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Catalysis and Mechanistic Insights in Contemporary Organic Chemistry

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Abstract

The current state of organic chemistry is based on the principles of catalysis and mechanistic knowledge, which allow performing efficient, selective, and sustainable transformations. In this review, recent progress in transition metal catalysis, organocatalysis, photoredox catalysis, and bio-inspired systems is highlighted, with a focus on how transition metal catalysis, organocatalysis, photoredox catalysis, and bio-inspired systems are guided by mechanistic knowledge in reaction design, optimization, and substrate scope. Kinetic analysis, spectroscopy, and computational modeling techniques are important in order to gain critical information about intermediates, transition states, and reaction pathways; hence, to develop rational catalysts. The issues of catalyst stability, mechanistic complexity and scalability are addressed, as well as the new trends in AI-driven prediction and green chemistry. Combining catalysis with mechanistic information is still broadening the horizons of present-day organic synthesis.

Key words: Catalysis, Mechanistic Insight, Organic Synthesis, Transition Metal Catalysis, Organocatalysis, Photoredox Catalysis.

Introduction

The core science of organic compounds, organic chemistry is important in the invention of pharmaceuticals, agrochemicals, polymers, and materials science. The complexity of synthetic targets has been steadily growing with the decades, attracting more effective, selective, and sustainable methodologies. Catalysis has become a pillar in the contemporary organic chemistry and has been fundamental in transformations that would otherwise be sluggish, ineffective, or even impossible in normal circumstances [1]. Catalysts equip chemists with the means by which to precisely, selectively and economically design a reaction by reducing the activation energies to the reaction and determining the pathways of a reaction. The strategic use of catalysis has, thus, changed the scene of organic synthesis; they provide avenues which reduce wastage, conserve energy and enable the formation of sophisticated molecules with fewer reaction stages [2].

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In addition to the simple use of catalysts, the explanation of the reaction mechanism has become more of a critical aspect. Mechanistic insights allow us to have the basic knowledge to rationally design new catalysts, enhance existing catalytic systems, and even predict the result of a reaction. By clarifying the stepwise changes happening at the molecular level, that is, the identification of intermediates, identifications of the transition states, and rate-limiting steps, chemists can optimize the reaction conditions, increase selectivity, and discover new reactivity effects [3]. Kinetic studies, isotopic labeling, spectroscopic monitoring and computational modeling are all techniques that have revolutionized the study of reaction mechanisms and made it possible to gain unprecedented clarity in the understanding of complex transformations [4].

In modern organic chemistry, catalysis and mechanistic investigations have been combined and have yielded important breakthroughs. Organocatalysis, transition metal catalysis, photoredox catalysis, and enzymatic catalysis have become the workhorse of a number of contemporary strategies in synthesis. Both catalytic domains have their advantages, and their application can be achieved rationally and with a strong emphasis on mechanistic knowledge [5]. An example is the discovery of asymmetric catalysis that is critical in the synthesis of enantiomerically pure products and is closely associated with the understanding of the molecular-scale interaction between chiral catalysts and substrates. On the same note, the structure of tandem or cascade reactions, which perform many transformations in a reaction step, requires careful mechanistic understanding to maintain compatibility and efficiency of each reaction step [6].

In this review, I will attempt to give a general overview of how catalysis and mechanistic investigation interrelate in present-day organic chemistry. It sheds light on how mechanistic knowledge does not only direct the generation of new catalytic strategies but also innovations that promote synthetic efficiency, selectivity and sustainability. The review highlights the essential role that catalysis and mechanistic understandings can currently contribute to the future of contemporary organic synthesis by covering recent innovations, problems, and opportunities [7].

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Principles of Catalysis in Organic Chemistry

Modern organic synthesis is built upon catalysis which can offer chemists potent methods to catalyze reactions, enhance selectivity, and can even provide reactions otherwise difficult or impossible under normal conditions. Fundamentally, catalysis is the ability to speed up a chemical reaction by the aid of a substance referred to as catalyst, which is not used up in the process. The catalysts increase the reaction efficiency by offering alternative reaction pathways with lower activation energies thereby reducing the amount of energy required and unwanted byproducts. It is this basic principle which forms the basis of a very large number of methods in modern organic chemistry, both small-molecule transformations and large multistep syntheses [8].

Organic chemistry Catalysts can broadly be grouped into a few categories depending on their composition and mechanism of action. Homogeneous catalysts are active in the same phase as the reactants, usually a solution, and have the benefit of excellent control of the molecule and easy mechanistic investigations. Homogeneous catalysts typically include transition metal complexes (like palladium, nickel or ruthenium based catalysts) that are used to catalyze cross-coupling reactions, hydrogenation, and C–H activation reactions [9]. By contrast, heterogeneous catalysts are in a separate phase with the reactants, usually in the form of a solid in contact with gaseous or liquid substrates. Metal oxides or supported metals are some of these catalysts, which are very popular in the industrial processes because they are robust, recyclable, and easily separated [10].

Other than metal-based system organocatalysis has been found to be a flexible, environmentally friendly method, in which small organic molecules are used to mediate reactions through non-covalent interactions, through enamine or iminium intermediates or by Brnsted/Lewis acid-base reactions. On the same note, biocatalysis, which uses enzymes or enzyme analogs, offers unparalleled chemo-, regio-, and stereoselectivity in mild conditions, which is in line with the tenets of green chemistry [11]. To gain a profound insight into the principles of catalysis one needs to know about such concepts as reaction kinetics, thermodynamics, and the character of transition states and intermediates. Catalysts are active due to stabilizing the high-energy transition states that subsequently reduces the energy barrier of a reaction. The exact catalyst-substrate interactions;

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coordination, hydrogen bonding or electronic effects determine the efficiency, selectivity and stereochemical product of the transformation. These interactions can only be explained by mechanistic studies such as kinetics, isotopic labelling, and modeling which are therefore necessary to create better catalysts rationally [12].

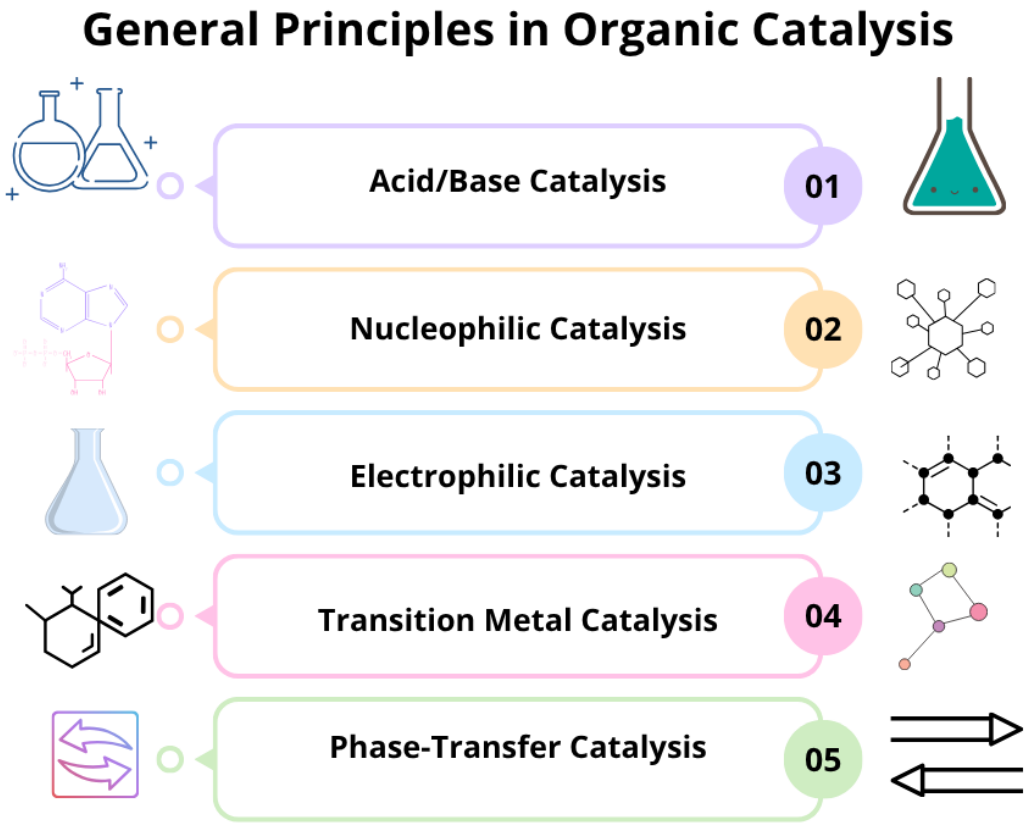


Figure: 1 showing general principles in organic catalysis

Generally, the principles of catalysis are the supporting bases of contemporary synthetic approach. Through understanding reaction mechanisms and reaction behavior with substrates, chemists can be able to design reactions that are more efficient, selective and sustainable. This underlying information does not only make it possible to be innovative in the development of reactions but also gives the skeleton of the mechanistic complexities that will be addressed in the subsequent paragraphs of this review [13].

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The Complications of Organic Reactions

The key to understanding the modern organic chemistry is the comprehension of the reaction processes as it provides the continuity between the visible and understandable phenomena and the intuitive knowledge of how to select reactions to suit a rational design. The reaction mechanism is the step-wise description of the process by which the reactants are turned into products and the processes involved in the transformation: the formations and the usage of intermediate products, the character of the transition states, and rate-limiting steps [14]. Mechanistic understanding does not only tell why a reaction occurs but also gives predictive capability of optimum reaction conditions, which enhance selectivity and plan novel transformations. In modern organic synthesis, such information cannot be dispensed with, in particular in the area of catalysis, where a small change in the catalyst or the reaction conditions can completely change the result [15].

The tools used in mechanistic studies are extensive in the breadth of experimental and computational tools. An example is kinetic analysis, which helps chemists to identify the orders of the reaction, the rate constant, and how the speed of a reaction depends on different factors. These studies can indicate the rate-limiting step and the nature of such reaction a concerted or a stepwise process. Isotopic labeling studies also enable one to trace the atoms in complex reactions and this gives a firsthand account of the bond breaking and bond forming reactions [16]. The methods of spectroscopy such as NMR, IR, UV-Vis and mass spectrometry can be used to monitor real-time the formation of reactive intermediates and provide a molecular picture of transient species that are frequently too short-lived to be isolated [17].

Computational chemistry has emerged in the recent decades as a fundamental complement to the experimental methods. Density functional theory (DFT) calculation, among other techniques, can be used to model potential energy surfaces, predict the transition states and estimate the activation barriers. Such computational clues can be used to rationalize observed selectivity's and develop new, more efficient and specific catalysts [18]. Mechanistic knowledge has far reaching practical consequences. Indicatively, the design of asymmetric catalysis, the key in the formation of chiral drugs, depends on the comprehensive understanding on the interaction of the chiral catalysts with

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the prochiral reactants. On the same note, to produce tandem or cascade reactions wherein several steps take place at a time, a profound comprehension of the interaction existing between catalysts and intermediates is necessary to ensure to avoid side reactions [19].

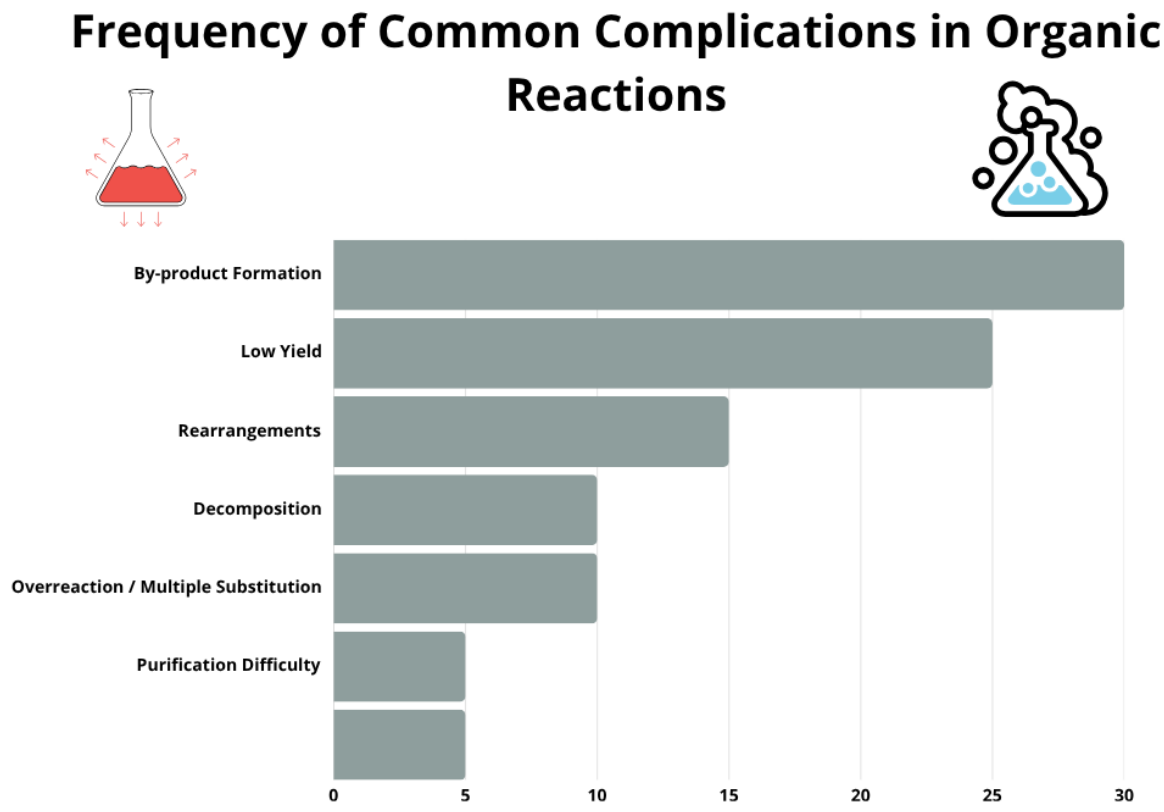


Figure: 2 showing frequency of common complications in organic chemistry

On the whole, mechanistic knowledge can be viewed as a blueprint of the modern organic synthesis that can teach chemists how rationally to design reactions, catalysts, and synthetic pathways. Making the finesse of molecular interactions, rearrangements of bonds, and profiles of energy a clearer concept, mechanistic studies transform trial and error methods into a systematic and predictable course of action, expediting innovation and making the creation of efficient, selective, and sustainable chemical reactions possible [20].

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Modern Catalytic Strategies

The field of modern organic chemistry is still being advanced through catalysis, which allows making efficient, selective and sustainable transformations. In the recent few decades, the catalytic strategies have gained considerable improvement and the toolkit of the chemist has increased and one can now build complex molecules with incredible precision [21]. The modern catalytic methods are broad and may include transition metal-based catalysts, all-organic and bio-inspired catalysts, with each having its own merits and mechanistic characteristics. One of the strongest tools in the use of organic synthesis is transition metal catalysis [22]. Palladium, nickel, copper, and ruthenium are capable of mediating a very diverse range of reactions, including cross-coupling, C -H activation, hydrogenation, and carbonylation. The mechanism of these catalysts is that they are capable of forming transient organometallic intermediates which promote bond formation or cleavage in a highly efficient manner. Chemists can optimize reactivity as well as selectivity, including regio- and stereocontrol, in complex molecular scaffolds due to their versatility and tunability, usually by ligand modification [23].

Organocatalysis, the use of small organic molecules as catalysts, has come out as a viable and metal-free alternative that is sustainable. These catalysts either mediate reactions via non-covalent interactions or hydrogen bonding or via covalent intermediates like enamines or iminium ions [24]. The idea of organocatalysis has proved especially useful in the field of asymmetric synthesis, where it allows achieving access to compounds with an enantiomeric enrichment without the use of costly and/or toxic metals. Photoredox catalysis is a relatively fast-developing area that involves the use of redox processes with the assistance of photoexcited catalysts using light energy. With this method, the changes are facilitated that are challenging in thermal conditions like radical-mediated bond formations and selective functionalizations in mild conditions. Transition metal catalysis or organocatalysis can also be used in a two-way photoredox catalyst, enhancing the breadth and performance of synthetic processes [25].

The biocatalysts possess remarkable chemo-, regio-, and stereoselectivity that is used in enzyme and bio-inspired catalysis. Nature or artificial enzymes provide an environmentally friendly

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environment, frequently in water, and can undergo transformations that are difficult to get conventional chemical catalysts to perform. To replicate these principles of catalysis in synthetic environments, bio-inspired catalysts exploit these enzymatic mechanisms to provide selective and efficient catalysis [26]. The efficiency, selectivity, sustainability, and scalability of catalytic strategy are considerations in the choice of catalytic strategy in modern organic synthesis. A combination of these knowledge with mechanistic understanding enables chemists to build reactions that yield its expected results with limited wastage. The constant improvement of catalytic schemes with the help of a high level of understanding of the mechanisms is the basis of the emergence of new synthetic strategies that serve the innovation of pharmaceuticals, materials science, and chemical biology [27].

Mechanism-Guided Development of Reactions

Mechanistic knowledge is a basic technique in the rational design of new organic reactions. Instead of depending on empirical experimentation, chemists now have turned increasingly to the aid of detailed information on reaction pathways, intermediates and transition states to design the construction of useful, selective, and innovative transformations. Tuning reaction conditions, catalyst structure and substrate scope with precise control is possible through mechanism-guided techniques which in the long run can be used to define synthetic strategies that can be predictable and reproducible [28]. Mechanistic insights have a major application in the design of selective transformations. Knowing which step in a reaction sequence is rate determinant, chemists can adjust catalysts, solvents, or temperature so as to enhance a preferred reaction pathway to the exclusion of other branch reactions [29]. The method is especially useful with stereoselective and asymmetric synthesis, in which small variations in the interactions between catalysts and substrates can determine the structure of the product. The nature of the effects of chiral catalysts on transition state geometry are studied in detail through a combination of kinetic and computational investigations, and can be used to rationally design catalysts that generate large enantiomeric excesses [30].

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Mechanism-directed methods are also useful in the generation of tandem and cascade reactions, where one and the same reaction vessel supports many transformations performed in sequence. Knowing the reactivity and compatibility of intermediates will make every step an efficient process without undesired side reactions. This will not only lead to increased overall yields but also results in better atom economy and less purification steps, which is in line with the concept of green chemistry [31]. The other useful use is in catalyst optimization. Understanding the catalyst-substrate interaction allows chemists to plan the rational design of ligands, alter the electronic or steric properties, and predict the consequences of the changes on the rate and selectivity of the reaction. Mechanistic understanding can also be used to determine the mechanisms of catalyst deactivation that allow the creation of stronger and reusable catalyst systems [32].

The mechanistic direction is necessary to increase the scope of reactions. Knowledge of the basic steps and possible constraints of a reaction allows chemists to manipulate experiment conditions to encompass more functional groups, heterocycles and complex molecular structures. This predictive power provides an acceleration to the generation of feasible synthetic protocols in pharmaceuticals, natural products and materials chemistry [33]. Mechanism directed reaction development changes the conventional approach to organic synthesis, which is more of an empirical effort to a rational and strategic endeavor. Through a combination of mechanistic understanding and catalytic design, chemists will be able to gain levels of efficiency, selectivity, and sustainability never before seen in the history of organic chemistry, which will serve as a source of innovation and push the limits of modern organic chemistry [34].

New Developments and Innovations

It is possible to state that the last ten years have seen incredible advances in fields such as catalysis and mechanistic insight, which resulted in the groundbreaking discoveries in the field of organic synthesis. New catalyst design, reaction engineering, and mechanistic understanding have increased the scale, efficiency and selectivity of chemical transformations, thereby giving chemists a greater control of complex molecular structures than ever before [35]. Transition metal catalysis is still a rich paradigm to be broken. Metal complexes and novel ligand structures have facilitated

unreachable transformations in the past, including C-H activation, remote functionalization, and selective cross-coupling reactions of sp 3 -hybridized centers. The developments are mostly influenced by mechanistic investigations that divulge minor electronic and steric impacts that can be carefully tailored to make changes in reactivity and selectivity. Also, dual-catalytic, where transition metals are used together with photoredox or organocatalysts, have provided access to previously inaccessible reaction pathways [36].

Organocatalysis has experienced a significant growth too, especially in asymmetric synthesis. New catalyst design approaches such as bifunctional and cooperative catalysts have enhanced enantioselectivity and increased the scope of substrates. The mechanism of high stereocontrol has been understood by mechanistic studies which in many cases include computational modeling to determine the non-covalent interactions and transition state geometry of the interactions that enable next-generation organocatalysts to be rationally designed [37]. Photoredox catalysis has transformed the industry because it allows light-driven radical reactions in a mild and sustainable condition. Recently, photoredox catalysis has been combined with transition metal catalysis enabling selective bond forming through single-electron transfer reactions. Radical generation, propagation and termination steps with a mechanistic understanding of radical reactions have played a paramount role in maximizing these reactions to be highly efficient and selective [38].

Enzyme and bio-inspired catalysis have undergone a lot of breakthrough as well. Functionalized active sites of engineered enzymes offer outstanding chemo-, regio-, and stereoselectivity, even with tricky synthetic substrates. Mechanistic enzyme-substrate interactions Mechanistic knowledge of enzyme-substrate interactions has enabled the design of synthetic mimics that incorporates the specificity of biocatalysis with the generality of chemical catalysis. Discovering new catalytic systems has become quicker due to progress in the field of computational chemistry and high-throughput screening. Machine learning and predictive modeling are supplementing conventional mechanistic studies and allow catalysts and reaction conditions to optimise quickly [39]. Combined all these new developments show the synergy between catalysis and mechanistic understanding. Experimental and computational methodologies have enabled chemists to design

reactions faster, more selective and environmentally friendly, and will form the basis of creating even more reactions faster, selective and environmentally friendly in the future [40].

Challenges and Limitations

The extraordinary progress in catalysis and in mechanistic insight notwithstanding, modern organic chemistry continues to encounter major problems, which restrain the full capacity of these strategies. Such limitations should be identified in order to direct future research as well as rational development of more efficient, selective and sustainable catalytic systems. Complexity of reaction mechanisms is one of the major challenges. Several organic changes, especially where several steps are involved or there are short-lived intermediates are mechanistically ambiguous [41]. It is not always easy to determine the short-lived intermediates or transition states even with sophisticated spectroscopic and computational analysis. Such ambiguity will frequently prevent the rational design of catalysts or reaction conditions, with the result that efficiency or selectivity will be suboptimal [42].

Also, there are practical limitations to catalyst stability and deactivation. Most of the high-activity catalysts, particularly the transition metal complexes, are susceptible to degradation during reaction or during impure crystal. Deactivation may take place by dissociation of the ligand, aggregation, or side reaction that is irreversible, and decreases catalytic efficiency and reproducibility. A continued challenge is designing strong and recyclable catalysts and in particular large scale or industrial-scale. The other restriction is compatibility of substrates and functional groups [43]. Although most catalytic systems are very effective with model substrates, their performance may drastically reduce with structurally diverse or sensitive molecules. This weakness limits the universality of some catalytic methods, particularly in the complex molecule synthesis, where several functional groups exist [44].

Other considerations are scalability and sustainability. Certain highly effective catalytic reactions that are challenging to scale-up include cost, catalyst availability, or reactivity to adverse environmental conditions. In addition, some of the reactions can be dependent on the toxic metals, dangerous solvents, or energy-demanding conditions, which restrict their compliance with the

principles of green chemistry. The predictability of the outcome of a reaction is also a challenge, and, particularly, for multi-step reactions, cascade reactions, or tandem reactions [45]. When the mechanistic pathways are not well studied or in situations where intermediates interact in complex ways then unintended side reactions, low yields or poor selectivity may be observed. To resolve these dilemmas, there is a need to have a synergistic effort of integrating high-level mechanistic research, computational modeling, and novel catalyst design. Through a well-organized discovery of limitations and approaches to resolve them, chemists will be able to enhance the strength, effectiveness, and sustainability of modern catalytic strategies, and push the boundaries of organic synthesis even higher [46].

Future Perspectives

The future of catalysis and mechanistic investigations in organic chemistry is bound to grow considerably, influenced by the complexity of synthetic targets, the need to have processes that are sustainable, and the sophistication of computer and analysis software. In the future, a number of new trends can be expected to influence the discipline, promoting innovation and enhancing the abilities of contemporary organic synthesis [47]. The collaboration of artificial intelligence (AI) and machine learning (ML) in reaction design and catalyst development is one of the potential paths. Predictive algorithms may process massive data sets of reaction products and reaction mechanisms to determine which conditions to use to achieve the best reaction, propose new catalytic systems, and predict reaction pathways. Such a strategy can radically decrease the trial and error experimentation, increasing discovery and enhancing reaction rate, selectivity and sustainability [48].

One of the primary areas of focus will remain sustainable and green catalysis. They are putting more emphasis on creating catalysts that work under mild conditions, feeds that are renewable and catalysts that produce minimal waste. Organocatalysts without metals, visible-light-driven photoredox systems and biocatalysts in the form of engineered proteins or enzymes are probably set to play a leading role in providing environmentally benign transformations with high efficiency and selectivity [49]. It will also be in future advances where mechanistic elucidation will be done

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on higher resolution. State-of-the-art spectroscopic methods, in situ methods and computer modeling are anticipated to offer a unique understanding of the reaction pathways, reaction intermediates, and reaction transition states. This more fundamental knowledge will allow the rational design of highly predictable, efficient and compatible catalysts and reactions that are compatible with complex molecular structures [50].

Moreover, the multidisciplinary approaches will gain more significance. Combining organic chemistry with materials science, computational chemistry, and chemical biology currently enables the creation of novel catalysts, dual catalytic systems, and cascade reactions in areas of pharmaceuticals to materials synthesis. Combination of bio-inspired concepts with synthetic chemistry is bound to increase the range of changes that can be made under mild and sustainable conditions [51]. Scalability and industrial applicability are the areas of focus in the future. Development of better, recyclable, and economical systems in catalysis will close the rift between the laboratory work and large-scale chemical production so that discoveries in organic synthesis can be practically applied in pharmaceuticals, agrochemicals, and advanced materials. It can be concluded that the interaction of advanced mechanistic knowledge, new catalyst design, and new technologies will transform the opportunities in organic chemistry [52]. The field is heading to future with reactions being highly predictable, sustainable and widely applicable, which opens the door to new horizons of chemical synthesis and new innovations in the field of molecules.

Conclusion

The new paradigms of modern organic chemistry have been catalysis and mechanistic understanding, which have essentially defined the way chemists think of chemical reaction design, management, and optimization. The combination of these two fields over the last decades has enabled the field of organic synthesis to shift away from being an empirical and trial-and-error science and turn into a predictive, rational science. The realization of how exactly catalysts can reflect on the reaction pathways and how intermediates and transition states dictate selectivity and efficiency, the chemists can now build up to the most sophisticated methodologies, which can solve issues on the ground and also on theory.

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In its different manifestations, such as transition metal catalysis, organocatalysis, photoredox catalysis and enzyme or bio-inspired catalysis, catalysis has given chemists greater control over chemical transformations than ever before. Various complex bond formations, including cross-coupling and C -H activation, previously viewed as highly challenging or even impossible, have become accessible using transition metal catalysts. The metal-free and environmentally benign organocatalysis has enabled asymmetric reactions with great stereocontrol and increased access to enantiomerically pure compounds, which are important in the pharmaceutical and agrochemical industries. Photoredox catalysis has provided completely new reaction paradigms by taking advantage of using light energy to produce reactive intermediates under mild conditions, and biocatalysis has provided the combination of precision with chemical versatility, reaction with incomparable chemo-, regio-, and stereoselectivity.

These catalytic systems have been optimized and rationalized by mechanical insights. Through the explanation of reaction pathways, determination of rate determining steps and the geometry of the transition states, chemists can predict and control the results of reactions with ever greater accuracy. Such tools as kinetic studies, isotopic labeling, and advanced spectroscopy, and computational modeling have helped elucidate long-standing mechanistic ambiguities and also informed the design of more selective, efficient, and robust catalysts. This mechanistic knowledge permits the generation of tandem and cascade reactions, asymmetric process optimization and substrate expansion, and waste reduction and atom economy, respectively, as dictated by the tenets of green chemistry.

Although these advances have been made, the challenges still persist, such as catalyst stability, mechanistic complexity and substrate compatibility and the ability to work at industrial scales. To solve these problems, further incorporation of experimental and computational methods, production of strong and recyclable catalysts and construction of environmentally friendly and sustainable reactions are all necessary. New technologies like artificial intelligence and machine learning will enable the discovery process to be faster and more efficient and predictive of the

reaction outcome, discover novel catalytic systems and optimize reaction conditions, making organic synthesis more accurate and efficient.

To sum up, the combination of catalysis and mechanistic knowledge has undergone a fundamental development of the current state of organic chemistry that has changed the way reactions are modeled, performed, and understood. The integrated use of these principles has facilitated chemists to attain high efficiency, selectivity, and sustainability in the synthesis of complex molecules and it has given strength upon the further innovations. With the current changes in the field, continued advancements in both the design of catalysts, mechanistic elucidation, and predictive technologies will push the frontiers of what can be synthetically attained leading to a new era of precision, sustainability, and creativity in organic synthesis. Catalysis and mechanistic understanding are not tools, but the principles that will keep on propelling change, innovation and discovery in the twenty first century of the chemistry profession.

References

[1]. Lakhani P, Bhanderi D, Modi CK. Nanocatalysis: recent progress, mechanistic insights, and diverse applications. Journal of Nanoparticle Research. 2024 Jul;26(7):148.

[2]. Zhang X, Chung LW, Wu YD. New mechanistic insights on the selectivity of transition-metal-catalyzed organic reactions: the role of computational chemistry. Accounts of chemical research. 2016 Jun 21;49(6):1302-10.

[3]. Blackmond DG. Kinetic profiling of catalytic organic reactions as a mechanistic tool. Journal of the American Chemical Society. 2015 Sep 2;137(34):10852-66.

[4]. Pinnoju P. Advanced Organic Chemistry-Reactions & Mechanics. Academic Guru Publishing House; 2025 Mar 21.

[5]. Carroll FA. Perspectives on structure and mechanism in organic chemistry. John Wiley & Sons; 2023 Apr 14.

[6]. Fey N, Lynam JM. Computational mechanistic study in organometallic catalysis: Why prediction is still a challenge. Wiley Interdisciplinary Reviews: Computational Molecular Science. 2022 Jul;12(4):e1590.

[7]. Okuyama T, Maskill H. Organic chemistry: a mechanistic approach. Oxford University Press; 2013.

[8]. Naher M, Gonzálvez MA, Williams CM, Bernhardt PV. Emerging applications and mechanistic insights of copper mediated electrocatalysts in organic transformations. Chemical Society Reviews. 2025.

[9]. Smajlagic I, Guest M, Durán R, Herrera B, Dudding T. Mechanistic Insight toward Understanding the Role of Charge in Thiourea Organocatalysis. The Journal of Organic Chemistry. 2019 Dec 2;85(2):585-93.

[10]. Buzzetti L, Crisenza GE, Melchiorre P. Mechanistic studies in photocatalysis. Angewandte Chemie International Edition. 2019 Mar 18;58(12):3730-47.

[11]. Blasco T. Insights into reaction mechanisms in heterogeneous catalysis revealed by in situ NMR spectroscopy. Chemical Society Reviews. 2010;39(12):4685-702.

[12]. Romero NA, Nicewicz DA. Mechanistic insight into the photoredox catalysis of anti-markovnikov alkene hydrofunctionalization reactions. Journal of the American Chemical Society. 2014 Dec 10;136(49):17024-35.

[13]. Loh CC. Synergistic catalysis: An emerging concept for selective carbohydrate synthesis. Chem Catalysis. 2024 Mar 21;4(3).

[14]. Cheng GJ, Zhang X, Chung LW, Xu L, Wu YD. Computational organic chemistry: bridging theory and experiment in establishing the mechanisms of chemical reactions. Journal of the American Chemical Society. 2015 Feb 11;137(5):1706-25.

[15]. Verma P, Patni PA, Sunoj RB. Mechanistic insights on N-heterocyclic carbene-catalyzed annulations: the role of base-assisted proton transfers. The Journal of Organic Chemistry. 2011 Jul 15;76(14):5606-13.

[16]. Jindal G, Kisan HK, Sunoj RB. Mechanistic insights on cooperative catalysis through computational quantum chemical methods. ACS Catalysis. 2015 Feb 6;5(2):480-503.

[17]. Vocadlo DJ, Davies GJ. Mechanistic insights into glycosidase chemistry. Current opinion in chemical biology. 2008 Oct 1;12(5):539-55.

[18]. Bonciolini S, Pulcinella A, Noël T. Tech-enhanced synthesis: exploring the synergy between organic chemistry and technology. Journal of the American Chemical Society. 2025 Aug 5;147(32):28523-45.

[19]. Lau YY, Zhai H, Schafer LL. Catalytic asymmetric synthesis of morpholines. Using mechanistic insights to realize the enantioselective synthesis of piperazines. The Journal of Organic Chemistry. 2016 Oct 7;81(19):8696-709.

[20]. Sreenithya A, Surya K, Sunoj RB. Hypercoordinate iodine (III) promoted reactions and catalysis: an update on current mechanistic understanding. Wiley Interdisciplinary Reviews: Computational Molecular Science. 2017 May;7(3):e1299.

[21]. Gong X, Caglayan M, Ye Y, Liu K, Gascon J, Dutta Chowdhury A. First-generation organic reaction intermediates in zeolite chemistry and catalysis. Chemical Reviews. 2022 Aug 10;122(18):14275-345.

[22]. Prieto Kullmer CN, Kautzky JA, Krska SW, Nowak T, Dreher SD, MacMillan DW. Accelerating reaction generality and mechanistic insight through additive mapping. Science. 2022 Apr 29;376(6592):532-9.

[23]. Schauermann S, Nilius N, Shaikhutdinov S, Freund HJ. Nanoparticles for heterogeneous catalysis: new mechanistic insights. Accounts of chemical research. 2013 Aug 20;46(8):1673-81.

[24]. Basheer H, Shamsi S, Qadir A, Sharma K, Azad CS, Kumar A, Khan IA. Kanamycin− Cu (II) Complex Catalyzed Ullmann Amine Synthesis at Room Temperature: A Tool for Mechanistic Insights into Methylene Blue Degradation. European Journal of Organic Chemistry. 2024 Aug 5;27(29):e202400328.

[25]. Michelet V, Toullec PY, Genêt JP. Cycloisomerization of 1, n-enynes: challenging metal-catalyzed rearrangements and mechanistic insights. Angewandte Chemie International Edition. 2008 May 26;47(23):4268-315.

[26]. Purushothaman A, Li S, Shilpa S, Bai ST, Sunoj RB. Mechanistic Insights into Rh-Catalyzed Regio-and Enantioselective Hydroformylation of Cyclopropyl-Functionalized Trisubstituted Alkenes. The Journal of Organic Chemistry. 2025 Jul 9;90(28):9892-902.

[27]. Garayalde D, Gómez-Bengoa E, Huang X, Goeke A, Nevado C. Mechanistic insights in gold-stabilized nonclassical carbocations: gold-catalyzed rearrangement of 3-cyclopropyl propargylic acetates. Journal of the American Chemical Society. 2010 Apr 7;132(13):4720-30.

[28]. Sigman MS, Harper KC, Bess EN, Milo A. The development of multidimensional analysis tools for asymmetric catalysis and beyond. Accounts of chemical research. 2016 Jun 21;49(6):1292-301.

[29]. Zhong S, Fu Y, Wang X, Liu X. Cyclization Reactions of N-Aminopyridinium Salts: Synthetic Scope and Mechanistic Insights. Advanced Synthesis & Catalysis. 2025 Sep 19:e70040.

[30]. Fiori KW, Du Bois J. Catalytic intermolecular amination of C− H bonds: method development and mechanistic insights. Journal of the American Chemical Society. 2007 Jan 24;129(3):562-8.

[31]. T. L A, P CA. Iron and Cobalt Catalyzed Homogeneous Hydrofunctionalization of Carbonyl Compounds: Recent Advances and Mechanistic Insights. ChemistrySelect. 2025 Jul;10(25):e02889.

[32]. Kalyani D, Deprez NR, Desai LV, Sanford MS. Oxidative C− H activation/C− C bond forming reactions: synthetic scope and mechanistic insights. Journal of the American Chemical Society. 2005 May 25;127(20):7330-1.

[33]. Wai JS, Marko I, Svendsen JS, Finn MG, Jacobsen EN, Sharpless KB. A mechanistic insight leads to a greatly improved osmium-catalyzed asymmetric dihydroxylation process. Journal of the American Chemical Society. 1989 Feb;111(3):1123-5.

[34]. Vedejs E, Denmark SE, editors. Lewis Base Catalysis in Organic Synthesis, 3 Volume Set. John Wiley & Sons; 2016 Oct 10.

[35]. Jindal G, Sunoj RB. Mechanistic insights on cooperative asymmetric multicatalysis using chiral counterions. The Journal of Organic Chemistry. 2014 Aug 15;79(16):7600-6.

[36]. Kaur P, Gurjar KK, Arora T, Bharti D, Kaur M, Kumar V, Parkash J, Kumar R. Efficient synthesis and mechanistic insights for the formation of imidazo [1, 2-a] pyridines via

multicomponent decarboxylative coupling using chitosan-supported copper catalysts. Molecular Catalysis. 2023 Nov 1;550:113582.

[37]. Chiu YH, Chang TF, Chen CY, Sone M, Hsu YJ. Mechanistic insights into photodegradation of organic dyes using heterostructure photocatalysts. Catalysts. 2019 May 9;9(5):430.

[38]. Porwal A, Rajendiran A, Alam P, Singh H, Singh K, Dubey A. Indole Moiety in Organic Synthesis: A Comprehensive Review of Methods and Mechanisms. International Journal of Pharmaceutical Investigation. 2024 Oct 1;14(4).

[39]. Milo A, Neel AJ, Toste FD, Sigman MS. A data-intensive approach to mechanistic elucidation applied to chiral anion catalysis. Science. 2015 Feb 13;347(6223):737-43.

[40]. Muralirajan K, Kancherla R, Maity B, Karuthedath S, Laquai F, Cavallo L, Rueping M. Mechanistic insights into excited-state palladium catalysis for C–S bond formations and dehydrogenative sulfonylation of amines. Nature Communications. 2023 Oct 19;14(1):6622.

[41]. Nagesh K, Reddy NS, Kareem S, Vali SR, Reddy BS. Recent advances in transition metal-catalyzed alkyne annulations: applications in organic synthesis. Organic & Biomolecular Chemistry. 2025;23(28):6665-82.

[42]. Kalar PL, Jain K, Agrawal S, Khan S, Vishwakarma R, Shivhare A, Deshmukh MM, Das K. Green synthesis of electrophilic alkenes using a magnesium catalyst under aqueous conditions and mechanistic insights by density functional theory. The Journal of Organic Chemistry. 2023 Dec 1;88(24):16829-44.

[43]. Wu S, Kaur J, Karl TA, Tian X, Barham JP. Synthetic molecular photoelectrochemistry: new frontiers in synthetic applications, mechanistic insights and scalability. Angewandte Chemie International Edition. 2022 Mar 14;61(12):e202107811.

[44]. Malapit CA, Prater MB, Cabrera-Pardo JR, Li M, Pham TD, McFadden TP, Blank S, Minteer SD. Advances on the merger of electrochemistry and transition metal catalysis for organic synthesis. Chemical reviews. 2021 Nov 19;122(3):3180-218.

[45]. Franzén J, Marigo M, Fielenbach D, Wabnitz TC, Kjærsgaard A, Jørgensen KA. A general organocatalyst for direct α-functionalization of aldehydes: stereoselective C− C, C− N, C− F, C− Br, and C− S bond-forming reactions. Scope and mechanistic insights. Journal of the American Chemical Society. 2005 Dec 28;127(51):18296-304.

[46]. Sohel A, Kovilakath MS, Gogoi PJ, Ansari H, Phukan P, Bag S, John NS, Baksi A. Mechanistic Insights into the Stabilization of In Situ Formed γ-NiOOH Species on Ni60Nb40 Nanoglass for Effective Urea Electro-Oxidation. Small. 2024 Nov;20(47):2405160.

[47]. Rowshanpour R, Gravel M, Dudding T. N-heterocyclic carbene organocatalyzed redox-active/ring expansion reactions: Mechanistic insights unveiling base cooperativity. The Journal of Organic Chemistry. 2022 Nov 30;87(24):16785-93.

[48]. Krupka J, Pasek J. Nitrile hydrogenation on solid catalysts–New insights into the reaction mechanism. Current Organic Chemistry. 2012 Apr 1;16(8):988-1004.

[49]. Korobkov SM, Birin KP, Tsivadze AY. Supremely high turnover numbers with a simple porphyrin photosensitizer: Kinetic and mechanistic insights into the oxidation of sulfides with singlet oxygen. Journal of Catalysis. 2025 May 1;445:116008.

[50]. Tak S, Grewal S, Shreya, Phogat P, Manisha, Jha R, Singh S. Mechanistic Insights and Emerging Trends in Photocatalytic Dye Degradation for Wastewater Treatment. Chemical Engineering & Technology. 2024 Nov;47(11):e202400142.

[51]. Pascanu V, González Miera G, Inge AK, Martín-Matute B. Metal–organic frameworks as catalysts for organic synthesis: a critical perspective. Journal of the American Chemical Society. 2019 Apr 11;141(18):7223-34.

[52]. Saigal, Sudheer N, Sahoo SC, Khan MM, Seth K. "In-Water" Three-Component One-Pot Reaction for the Facile Synthesis of Densely Functionalized 2, 3-Dihydro-1 H-pyrrol-2-ols and Mechanistic Insight. ACS Sustainable Chemistry & Engineering. 2024 Aug 22;12(35):13336-51.