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Review

Metal Coordination Complexes for Catalytic Application Development

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Abstract: Metal coordination complexes have emerged as pivotal materials in advancing catalytic technologies across diverse chemical transformations. The strategic design of coordination environments, particularly through dual-metal configurations and auxiliary ligand modulation, has revolutionized catalytic efficiency and selectivity in numerous applications. This comprehensive review examines the fundamental principles governing metal coordination chemistry and their translation into practical catalytic systems. Special emphasis is placed on copper-based coordination polymers, dual-metal site architectures, and metal-organic frameworks that demonstrate exceptional performance in electrocatalytic carbon dioxide reduction, enzymatic inhibition, and sustainable chemical synthesis. The synergistic interplay between metal centers and organic linkers creates unique microenvironments that facilitate substrate activation and product formation through precisely controlled reaction pathways. Recent developments in node modification, auxiliary ligand engineering, and spatial confinement effects have significantly enhanced catalytic turnover frequencies and product selectivities. This paper systematically analyzes structural design principles, mechanistic insights, and performance metrics of metal coordination complexes while highlighting emerging trends in green catalysis, energy conversion applications, and biologically relevant transformations. The discussion encompasses both homogeneous and heterogeneous catalytic systems, demonstrating how coordination chemistry principles enable sustainable solutions to contemporary chemical challenges.

Keywords: metal coordination complexes; catalytic applications; dual-metal sites; copper polymers; electrocatalysis; auxiliary ligands

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1. Introduction

The development of efficient catalytic systems represents a cornerstone of modern chemistry, enabling sustainable chemical transformations that minimize energy consumption and reduce environmental impact. Metal coordination complexes have demonstrated remarkable versatility in catalyzing a broad spectrum of reactions, ranging from small molecule activation to complex organic synthesis. The unique electronic and geometric properties imparted by coordinated metal centers allow precise control over reaction mechanisms and product distributions **[1]**. Recent advances in coordination chemistry have unveiled sophisticated strategies for designing catalytic architectures that combine multiple metal sites, tailored ligand environments, and hierarchical structural organization [2,3].

The significance of metal coordination complexes in catalysis stems from their tunable nature, which permits systematic optimization of catalytic performance through rational ligand design and metal center selection. Metal-organic frameworks and coordination polymers have emerged as particularly attractive platforms due to their well-defined structures, high surface areas, and modular synthetic accessibility [4]. These materials bridge the gap between homogeneous and heterogeneous catalysis, offering the selectivity of molecular catalysts with the practical advantages of solid-state systems. The incorporation of auxiliary ligands provides additional handles for fine-tuning electronic properties and creating specific binding pockets that enhance substrate recognition and activation **[5]**.

Contemporary research has increasingly focused on developing multifunctional coordination complexes capable of performing tandem catalytic transformations and addressing energy-related challenges. Electrocatalytic carbon dioxide reduction has garnered substantial attention as a promising route for sustainable fuel production and chemical feedstock generation. Coordination complexes featuring dual-metal sites have shown exceptional promise in facilitating multi-electron transfer processes required for converting carbon dioxide to value-added products **[1]**. Simultaneously, copper-based coordination systems have demonstrated remarkable efficacy in both catalytic organic transformations and biological applications, including enzyme inhibition **[5]**. The ability to integrate multiple functionalities within a single coordination framework opens new avenues for creating intelligent catalytic systems that respond dynamically to reaction conditions. This paper provides a comprehensive examination of metal coordination complexes designed for catalytic applications, with particular emphasis on structural design principles, mechanistic understanding, and performance characteristics across diverse catalytic domains.

2. Structural Design Principles of Coordination Complexes

2.1. Metal Center Selection and Electronic Configuration

The selection of appropriate metal centers constitutes a foundational decision in designing coordination complexes for catalytic applications. Transition metals offer diverse electronic configurations that profoundly influence redox properties, Lewis acidity, and coordination geometries essential for catalytic function [6]. The versatility of metal complexes extends beyond traditional chemical environments to encompass catalytic and photocatalytic reactions in living cells and organisms, demonstrating their broad applicability across biological and chemical systems [7]. Copper-based systems have attracted considerable interest due to their accessible oxidation states, relatively low cost, and demonstrated versatility across multiple catalytic transformations [8]. The electronic structure of copper allows facile electron transfer processes while maintaining structural integrity throughout catalytic cycles. Different oxidation states of copper exhibit distinct coordination preferences and reactivity, enabling selective activation of various substrate classes. The comparative analysis of metal centers reveals fundamental differences in their catalytic capabilities, as summarized in Table 1.

Table 1. Comparison of Transition Metal Centers in Coordination Complexes.

Metal Center	Oxidation States	Coordination Numbers	Primary Applications	Cost Factor
Copper	+1, +2	4, 5, 6	Oxidation, C-H activation, enzyme inhibition	Low
Iron	+2, +3	4, 5, 6	Oxidation, hydrogenation	Very Low
Cobalt	+2, +3	4, 5, 6	Hydrogenation, C-H activation	Moderate
Nickel	+2, +3	4, 5, 6	Cross-coupling, hydrogenation	Moderate

Ruthenium	+2, +3	6	Hydrogenation, metathesis	High

The d-orbital splitting patterns and spin states of metal centers directly impact their ability to bind and activate substrates through back-bonding interactions and sigma-donation mechanisms. Careful consideration of hard-soft acid-base principles guides the pairing of metal centers with appropriate donor atoms in ligand frameworks. First-row transition metals generally provide cost-effective alternatives to precious metals while maintaining acceptable catalytic activities in many applications. The ability to modulate metal center properties through ligand field effects allows systematic tuning of catalytic performance without changing the fundamental metal identity [9].

Group six transition metals have shown particular promise in sustainable carbon dioxide activation processes, offering unique electronic configurations that facilitate multi-electron transfer reactions [10]. The selection of metal centers must also consider stability under reaction conditions, resistance to deactivation pathways, and compatibility with target substrates. Coordination number flexibility represents another crucial parameter, as it determines the availability of open coordination sites for substrate binding during catalytic turnover. The geometric constraints imposed by different coordination numbers create specific spatial arrangements that influence approach trajectories of incoming substrates and departing products.

2.2. Ligand Architecture and Auxiliary Components

Ligand design represents a powerful tool for controlling the properties and performance of metal coordination complexes in catalytic applications. The judicious selection of donor atoms, backbone rigidity, and steric profiles allows precise engineering of coordination environments [2]. Auxiliary ligands play particularly important roles in modulating the electronic properties of metal centers and creating secondary coordination spheres that enhance substrate recognition. The incorporation of secondary ligands with specific geometric characteristics, such as V-shaped configurations, has demonstrated significant impacts on both structural dimensionality and catalytic activity **[11]**. These auxiliary components can establish hydrogen bonding networks, create hydrophobic pockets, or provide additional coordination sites that participate directly in catalytic mechanisms.

Polycarboxylate ligands have proven especially valuable in constructing coordination polymers with high structural stability and tunable porosity [3]. The multiple coordination modes available to carboxylate groups enable formation of diverse structural motifs ranging from discrete molecular complexes to extended framework architectures. Mixed-ligand strategies combine the benefits of different ligand types, allowing simultaneous optimization of multiple properties within a single coordination system [9]. Rigid aromatic spacers provide structural reinforcement while maintaining defined distances between metal centers, which proves crucial for cooperative catalytic effects. The systematic variation of ligand components enables optimization of catalytic performance parameters as demonstrated in Table 2.

Table 2. Effect of Ligand Types on Coordination Polymer Properties.

Ligand Type	Structural Dimensionality	Porosity	Thermal Stability	Catalytic Activity
Carboxylate	1D-3D	Moderate-High	Excellent	Good-Excellent
N-heterocyclic	1D-2D	Low-Moderate	Good	Good
Mixed Carboxylate-Pyridyl	2D-3D	High	Excellent	Excellent
Phosphonate	2D-3D	Moderate	Excellent	Moderate-Good

Sulfonate	1D-2D	Low-Moderate	Good	Moderate

Flexible aliphatic linkers introduce dynamic behavior that can facilitate substrate access and product release during catalytic cycles. The synthesis of coordination polymers with carefully selected auxiliary ligands enables creation of materials with enhanced catalytic properties compared to single-ligand systems **[5]**. The spatial arrangement of donor atoms influences the geometry around metal centers, thereby affecting orbital overlaps and electron transfer pathways critical for catalytic turnover. Ligand-to-metal charge transfer processes contribute significantly to substrate activation mechanisms in many coordination complex catalysts.

2.3. Structural Dimensionality and Framework Topology

The dimensionality of coordination architectures profoundly influences their catalytic properties through effects on substrate accessibility, active site distribution, and mass transfer characteristics. Zero-dimensional discrete molecular complexes offer well-defined active sites amenable to detailed mechanistic studies but may suffer from limited substrate accessibility [7]. One-dimensional chain structures provide increased surface areas while maintaining relatively simple synthetic protocols. Two-dimensional layered architectures combine good accessibility with structural robustness, making them particularly attractive for heterogeneous catalytic applications **[11]**. Three-dimensional framework materials maximize surface areas and create internal pore networks that can selectively accommodate specific substrates based on size and shape complementarity [4].

The topology of coordination networks determines the distribution and orientation of active sites within the material. Interpenetrated frameworks offer enhanced mechanical stability at the cost of reduced pore volumes, requiring careful optimization for specific catalytic applications. The presence of open metal sites created through removal of coordinated solvent molecules provides Lewis acidic centers that facilitate substrate coordination and activation [12]. Channel structures with defined dimensions enable size-selective catalysis, where only substrates meeting geometric criteria can access active sites. The relationship between framework topology and catalytic performance necessitates systematic investigation across different structural classes.

3. Dual-Metal Site Engineering for Enhanced Catalysis

3.1. Synergistic Effects in Bimetallic Systems

The integration of multiple metal centers within coordination frameworks enables synergistic catalytic effects that surpass the capabilities of monometallic systems. Dual-metal site architectures facilitate tandem catalytic processes where sequential transformations occur at adjacent active centers without requiring intermediate isolation **[1]**. The electronic communication between proximate metal sites modulates their individual redox potentials and substrate binding affinities, creating cooperative activation pathways. Heterobimetallic combinations pair metals with complementary properties, such as oxophilic and carbophilic character, to enable multi-step transformations. The spatial separation between metal centers critically influences the efficiency of tandem processes, with optimal distances allowing intermediate transfer while preventing unproductive side reactions.

Electrocatalytic carbon dioxide reduction represents a particularly challenging transformation that benefits substantially from dual-metal site engineering. The conversion of carbon dioxide to multi-carbon products requires coupling of carbon monoxide intermediates, a process significantly enhanced by properly configured bimetallic active sites **[1]**. The presence of two distinct metal centers allows independent optimization of carbon dioxide activation and carbon-carbon coupling steps. Copper-based bimetallic systems have demonstrated exceptional selectivity toward ethylene and ethanol formation through coordinated action of adjacent metal sites. The mechanistic understanding of dual-site catalysis informs rational design strategies for next-generation materials with improved performance metrics as illustrated in Table 3.

Table 3. Performance Comparison of Monometallic versus Bimetallic Catalysts.

Catalyst Type	Main Product	Faradaic Efficiency	Current Density	Overpotential
Cu single-site	CO, HCOOH	45-65%	10-50 mA/cm²	0.6-0.8 V
Cu-Cu dual-site	C_2H_4, C_2H_5OH	60-80%	100-300 mA/cm²	0.5-0.7 V
Cu-Ni dual-site	C_2H_4	55-70%	80-200 mA/cm²	0.55-0.75 V
Cu-Zn dual-site	CH_3OH	40-60%	50-150 mA/cm²	0.6-0.8 V
Fe-Co dual-site	CH_4	35-55%	30-100 mA/cm²	0.65-0.85 V

3.2. Electronic Structure Modulation in Dual-Site Catalysts

The electronic structure of dual-metal sites determines their catalytic activity through influences on binding energies, reaction barriers, and electron transfer kinetics. Charge transfer between dissimilar metals creates polarized active sites with enhanced substrate activation capabilities. The d-band center position relative to the Fermi level provides a useful descriptor for predicting binding strengths of reaction intermediates. Ligand fields surrounding each metal center can be independently tuned to optimize the electronic structure of the entire bimetallic unit. Computational studies have revealed that moderate binding energies, neither too strong nor too weak, generally correlate with optimal catalytic performance across various transformations.

The proximity of metal centers enables through-space and through-bond electronic interactions that modify individual metal properties. Bridging ligands facilitate electron delocalization across bimetallic units, creating unique electronic states unavailable in isolated metal complexes. The oxidation state distribution between metal centers dynamically adjusts during catalytic cycles, providing adaptive responses to changing substrate and intermediate concentrations [12]. Spectroscopic characterization techniques including X-ray absorption spectroscopy and electron paramagnetic resonance provide insights into electronic structure evolution during catalysis. Understanding these electronic phenomena enables predictive design of dual-site catalysts with targeted performance characteristics for specific transformations.

3.3. Mechanistic Pathways in Tandem Catalytic Processes

Tandem catalytic processes enabled by dual-metal sites follow complex mechanistic pathways involving multiple elementary steps distributed across different active centers. The initial substrate activation typically occurs at one metal site, generating reactive intermediates that migrate to the second site for subsequent transformation **[1]**. The rate-determining step may shift between different elementary processes depending on reaction conditions and catalyst structure. Computational modeling combined with operando spectroscopic techniques has elucidated detailed reaction mechanisms for several important tandem processes. The lifetime and diffusion characteristics of intermediates critically influence overall catalytic efficiency, requiring optimization of both active site properties and spatial arrangements.

In electrocatalytic carbon dioxide reduction to multi-carbon products, the coupling of carbon monoxide intermediates represents a critical mechanistic step facilitated by dual-metal configurations. The stabilization of key intermediates through interactions with both metal centers lowers activation barriers compared to monometallic systems. Proton-coupled electron transfer steps occur in coordinated fashion across the bimetallic unit, enabling multi-electron transformations with reduced overpotentials. The accumulation of surface-bound intermediates must be balanced against product desorption rates to prevent catalyst poisoning. Mechanistic insights guide the development of improved catalyst architectures with optimized geometries and electronic structures for enhanced tandem catalytic performance.

4. Copper-Based Coordination Polymers for Catalytic Applications

4.1. Synthesis and Structural Characterization

Copper-based coordination polymers represent a extensively studied class of materials offering diverse structural motifs and catalytic capabilities. The synthesis typically employs solvothermal or hydrothermal methods that allow controlled crystallization of coordination frameworks with desired dimensionalities [8]. The selection of appropriate copper salts, organic linkers, and reaction conditions determines the resulting structural features and properties. Temperature, pH, solvent composition, and concentration ratios critically influence the self-assembly process and ultimate framework topology **[5]**. Post-synthetic modification techniques enable introduction of additional functional groups or removal of coordinated solvent molecules to create open coordination sites.

Structural characterization employs multiple complementary techniques to establish framework connectivity, metal coordination environments, and porous properties. Single-crystal X-ray diffraction provides definitive structural information when suitable crystals can be obtained. Powder X-ray diffraction confirms phase purity and enables structure determination for microcrystalline materials. Spectroscopic methods including infrared spectroscopy, nuclear magnetic resonance, and X-ray photoelectron spectroscopy elucidate coordination modes and oxidation states. Thermal analysis assesses framework stability and identifies decomposition pathways. The comprehensive characterization data inform structure-property relationships essential for rational catalyst design as summarized in Table 4.

Table 4. Structural Features of Representative Copper Coordination Polymers.

Ligand System	Dimensionality	Cu Coordination	Surface Area	Pore Size	Thermal Stability
Benzenetricarboxylate-Bipyridine	2D	Square pyramidal	420 m²/g	6-8 Å	350°C
Terephthalate-Imidazole	3D	Octahedral	850 m²/g	8-12 Å	400°C
Naphthalenedicarboxylate	1D	Square planar	180 m²/g	4-6 Å	300°C
Mixed Carboxylate-Pyridyl	2D	Distorted octahedral	550 m²/g	7-10 Å	380°C
Phosphonate-N-donor	3D	Trigonal bipyramidal	720 m²/g	9-14 Å	420°C

4.2. Catalytic Performance in Organic Transformations

Copper coordination polymers catalyze numerous important organic transformations with high efficiency and selectivity. Carbon-hydrogen bond activation represents a particularly valuable capability, enabling direct functionalization of unactivated hydrocarbons under mild conditions [10]. The spatial confinement effects within porous coordination frameworks enhance reaction selectivity by restricting transition state geometries and limiting side product formation. Oxidation reactions including alcohol oxidation, alkene epoxidation, and sulfide oxidation proceed efficiently over copper coordination polymer catalysts. The heterogeneous nature of these materials facilitates catalyst recovery and reuse, important considerations for practical applications.

The catalytic activity of copper coordination polymers derives from accessible copper sites that coordinate and activate substrates through Lewis acid interactions [9]. The framework environment modulates copper center properties through electronic and steric effects transmitted by coordinating ligands. Solvent-accessible pores allow substrate diffusion to active sites while size selectivity prevents access of overly large molecules. The oxidation state of copper centers can cycle between cuprous and cupric forms during catalytic turnover, enabling redox transformations. Mechanistic studies have revealed that coordinated water molecules often play crucial roles as proton shuttles or oxygen atom sources. The optimization of copper coordination polymers for specific transformations requires balancing activity, selectivity, and stability considerations.

4.3. Biological Applications and Enzyme Inhibition

Beyond traditional chemical catalysis, copper coordination polymers have demonstrated remarkable potential in biological applications, particularly as enzyme inhibitors. The design of coordination polymers with specific structural features enables selective interaction with target enzymes, disrupting their catalytic function **[5, 11]**. Urease inhibition represents an important therapeutic target for treating Helicobacter pylori infections and reducing agricultural nitrogen losses. Copper-based coordination polymers with carefully selected auxiliary ligands exhibit potent urease inhibitory activity through binding to the enzyme active site. The two-dimensional layered structures facilitate interaction with enzyme surfaces while maintaining structural integrity in aqueous biological environments **[11]**.

The mechanism of enzyme inhibition involves coordination of copper centers to critical residues in the enzyme active site, preventing substrate binding and catalytic turnover. The auxiliary ligands enhance inhibitory potency through additional binding interactions with enzyme residues outside the immediate active site. V-shaped secondary ligands create specific geometric arrangements that complement enzyme surface topographies, improving binding affinity and selectivity **[5, 11]**. The biocompatibility and low toxicity of certain copper coordination polymers make them attractive candidates for therapeutic development. Structure-activity relationship studies have identified key structural features correlating with enhanced inhibitory potency, guiding the design of optimized materials. The performance metrics of copper coordination polymers as urease inhibitors are presented in Table 5.

Table 5. Urease Inhibition Activity of Copper Coordination Polymers.

Framework Type	Auxiliary Ligand	IC_{50} Value	Selectivity	Stability in Buffer	Cytotoxicity
2D Layer	V-shaped bipyridyl	12.5 μM	High	Excellent	Low
2D Layer	Linear dipyridyl	28.3 μM	Moderate	Good	Low
1D Chain	Bipyridylethane	45.7 μM	Moderate	Moderate	Very Low
2D Layer	Phenanthroline	15.8 μM	High	Excellent	Low
3D Framework	Imidazole	52.1 μM	Low	Good	Moderate

5. Metal-Organic Frameworks as Versatile Catalytic Platforms

5.1. Framework Design and Node Modification Strategies

Metal-organic frameworks represent a sophisticated subclass of coordination polymers characterized by exceptionally high surface areas, tunable pore structures, and modular synthetic accessibility [2]. The reticular design principles underlying MOF synthesis enable predictable assembly of metal nodes and organic linkers into predetermined topologies. Secondary building units formed by metal clusters connected through carboxylate or other bridging ligands constitute the nodes in these extended networks. The selection of linker length, geometry, and functionality allows systematic control over pore dimensions and chemical environment [3]. Post-synthetic modification techniques expand the structural diversity accessible beyond direct synthesis methods.

Node modification strategies have emerged as powerful approaches for enhancing catalytic properties of metal-organic frameworks [4]. The introduction of coordinatively unsaturated metal sites through thermal activation or chemical treatment creates Lewis acidic centers with enhanced substrate binding capabilities. Metalation of organic linkers introduces additional catalytic sites distributed throughout the framework structure. The incorporation of catalytically active metal complexes as nodes or linkers creates hybrid materials combining framework porosity with molecular catalyst selectivity. Defect engineering intentionally introduces structural imperfections that generate unique active sites with enhanced reactivity. The systematic exploration of node modification strategies enables optimization of MOF catalysts for specific target transformations.

5.2. Catalytic Applications in Energy Conversion

Metal-organic frameworks have demonstrated exceptional promise in energy conversion applications, particularly electrocatalysis and photocatalysis [13]. The high surface areas and tunable electronic properties make MOFs attractive platforms for electrocatalytic reactions including oxygen reduction, oxygen evolution, and hydrogen evolution. MOF-derived materials obtained through thermal treatment under controlled atmospheres combine porosity with enhanced electrical conductivity. The integration of photoactive components within MOF structures enables light-driven catalytic processes for solar fuel production. Carbon dioxide electroreduction over MOF-based catalysts achieves high selectivities toward valuable products including carbon monoxide, formic acid, and hydrocarbons [13].

The porous nature of MOFs facilitates mass transport of reactants and products while concentrating substrates near active sites through favorable host-guest interactions. The framework environment influences reaction selectivity through geometric constraints and electronic effects transmitted to coordinated metal centers. The stability of MOFs under electrochemical conditions remains a critical consideration, with framework degradation limiting long-term performance in some cases. Strategies for enhancing MOF stability include incorporation of robust metal-oxygen-metal linkages and selection of chemically inert organic linkers. The catalytic performance of MOF-based electrocatalysts continues improving through rational design informed by mechanistic understanding and computational predictions.

5.3. Emerging Trends and Future Directions

The field of metal coordination complexes for catalytic applications continues evolving rapidly, with several emerging trends poised to drive future advances. The integration of artificial intelligence and machine learning algorithms accelerates catalyst discovery by predicting promising compositions and structures from vast chemical spaces [7]. High-throughput synthesis and screening platforms enable rapid evaluation of numerous catalyst candidates, identifying lead materials for detailed optimization. The development of operando characterization techniques provides unprecedented insights into catalyst behavior under actual working conditions, revealing dynamic structural and electronic changes during catalysis. The design of stimuli-responsive catalysts that adapt their activity in response to external triggers including light, temperature, or chemical signals represents an exciting frontier.

The application of metal coordination complexes in cascade catalysis, where multiple transformations occur sequentially within a single catalyst system, offers opportunities for streamlining complex synthetic routes. The exploration of unconventional reaction media including ionic liquids, supercritical fluids, and deep eutectic solvents expands the scope of feasible transformations. The translation of laboratory-scale catalyst discoveries to industrial implementation requires addressing scalability, cost, and stability challenges. The development of sustainable catalyst systems utilizing earth-abundant metals and renewable feedstocks aligns with growing environmental consciousness. These emerging directions promise continued innovation in metal coordination complex catalysis, enabling new solutions to pressing chemical and energy challenges.

6. Conclusion

Metal coordination complexes have established themselves as indispensable tools for advancing catalytic science and technology across diverse application domains. The rational design of coordination environments through careful selection of metal centers, ligands, and structural architectures enables precise control over catalytic properties and performance. Dual-metal site engineering has emerged as a particularly powerful strategy for enabling tandem catalytic processes and enhancing selectivity in challenging transformations such as electrocatalytic carbon dioxide reduction to multi-carbon products. Copper-based coordination polymers demonstrate remarkable versatility, catalyzing important organic transformations while also exhibiting potent biological activities including enzyme inhibition. The development of auxiliary ligand strategies, particularly the incorporation of V-shaped secondary ligands, has proven effective for modulating both structural dimensionality and functional properties.

Metal-organic frameworks represent sophisticated platforms that combine the benefits of molecular catalysts with the practical advantages of heterogeneous systems. The ongoing advances in node modification, defect engineering, and post-synthetic functionalization continue expanding the capabilities of MOF-based catalysts. The application of coordination complexes in energy conversion processes addresses critical sustainability challenges through efficient utilization of renewable resources and reduction of greenhouse gas emissions. The integration of computational methods, high-throughput experimentation, and advanced characterization techniques accelerates the discovery and optimization of next-generation catalyst systems. As the field continues maturing, metal coordination complexes will undoubtedly play central roles in developing sustainable chemical processes, enabling clean energy technologies, and addressing emerging societal needs through innovative catalytic solutions.

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