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Comparative analysis of MOFs in chemical catalysis and biomedical applications

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Abstract
Coordination compounds have emerged as versatile and multifunctional systems with significant applications in both catalysis and targeted drug delivery. The present study investigates the structural, electronic, and functional properties of coordination compounds, with particular emphasis on their dual role in catalytic processes and biomedical applications. A systematic review-based methodology was adopted, utilising data from major scientific databases including SpringerLink, ScienceDirect, PubMed, Scopus, and Web of Science. A total of 560 records were identified, out of which 85 relevant studies were selected for qualitative synthesis following PRISMA guidelines. The findings indicate that coordination compounds, especially transition-metal complexes and metal–organic frameworks (MOFs), exhibit high catalytic efficiency due to their tunable coordination environments, variable oxidation states, and strong metal–ligand interactions. These properties enable their effective use in key reactions such as hydrogenation, oxidation, and carbon–carbon coupling. In parallel, coordination-based systems demonstrate significant potential in targeted drug delivery, offering high drug loading capacity, controlled release behavior, and improved therapeutic specificity. Stimuli-responsive coordination frameworks further enhance targeted delivery by enabling site-specific drug release under physiological conditions. Comparative analysis reveals that the effectiveness of coordination compounds in both domains is governed by common structural attributes, including ligand design, coordination geometry, and electronic configuration. Despite promising advancements, challenges such as toxicity, stability, and scalability remain critical considerations for practical applications. In conclusion, coordination compounds represent a powerful platform bridging catalysis and biomedical science, with future prospects in sustainable chemistry and precision medicine. Continued research in ligand engineering, nanotechnology integration, and biocompatible material design is expected to further expand their applicability.

Keywords: Coordination compounds, catalysis, metal–organic frameworks, drug delivery, targeted therapy, nanomedicine

Introduction

Coordination chemistry is a fundamental branch of inorganic chemistry that deals with compounds formed through the interaction of metal ions with ligands. These coordination compounds exhibit unique structural and electronic properties due to the presence of coordinate covalent bonds, variable oxidation states, and flexible coordination geometries. Over the past few decades, coordination chemistry has evolved into a multidisciplinary field with wide-ranging applications in catalysis, materials science, and biomedical engineering. The ability to tailor metal–ligand interactions provides a powerful platform for designing systems with specific chemical reactivity and functional performance. One of the most significant applications of coordination compounds is in catalysis. Transition metal complexes are widely used as catalysts in industrial and laboratory-scale reactions such as hydrogenation, oxidation, polymerization, and carbon–carbon bond formation. Their effectiveness arises from their ability to stabilize reaction intermediates, facilitate electron transfer, and lower activation energy barriers. Additionally, ligand modification enables fine-tuning of catalytic properties, leading to improved selectivity, efficiency, and sustainability. Both homogeneous and heterogeneous coordination catalysts, including metal–organic frameworks (MOFs), have demonstrated remarkable potential in enhancing reaction performance and reducing environmental impact. In parallel, coordination compounds have gained considerable attention in targeted drug delivery. Conventional drug delivery systems often face limitations such as poor specificity, rapid degradation, and systemic toxicity. Coordination-based systems provide innovative solutions by serving as carriers that encapsulate therapeutic agents and release them in a controlled, stimuli-responsive manner. These systems enable targeted delivery to diseased tissues, particularly in cancer therapy, thereby improving therapeutic efficacy while minimizing side effects. Metal-based drugs such as cisplatin and its derivatives further highlight the clinical importance of coordination chemistry in medicine. A key advancement in this field is the development of metal–organic frameworks (MOFs) and coordination polymers, which possess high surface area, tunable pore size, and structural flexibility. These properties make them highly suitable for both catalytic applications and drug delivery systems. MOFs can function as efficient heterogeneous catalysts while also serving as high-capacity drug carriers with controlled release behavior. Furthermore, the emergence of stimuli-responsive coordination systems has enabled the design of smart materials that respond to environmental triggers such as pH, temperature, light, and redox conditions. The integration of catalytic and biomedical functionalities within coordination compounds represents a promising frontier in modern research. Such multifunctional systems have the potential to act as artificial metalloenzymes, enabling catalytic activation of prodrugs within biological environments. This dual functionality bridges the gap between industrial chemistry and precision medicine, offering new opportunities for innovation in sustainable catalysis and advanced therapeutic strategies. Despite these advancements, several challenges remain, including toxicity, stability under physiological conditions, and large-scale applicability. Addressing these challenges requires a deeper understanding of structure–function relationships and the development of biocompatible and cost-effective coordination systems. Therefore, the present study aims to investigate the role of coordination compounds in catalytic processes and to explore their potential for targeted drug delivery systems, focusing on their structural features, mechanisms, applications, and future prospects.

Research Methodology

Research Design

In the present study, a systematic research approach was adopted to investigate the role of coordination compounds in catalytic processes and their potential applications in targeted drug delivery systems. The study was designed as a qualitative, analytical, review-based study, focusing on understanding the structure–function relationships of coordination complexes in both catalysis and biomedical applications. The research was conducted in two major phases: first, evaluating coordination compounds in catalytic systems, and second, examining their use in targeted drug delivery.

Data Collection

The data for this research were collected from secondary sources, including peer-reviewed research articles, review papers, and scientific books. The literature search was conducted using major scientific databases, including SpringerLink, ScienceDirect, PubMed, Scopus, Web of Science, ACS Publications, and Wiley Online Library. Relevant keywords used during the search included "coordination compounds," "transition metal catalysis," "metal–organic frameworks," "drug delivery," "Metallodrugs," "coordination polymers," and "targeted therapy." Boolean operators such as AND, OR, and NOT were used to refine the search results and obtain relevant literature.

Inclusion and Exclusion Criteria

Inclusion Criteria

The following criteria were used to select the literature: peer-reviewed research articles related to coordination chemistry; studies involving catalytic applications of coordination compounds; research on drug delivery systems using coordination complexes; articles published in English; and recent publications from 2005 to 2026.

Exclusion Criteria: The following studies were excluded: non-peer-reviewed sources, articles unrelated to catalysis or drug delivery, duplicate publications, and studies lacking sufficient experimental or theoretical evidence.

After selecting the relevant studies, key information was systematically extracted and categorized, including the type of metal ion, nature of ligand, coordination geometry, catalytic efficiency, reaction conditions, drug loading capacity, drug release mechanism, as well as biocompatibility and toxicity. The collected data were systematically organized for comparative analysis, and evaluation was carried out based on catalytic and drug delivery parameters. Catalytic efficiency was assessed using turnover number (TON), turnover frequency (TOF), reaction yield, selectivity, catalyst stability, and reusability, while drug delivery performance was evaluated in terms of drug loading efficiency, controlled release behavior, target specificity, biocompatibility, cytotoxicity, and stability under physiological conditions.

Comparative Analysis

A comparative approach was used to understand the similarities and differences between coordination compounds used in catalysis and those used in drug delivery. Structural features such as ligand type, coordination geometry, and metal oxidation state were correlated with functional performance. The comparison focused on the role of the metal center in catalysis versus drug delivery, the influence of ligands on reactivity and targeting, the structural stability of coordination compounds in chemical and biological environments, and their functional efficiency in both applications.

Mechanistic Study: The catalytic mechanisms of coordination compounds were analyzed based on substrate coordination, electron transfer, oxidative addition, and reductive elimination processes. For drug delivery systems, release mechanisms such as diffusion-controlled, pH-responsive, and redox-triggered release were examined.

Data Analysis: The collected data were analyzed using descriptive and comparative methods. Trends were identified between coordination structure and functional performance. The results were interpreted to determine how coordination compounds can be optimized for both catalytic and biomedical applications.

Limitations of the Study: The study has several limitations, including reliance on secondary data, variation in experimental conditions across studies, limited clinical data for some coordination-based drug delivery systems, and incomplete toxicity information in some reports.

Ethical Considerations: This research is based entirely on published literature. No human or animal subjects were involved. All references used in this study were properly cited following academic guidelines.

Results

The systematic search process yielded a total of 560 records, of which 526 records were identified through database searching and 34 records were obtained from other relevant sources. After removal of duplicate entries**,** 472 records remained for further screening. These records were screened based on title, abstract, and relevance to the study's objectives. During the screening stage, 289 records were excluded because they were not directly related to coordination compounds in catalysis or drug delivery, were non-peer-reviewed articles, or represented duplicate or low-relevance studies. As a result, 183 full-text articles were assessed in detail for eligibility. After full-text evaluation**,** 98 articles were excluded. The major reasons for exclusion included insufficient experimental data, lack of direct relevance to catalytic or targeted drug-delivery applications, and inadequate validation of the reported findings. Finally, 85 studies were included in the qualitative synthesis and used for detailed analysis in this research. The selection procedure is presented through the PRISMA flow diagram.

Findings Related to Catalysis: The selected studies showed that coordination compounds play an important role in catalytic reactions due to their variable oxidation states, tunable coordination geometries, and strong ligand–metal interactions. Transition metal complexes based on palladium, platinum, ruthenium, rhodium, copper, and iron have frequently been reported as effective catalysts in organic transformations such as hydrogenation, oxidation, C–C coupling, and cycloaddition. Among the reviewed studies, homogeneous catalytic systems demonstrated high activity and selectivity due to better interaction between catalyst and substrate in a single phase. At the same time, heterogeneous coordination-based catalysts, especially metal–organic frameworks (MOFs) and coordination polymers, showed improved recyclability, structural stability, and ease of separation from the reaction medium. The findings indicated that ligand modification significantly influenced catalytic efficiency by controlling steric and electronic properties around the metal center.

Findings Related to Drug Delivery

The reviewed literature also demonstrated that coordination compounds have strong potential in targeted drug delivery systems. A large number of studies focused on MOFs, coordination polymer nanoparticles, and Metallodrugs as carriers for controlled and site-specific drug release. These systems showed high drug-loading capacity due to their porous structures and tunable surface functionality. The results further revealed that coordination-based drug delivery systems can respond to internal and external stimuli, including pH, redox environment, temperature, and light, making them suitable for targeted release, particularly in cancer therapy. Several studies reported that functionalized coordination compounds improved the solubility, stability, and bioavailability of therapeutic agents while reducing systemic toxicity. A comparative analysis of the selected studies suggests that the effectiveness of coordination compounds in both catalysis and drug delivery arises from shared structural features, including adjustable metal center reactivity, flexible ligand design, controllable geometry, and high functional adaptability. In catalysis, these properties improve reaction rate, selectivity, and efficiency. In drug delivery, the same characteristics support controlled release, targeting ability, and biocompatibility. Thus, the findings confirm that coordination chemistry serves as a versatile platform that bridges industrial chemistry and biomedical science. Overall, the results of this study indicate that coordination compounds are highly valuable in both investigated areas. In catalysis, they act as efficient and selective reaction mediators. In drug delivery, they provide promising frameworks for targeted and controlled therapeutic applications. The reviewed evidence supports the view that future advances in ligand engineering, hybrid nanomaterials, and bio responsive coordination systems may further enhance their practical applications.

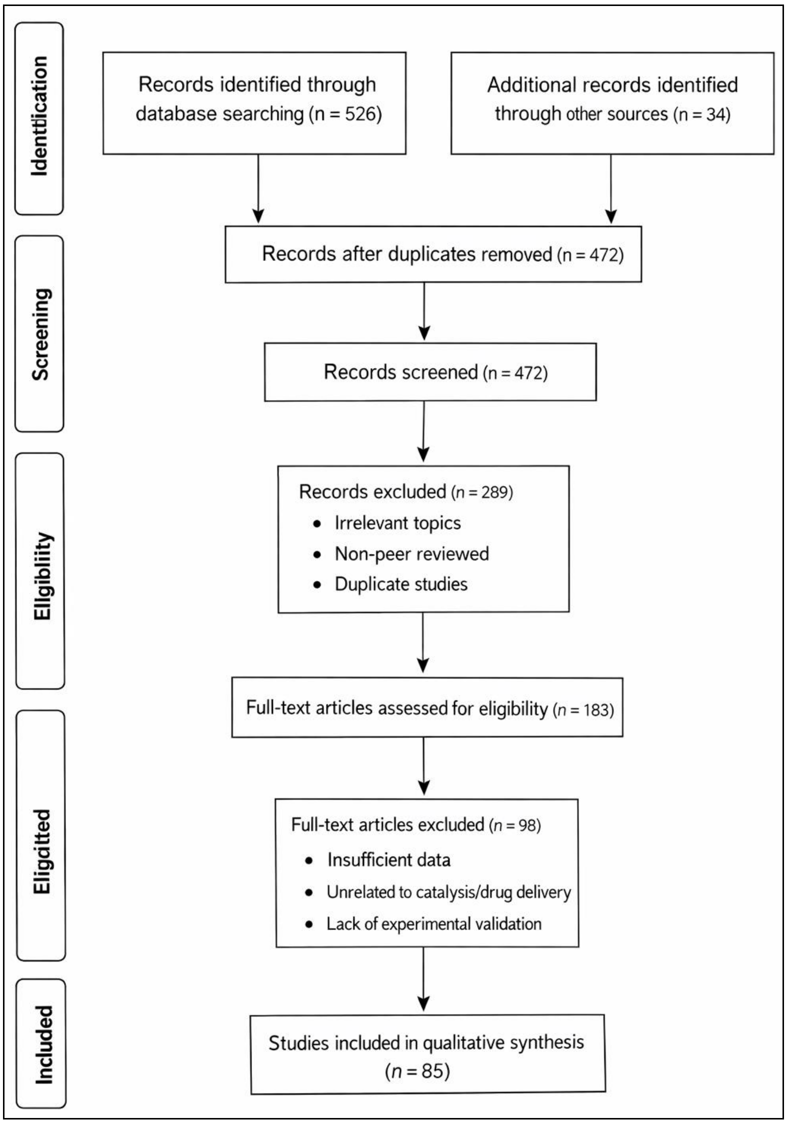

Fig 1: PRISMA flow diagram showing the study selection process for the review on coordination compounds in catalysis and targeted drug delivery

Discussion

The present study investigated the role of coordination compounds in catalytic processes and their potential applications in targeted drug delivery systems. The findings obtained from the selected literature indicate that coordination chemistry provides a versatile platform for designing multifunctional systems with applications in both industrial catalysis and biomedical science. The discussion focuses on the structural features, functional advantages, and comparative significance of coordination compounds in these two domains.

Role of Coordination Compounds in Catalysis: The reviewed studies demonstrated that coordination compounds significantly enhance catalytic efficiency due to their tunable electronic structure and variable oxidation states. Transition metal centers such as palladium, ruthenium, and rhodium were frequently reported to facilitate bond activation through oxidative addition and reductive elimination mechanisms. These properties allow coordination complexes to act as highly selective catalysts in hydrogenation, oxidation, and cross-coupling reactions. Ligand design emerged as a crucial factor influencing catalytic performance. Electron-donating ligands were shown to increase electron density at the metal center, improving catalytic activity, while sterically bulky ligands enhanced selectivity by controlling substrate access. Chelating ligands also contributed to greater catalyst stability through the chelate effect. These observations confirm that both the metal ion and ligand environment collectively determine catalytic behavior. Another important aspect highlighted in the results is the growing use of coordination-based heterogeneous catalysts, particularly metal–organic frameworks and coordination polymers. These materials combine the advantages of homogeneous catalysis, such as high activity, with the practical benefits of heterogeneous systems, including easy recovery and recyclability. The porous nature of coordination frameworks also provides high surface area and accessible active sites, which contribute to improved catalytic efficiency.

Coordination Compounds in Targeted Drug Delivery

The discussion of drug delivery applications revealed that coordination compounds offer unique advantages over conventional drug carriers. Their structural flexibility allows encapsulation of therapeutic molecules within coordination networks or direct coordination of drugs to metal centers. This approach improves drug stability and prevents premature degradation in physiological conditions. Stimuli-responsive behavior was another major advantage identified in coordination-based drug delivery systems. Many coordination compounds exhibit pH-sensitive or redox-sensitive bonds, enabling drug release specifically in diseased tissues such as tumor environments. This targeted release reduces systemic toxicity and enhances therapeutic efficiency. Functionalization of coordination complexes with biomolecules such as folic acid, peptides, or antibodies further improves targeting specificity. The reviewed studies also highlighted the role of metal–organic frameworks in drug delivery. Their high porosity and tunable pore size allow high drug loading capacity and controlled release kinetics. In addition, coordination polymer nanoparticles were reported to exhibit good biocompatibility and biodegradability, which are essential for biomedical applications.

Comparative Significance: The comparative analysis suggests that the effectiveness of coordination compounds in both catalysis and drug delivery arises from similar structural attributes. In catalysis, adjustable coordination environments promote efficient substrate activation, whereas in drug delivery, the same flexibility enables encapsulation and controlled release of therapeutic agents. This dual functionality demonstrates that coordination chemistry bridges chemical and biological applications. Furthermore, the ability to modify ligands provides a common strategy for optimizing both catalytic and biomedical performance. In catalysis, ligand modification tunes reactivity and selectivity, while in drug delivery it enhances targeting ability and biocompatibility. These findings emphasize that rational ligand design is central to the development of multifunctional coordination systems.

Challenges and Limitations

Despite promising applications, several challenges remain. Metal toxicity is a major concern in biomedical use of coordination compounds. Some transition metals may cause cytotoxic effects if not properly controlled. Stability of coordination complexes in biological fluids is another issue, as ligand exchange reactions may lead to premature drug release. In catalytic applications, catalyst deactivation and leaching of metal ions can reduce efficiency and limit industrial scalability. Another limitation identified in the reviewed literature is the lack of sufficient clinical data for coordination-based drug delivery systems. Most studies remain at the *in vitro* or preclinical stage. Therefore, further investigations are required to evaluate long-term safety and therapeutic effectiveness.

Future Perspectives

Future research should focus on developing biocompatible coordination compounds using less toxic metals such as iron, zinc, and magnesium. Integration of coordination chemistry with nanotechnology and biomaterials may lead to advanced multifunctional systems capable of simultaneous catalysis, imaging, and therapy. Additionally, computational modeling and artificial intelligence-assisted ligand design may accelerate the development of optimized coordination complexes. Overall, the discussion confirms that coordination compounds offer significant advantages in both catalytic processes and targeted drug delivery. Their structural diversity, tunable reactivity, and multifunctionality make them promising candidates for sustainable chemical transformations and precision medicine. Continued research in coordination chemistry is expected to expand their applications and overcome existing limitations, ultimately contributing to advances in both industrial and biomedical fields.

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