



A Comprehensive Review of Metal Complexes: Synthesis, Characterization, and Applications

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Abstract

Metal complexes, formed through the coordination of central metal ions with surrounding ligands, occupy a central position in modern chemical research owing to their structural versatility and functional diversity. This review provides a consolidated account of the synthesis, characterization, and applications of metal complexes reported largely within the last decade. The introduction outlines the fundamental principles of coordination chemistry, the historical evolution of the field, and the significance of metal complexes across chemical, biological, and industrial domains. The literature review is organized around four themes: synthetic strategies, including classical, green, and template-assisted routes; spectroscopic and structural characterization techniques such as UV-Vis, FT-IR, NMR, EPR, and X-ray diffraction; biomedical applications encompassing antimicrobial, anticancer, antioxidant, and DNA-binding activities; and catalytic, industrial, and materials-oriented applications such as cross-coupling catalysis, metal-organic frameworks, sensing, and energy conversion devices. Four summary tables consolidate representative examples drawn from the literature. A research methodology section describes the review's literature-search and synthesis approach, followed by a conclusion that draws together recurring structure-activity relationships, and a future work section that identifies emerging directions, including green and sustainable synthesis, artificial-intelligence-assisted complex design, and multifunctional theranostic agents. Collectively, the review underscores that rational ligand design and precise structural characterization remain the two pillars on which the expanding application landscape of metal complexes rests.

Keywords: metal complexes; coordination chemistry; Schiff base; spectroscopic characterization; catalysis; biomedical applications; metal-organic frameworks

1. Introduction

1.1 Background and Significance of Metal Complexes

Metal complexes, also known as coordination compounds, consist of a central metal atom or ion bonded to a surrounding array of molecules or ions called ligands. This coordination arises from the donation of electron pairs from ligand donor atoms, typically nitrogen, oxygen, sulfur, or phosphorus, into vacant orbitals of the metal center. The resulting compounds display an extraordinary range of geometries, oxidation states, and electronic configurations, which in turn govern their color, magnetism, reactivity, and stability. Because the properties of a metal complex can be tuned almost continuously by varying the identity of the metal, its oxidation state, and the structure of the coordinating ligand, coordination

chemistry has become an indispensable toolkit for chemists working across disciplines as varied as medicinal chemistry, materials science, environmental remediation, and industrial catalysis.

The importance of metal complexes is further amplified by their presence in biological systems, where metal ions such as iron, zinc, copper, and cobalt are coordinated within enzymes and proteins to perform essential functions including oxygen transport, electron transfer, and catalysis of metabolic reactions. This natural precedent has inspired the design of synthetic metallodrugs and biomimetic catalysts that borrow principles from nature while introducing new metal-ligand combinations not found in biological systems. Coordination compounds with transition metal ions have found extensive application in the chemical industry, ranging from catalysis to materials synthesis, reflecting the breadth of their utility beyond the laboratory bench (Malinowski et al., 2020).

1.2 Fundamentals of Coordination Chemistry

The theoretical foundation of coordination chemistry rests upon several complementary models, including crystal field theory, ligand field theory, and molecular orbital theory, each of which explains different aspects of metal-ligand bonding and the resulting spectroscopic and magnetic behavior. Ligands are classified according to their denticity, the number of donor atoms that simultaneously bind to a metal center, ranging from monodentate ligands such as water and ammonia to polydentate chelating ligands such as ethylenediaminetetraacetic acid. Chelating ligands generally confer enhanced thermodynamic stability to the resulting complex, an effect commonly referred to as the chelate effect. Coordination number and geometry, which typically range from four-coordinate tetrahedral or square planar arrangements to six-coordinate octahedral geometries, are dictated by the electronic configuration of the metal ion, steric requirements of the ligands, and crystal field stabilization energy considerations.

Schiff base ligands, formed through the condensation of primary amines with aldehydes or ketones to generate an imine functional group, represent one of the most extensively studied classes of chelating ligands in coordination chemistry. Their synthetic accessibility, structural tunability, and ability to stabilize metal ions in a variety of oxidation states have made them a recurring motif throughout the synthetic and biomedical literature reviewed in this paper (Abu-Dief et al., 2021).

1.3 Historical Development of Metal Complex Research

The systematic study of coordination compounds traces its origins to the work of Alfred Werner in the late nineteenth century, whose coordination theory explained the structure of complex salts such as cobalt-ammine chlorides and laid the conceptual groundwork for modern inorganic chemistry. Through the twentieth century, the development of crystal field theory and molecular orbital theory provided increasingly sophisticated explanations for the electronic structure of metal complexes, while advances in X-ray crystallography enabled the direct determination of three-dimensional molecular structures. The latter half of the twentieth century witnessed the emergence of organometallic chemistry and homogeneous catalysis, exemplified by landmark discoveries such as Wilkinson's catalyst and Ziegler-Natta



polymerization catalysts, which demonstrated the industrial relevance of metal complexes on a large scale.

In the twenty-first century, research has increasingly focused on sustainable and green synthetic methodologies, biomedical applications of metal-based drugs following the success of cisplatin, and the design of porous coordination materials such as metal-organic frameworks. Concurrently, the integration of computational tools, including density functional theory and, more recently, artificial-intelligence-assisted screening, has accelerated the rational design of new metal complexes with tailored properties, reflecting a broader shift from empirical trial-and-error synthesis toward predictive, structure-guided design.

1.4 Scope and Objectives of the Review

This review aims to provide an integrated overview of metal complexes by drawing together three interconnected aspects of the field: the synthetic strategies employed to prepare them, the analytical techniques used to characterize their structure and purity, and the diverse applications that have been reported in the literature published predominantly between 2015 and 2024. The specific objectives of this review are: first, to summarize classical and emerging synthetic routes for metal complex preparation, including conventional reflux methods, green and sustainable approaches, and template-directed synthesis; second, to consolidate the principal spectroscopic and structural characterization techniques and the type of information each technique provides; third, to survey representative biomedical applications, including antimicrobial, anticancer, antioxidant, and DNA-interaction studies; and fourth, to review catalytic, industrial, and materials-science applications of metal complexes, including cross-coupling catalysis, metal-organic frameworks, luminescent sensing, and energy-conversion devices. By organizing the literature into these four thematic categories and presenting representative examples in tabular form, this review is intended to serve as a practical reference for researchers entering the field of coordination chemistry.

2. Literature Review

2.1 Synthetic Methods for Metal Complexes

The synthesis of metal complexes has traditionally relied on straightforward solution-based methods in which a metal salt, typically a chloride, nitrate, or acetate, is reacted with a stoichiometric quantity of ligand under reflux in a polar solvent such as ethanol or methanol. This conventional approach remains widely used because it is operationally simple, scalable, and compatible with a broad range of ligand functionalities. For instance, series of transition metal complexes of thiol-substituted triazole ligands have been prepared in alcoholic media under reflux, yielding complexes subsequently confirmed by elemental analysis and spectroscopic methods. Similarly, transition metal complexes of the nonsteroidal anti-inflammatory drug naproxen have been synthesized through direct reaction of the sodium salt of the drug with metal ions, illustrating how existing pharmaceutical scaffolds can be repurposed as ligands for coordination chemistry (Hasan et al., 2016).

Beyond conventional reflux synthesis, a growing body of literature has emphasized environmentally sustainable synthetic methodologies that minimize the use of hazardous solvents, reduce energy consumption, and employ renewable reducing or capping agents.

Green synthesis routes frequently exploit biological extracts derived from plants, algae, or microorganisms, which contain reducing and capping biomolecules such as flavonoids and phenolic compounds capable of converting metal ions into stable nanostructured or coordination products under mild, ambient conditions (Md Ishak et al., 2019). Such approaches are particularly attractive for the preparation of metal and metal oxide nanoparticles intended for antimicrobial and catalytic applications, as they avoid the toxic byproducts associated with conventional chemical reduction methods.

Template-directed and mixed-ligand synthetic strategies represent a further refinement of synthetic methodology, in which auxiliary or co-ligands are deliberately introduced to control the coordination geometry, stoichiometry, or solubility of the resulting complex. Mixed-ligand copper and nickel complexes bearing tridentate donor sets alongside auxiliary imidazole ligands have been synthesized in this manner to enhance aqueous solubility while retaining biological activity. Metal-organic framework synthesis extends this template concept further, employing polytopic organic linkers and metal nodes or clusters that self-assemble into extended, often porous, crystalline architectures; node modification strategies applied after initial framework assembly allow post-synthetic tuning of catalytic and adsorption properties without requiring a completely new synthesis. Across these methods, common variables that determine the outcome of synthesis include solvent polarity, reaction temperature and time, metal-to-ligand stoichiometric ratio, and the pH of the reaction medium, all of which must be optimized empirically or, increasingly, guided by computational prediction. A comparative summary of representative synthetic approaches is presented in Table 1.

Table 1. Representative synthetic methods for metal complexes

Synthetic Method	Typical Conditions	Representative Metal/Ligand System	Key Reference
Conventional reflux (solution) synthesis	Ethanol/methanol, reflux, 2-6 h	Ni(II), Cu(II), Zn(II) triazole-thiol complexes	Related to Abu-Dief et al. (2021)
Schiff base condensation route	Ethanol, room temperature to reflux, metal salt added post-condensation	Zn(II), Pd(II), Cr(III), VO(II) Schiff base complexes	Abu-Dief et al. (2021)
Green/plant-extract-mediated synthesis	Aqueous plant extract, ambient to mild heating, no organic solvent	Ag, Au, ZnO, Cu metal/metal-oxide nanoparticles	Md Ishak et al. (2019)
Mixed-ligand/template synthesis	Co-ligand introduced to	Water-soluble Ni(II)/Cu(II) mixed-	Related to Abdel-Rahman et al.

Synthetic Method	Typical Conditions	Representative Metal/Ligand System	Key Reference
	control geometry and solubility	ligand complexes	(2022)
Self-assembly (metal-organic framework) synthesis	Solvothermal, metal node + polytopic organic linker	Cu(II) MOFs for CO ₂ capture and catalysis	Wang & Astruc (2020)

2.2 Spectroscopic and Structural Characterization Techniques

Rigorous characterization is essential to confirm the successful formation, purity, and structural identity of a newly synthesized metal complex. Elemental analysis remains the starting point in most studies, providing quantitative information on the carbon, hydrogen, nitrogen, and, where applicable, sulfur content of the isolated solid, which is compared against theoretical values calculated for the proposed molecular formula; this technique is particularly valuable for compounds not amenable to high-performance liquid chromatography analysis. Ultraviolet-visible spectroscopy is used to probe electronic transitions within the complex, including ligand-centered pi to pi-star transitions, ligand-to-metal or metal-to-ligand charge-transfer bands, and, for many transition metal ions, d-d transitions that report directly on coordination geometry and ligand field strength.

Fourier-transform infrared spectroscopy is routinely employed to identify shifts in characteristic vibrational bands upon complexation, most notably the shift of the imine carbon-nitrogen stretching frequency in Schiff base complexes, which provides direct evidence of coordination through the azomethine nitrogen. Nuclear magnetic resonance spectroscopy, encompassing both proton and carbon-13 experiments, offers detailed information on the diamagnetic ligand environment and, in favorable cases, can be used to monitor coordination-induced shifts in resonance signals, while electron spin resonance spectroscopy is applied specifically to paramagnetic complexes, such as those of copper(II) or vanadyl ions, to elucidate the symmetry of the metal coordination environment. Magnetic susceptibility measurements complement these spectroscopic techniques by providing the number of unpaired electrons and, therefore, insight into oxidation state and geometry, while molar conductivity measurements in solution distinguish electrolytic from non-electrolytic complexes.

Thermogravimetric analysis is frequently used to establish the thermal stability of a complex and to confirm the presence and number of coordinated or lattice water molecules, information that is often corroborated by mass spectrometry, which additionally confirms the molecular ion peak and overall stoichiometry of the complex. Where single crystals of sufficient quality can be obtained, single-crystal X-ray diffraction provides the unambiguous three-dimensional molecular structure, including precise bond lengths, bond angles, and coordination geometry, while powder X-ray diffraction is used for polycrystalline or nanostructured samples to establish phase identity and crystallite size. Increasingly, density

functional theory calculations are performed alongside experimental characterization to rationalize electronic structure, predict frontier molecular orbital energies, and support molecular docking studies relevant to biological activity (Abdel-Rahman et al., 2022). A summary of these techniques and the structural information they provide is given in Table 2.

Table 2. Principal characterization techniques used for metal complexes

Technique	Information Obtained	Typical Application	Key Reference
Elemental (CHNS) analysis	Elemental composition and purity	Confirming proposed molecular formula	Malinowski et al. (2020)
UV-Vis spectroscopy	Electronic transitions, charge-transfer and d-d bands	Geometry and ligand-field assessment	Abu-Dief et al. (2021)
FT-IR spectroscopy	Vibrational shifts on coordination (e.g., C=N stretch)	Identifying ligand donor atoms	Abdel-Rahman et al. (2022)
¹ H/ ¹³ C NMR spectroscopy	Ligand environment, coordination-induced shifts	Diamagnetic complex structure elucidation	Hasan et al. (2016)
EPR/ESR spectroscopy	Symmetry of paramagnetic metal centers	Cu(II), VO(II) complex geometry	Abdel-Rahman et al. (2022)
Single-crystal/powder XRD	Bond lengths, angles, phase identity	Definitive molecular/crystal structure	Loginova et al. (2022)
Thermogravimetric analysis	Thermal stability, hydration state	Confirming coordinated/lattice water	Malinowski et al. (2020)
DFT computational analysis	Frontier orbitals, reactivity descriptors	Rationalizing electronic structure and docking	Abdel-Rahman et al. (2022)

2.3 Biomedical Applications of Metal Complexes

The biomedical relevance of metal complexes has expanded considerably since the clinical success of the platinum-based anticancer drug cisplatin, prompting extensive investigation of alternative metal centers and ligand frameworks with improved selectivity and reduced toxicity. Schiff base metal complexes, in particular, have been widely reported to exhibit potent antimicrobial activity against both Gram-positive and Gram-negative bacterial strains as well as fungal pathogens, with the coordinated metal ion generally enhancing the lipophilicity of the parent ligand and thereby improving penetration through microbial cell

membranes. Copper(II) and zinc(II) complexes of Schiff bases derived from sulfonamide and benzoin precursors have shown pronounced antifungal and antibacterial efficacy, respectively, underscoring how the choice of metal ion can be tuned to target specific classes of pathogens. Silver(I) complexes, benefiting from the intrinsic antimicrobial character of the silver ion itself, have similarly been coordinated with phenolic Schiff base and salicylic acid derivative ligands to yield compounds with enhanced antibacterial evaluation profiles and favorable interactions with biomolecules such as serum albumin (Loginova et al., 2022).

In the context of anticancer research, metal complexes of cobalt, ruthenium, copper, and vanadium coordinated to pyrimidine- and quinazoline-based Schiff base ligands have demonstrated cytotoxic activity against a range of human cancer cell lines, including breast, lung, colon, and liver carcinoma cells, in several cases exhibiting lower half-maximal inhibitory concentration values than the coordinated free ligand alone (Alkis et al., 2021). The antibacterial activity of metal complexes containing 1,10-phenanthroline has also been highlighted as a promising avenue for combating antibiotic-resistant pathogens, given the ability of phenanthroline-based ligands to intercalate with bacterial DNA and disrupt essential cellular processes (Viganor et al., 2017). Complementing these cytotoxicity studies, DNA-binding and DNA-cleavage assays are routinely performed to probe the mechanism of biological action, while molecular docking simulations increasingly accompany experimental bioassays to predict the binding mode of a candidate complex within a target protein or nucleic acid active site.

Beyond antimicrobial and anticancer activity, metal complexes have also been explored as antioxidant agents capable of scavenging reactive oxygen species, as optical probes for cellular imaging and DNA sensing exploiting the rich photophysical properties of transition metal and lanthanide centers (Berrones Reyes et al., 2021), and as coordination compounds of nonsteroidal anti-inflammatory drugs designed to mitigate the gastrointestinal side effects associated with the free drug while retaining or enhancing its therapeutic action (Santos et al., 2022). Collectively, these findings illustrate that metal coordination is not merely a means of stabilizing a bioactive ligand but can itself introduce new modes of biological action, positioning metal complexes as a distinct and expanding class of therapeutic and diagnostic agents. Representative biomedical applications are summarized in Table 3.

Table 3. Representative biomedical applications of metal complexes

Application	Metal/Ligand System	Reported Biological Outcome	Key Reference
Antibacterial/antifungal activity	Cu(II), Zn(II) sulfonamide/benzoin Schiff bases	Selective activity against bacterial and fungal strains	Abdel-Rahman et al. (2022)
Antibiotic-resistance combating agents	Metal-phenanthroline complexes	Disruption of bacterial DNA function	Viganor et al. (2017)

Application	Metal/Ligand System	Reported Biological Outcome	Key Reference
Anticancer cytotoxicity	Co(II)/Ru(II) pyrimidine Schiff base complexes	Reduced IC ₅₀ vs. free ligand in cancer cell lines	Alkis et al. (2021)
Antibacterial/biofilm inhibition	Ag(I) phenolic Schiff base and salicylate complexes	Antibacterial evaluation, biomolecule interaction	Loginova et al. (2022)
NSAID-based coordination therapeutics	Metal-NSAID (e.g., naproxen) complexes	Enhanced/retained anti-inflammatory action	Santos et al. (2022)
DNA sensing and cellular imaging	Re(I), Ru(II), Ir(III), Eu(III), Tb(III) luminescent complexes	Selective binding to non-duplex DNA topologies	Berrones Reyes et al. (2021)

2.4 Catalytic, Industrial, and Materials Applications

Transition metal complexes occupy a central role in homogeneous and heterogeneous catalysis, underpinning a wide array of industrially important transformations. Palladium and copper complexes have long served as catalysts for cross-coupling reactions such as the Sonogashira coupling, enabling carbon-carbon bond formation between aryl or vinyl halides and terminal alkynes under comparatively mild conditions, a transformation extensively applied in the synthesis of pharmaceuticals, natural products, and conjugated organic materials. First-row transition metal complexes, particularly those of iron and manganese bearing pincer-type ligands, have gained prominence as more earth-abundant and cost-effective alternatives to precious-metal catalysts for hydrogenation and dehydrogenation reactions, with iron complexes shown to catalyze a broad scope of reduction and hydrometalation reactions through metal-ligand cooperative mechanisms (Wei & Darcel, 2019). Bimetallic and heterobimetallic complexes have further extended catalytic scope to challenging transformations such as the hydrogenation of carbon dioxide to formate, exploiting synergistic activation between two distinct metal centers within a single molecular framework (Fickenscher et al., 2023).

Metal-organic frameworks, constructed from metal ions or clusters connected by polytopic organic linkers, represent one of the most rapidly growing application areas for coordination chemistry, owing to their high surface area, tunable pore architecture, and chemically addressable metal nodes. These materials have been applied extensively as heterogeneous catalysts for organic transformations, including carbon dioxide fixation into cyclic carbonates, as well as in gas storage, separation, and, more recently, as antimicrobial materials that exploit the sustained release of metal ions and generation of reactive oxygen species (Wang & Astruc, 2020). The compositional flexibility of metal-organic frameworks,

combined with post-synthetic node and linker modification strategies, allows their catalytic and adsorptive properties to be fine-tuned for specific target reactions or analytes without requiring an entirely new synthetic scaffold.

In the domain of materials science and energy conversion, metal complexes function as photosensitizers in dye-sensitized solar cells, where ruthenium polypyridyl complexes have historically dominated the field owing to their favorable light-harvesting and charge-injection properties, while more recent research has focused on earth-abundant copper complexes as cost-effective alternatives capable of serving as both photosensitizers and redox mediators (Colombo et al., 2021). Luminescent lanthanide complexes, prized for their long excited-state lifetimes and narrow, line-like emission bands, have found application as responsive sensors and probes for anions, biomolecules, and reactive oxygen or nitrogen species in complex biological media, exploiting time-gated detection methods that discriminate lanthanide-centered emission from short-lived background autofluorescence (Bodman & Butler, 2021; Parker et al., 2021). Coordination compounds with transition metal ions additionally find application throughout the broader chemical industry, spanning pigments, catalysts for polymerization, and precursors for the deposition of thin-film materials (Malinowski et al., 2020). Representative catalytic, industrial, and materials applications are summarized in Table 4.

Table 4. Representative catalytic, industrial, and materials applications of metal complexes

Application	Metal/Ligand System	Functional Role	Key Reference
Cross-coupling catalysis	Pd/Cu complexes (Sonogashira-type coupling)	C-C bond formation catalyst	Related MOF/catalysis literature
Hydrogenation/dehydrogenation catalysis	Fe, Mn pincer complexes	Earth-abundant redox catalyst	Wei & Darcel (2019)
CO ₂ hydrogenation catalysis	Heterobimetallic Mo-Ir/Rh complexes	Synergistic bimetallic activation	Fickenscher et al. (2023)
Heterogeneous catalysis/gas capture	Cu(II) metal-organic frameworks	Lewis-acid catalytic sites, CO ₂ capture	Wang & Astruc (2020)
Dye-sensitized solar cells	Cu(I)/Ru(II) polypyridyl photosensitizers	Light harvesting and redox mediation	Colombo et al. (2021)
Luminescent chemosensing	Eu(III), Tb(III)	Selective	Bodman &



Application	Metal/Ligand System	Functional Role	Key Reference
	lanthanide complexes	anion/biomolecule detection	Butler (2021)

3. Research Methodology

This review was compiled using a structured narrative literature review methodology rather than a formal systematic review protocol, reflecting its objective of providing a broad, thematically organized synthesis of the coordination chemistry literature rather than an exhaustive, quantitatively pooled analysis. Relevant peer-reviewed articles, predominantly published between 2015 and 2024, were identified through searches of major scientific databases and publisher platforms, including ScienceDirect, PubMed, Springer, the American Chemical Society Publications platform, and the Royal Society of Chemistry publishing platform, using combinations of keywords such as "metal complex synthesis," "Schiff base coordination compound," "metal complex characterization," "anticancer metal complex," "antimicrobial metal complex," and "metal-organic framework catalysis."

Articles were selected for inclusion based on their relevance to the synthesis, spectroscopic or structural characterization, or application of metal complexes, with priority given to peer-reviewed original research articles and review articles published in reputable, indexed journals. Studies published prior to 2015 were generally excluded unless they represented seminal or historically foundational contributions necessary to contextualize the development of the field, as noted explicitly in the relevant sections of the introduction. For each selected study, key information was extracted, including the metal ion and ligand system employed, the synthetic method used, the characterization techniques applied, and the principal application or biological/catalytic outcome reported. This extracted information was subsequently organized into four thematic categories, namely synthetic methods, characterization techniques, biomedical applications, and catalytic or materials applications, and consolidated into the summary tables presented in the literature review section to facilitate direct comparison across studies. Where multiple studies reported comparable findings, representative examples were selected for detailed discussion and tabulation to avoid unnecessary repetition while still capturing the diversity of metal-ligand systems reported in the literature.

4. Conclusion

This review has traced the interconnected threads of synthesis, characterization, and application that define contemporary research on metal complexes. Across the literature surveyed, several consistent themes emerge. First, ligand design remains the primary lever through which researchers tune the properties of a metal complex, with Schiff base ligands in particular offering a synthetically accessible and structurally versatile platform for introducing a wide variety of donor atom combinations and functional substituents. Second, no single characterization technique is sufficient to establish the structure and purity of a



newly synthesized complex; rather, a complementary combination of elemental analysis, spectroscopic methods, magnetic and conductivity measurements, and, where possible, X-ray diffraction is required to build a complete structural picture, increasingly supported by density functional theory calculations. Third, the applications of metal complexes have diversified substantially beyond their traditional role as catalysts, now spanning antimicrobial and anticancer therapeutics, DNA and biomolecule sensing, dye-sensitized solar cells, and porous framework materials for gas capture and heterogeneous catalysis.

A recurring structure-activity relationship observed throughout the literature is that coordination to a metal ion frequently enhances the biological or catalytic activity of the parent ligand, often attributed to increased lipophilicity, altered redox behavior, or the introduction of an entirely new mode of action associated with the metal center itself. At the same time, the reviewed literature highlights that the translation of promising laboratory-scale metal complexes into clinically or industrially deployed products remains constrained by challenges related to solubility, stability under physiological or process conditions, reproducibility of large-scale synthesis, and, in some cases, cost or toxicity of the metal ion employed. Addressing these constraints will require continued collaboration between synthetic chemists, structural biologists, and materials engineers, underscoring that metal complex research is, and will likely remain, an inherently interdisciplinary endeavor.

5. Future Work

Building on the trends identified in this review, several directions appear particularly promising for future research. Continued development of green and sustainable synthetic methodologies, including plant-extract-mediated synthesis, solvent-free mechanochemical routes, and microwave-assisted synthesis, will be important for reducing the environmental footprint of metal complex preparation while maintaining or improving yield and purity. Expanded use of computational and artificial-intelligence-assisted approaches, including machine-learning-guided prediction of ligand-metal binding affinities and density functional theory screening of candidate complexes prior to synthesis, is likely to accelerate the discovery of new complexes with targeted properties and reduce reliance on trial-and-error experimentation.

In the biomedical domain, future work should prioritize the design of multifunctional theranostic metal complexes that combine therapeutic activity, such as anticancer cytotoxicity, with diagnostic imaging capability within a single molecular scaffold, alongside more rigorous investigation of pharmacokinetics, selectivity toward diseased versus healthy cells, and long-term toxicity profiles to support eventual clinical translation. Further exploration of earth-abundant first-row transition metals, such as iron, manganese, cobalt, and copper, as substitutes for precious and often more toxic metals such as platinum, ruthenium, and palladium, represents an important direction for both economic and environmental sustainability across catalytic and biomedical applications alike. Finally, continued development of metal-organic frameworks and related porous coordination materials for applications in carbon capture, hydrogen storage, and environmental remediation, coupled with improved understanding of their long-term structural stability

under operational conditions, will be essential for translating laboratory-scale successes into deployable technologies addressing pressing energy and environmental challenges.

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