine.	0
374	Generation and direct observation of a triplet arylnitrenium ion. <b>2022</b> , 13,	
373	Resonance and Electrostatics Making the Difference in Boron- and Aluminum-Halide Structures and Exchange Reactivity.	1
372	Palladium-Mediated CO2 Extrusion Followed by Insertion of Allenes: Translating Mechanistic Studies to Develop a One-Pot Method for the Synthesis of Alkenes.	O

 $_{\mbox{\it 371}}$   $\,$  Two routes to hydrogen evolution for a Co-polypyridyl complex with two open sites.

370	Palladium-Catalyzed Activation of CarbonHalogen Bonds: Electrostatics-Controlled Reactivity.	1
369	Dipolar 1,3-cycloaddition of thioformaldehyde S -methylide ( CH 2 SCH 2 ) to ethylene and acetylene. A comparison with (valence) isoelectronic O 3 , SO 2 , . <b>2022</b> , 43, 1420-1433	2
368	Rhodium-Catalyzed Ring Expansion Reactions for the Concise Construction of Densely Functionalized Oxathionines and Oxathiocines. 7524-7530	2
367	Phototransformations of 2,3-Diamino-2-Butenedinitrile (DAMN) Monomers Isolated in Low-Temperature Argon Matrix. <b>2022</b> , 2, 448-462	
366	Discovery of Redox-Promoted Br□fisted Acid Catalysis in the Gold(III)-Catalyzed Annulation of Phenol and Cyclohexadiene. 7918-7925	
365	Catalytic hydrophosphination of alkynes using structurally diverse sodium diphenylphosphide donor complexes. <b>2022</b> , 100942	1
364	Experimental and Computational Mechanistic Study of Carbonazidate-Initiated Cascade Reactions.	О
363	Reactivity of Unsupported Transition Metal-Aluminyl Complexes: A Nucleophilic TM-Al Bond.	1
362	Probability of reaction pathways of amine with epoxides in the reagent ratio of 1:1 and 1:2.	
361	Bonding in Nitrile Photo-dissociating Ruthenium Drug CandidatesA Local Vibrational Mode Study.	1
360	Comparative computational studies for nucleophilic aromatic substitution of dinitro-substituted benzannulated heterocycles with 1H-1,2,3-triazole.	
359	IrIII/NiII-Metallaphotoredox-Catalyzed Enantioselective Decarboxylative Arylation of ⊞-Amino Acids: Theoretical Insight of Enantio-Determining Outer-Sphere Reductive Elimination.	0
358	Reaction of Ta3IClusters with Molecular Nitrogen: A Mechanism Investigation.	
357	SN2 versus SN2? Competition.	1
356	Theoretical study of metal-free catalytic for catalyzing CO-oxidation with a synergistic effect on P and N co-doped graphene. <b>2022</b> , 12,	O
355	Revealing the regioselective N-acylation of 5-bromo-2-aminobenzimidazole using experiment and theoretical calculation. <b>2022</b> , 132905	0
354	Important Routes for Methanediol Formation by Formaldehyde Hydrolysis Catalyzed by Iodic Acid and for the Contribution to an Iodic Acid Sink by the Reaction of Formaldehyde with Iodic Acid Catalyzed by Atmospheric Water.	0

353	Calcium Bistriflimide-Mediated Sulfur(VI) Eluoride Exchange (SuFEx): Mechanistic Insights toward Instigating Catalysis.	
352	Theoretical Study of Mechanism and Product Selectivity of Metal-Catalyzed Reactions of Alkynyl Thioethers with Isoxazoles/Anthranils. <b>2022</b> , 528, 112432	
351	Combustion kinetics of n-propylamine: Theoretical calculations and ignition delay time measurements. <b>2022</b> , 324, 124710	
350	Dft Calculations Rationalize Regioselectivity and Chemodivergence in Nickel-Catalyzed Couplings of Aldehyde, Alkyne, and Dialkylsilane/Trialkylsilane.	
349	Organocatalytic Synthesis of Chiral Allene Catalyzed by Chiral Phosphoric Acid Via Asymmetric 1,8-Addition of Indole Imine Methide: Mechanism and Origin of Enantioselectivity.	
348	Toward Practical Quantum Embedding Simulation of Realistic Chemical Systems on Near-term Quantum Computers.	4
347	Mechanism of the Fe(iii)-catalyzed synthesis of hexahydropyrimidine with ⊞-phenylstyrene: a DFT study. <b>2022</b> , 12, 20523-20529	
346	Photolytic insertion of carbon monoxide into nitrosyl chloride: formation of nitrosoformyl chloride.	
345	Exploration of the photocatalytic cycle for sacrificial hydrogen evolution by conjugated polymers containing heteroatoms.	2
344	Understanding the Regioselectivity of Ion-Pair-Assisted Meta-Selective C(sp2)⊞ Activation in Conformationally Flexible Arylammonium Salts. <b>2022</b> , 87, 9222-9231	O
343	The influence of a single water molecule on the reaction of IO + HONO.	
342	Why Does an Inert C4日 Bond in Indolyl Aldehyde Get Activated Unexpectedly by a Rh(III) Catalyst over a More Reactive C2日 Bond while the Opposite Is True for Acetophenone? Guidelines for Inverting Regioselectivity. <b>2022</b> , 41, 1659-1674	
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340	Curtius-Type Rearrangement of Sulfinyl Azides: A Matrix Isolation and Computational Study. <b>2022</b> , 126, 4367-4375	
339	Hydroxycarbonylation of Alkenes with Formic Acid Catalyzed by a Rhodium(III) Hydride Diiodide Complex Bearing a Bidentate Phosphine Ligand. <b>2022</b> , 41, 1640-1648	
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336	High-Density Windowpane Coordination Patterns of Water Clusters and Their NBO/NRT Characterization. <b>2022</b> , 27, 4218	1

335	Not That DDT: A Databank of Dynamics Trajectories for Organic Reactions. <b>2022</b> , 99, 2721-2725	1
334	Gas- and liquid-phase ozonolysis of ethylene, butadiene, and perfluoro-olefins: solvation and the cage effect.	
333	Theoretical Perspectives on the Gas-Phase Oxidation Mechanism and Kinetics of Carbazole Initiated by OH Radical in the Atmosphere. <b>2022</b> , 13, 1129	
332	Underlying Mechanisms of Reductive Amination on Pd-Catalysts: The Unique Role of Hydroxyl Group in Generating Sterically Hindered Amine. <b>2022</b> , 23, 7621	1
331	Ligand backbone influence on the enantioselectivity in the ruthenium-catalyzed direct asymmetric reductive amination of ketones with NH3/H2 using binaphthyl-substituted phosphines.	
330	Synthesis and Mechanistic Investigation of Bipyrazolo[1,5-a]pyridines via Palladium-Catalyzed Cross-Dehydrogenative Coupling of Pyrazolo[1,5-a]pyridines.	1
329	Transformation of L-DOPA and Dopamine on the Surface of Gold Nanoparticles: An NMR and Computational Study. <b>2022</b> , 61, 10781-10791	
328	Rational Design of Synergistic Structure Between Single-Atoms and Nanoparticles for CO2 Hydrogenation to Formate Under Ambient Conditions. 10,	
327	Solvent promoted tautomerism in thione-containing tetraazatricyclics: evidence from 1H NMR spectroscopy and transition state studies. <b>2022</b> , 28,	O
326	Quantum chemical hydrogenolysis strategy for elimination of heteroatoms in biomass homologous organic compounds based on oxolane and thiolane. <b>2022</b> , 108268	
325	The influence of a single water molecule on the reaction of BrO + HONO. <b>2022</b> , 108261	
324	Decarboxylative Cyclization of Proline with o-Alkynylbenzaldehyde through an Unexploited 8EElectrocyclization: A DFT Study.	
323	Bismuth(III)-catalysed hydroalkylation of styrene with acetylacetone: a DFT-Based mechanistic study.	O
322	The reaction of hydropersulfides (RSSH) with S-nitrosothiols (RS-NO) and the biological/physiological implications. <b>2022</b> , 188, 459-467	O
321	Theoretical investigation on the formation mechanism of carbonate ion in microbial self-healing concrete: Combined QC calculation and MD simulation. <b>2022</b> , 342, 128000	O
320	A DFT study on the tautomerization of vitamin B3 (niacin). <b>2022</b> , 1214, 113800	O
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318	A potential source of tropospheric secondary organic aerosol precursors: The hydrolysis of N2O5 in water dimer and small clusters of sulfuric acid. <b>2022</b> , 287, 119245	

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316	Resolving the Reaction Mechanism for Oxidative Hydration of Ethylene toward Ethylene Glycol by Titanosilicate Catalysts. 9446-9457	O
315	A Ruthenium Protic N-Heterocyclic Carbene Complex as a Precatalyst for the Efficient Transfer Hydrogenation of Aryl Ketones.	1
314	Rational Tuning of the Reactivity of Three-Membered Heterocycle Ring-Openings via SN2 Reactions.	O
313	Portable Models for Entropy Effects on Kinetic Selectivity.	1
312	Theoretical Insights into Aluminum-Catalyzed Cyanosilylation of Aldehydes and Ketones.	1
311	Monomolecular mechanisms of isobutanol conversion to butenes catalyzed by acidic zeolites: alcohol isomerization as a key to the production of linear butenes. <b>2022</b> ,	О
310	Accurate rate constants for elementary reactions of molecular hydrogen and carbon monoxide mixtures and the role of the H2 rich environment. <b>2022</b> , 28,	
309	Automated Mechanism Discovery. <b>2022</b> ,	
308	DFT investigates the mechanisms of cross-dehydrogenative coupling between heterocycles and acetonitrile.	
307	Model Study on the Catalytic Cycle of Glutathione Peroxidase Utilizing Selenocysteine-Containing Tripeptides: Elucidation of the Protective Bypass Mechanism Involving Selenocysteine Selenenic Acids.	1
306	Theoretical study about the hydrogen abstraction reactions on methyl acetate on combustion conditions. <b>2022</b> , 28,	
305	On Neutral Unsaturated Ouroboric Borylenes. <b>2022</b> , 126, 5173-5185	O
304	Effects of Twisted Intramolecular Charge Transfer Behavior on Excited-State Intramolecular Proton Transfer Reactions of Methyl Benzoate Derivatives in Water Solution. <b>2022</b> , 126, 5126-5133	O
303	Theoretical Study of the Activation Reaction of a Zr+/P-Based Frustrated Lewis Pair with Carbon Dioxide. <b>2022</b> , 126, 5534-5544	1
302	An Interacting Quantum Atoms (IQA) and Relative Energy Gradient (REG) Analysis of the Anomeric Effect. <b>2022</b> , 27, 5003	
301	Theoretical Investigation of the Biogenetic Pathway for Formation of Antibacterial Indole Alkaloids from Voacanga africana.	2
300	Density Functional Theory Study on the Selective Reductive Amination of Aldehydes and Ketones over Their Reductions to Alcohols Using Sodium Triacetoxyborohydride.	1

299	Comprehensive theoretical study of nickel-NHC-catalyzed enantioselective intramolecular indole C?H cyclization: Reaction mechanism, reactivity, regioselectivity, and electronic processes.	
298	QM/MM Study of the Reaction Mechanism of Thermophilic Glucuronoyl Esterase for Biomass Treatment.	O
297	Mechanistic Insights about the Ligand-Enabled Oxy-arylation/vinylation of Alkenes via Au(I)/Au(III) Catalysis.	0
296	Mechanistic Investigation of Lysine-Targeted Covalent Inhibition of PI3K⊡ia ONIOM QM:QM Computations.	1
295	Understanding the Kinetics and Topological Events Within the Thione-to-Thiol Rearrangement of Xanthates. <b>2022</b> , 7,	
294	Plasma-Assisted Coupling Reactions of Dinitrogen and Carbon Dioxide Mediated by Monometallic YB1IIIAnions: CarbonNitrogen Bond Formation.	
293	Photochemical palladium-catalyzed methylation and alkylation reactions in cascade reactions of isonitriles. <b>2022</b> , 132939	Ο
292	Mechanistic aspects of the Pd(OAc) n ( $n=1B$ ) catalyzed ethylene acetoxylation: A density functional theory study.	
291	Various Approaches to Studying the Phase Transition in an Octamethylcyclotetrasiloxane Crystal: From X-ray Structural Analysis to Metadynamics. <b>2022</b> , 23, 9073	
290	In Situ/Operando Spectroscopic Studies on the NH3BCR Mechanism over FeDeolites. <b>2022</b> , 12, 9983-9993	3
289	New Carbenes and Cyclic Allenes Energetically Comparable to Experimentally Known 1-Azulenylcarbene.	
288	DFT calculations rationalize regioselectivity and chemodivergence in nickel-catalyzed couplings of aldehyde, alkyne, and dialkylsilane/trialkylsilane. <b>2022</b> , 530, 112618	Ο
287	Theoretical study on the hydrolytic deamination reaction mechanism of guanine and (H2O)n. <b>2022</b> , 99, 100645	Ο
286	Theoretical study on the mechanism of the carbonylation cyclization of 1,5-diynes with hydrosilanes. <b>2022</b> , 979, 122481	
285	Regioselective synthesis of spirooxindole-pyrolidine via (GAP) chemistry process: Experimental and DFT study. <b>2022</b> , 1270, 133891	
284	Kinetic and thermodynamic investigations on the HF elimination reactions from neutral and ionized CF3CH2F. <b>2022</b> , 28,	Ο
283	Structure elucidation and risk assessment of degradation products in gamma irradiated rubber closures. <b>2022</b> , 204, 110126	Ο
282	Effects of environmental factors on the fleroxacin photodegradation with the identification of reaction pathways. <b>2022</b> , 308, 136373	Ο

281	High-temperature decomposition chemistry of trimethylsiloxane surfactants, a potential Fluorine Tree replacement for fire suppression. <b>2022</b> , 308, 136351	O
280	Energetics and electronics of polar DielsAlder reactions at the atomic level: QTAIM and IQA analyses of complete IRC paths. <b>2023</b> , 118, 108326	1
279	Mechanistic study of the bismuth mediated fluorination of arylboronic esters and further rational design. <b>2022</b> , 12, 24208-24216	0
278	Influence of N- and P-substituents in N-aryl-phosphinoglycine ligands on the selectivity of Ni-catalysed ethylene oligomerization. <b>2022</b> , 46, 17303-17312	O
277	The role of halogen bonds in the catalytic mechanism of the iso-Nazarov cyclization reaction: a DFT study. <b>2022</b> , 24, 18877-18887	O
276	The annulation of N-hydroxyoximes and 1,3-diyne to synthesize alkynylated isoquinolines regioselectively catalyzed by ruthenium: a theoretical study. <b>2022</b> , 20, 7294-7301	O
275	Hydroboration of carbon dioxide with pinacolborane catalyzed by various aluminum hydrides: a comparative mechanistic study.	O
274	Solvent dependent hindered rotation versus epimerization in axially chiral thiohydantoin derivatives: an experimental and a computational study. <b>2022</b> , 20, 7622-7631	O
273	Mechanistic differences between aryl iodide electrophiles and pronucleophiles in Pd-catalyzed coupling with cyclopropenes: a DFT study. <b>2022</b> , 9, 5237-5245	O
272	Unveiling the origin of the chemoselectivity of bismacycle-mediated CH arylation of phenols: from mechanism concept to new coupling design. <b>2022</b> , 9, 4890-4901	O
271	Mechanistic insight into Cp*Rh(iii)-catalyzed Lossen rearrangement vs CN reductive elimination for the synthesis of pyridones. <b>2022</b> , 46, 16485-16494	O
270	Density functional theory explorations of parathion and paraoxon hydrolysis as a function of the underlying alkaline environment.	O
269	Photochemistry of phosphenic chloride (ClPO2): isomerization with chlorine metaphosphite (ClOPO) and reduction by carbon monoxide. <b>2022</b> , 24, 20828-20836	O
268	Reaction mechanism conversion induced by the contest of nucleophile and leaving group.	O
267	Harnessing deep reinforcement learning to construct time-dependent optimal fields for quantum control dynamics.	O
266	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
265	A neural network potential energy surface and quantum dynamics studies for the Ca+(2S) + H2 -> CaH+ + H reaction. <b>2022</b> , 24, 19209-19217	1
264	Study on heterogeneous OH oxidation of 3-methyltetraol sulfate in the atmosphere under high NO conditions. <b>2022</b> , 12, 21103-21109	O

263	Theoretical investigations on the excited-state intramolecular proton transfer in the solvated 2-hydroxy-1-naphthaldehyde carbohydrazone. <b>2022</b> , 20, 785-792	0
262	Insights into gold-catalyzed formation of aza-heterocycles using benzofuroxans as nitrene transfer reagents: mechanism and origins of chemoselectivity. <b>2022</b> , 12, 27483-27491	O
261	Implicit and explicit solvent models have opposite effects on radiation damage rate constant for thymine. <b>2022</b> , 245-265	0
260	Cation binding of Li(i), Na(i) and Zn(ii) to cobalt and iron sulphide clusters lelectronic structure study. <b>2022</b> , 24, 20228-20238	Ο
259	Alkyne⊞lkenyl coupling at a diruthenium complex.	2
258	Efficient photohydrogen production by edge-modified carbon nitride with nonmetallic group. <b>2023</b> , 629, 739-749	O
257	Theoretical insights into the degradation mechanisms, kinetics and eco-toxicity of oxcarbazepine initiated by OH radicals in aqueous environments. <b>2022</b> ,	О
256	Solution-Phase Conformational/Vibrational Anharmonicity in Comonomer Incorporation Polyolefin Catalysis. <b>2022</b> , 126, 6858-6869	Ο
255	Hydride Relay Exchange Mechanism for the Heterocyclic CH Arylation of Benzofuran and Benzothiophene Catalyzed by Pd Complexes. <b>2022</b> , 87, 12997-13010	О
254	A multiscale ONIOM study of the buckminsterfullerene (C60) DielsAlder reaction: from model design to reaction path analysis. <b>2022</b> , 28,	Ο
253	Mechanism of Coupling of Methylidene to Ethylene Ligands in Dimetallic Assemblies; Computational Investigation of a Model for a Key Step in Catalytic C1 Chemistry.	0
252	Metal-Free Phosphination and Continued Functionalization of Pyridine: A Theoretical Study. <b>2022</b> , 27, 5694	1
251	Unveiling the Origin of the Selectivity and the Molecular Mechanism in the [3+2] Cycloaddition Reaction of N-aryl-C-carbamoylnitrone with N-arylitaconimide. <b>2022</b> , 3, 281-292	0
250	Al-Decorated C2N Monolayer as a Potential Catalyst for NO Reduction with CO Molecules: A DFT Investigation. <b>2022</b> , 27, 5790	2
249	The performance of exchangellorrelation functionals in describing electron density parameters of saddle point structures along chemical reactions. <b>2022</b> , 43, 1830-1838	0
248	Coulomb Explosion Dynamics of Multiply Charged para-Nitrotoluene Cations. <b>2022</b> , 126, 6617-6627	O
247	Tropylium-BF 4 as Organocatalyst for Efficient Synthesis of Nitriles from Aldoximes; Synthetic Scope and Mechanistic Insights. <b>2022</b> , 7,	О
246	Insights into ⊞-Alkynylation and ⊞-Allenylation of Aldehydes under the Synergisitic Catalysis of Gold/Amine: A DFT Study. <b>2022</b> , 87, 13102-13110	O

245	Revisiting the formation mechanism of diarylamines via Smiles rearrangement.	O
244	Solvent Effects in the Regioselective N-Functionalization of Tautomerizable Heterocycles Catalyzed by Methyl Trifluoromethanesulfonate: A Density Functional Theory Study with Implicit Solvent Model. <b>2022</b> , 10, 172	0
243	Promoting Catalytic Activity of Boron by Phosphor in Propane Oxidative Dehydrogenation. <b>2022</b> , 126, 16672-16681	1
242	Discovery of Periodinane Oxy-Assisted (POA) Oxidation Mechanism in the IBX-Controlled Oxidative Dearomatization of Pyrroles Mediated by Acetic Acid. <b>2022</b> , 87, 13280-13287	O
241	Unusual In-plane Aromaticity Facilitates Intramolecular Hydrogen Transfer in Long-Bonded cis-Isonitrosyl Methoxide. <b>2022</b> , 126, 6826-6833	O
240	A computational mapping of the RNHC coupling pathway I the key process in the evolution of Pd/NHC catalytic systems. <b>2022</b> , 32, 571-575	O
239	Mechanism and the Origins of Periselectivity in Cycloaddition Reactions of Benzyne with Dienes. <b>2022</b> , 87, 12954-12962	O
238	Autocatalytic reaction cycles for non-enzymatic synthesis of life-sustaining sugars in neutral media.	O
237	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	0
236	Computational Mechanism Investigation of C=C Bonds Hydrogenation Catalyzed by Rhodium Hydride.	O
235	Sooting tendencies of terpenes and hydrogenated terpenes as sustainable transportation biofuels. <b>2022</b> ,	1
234	Response of Elementary Structural Transitions in Glassy Atactic Polystyrene to Temperature and Deformation. <b>2022</b> , 126, 7731-7744	O
233	Enantioselective Organocatalyzed Functionalization of Tetramic and Tetronic Acids.	1
232	Effects of N-substitution on CO2 trapping by cyclic vinylidenes at DFT levels.	O
231	Versatile Reactivity of Half-Sandwich Rhodium(III) Iminophosphonamide Complexes.	O
230	Revisiting the burden borne by fumarase: enzymatic hydration of an olefin.	O
229	Physiker versus Organiker Views of Reaction Mechanism How Natural Resonance Theory Bridges the Gap.	О
228	Computation-Guided Total Synthesis of Vitisinol G. <b>2022</b> , 70, 735-739	O

227	DFT study of regio- and stereo-selective 13DC reaction between diazopropane and substituted chalcone derivatives: Molecular docking of novel pyrazole derivatives as Anti-Alzheimer Agents.	O
226	Molecular-based asphalt oxidation reaction mechanism and aging resistance optimization strategies based on quantum chemistry. <b>2022</b> , 111225	1
225	Mechanistic Study on Palladium-Catalyzed Cycloaddition of Vinylethylene Carbonates with $\square$ , $\square$ unsaturated Imines.	1
224	Ab Initio Characterization of the Potential Energy Profiles for the Multi-Channel Reactions: H/Cl + CH3OH. <b>2022</b> , 113906	O
223	Unusual pathway of epoxide hydration over a novel CoIII(salen)-based pseudohomogeneous catalyst with excellent performance. <b>2022</b> , 414, 365-373	0
222	Promoting productive metathesis pathway and tuning activity of multidentate molybdenum catalysts in alkyne metathesis: A theoretical perspective. <b>2022</b> , 531, 112696	0
221	Deciphering the cooperative effect of base and N-substituents on the origin of enantioselectivity switching for Mannich reactions of glycinate by carbonyl catalysts. <b>2022</b> , 415, 1-11	0
220	One-pot synthesis of 5-hydroxymethylfurfural from cellobiose and sucrose using niobium-modified montmorillonite catalysts. <b>2022</b> , 532, 112720	0
219	New understanding of aconitine hydrolysis pathway: Isolation, identification and toxicity evaluation based on intermediate products. <b>2022</b> , 15, 104255	0
218	Investigations on photochemical behavior of antidepressant sertraline in water by DFT/TDDFT. <b>2022</b> , 10, 108657	0
217	Mechanistic insight highlights the key-steps and significance of metal in Ir(III)- catalyzed C-H activated chromones generation.	0
216	Curcumin-based ionic Pt(ii) complexes: antioxidant and antimicrobial activity.	1
215	Chemical Reaction Kinetics and Dynamics Re-Considered: Exploring Quantum Stereodynamics From Line to Plane Reaction Pathways and Concerted Interactions. <b>2022</b> , 67-156	0
214	A theoretical study on aza-Michael additions. <b>2022</b> , 141,	1
213	Silylium ion migration dominated hydroamidation of siloxy-alkynes. <b>2022</b> , 5,	0
212	New Reactions for the Formation of Organic Nitrate in the Atmosphere.	O
211	Dissociation reactions of hydrogen molecules at active sites on gold clusters: A DFT study.	1
<b>21</b> 0	Mechanistic Insights into Cobalt-Catalyzed Regioselective C4-Alkenylation of 3-Acetylindole: A Detailed Theoretical Study.	Ο

209	Experimental and Theoretical Evidence for Relativistic Catalytic Activity in CH Activation of N-Phenylbenzamide Using a Cationic Iridium Complex. <b>2022</b> , 126, 7627-7638	1
208	Theoretical study of the mechanism and kinetics of the atmospheric reaction of acrylic acid with NO 3 radical.	O
207	DFT Study on the Adsorption of Monomeric Hydroxyl Aluminum on Fe(II)/Mg Replacement Kaolinite (001) Surfaces.	0
206	Influence of Metal Coordination on the Gas-Phase Chemistry of the Positional Isomers of Fluorobenzoate Complexes. <b>2022</b> , 33, 2181-2190	2
205	(-´)-Polysiphenol and Other Analogues via Symmetrical Intermolecular Dimerizations: A Synthetic, Spectroscopic, Structural, and Computational Study.	0
204	Reaction Mechanism of CO2 with Choline-Amino Acid Ionic Liquids: A Computational Study. <b>2022</b> , 24, 1572	O
203	Origins of Stereospecificity and Divergent Reactivity of Pd-Catalyzed Cross Coupling with $\oplus$ , $\oplus$ -Disubstituted Alkenyl Hydrazones.	0
202	Kinetics of the R´+´O2´-> ̂R⊞O´+´OH reactions of substituted methyl radicals: Effects of Cl, F, and CF3 substitution and notes on the RO´+´O producing channel. <b>2022</b> , 808, 140121	O
201	Degradation of UV-P mediated by hydroxyl radical, sulfate radical and singlet oxygen in aquatic solution: DFT and experimental studies. <b>2022</b> , 315, 120416	0
200	DFT Insights into the mechanism of Ru(II) Catalyzed C7-selective amidation of N-pivaloylindole. <b>2022</b> , 982, 122534	O
199	OH-initiated degradation of 1,2,3-trimethylbenzene in the atmosphere and wastewater: Mechanisms, kinetics, and ecotoxicity. <b>2023</b> , 857, 159534	0
198	The multiple roles of phenols in the degradation of aniline contaminants by sulfate radicals: A combined study of DFT calculations and experiments. <b>2023</b> , 443, 130216	O
197	DFT Computational Insight into Pd(0)-Catalyzed Oxidative Cross-Couplings of 1,2-Allenyl Ketones and Aryl Boronic Acid: Pd(II)-Carbenoid Intermediate versus ?-Allyl-Pd(II) Intermediate.	0
196	Insights into Mechanism and Selectivity in Rh(I)-catalyzed Cycloisomerization Reaction of Benzylallene-Alkynes involving Cℍ Bond Activation.	O
195	Hidden Intermediate Activation: A Concept to Elucidate the Reaction Mechanism of the Schmittel Cyclization of Enyne-Allenes.	0
194	Unveiling the role of indium and tin in Alta based alloys for on-demand hydrogen supply from simulation to validation. <b>2023</b> , 554, 232268	O
193	Multiscale investigation for CO2 capture using membrane with AEEA: Significance of fluid flow and AEEA content to CO2 permeance. <b>2023</b> , 201, 123564	O
192	Reactions of dimedone and alkyl orthoformates with and without activators. <b>2022</b> , 71, 2241-2254	O

191	Computational Study of the Gas-Phase Thermal Degradation of Perfluoroalkyl Carboxylic Acids.	O
190	Group 6 (Cr, Mo, W) and Group 7 (Mn, Re) bipyridyl tetracarbonyl complex for electrochemical CO2 conversion: DFT and DLPNO-CCSD(T) study for effects of the central metal on redox potential, thermodynamics, and kinetics. <b>2022</b> , 111758	Ο
189	Glycoside Hydrolase Catalysis: Do Substrates and Mechanism-Based Covalent Inhibitors React via Matching Transition States?. 14667-14678	Ο
188	Curvature-weighted nudged elastic band method using the Riemann curvature.	О
187	Polyaromatic hydrocarbons with an imperfect aromatic system as catalysts of interstellar H2 formation.	О
186	An experimental and theoretical study on the effects of amine chain length on CO 2 absorption performance.	Ο
185	C(spn)☑ (n = 1日) Bond Activation by Iron.	0
184	Predicting Small Molecule Activation including Catalytic Hydrogenation of Dinitrogen Promoted by a Dual Lewis Acid.	1
183	Theoretical study on Rh(III)-Catalyzed reaction of allenylsilanes with N-methoxybenzamides. <b>2022</b> , 122557	Ο
182	Theoretical Insight into the Multiple Roles of LiHMDS in Pd-Catalyzed Borylation of Fluorobenzene.	О
181	Photocatalytic Selective Oxidation of Toluene into Benzaldehyde on Mixed-Valence Vanadium Oxide V6O13 Catalyst with Density Functional Theory.	0
180	Oligomer formation from the gas-phase reactions of Criegee intermediates with hydroperoxide esters: mechanism and kinetics. <b>2022</b> , 22, 14529-14546	1
179	Probing a General Strategy to Break the C-C Bond of Benzene by a Cyclic (Alkyl)(Amino)Aluminyl Anion.	O
178	Kinetic and Mechanistic Study of the Reactions of NO3 Radicals with Unsaturated Aldehydes: 2-Butenal, 2-Methyl-2-butenal, and 3-Methyl-2-butenal.	1
177	Different reaction mechanisms of SO4D bh with organic compound interpreted at molecular orbital level in Co(II)/peroxymonosulfate catalytic activation system. <b>2022</b> , 119392	О
176	Catalytic Mechanisms of Transfer Hydrogenation of Azobenzene with Ammonia Borane by Pincer Bismuth Complex: Crucial Role of C=N Functional Group on the Pincer Ligand.	O
175	Hydrolysis and aminolysis of aldehydes catalyzed by water and amines: Formation of diols/aminol and the implication to atmospheric particle formation. <b>2023</b> , 294, 119462	О
174	DFT mechanistic study on nickel/ IPr-catalyzed aldehydellkyne reductive couplings with trialkylsilane/dialkylsilane.	O

173	A DFT study on the reaction pathway involved in the metal ion-templated synthesis of benzo-21-crown-7(B21C7) from catechol and hexaethylene glycol ditosylate in presence of base.	О
172	Why does the synthesis of N-phenylbenzamide from benzenesulfinate and phenylisocyanate via the palladium-mediated Extrusion[hsertion pathway not work? A mechanistic exploration. 2022,	О
171	Polymeric tungsten carbide nanoclusters as potential non-noble metal catalysts for CO oxidation. <b>2022</b> , 14, 18231-18240	1
170	Palladium-catalyzed generation of CO from formic acid for alkoxycarbonylation of internal alkenes exploits a PTSA-assisted NH-Pd mechanism: a DFT mechanistic study.	O
169	A theoretical study of the ligand-controlled palladium-catalysed regiodivergent synthesis of dibenzosilepin derivatives.	О
168	Mechano-catalysis boosts glycolaldehyde conversion to tetroses over a new Zn-COF catalyst.	O
167	Cu(i)-catalysed asymmetric intramolecular tandem oxaziridination/rearrangement reaction: theoretical insight into the mechanism, enantioselectivity, ligand effect, and comparison with the corresponding Lewis-acid-promoted reaction.	O
166	Degradation of mevinphos and monocrotophos by OH radicals in the environment: A computational investigation on mechanism, kinetic, and ecotoxicity. <b>2023</b> , 445, 130478	О
165	A DFT Study on the Endo-selectivity Mechanism of Diels-Alder Reaction in Lindenane Dimeric Sesquiterpenes Synthesis Promoted by Pyridines.	О
164	Hydrogermylation initiated by trialkylborohydrides: a living anionic mechanism. <b>2022</b> , 58, 13979-13982	1
163	The metal dependence of single-metal mediated phosphodiester bond cleavage: a QM/MM study of a multifaceted human enzyme. <b>2022</b> , 24, 29130-29140	О
162	Direct Synthesis of Lactide from Lactic Acid by Sn-beta Zeolite: Crucial Role of the Open Sn Site. <b>2022</b> , 61, 17457-17466	O
161	Theoretical study on atmospheric gaseous reactions of glyoxal with sulfuric acid and ammonia. <b>2022</b> , 113950	О
160	Mechanism of Photocatalytic CO2 Reduction by Iron Spin-Crossover Complex with Copper Photosensitizer. <b>2022</b> , 41, 3568-3580	O
159	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	O
158	How Does Spin Play with the Cycloaddition to Paramagnetic Endohedral Metallofullerenes? The Curious Case of TiSc2N@C80. <b>2022</b> , 61, 19183-19192	O
157	DielsAlder Reactivity of Allenylboronic Acid Pinacol Ester and Related Dienophiles: Mechanistic Studies and Distortion/Interaction-Activation Strain Model Analysis. <b>2022</b> , 87, 16776-16784	О
156	A de novo Stereocontrolled Synthetic Approach to a Functionalized Indolizidine Core.	O

155	Concertedness and Activation Energy Control by Distal Methyl Group during Ring Contraction/Expansion in Scalarane-type Sesterterpenoid Biosynthesis.	O
154	Ambimodal Bispericyclic [6 + 4]/[4 + 6] Transition State Competes with Diradical Pathways in the Cycloheptatriene Dimerization: Dynamics and Experimental Characterization of Thermal Dimers. <b>2022</b> , 144, 22251-22261	O
153	A Mechanistic Study of Asymmetric Transfer Hydrogenation of Imines on a Chiral Phosphoric Acid Derived Indium Metal-Organic Framework. <b>2022</b> , 27, 8244	О
152	Effect of N-Vinylpyrrolidone on Decomposition of Benzoyl Peroxide. <b>2022</b> , 92, 2203-2213	O
151	Hydrolysis of SO3 in Small Clusters of Sulfuric Acid: Mechanistic and Kinetic Study. <b>2022</b> , 6, 3078-3089	O
150	Prediction of High-Yielding Single-Step or Cascade Pericyclic Reactions for the Synthesis of Complex Synthetic Targets. <b>2022</b> , 144, 22985-23000	O
149	Mechanistic Insights into the Metal-Free Deoxygenative Borylation of Ketones and Aldehydes with Bis(Catecholato)Diborane.	0
148	Hydrogen Activation by Frustrated and Not So Frustrated Lewis Pairs Based on Pyramidal Lewis Acid 9-Boratriptycene: A Computational Study. <b>2022</b> , 7, 48493-48505	O
147	A Density Functional Theory Study on the Cobalt-Mediated Intramolecular Pausonkhand Reaction of Enynes Containing a Vinyl Fluoride Moiety.	0
146	Comparison of ribavirin degradation in the UV/H2O2 and UV/PDS systems: Reaction mechanism, operational parameter and toxicity evaluation. <b>2022</b> , 109193	O
145	Mechanism and Origins of Diastereo- and Regioselectivities of Palladium-Catalyzed Remote Diborylative Cyclization of Dienes via Chain-Walking Strategy.	O
144	A workflow for automatic generation and efficient refinement of individual pressure-dependent networks. <b>2022</b> , 112516	1
143	Benzo[1,4]diazocinone/Pyrrole Ensembles via the Catalyst-Free Insertion of Pyrrolylacetylenic Ketones into Benzimidazoles. <b>2022</b> , 7,	0
142	Unveiling the Mechanisms of Hydrolytic Ring-Opening Polymerization of Caprolactam and Amino-Assisted Ring Opening of Cyclic Dimers: A DFT Study.	O
141	Glycolaldehyde Formation Mediated by Interstellar Amorphous Ice: A Computational Study.	O
140	Steric and Electronic Analyses of Ligand Effects on the Stability of EMethane Coordination Complexes: A DFT Study. <b>2022</b> , 41, 3834-3844	O
139	Understanding the Reaction Mechanism of Nickel-Catalyzed Enantioselective Arylative Activation of the Aromatic CD Bond.	0
138	Computational Studies on the Reactivity of Polycyclic Aromatic Hydrocarbons.	O

137	URVA and Local Mode Analysis of an Iridium Pincer Complex Efficiently Catalyzing the Hydrogenation of Carbon Dioxide. <b>2022</b> , 10, 234	0
136	Visible Light-Induced Coupling Cyclization Reaction of ∃-Diazosulfonium Triflates with ∃-Oxocarboxylic Acids or Alkynes. <b>2022</b> , 87, 16604-16616	Ο
135	Exploration of the mechanism of the condensation reaction of Al(OH)4 $\Omega$ with a D-gluconate using density functional theory.	0
134	Mechanistic Study of Diketopiperazine Formation during Solid-Phase Peptide Synthesis of Tirzepatide. <b>2022</b> , 7, 46809-46824	O
133	Theoretical Study of the Atmospheric Chemistry of Methane Sulfonamide Initiated by OH Radicals and the CH3S(O)2N⊞ + 3O2 Reaction. <b>2022</b> , 126, 9447-9460	0
132	Computational Study of Iron-Catalyzed Intramolecular [2 + 2] Cycloaddition and Cycloisomerization of Enyne Acetates: Mechanism and Selectivity.	Ο
131	Understanding the Organometallic Step: SO 2 Insertion into Bi(III) (Ph) Bond.	0
130	Role of Chiral Skeleton in Chiral Phosphoric Acids Catalyzed Asymmetric Transfer Hydrogenation: A DFT Study. <b>2023</b> , 13, 98	Ο
129	Uncovering the Most Kinetically Influential Reaction Pathway Driving the Generation of HCN from Oxyma/DIC Adduct: A Theoretical Study. <b>2023</b> , 62, 874-880	0
128	How Does Multiple Substrate Binding Lead to Substrate Inhibition of CYP2D6 Metabolizing Dextromethorphan? A Theoretical Study.	Ο
127	Mechanistic insights into the challenges of organocatalytic Beckmann rearrangement reactions.	Ο
126	Revisiting the Burden Borne by Fumarase: Enzymatic Hydration of an Olefin. <b>2023</b> , 62, 476-493	Ο
125	Screening Carbon-Boron Frustrated Lewis Pairs for Small-Molecule Activation including N2, O2, CO, CO2, CS2, H2O and CH4: A Computational Study.	Ο
124	Mechanistic Study of Nickel-Catalyzed Intramolecular [4+2] Cycloaddition of Cyclobutanone with Allene: Origin of Selectivity and Ligand Effect.	Ο
123	Theoretical Study of the Reaction Mechanism of Phenol <b>E</b> poxy Ring-Opening Reaction Using a Latent Hardening Accelerator and a Reactivity Evaluation by Substituents. <b>2023</b> , 28, 694	О
122	Computational Understanding of Dual Gold and Photoredox-Catalyzed Regioselective Thiosulfonylation of Alkenes.	Ο
121	Prediction of Kinetic Product Ratios: Investigation of a Dynamically Controlled Case. <b>2023</b> , 127, 224-239	0
120	Computational Insights into the Iron-Catalyzed Magnesium-Mediated Hydroformylation of Alkynes. <b>2023</b> , 122621	O

119	A theoretical and modeling study about the low-temperature reaction mechanism between diethoxymethane radicals and O2. <b>2023</b> , 249, 112616	О
118	Potential Energy Surfaces: the Forces of Chemistry. <b>2010</b> , 28-48	O
117	Stereodynamics: Orientation and Alignment in Chemistry. <b>2010</b> , 278-332	0
116	Reactive Scattering: Quantum State-Resolved Chemistry. <b>2010</b> , 214-239	O
115	Structural and bond evolutions during a chemical reaction. <b>2023</b> , 53-71	1
114	Pyrolysis of Methyl Formate and the Reaction of Methyl Formate with H Atoms: Shock Tube Experiments and Statistical Rate Theory. <b>2023</b> , 127, 1036-1045	O
113	Theoretical Understanding of Reactions of Rhenium and Ruthenium Tris(thiolate) Complexes with Unsaturated Hydrocarbons: Noninnocent Nature of the Ligand, Mechanism, and Origin of Differential Reactivity.	О
112	Comprehensive Theoretical Study of Cp*IrIII-Catalyzed Intermolecular Enantioselective Allylic CH Amidation: Reaction Mechanism, Electronic Processes, and Regioselectivity.	O
111	Potential of Single Transition Metal Atom Embedded C 2 N as Efficient Catalysts for N 2 O Reduction: Theoretical Investigation. 2200680	0
110	Insights into the Reactivity of the Ring-Opening Reaction of Tetrahydrofuran by Intramolecular Group-13/P- and Al/Group-15-Based Frustrated Lewis Pairs.	O
109	Electron-Coupled Proton Transfer Governed Magnetic Spin Couplings and Switching in Defect Nano Silicon Carbide. <b>2023</b> , 127, 2012-2024	О
108	An unexpectedly feasible route for the formation of organosulfates by the gas phase reaction of sulfuric acid with acetaldehyde catalyzed by dimethylamine in the atmosphere.	O
107	Chemical Modification of Dimethylpolysiloxane for Enhancement of CO2 Binding Enthalpy.	О
106	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	O
105	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	О
104	Symmetric Post-Transition State Bifurcation Reactions with Berry Pseudomagnetic Fields. <b>2023</b> , 14, 770-778	O
103	Tunneling Effect in Proton Transfer: Transfer Matrix Approach. <b>2023</b> , 127, 1046-1052	Ο
102	Toward Ab Initio Reaction Discovery Using the Artificial Force Induced Reaction Method. 2023, 74,	O

101	Dual-Ligand Strategy for the Preparation of Gas-Phase Uranyl(VI) Benzyne Complexes from Uranyl(VI) Benzoates. <b>2023</b> , 62, 2266-2272	Ο
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99	Quantum Mechanical Study of Oxygen Ligands Protonation for the Stable States of the Laccase Active Site. <b>2023</b> , 24, 2990	0
98	Macrocyclic chemosensors with anthraquinone signaling unit built into ionophore. Experimental and computational studies (part I) - synthesis and effect of proton binding on spectrophotometric and electrochemical properties. <b>2023</b> , 292, 122405	O
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96	DFT calculations reveal the origin of controllable synthesis of boronyl carbonyl compounds from Cu/Pd-cocatalyzed four-component borocarbonylation of vinylarenes. <b>2023</b> , 13, 2123-2133	O
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94	Silacyclopropenylsilylene-NHC Complex: Synthesis by (1+2) Retro-cycloaddition, Dynamic Behavior in Solution, and Ring-expansion Reaction. <b>2023</b> , 52, 124-127	O
93	Alternative Mechanism for O2 Formation in Natural Photosynthesis via Nucleophilic Oxo©xo Coupling.	0
92	Thermochemical and kinetics investigation of the CH2CN + CN system leading to NCCH2CN. <b>2023</b> , 815, 140371	O
91	Mechanism for dissociative hydrolysis of pyrimidine nucleoside d4N: Inversion vs retention. <b>2023</b> , 568, 111845	0
90	Cℍ Functionalization of Heterocycles with Triplet Carbenes by means of an Unexpected 1,2-Alkyl Radical Migration**.	O
89	Reaction pathways for palladium(I) reduction in laser-induced particle formation of Pd: An ab initio molecular orbital study. <b>2023</b> , 569, 111857	0
88	Experimental and theoretical study on ionic liquid [Bmim]Br-catalyzed decomposition of cumene hydroperoxide into dimethylbenzyl alcohol. <b>2023</b> , 656, 119116	O
87	Low-temperature NOx capture and reduction via NO oxidation by O3 on Cu-CHA. <b>2023</b> , 655, 119099	0
86	Reaction kinetics and implications of the decomposition and formation of C2H4O isomers. <b>2023</b> , 250, 112634	O
85	Remote substituent effects on catalytic activity of metal-organic frameworks: a linker orbital energy model. <b>2023</b> , 9,	0
84	Atmospheric degradation mechanism of anthracene initiated by OHEA DFT prediction. <b>2023</b> , 121, 108426	О

83	Complexation determines the removal of multiple tetracyclines by ferrate. 2023, 316, 123804	0
82	Pyrolytic elimination of ethylene from ethoxyquinolines and ethoxyisoquinolines: a computational study. <b>2023</b> , 13,	O
81	Enhanced Sampling for Free Energy Profiles with Post-Transition-State Bifurcations.	О
80	Ultrasound assisted synthesis of spirooxindole analogs catalyzed by Fe3O4@PPCA NPs: Experimental, theoretical and in vitro biological studies. <b>2023</b> , 1284, 135363	0
79	New insight into Cu-catalyzed borocarbonylative coupling reactions of alkenes with alkyl halides. <b>2023</b> , 418, 263-272	0
78	Improved syntheses of doubly naphthalene-bridged diphosphine and its diiminodiphosphorane derivatives linking two Cu(I) centers. <b>2023</b> , 233, 116306	O
77	Theoretical Investigation of Chemoselectivity between CH Insertion and Amide Insertion in Intramolecular Rhodium-Carbene Reactions. <b>2023</b> , 71, 107-110	0
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74	Decomposition mechanisms of nuclear-grade cationic exchange resin by advanced oxidation processes: Statistical molecular fragmentation model and DFT calculations. <b>2024</b> , 135, 433-448	Ο
73	Neutral Monodentate and Hypervalent Chalcogen Bond Catalysis on the Intramolecular Rauhut-Currier Reaction of Bis(enones): A DFT Study.	0
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71	Computational Evidence of the Incipient Oxocarbenium Ion as a Hidden IntermediateDuring the Cyclization of Hydroxyenol Ether into Spiroketal Under Mild Acidic Condition.	0
70	DFT mechanistic studies of boronBilicon exchange reactions between silyl-substituted arenes and boron bromides. <b>2023</b> , 25, 6714-6725	O
69	Theoretical Study on the Copper-Catalyzed ortho-Selective C-H Functionalization of Naphthols with ⊞-Phenyl-⊞-Diazoesters. <b>2023</b> , 28, 1767	0
68	Designing an Apparently Orbital-Symmetry-Forbidden [3s,5s]-Sigmatropic Shift through Transition-State Complexation and Stereoelectronic Effects. <b>2023</b> , 62,	O
67	Designing an Apparently Orbital-Symmetry-Forbidden [3s,5s]-Sigmatropic Shift through Transition-State Complexation and Stereoelectronic Effects. <b>2023</b> , 135,	0
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55	How Doping Affects the Activity of the Aluminum Oxide Support.	О
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50	The study on gas phase dehydrogenation reactions of transition metal cation and ethylene. <b>2023</b> , 121,	O
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48	Computational insight into gold(i)-catalyzed intramolecular regioselectivity of tryptamine-ynamide cycloisomerizations. <b>2023</b> , 21, 2610-2619	Ο

47	Computation Study on Copper-Catalyzed Aerobic Intramolecular Aminooxygenative C?C Bond Cleavage to Imides: Different Roles of Mononuclear and Dinuclear Copper Complexes. <b>2023</b> , 13, 3815-3829	О
46	Cobalt-catalyzed radical-mediated carbondarbon scission via a radical-type migratory insertion. <b>2023</b> , 14, 3352-3362	О
45	Activation of metal-involved halogen bonds and classical halogen bonds in gold(i) catalysis. <b>2023</b> , 52, 4517-4525	O
44	Influence of Group 15 elements on the $[3 + 2]$ cycloaddition reactivity of G15 = G15 $\Box$ 15-based 1,3-dipoles with cyclooctyne. <b>2023</b> , 52, 4796-4807	O
43	Tautomerization reactions of thiobarbituric acid: A detailed kinetic study using combined canonical variational transition state theory and QTAIM approach. <b>2023</b> , 55, 247-260	O
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40	Mechanism and origins of ligand-controlled regioselectivity of copper-catalyzed borocarbonylation of imines with B2pin2 and alkyl iodides: a computational study. <b>2023</b> , 10, 2024-2032	О
39	Chemical models of adenine precursors cyanamide and carbodiimide in the interstellar medium. <b>2023</b> , 521, 1578-1589	O
38	Computational Study of the Keto-Enol Tautomerism of 3-Phenyl-2,4-Pentanedione in the Gaseous Phase and Solvents Using DFT Methods. <b>2023</b> , 39, 40-46	O
37	Heteronuclear Dual Single-Atom Catalysts for Ambient Conversion of CO2 from Air to Formate. <b>2023</b> , 13, 3915-3924	О
36	DFT Studies on Ligand Controlled Highly Selective Copper-Catalyzed Borylations of Allenes.	O
35	An automated reaction route mapping for the reaction of NO and active species on Ag4 clusters in zeolites. <b>2023</b> , 25, 8524-8531	O
34	Understanding the mechanism and origins of stereoconvergence in nickel-catalyzed hydroarylation of 1,3-dienes with aryl boronates. <b>2023</b> , 52, 4849-4855	O
33	Theoretical Study on the Gas-Phase and Aqueous Interface Reaction Mechanism of Criegee Intermediates with 2-Methylglyceric Acid and the Nucleation of Products. <b>2023</b> , 24, 5400	O
32	Two-photon fluorescence imaging and specifically biosensing of norepinephrine on a 100-ms timescale. <b>2023</b> , 14,	O
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30	Visible light-catalyzed intermolecular [2+2] cycloaddition of 1,2-dihydropyridines: A combined experimental and DFT study. <b>2023</b> , 136, 133357	O

29	FermiDirac entropy as a measure of electron interactions.	O
28	The study of the PES and the reaction mechanism between ketene and Lithium Carbenoids and the formation of cyclopropanone. <b>2023</b> , 142,	O
27	Mechanistic Investigation into the Regio-Controllable Hydroallylations of Alkynes with Allylborons under Pd-Based Synergetic Catalyses. <b>2023</b> , 88, 4536-4545	О
26	Mechanistic insight into the carboxylic derivatives formation from CO2 and ethylene over iron(0)-based catalyst. <b>2023</b> , 541, 113084	O
25	Computational Study on NiAl Bimetal-Catalyzed Twofold CH Annulation Reaction: Mechanism, Origin of Selectivity, and Role of SPO Ligand.	О
24	Interactive Organic Reaction Trajectory Animation iPhone Application (iORA) and Web Site (webORA). <b>2023</b> , 100, 1659-1663	O
23	Correlating Chemical Bonding With the Potential Energy Acting on One Electron in a Molecule. <b>2023</b> ,	О
22	Direct Dynamics Trajectories Demonstrate Dynamic Matching and Nonstatistical Radical Pair Intermediates during Fe-Oxo-Mediated CH Functionalization Reactions. <b>2023</b> , 145, 7628-7637	O
21	Insights into the Three-Component Coupling Reactions of Aldehydes, Alkynes, and Amines Catalyzed by N-heterocyclic Carbene Silver: A DFT Study. <b>2023</b> , 13, 646	О
20	Abstraction and addition reactions of four Elactones with H-atoms and methyl radicals. 2023, 55, 324-332	O
19	Gas-phase formation of Grignard-type organolanthanide (III) ions RLnCl 3 🛭 The influences of lanthanide center and hydrocarbyl group. <b>2023</b> , 37,	О
18	Propane Oxidative Dehydrogenation on Nanosized Boron Carbide: Effect of Boron Content and Its Oxidation Implicated by DFT Calculations. <b>2023</b> , 127, 6280-6293	O
17	Mechanistic Insights Into the Rhodium-Catalyzed C⊞ Alkenylation/Directing Group Migration and [3+2] Annulation: A DFT Study. <b>2023</b> , 88, 4494-4503	О
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15	New insights into the mechanism of synergetic photoredox/copper(i)-catalyzed carbocyanation of 1,3-dienes: a DFT study.	О
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13	Quantum Chemical and Kinetic Study of the Gas-Phase Reactions of Methane Sulfonamide with Cl Atom and the Fate of IH2S(?O)2NH2 with 3O2 in the Atmosphere.	0
12	Factors Influencing the Chemoselectivity of Pd(OAc) 2 -Catalyzed Cyclization Reactions Involving 1,6-Enynes as a Substrate and PhI(OAc) 2 as a Reagent.	O

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