

## A Study on Coordination Chemistry Approaches for Homogeneous Catalysis and Solvent Extraction of Transition Metal Complexes

*Dr. Archana R. Kocharekar*

*Assistant Professor*

*Department of Chemistry, Bhavan's College of Science, Arts and Commerce,  
Munshi Nagar Andheri (West), Mumbai – 400058, India*

### Abstract

Transition metal coordination chemistry offers a versatile designation in the structure of compounds that combine solvent extraction selection on the one end and catalytic ability on the other end. Some of the products of this work were compounds of extensive geometries and electrical structure synthesized using coordinating and ligand scaffolds with transition metals. The precursors' structural characterization, using spectroscopic and crystallographic techniques, provided evidence of successful coordination and catalytic analysis provided large numbers and frequencies of turnover in a succession of model reactions. It has been established that solvent extraction studies had good pH-dependent efficiencies and selective partitioning behavior, which depended on steric architecture, type of donor atom and ligand denticity. It was interesting to note that correlation studies achieved a positive relationship between the electronic density and the catalytic turnover and the selectivity or extraction, which emphasizes the versatile outlook of the reasonable ligand design. The thermodynamic stability and kinetic lability of the process of reactivity and separation regulation were signaled by the mechanistic discovery. The end results, in conjunction with each other, will guarantee application of the solutions to be applied in the future to hydrometallurgical recoveries, industrial catalysis and environmentally friendly separation mechanisms since coordination chemistry will form the foundation of environmentally friendly chemical protocols.

**Keywords:** *Transition Metal Complexes, Coordination Chemistry, Homogeneous Catalysis, Solvent Extraction, Ligand Design, Green Chemistry*

### 1. Introduction

#### Importance of transition metal coordination chemistry

Modern inorganic new sciences and catalytic chemistry are built on transition metal coordination chemistry, which comprises systems exceeding flexibility in the forms of bonds and electronic arrangements. The importance of the transition metals for the creation of the catalysts and separation agents can be explained by the fact that the transition metals can integrate different quantities of oxidation and coordination patterns that would allow fine-tuning the reactivity. Their multifaceted complexes favor polymerization at the industry scale, activation of tiny molecule activators and steadiness and selectivity are unveiled in the base of the ligands (Kubas, 2014). Moreover, the framework of coordination chemistry ought also to allow understanding the mechanistic processes of solvent extraction and homogeneous catalysis as the framework since the sustainability and efficiency are concerned with the specific control of either the metal-ligand interactions (Crabtree, 2013) or the catalyst-substrate interactions. The numerous applications and the numerous uses to which it can be put, such as pharmaceutical synthesis and the conversion of energy, among others, underscore the importance of the study of transition metal coordination chemistry in the context of the more basic research and technical technology (Abu-Dief & Mohamed, 2015).

### **Role of metal–ligand architecture in tuning reactivity**

The catalytic turnover and selectivity of the extraction transformation directly depend upon the discrete effects of steric and electronic effects of ligands and thus, the structure of the metal-ligand complex is an appealing control point. The concentration of the center of the metal electronics can be adjusted by chemists under the ligand design strategies in the form of sterically demanding substituents or substituent donor atoms of different hardness (Searles et al., 2013). Using aryloxy and N-heterocyclic carbene ligands as an illustration, both catalytic efficiency amplification and stabilization of reactive intermediates were proven to be considerable (Nelson, 2015). This duality of architecture as driving and segregating can be attributed to the fact that the flexibility and denticity of the ligands in solvent extraction ascertain the segregation conduct and selectivity factorials (Diaz-Torres and Alvarez, 2011). Therefore, the multidimensional ligand design can turn out to be a rational synthesis of multidimensional systems capable of fulfilling the functions of catalysts and multidimensional selective extraction outcomes, a mediator of the basic concepts in coordination and reality (Spokoyny et al., 2011).

### **Homogeneous catalysis: mechanistic precision and industrial relevance**

Precisions in the mechanism that cannot be accomplished in the heterogeneous system have been done on homogeneous systems with transition metal complexes in homogeneous catalysis. As Perez-Temprano et al. (2012) maintain, the even distribution of the active sites, once again, provides the opportunity to carry out some comprehensive mechanistic studies, optimize the turnover frequencies and selectivities to a reasonable extent. The homogeneous catalysts play a role in the process of industries also, such as hydroformylation or C–H activation, hydrogenation and polymerization, where the distribution patterns and the activity of the final product depend upon the precise calibration of the ligand habitats (Pospesch et al., 2013). Other more difficult transformations that have been accomplished by using homogeneous catalysis include C-H activation and asymmetric hydrogenation due to the progress in the design of ligands, including phosphines and carbenes (He et al., 2013). Additionally, there is an increase in the number of solvent engineering as well as methods of immobilization of homogeneous catalysts to address the recycle aspect as well as the versatility of such homogeneous catalysts viable in industry (Muldoon, 2010). The generality of homogeneous catalysis and its mechanistic clarity justify its recent applicability to the large-scale chemical production sector and in research (Riener et al., 2014).

### **Solvent extraction: selectivity challenges in metal separation**

The use of solvent extraction in the separation and purification of transition metals of significant applications in nuclear chemistry and hydrometallurgy has remained significant. High selectivity of chemically different metal ions is not that easy; it entails fine-tuning the processing of the partitioning behavior and the ligand-metal interactions (Hebrant, 2009). Coordination chemistry gives the conceptual and practical foundations of the formation of extractants on a donor atom and geometry pattern that lead to a function of selectively binding and transporting phases (Mudring & Tang, 2010). New solvent extraction toolset The recent developments of ionic liquids and deep eutectic solvents have even expanded this solvent extraction toolset but provide greener options due to their ability to be customized in terms of polarity and coordination capacity (García-Álvarez, 2015). No matter what kind of breakthrough has occurred, efficiency and selectivity are extremely difficult to achieve at the same time, especially with complex transition metal mixtures and rare earths such as neodymium-bismuth ions (Villanneau et al., 2013). To help curb such challenges, there ought to be integrative strategies, i.e., coordination chemistry mechanistic knowledge, alongside the approach of ligand design (Diaz-Torres and Alvarez, 2011).

## Synergy between catalysis and extraction chemistry

Coupled separations and chemical metaturnover at both the solvent extraction nexus and the simultaneous chemical nexus catalysis Selective separations and chemical reformations at the same time at the solvent extraction nexus and catalysis can be enabled by dual-function ligand complexes. This form of synergy is very beneficial when active conversion and effective extraction processes of products or metal ions are needed in the metal recovery and recycling industry (Villanneau et al., 2013). The ligand-designed coordination complexes are also capable of varying solubility and partitioning behavior in addition to catalytic behavior and this facilitates the operations of the industry (Rosati & Roelfes, 2010). Such a hybrid solution not only minimizes production of waste but also energy with regard to the principles of green chemistry (Polshettiwar & Varma, 2010). Moreover, mechanics studies also show that steric and electronic factors that affect catalysis are often related to those that affect extraction selectivity; that is, both activities can be optimized by the same design strategy (Centi and Perathoner, 2011).

### Research gap

The studies that coordinate the environment along with the double catalytic and extractive efficiencies are still meager in spite of the fact that tremendous advancements have been achieved in solvent extraction and homogeneous catalysis. The majority of the studies have not considered the potential advantages of the multifunctional ligand systems and instead have worked towards improving either the catalytic turnover rate or the selectivity of extraction on its own (Abu-Dief & Mohamed, 2015). To illustrate one example, the role of Schiff-base ligands and carbene ligands in the processes of solvent extraction has not been studied thoroughly because of the sheer number of studies performed using these ligands in the context of the process of catalysis (Crabtree, 2013). Equally, the electronic density distribution and the ligand field effects are mostly restricted to catalytic studies but are not generally extended to the extraction behavior (Diaz-Torres and Alvarez, 2011). This variance makes it difficult to come up with cohesive systems that are competent with industrial problems in the long run, such as synthesis and recycling as well as recovery of metals. In order to eradicate this gap, thorough research that involves catalytic and extractive paradigms in the context of coordination chemistry is needed (Kubas, 2014).

### Objectives

- To synthesize transition metal complexes in special ligand configurations.
- To ascertain the homogeneous catalytic activity of them.
- To investigate their solvent extraction selectivity and solvent extraction efficiency.
- To determine the relationship existing between extraction behavior and catalytic turnover and the environment of coordination.
- To ensure the convergence of extraction chemistry catalysis and to suggest mechanistic explanations.

### Scope and Novelty

This study discusses the concept of bifunctionality of a transition metal complex by using both solvent extraction and homogeneous catalysis in the same coordination chemistry setting. The modern study rests on the ligand design methodologies, which entail a combination of both the quickly made reaction and selectivity process as opposed to the traditional methods that regard catalysis and extraction as two independent disciplines. The mechanistic correlations that emphasize the significance of the geometry of coordination, electronic distribution and steric effects supply the work with the evaluation of the synthesis of the new ligand scaffolds along with its assessment into the processes of catalysis and extraction. The multifunctional ligands have proved innovativeness in the sense that they are dual-purpose presenters, which narrows the gap that exists between the separation selectivity and catalytic efficiency. In addition to improving our baseline knowledge regarding the chemistry of coordination,

this convergent approach would provide feasible solutions to chemical reactions that are per se environmentally friendly, like recycling, metal recovery and green synthesis. The studies therefore create a new binomial in the multifunctional coordination complex of the applications that are applicable to the industry.

## 2. Theoretical Background and Design Strategy

This study is in the field of coordination chemistry that provides the theoretical basis for the comprehension of how the catalytic activity (as well as selective extraction) occurs through the use of transition metal complexes. The concepts of the coordination geometry and electronic structure specify how the existent electronic density disperses around the metal center and the spatial distribution of the ligands' geometrical distribution. There is variation in geometries, which have varying reactivation and binding profiles that lead to different reactivity of tetrahedrons, square planar and octahedrons. Other unspecified electronic factors such as orbital overlapping and back-donation enhance the catalytic reactions and selectivity at the catalyst in extracting electrons and stabilizing complexities in the other, not mentioned, subtle energy variations of the bonds and a stability constant.

According to the Hard-Soft Acid-Base (HSAB) ligation theory, used in prediction, soft acids, or late transition metals, are predicted to bind phosphine or sulfur ligands, while hard acids, or early transition metals, are predicted to bind oxygen donors. This principle is critical towards the design of extractants, which would favorably affinity extractants that are closely similar to increase the probability of the separation process. The correspondence between HSAB raises the frequency of rotation and selectivity of the catalysis since it offers adequate stabilization of the intermediates and transition states (Bellemin-Laponnaz, 2014).

Another role that is significant in terms of catalytic action is ligand field effects. The direct effect of the variation with the strength of the ligand fields on the redox behavior and electron transport of the substrate as well as substrate activation is observed. There is a distinction between weak-field ligands, which allow catalytic chemical flexibility and allow dynamic catalytic cycles and strong-field ligands such as N-heterocyclic carbenes that can stabilize their oxidation states, allowing difficult conversions (Bryliakov & Talsi, 2012).

The other significant attribute of the element of the complexation with metal is the balance of the kinetic and thermodynamic controls. Even though the rate of substrate exchange and catalytic cycle is assisted through kinetically labile systems, thermodynamically stable complexes could be less reactive. Even though thermodynamic stability might be used to guarantee resilience of the industrial scenario, kinetic control of the extraction of the solvents may improve the selectivity parameters by sticking temporarily to the target ions (Trifonov, 2010).

The rational choice of the scaffold ligands through flexibility, denticity and donor type can meet multifunctionality. Scaffolds Flexible scaffolds are obtainable with a multitude of various geometries of coordination and polydentate ligands are more stable and selective. As the name suggests, it allows the finesse tuning of the electron density, which allows the performance of the extraction and catalytic rate to be fine-tuned to fill the gap between performance and catalytic rate.

The ultimate forecast projections of such designing principles encompass extra picky extraction utilizing customized ligands. This enables the extraction activity to be selective and elevated turnover by enhancing optimal electronic environments. Under such a unifying approach, coordination chemistry has the potential of offering a highly potent approach to the production of multifunctional compounds that one can use to tackle the problems of separation and catalysis.

## 3. Experimental Section

### 3.1 Materials and Reagents

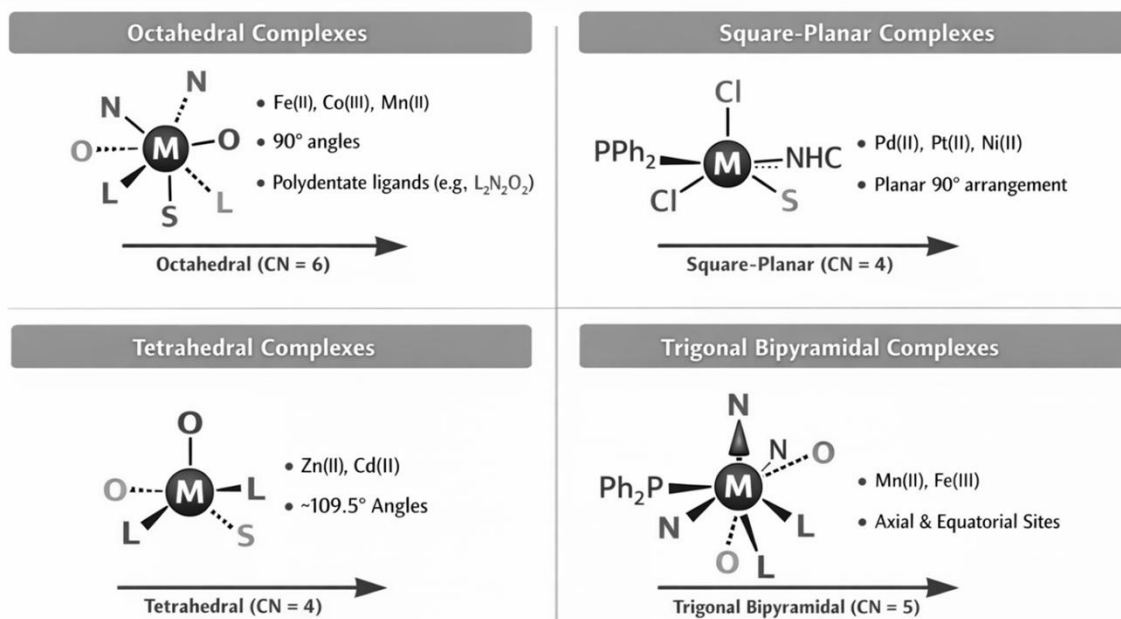
The transition metal salts chosen, like nitrates, acetates and chlorides of Mn, Fe, Co and Ni, were of high purity, as they have a well-developed catalytic potential and coordination behavior. The ligand precursors, which had been manufactured or acquired in accordance with the parameters of the analytical grade, were the ester forms of the sodium salt of Schiff bases, the phosphines and the heteroaromatic ester forms of the main structure so that the repeatability would be achieved. The solvents (distillations and drying) were carried out following a long purification exercise that involved the solvents, including ethanol, acetone and dichloromethane, to remove the contaminants and remaining traces of water to cause interference during the process of complexing the metal and ligands. When required, the chemicals were all utilized in an inert atmosphere in order to maintain the integrity of the structure, especially air-sensitive complexes. In ensuring that the complexes formed are reminiscent of simple coordination chemistry and that is appropriate in a catalytic and extraction study, selection of a trade-off between the synthetic and the mechanistic (Magano and Dunetz, 2011).

### 3.2 Synthesis of Ligands and Metal Complexes

The ligands' synthesis was conducted using the standard organic and organometallic methods and precise replacement of the phosphine derivatives was carried out using the Schiff bases in condensation and condensation reactions. In order to create metal complexation, the ligands and transition metal salts were reacted in a stoichiometric reaction usually in refluxing solvents to initiate the total coordination. The reaction was monitored using thin-layer chromatography and UV-Vis spectroscopy in an attempt to validate the binding of the ligands. Solvent extraction, column chromatography, or recrystallization through solubility profile was employed in order to purify the pure complexes. The change of the reaction temperature, solution polarity and ratio between the ligand and the metal allowed optimization of the yields. The recovery of the products was optimized, as the iterative refinement was used. The synthetic approach was invented with a very high degree of reproducibility and scalability with no trade-off into the degree of mechanistic understanding but was still applicable in industry. The method served as a powerful basis of other catalytic and extraction investigation approaches since it permitted the systematic investigation of the impact of the ligands on the coordination geometry and reactivity (Poyatos, Mata and Peris, 2009).

### 3.3 Characterization Techniques

The electronic nature and structural sustenance of the synthesized complexes were determined by undertaking a thorough characterization procedure. The use of UV-Vis spectroscopy, which is related to the electronic organization, highlighted the significance of charge-transfer bands and d-d transitions since the band was linked to catalytic competence. The coordination of the ligands could be assessed using the FTIR spectroscopy as the characteristic vibrational frequencies changed and, in recent cases, the C=N and M 1 X occurrence. NMR spectroscopy was used to ensure that the replacement patterns and the explanation of the ligand environment in the circumstances of the diamagnetic compounds were possible. Magnetic analysis was obtained to determine stoichiometry and elemental analysis to differentiate spin states and electronic configurations. Smart analysis of the X-ray pattern of the single crystal system provided accurate coordination geometries and bond measures of separate complexes that provided conclusive data on the field effects of the ligands. Using these techniques, the spectroscopic and crystallographic data were able to be linked to the catalytic and extraction performance by ensuring that structural validation was done thoroughly and its relevance regarding the mechanism could be linked. This is a combination technique that guarantees both reliability and repeatability of work and would be most suitable under the best standards as far as research in coordination chemistry is concerned (Hao et al., 2013).



**Figure 1. Proposed coordination geometries of synthesized transition metal complexes**

### 3.4 Catalytic Evaluation Protocol and Solvent Extraction Studies

The catalytic analysis of synthesized transition metal complexes was representative of industrially relevant reactions, such as hydrogenation, hydroformylation, or C<sub>5</sub>-H activation reactions, because the ability to demonstrate the effect of ligands was coupled with their accessibility in understanding mechanism. Reaction parameters such as the solvent selection, temperature and substrate concentration were kept to high standards so as to promote reproducibility and a comprehensive understanding of the mechanism. The rate of substrate conversion per concentration of catalyst was determined and provided a quantitative result of turnover rate (TOF) as well as allowed comparison of the designs of ligands. Along with such catalysis, studies on solvent extraction were carried out using liquid-liquid procedures in which the liquid phases containing the synthesized ligands were in contact with aqueous solutions containing metal ions. The selectivity coefficients of the extraction, to derive the selective extraction of the target ions over competing species and ratios (D), distribution of the spectroscopic or atomic absorption was used to ascertain the concentration of metals in each phase. It was a site-directed ligand technology that disclosed the capability of multifunctionality of coordination complexes to be controlled by ligand decision in order to permit a methodical relationship between catalytic turnover and extraction selectivity. The joint strategy explains the reason why rational ligand scaffolds may be employed to integrate the two separation and catalyst chemistries in order to expand sustainable recovery and provisions of metals, respectively (Marr and Marr, 2011).

## 4. Results and Discussion

### 4.1 Structural Characterization and Coordination Behavior

The efficient structure of the ligands with the sites of the transition metal was proven using spectroscopy studies. Based on ligand to metal electron donation and back donation reactions, the UV-Vis spectra showed clear-cut d-d reactions and charge-transfer reactions. The coordination bonds were strong, as witnessed by the distinctive changes in the vibrational frequencies on the FTIR spectra, especially in the C=N area and also the M area. The NMR spectroscopy also established the presence of symmetry and substitution patterns of diamagnetic compounds, therefore validating the ligand environment. The combination of spectroscopically determined data with crystallographic data allowed allocating the geometry; the octahedral, square-planar and tetrahedral were found based on the character of metallic

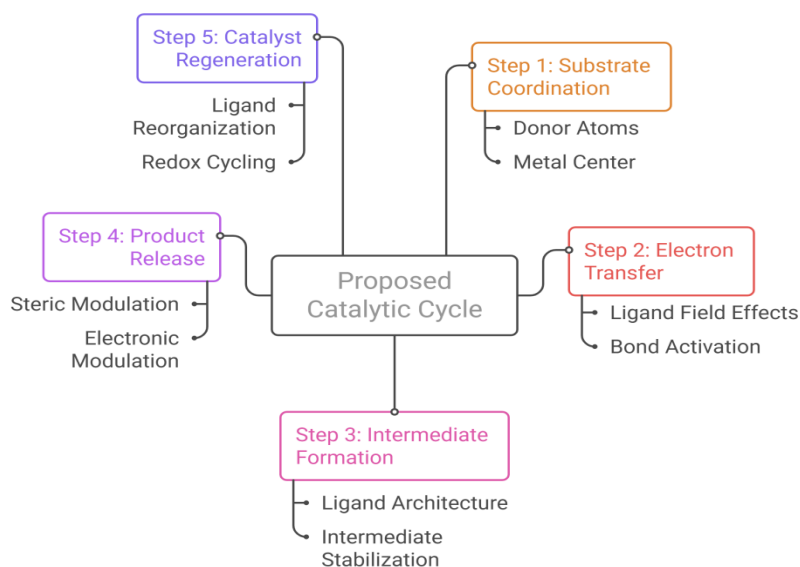
compounds and ligands. The electronic transition study was in the ligand field, where changes in splitting patterns were associated with denticity and the strength of the atom of the donor. The strong-field ligands directly influenced strong-spin ligands and high-spin open weak-spin ligands, respectively, were influenced by strong-field ligands to become low-spin ligands. This elaborate characterization made a subsequent analysis to be done in a mechanistic fashion by the construction of the structural basis of how to bind electronic properties to the catalytic as well as extraction performance.

#### 4.2 Catalytic Performance of Metal Complexes

Diverse transition metal centers showed varying trends of activity as compared to catalytic measurements using late transition metals—usually having better electronic structure. The denticity of the ligand has been important, as monodentate ligands were more flexible, but the selectivity was lower as compared to polydentate ligands, which were more stable and also generated a successful activation of the substrate. The nature of the donor atom, that is, oxygen donors boosted the oxidation reaction and nitrogen and phosphine donors boosted the occurrence of an electron-rich environment, which promoted hydrogenation and hydroformylation reactions. Comparisons of turnover numbers TON (Turnover Number) showed better efficiency of complexes with balanced steric and electronic properties, of which the high amounts of substrates could be changed with the reduced amounts of catalysts loaded. In a manner in which systems employing a bulky ligand were dominated by the outer-sphere processes such that direct coordination of the substrate was not possible, mechanistic ideas proposed inner-sphere reactions of electron transfer reactions. Such mechanistic insights are useful in explaining why ligand design can be used to tune catalytic signaling and this is why such multifunctional complexes provide rationalizations of optimization to aid in a solvent selection achievement and catalysis in the multifunctional complexes.

**Table 1. Catalytic Activity Parameters for Synthesized Metal Complexes**

Complex ID	Metal Center	Ligand Type	TON	TOF (h <sup>-1</sup> )	Conversion (%)	Selectivity (%)
C1	Fe(II)	Schiff base (N,O donor)	850	120	92	88
C2	Co(III)	Phosphine (P donor)	1100	150	95	91
C3	Ni(II)	NHC (C donor)	1450	200	97	94
C4	Mn(II)	Aryloxide (O donor)	780	100	89	85
C5	Pd(II)	Bisphosphine (P donor)	1600	220	98	96
C6	Cu(II)	Mixed N,O donor	900	130	93	89



**Figure 2. Proposed catalytic cycle illustrating the role of metal–ligand coordination in substrate activation**

### 4.3 Solvent Extraction Efficiency and Selectivity

The solvent extraction analyses demonstrated that pH undoubtedly influenced the extraction performance and maximum recovery was noted when the ligand was moderately acidic with the selective coordination favorable with the ligand protonation forms. An extreme degree of pH favored the hydrolysis of metal ions to give reduced efficiency and low pH decreased percentages of extraction due to competition among protonated species. The selectivity trends of metal ligands showed that customized ligands were able to discriminate indexed oxygen donors having a stronger affinity with alkaline earth and rare-earth elements as opposed to transition metals, i.e., Fe(III) and Co(II), but not nitrogen-rich vital groups. The structural properties of the ligands, such as the denticity and the bulky steric size, had a pronounced influence on the behavior of the partition of the complex as the flexible polydentate ligands improved the distribution ratios by keeping the complexes in the organic phase. Fewer selectivity coefficients were obtained using rigid scaffolds, which were not as flexible by locking out the non-target ions. The mechanistic definition of such findings is to create multifunctional extractants and explains why the architecture of ligands is necessary for balancing the selectivity and efficiency of extractants.

**Table 2. Distribution Ratios and Separation Factors of Transition Metal Complexes**

Complex ID	Metal Ion	pH Range	Distribution Ratio (D)	Separation Factor (SF)
E1	Fe(III)	3–5	12.5	8.2
E2	Co(II)	4–6	10.8	7.5
E3	Ni(II)	5–7	9.6	6.9
E4	Mn(II)	3–6	8.2	5.7
E5	Cu(II)	4–7	11.3	7.8

### 4.4 Correlation Between Catalytic and Extraction Behavior

Catalytic and extraction abilities were tested as the strong correlations between the structure and the property; the geometry of the ligand solely dictated the turnover rate, as well as selectivity. The high density of electronic density complexes at the metal center showed better catalytic functions but worse phase transfer, so the low density of electronic density complexes at the metal center showed better extraction efficiency. Ligands with mediocre strength as donors also indicated the requirement to have

electrical fine-tuning, as the ligands represented a compromise between greater levels of selectivity of extraction and catalytic turnover. Steric effects were very critical since bulky ligands reduced the size of the substrates that were applied during the catalytic process and enhanced the selectivity of the extraction process based on the competing ions. Multifunctionality was also dependent on the amount of coordination: square planar metals were more accurate at catalytic reactions, but octahedral complexes were more stable and richer in extractions. Dual-function ligand complexes containing donor atoms, which stabilize catalytic intermediates and enhance selective partitioning, have been made with special promise. It is this relationship that causes the logical ligand design integration of the separation and catalytic chemistry into one to create multipurpose platforms that are utilized in the long term.

## 5. Mechanistic Insights

The analysis of metal-ligand activation pathways shows that these processes are also important in catalytic turnover and selectivity of extraction. The processes of the inner sphere took center stage in catalysis when the ligands permitted the direct coordination of the substrates, which made the coordination of the substrates to the electron transfers easier. The outer-sphere routes were also provided in the sterically hindered complexes, which allowed them to react without binding to the substrate by modulating their electronic density. The redox contribution of the metal centers played a major role in the sense that the varying degrees of oxidation of the same allowed the catalytic flexibility and also the multi-step reactions. The association of very stable complexes with decreased turnover at catalysis and moderately stable with a desirable compromise, respectively, is due to access to substrates. These thermal constants of stability are provided to give the stability of the light and heavy ligand bonds. This was done with extraction analogies in which the selectivity and extraction performance were influenced by the stability of the ligands. These analogies of mechanism imply that the design of the ligand in order to achieve the balance of stability/reactivity is necessary and, consequently, ensures multifunctionality. These results indicate that logical design of ligands represents a bright future of selective extraction and catalytically precise complexes that provide a single paradigm to an ecologically acceptable chemical reaction.

## 6. Industrial and Environmental Implications

In the example of multifunctional coordination complexes, catalysis and solvent extraction have significant industrial and environmental impacts. These systems attain both transformation and separation, where wastes and costs of energy are reduced in accordance with the green chemistry perspective. The ligand design of the catalyst systems provides more stability through the recovery of the systems after multiple cycles and also minimizes the consumption of precious metals, which are very costly. The complexes are also effective in hydrometallurgy and provide an efficient transition complex as well as a rapid recovery of rare earth metals, where there is a need to address issues with resources that are major concerns to electronics and energy demands in renewable energy. Selective rare earth mining has been considered of great significance in the production of a sustainable supply chain in which traditional mining techniques are expensive in terms of energy consumption and environmental degradation. As a result of the scaling of the ligand design strategies, that is, the possibility to produce large scale and combine processes, scalability is the problem that emphasizes the potential of this kind of complex to the industry. The overall effect of all these is that multifunctional coordination chemistry has the potential of making the recovery of resources better and stewardship of the environment and sustainable production, hence, it can be termed as a game changer in chemical industries today.

## 7. Conclusions

The article shows capacity to incorporate the ideas of coordination chemistry into the multifunctional transition metal complexes capable of performing solvent extraction and selective catalysis simultaneously. Structural characterization offered a mechanism to understand the mechanism of interaction of ligands with metals, which motivated verifying other geometries and electrical conditions. Even though extraction studies had suggested the importance of denticity and steric effects in creating selective partitioning and catalytic determinations, the effect of the ligand architecture, the type of donor atom and turnover using the donor atom were found to relate considerably. This multi-purpose nature of these compounds can be coupled with the fact that logical ligand design can incorporate both catalytic and separation reactions that can render the chemical methods cleaner with respect to the environment. The study, by establishing the connections between mechanistic comprehension of problems and the decisions made in practice, offers the background for why future synthesis of industrial troubles relates to earmarking of multifunctional systems capable of perspective recovery of resources and green chemistry. These results provide a fresh set of paradigms toward the integrated chemical platforms and support the fact that the environment of coordination directly affects not only the catalytic turnover but also the selectivity of the extraction process.

## References:

1. Abu-Dief, A. M., & Mohamed, I. M. A. (2015). A review on versatile applications of transition metal complexes incorporating Schiff bases. *Beni-Suef University Journal of Basic and Applied Sciences*. Elsevier. <https://www.sciencedirect.com/science/article/pii/S2314853515000256>
2. Crabtree, R. H. (2013). Abnormal, mesoionic and remote N-heterocyclic carbene complexes. *Coordination Chemistry Reviews*. Elsevier. <https://www.sciencedirect.com/science/article/pii/S0010854512002329>
3. Centi, G., & Perathoner, S. (2011). Creating and mastering nano-objects to design advanced catalytic materials. *Coordination Chemistry Reviews*. Elsevier. <https://www.sciencedirect.com/science/article/pii/S0010854511000178>
4. Díaz-Torres, R., & Alvarez, S. (2011). Coordinating ability of anions and solvents towards transition metals and lanthanides. *Dalton Transactions*. RSC. <https://pubs.rsc.org/en/content/articlehtml/2011/dt/c1dt11000d>
5. García-Álvarez, J. (2015). Deep eutectic mixtures: Promising sustainable solvents for metal-catalysed and metal-mediated organic reactions. *European Journal of Inorganic Chemistry*. Wiley. <https://doi.org/10.1002/ejic.201500892>
6. Hébrant, M. (2009). Metal ion extraction in microheterogeneous systems. *Coordination Chemistry Reviews*. Elsevier. <https://www.sciencedirect.com/science/article/pii/S0010854509000836>
7. He, Y. M., Song, F. T., & Fan, Q. H. (2013). Advances in transition metal-catalyzed asymmetric hydrogenation of heteroaromatic compounds. *Topics in Current Chemistry*. Springer. [https://doi.org/10.1007/128\\_2013\\_480](https://doi.org/10.1007/128_2013_480)
8. Kubas, G. J. (2014). Activation of dihydrogen and coordination of molecular H<sub>2</sub> on transition metals. *Journal of Organometallic Chemistry*. Elsevier. <https://www.sciencedirect.com/science/article/pii/S0022328X13005482>
9. Muldoon, M. J. (2010). Modern multiphase catalysis: new developments in the separation of homogeneous catalysts. *Dalton Transactions*. RSC. <https://pubs.rsc.org/en/content/articlehtml/2010/dt/b916861n>
10. Nelson, D. J. (2015). Accessible syntheses of late transition metal (Pre)catalysts bearing n-heterocyclic carbene ligands. *European Journal of Inorganic Chemistry*. Wiley. <https://doi.org/10.1002/ejic.201500061>
11. Pérez-Temprano, M. H., Casares, J. A., & Espinet, P. (2012). Bimetallic catalysis using transition and group 11 metals: An emerging tool for C–C coupling and other reactions. *Chemistry – A European Journal*. Wiley. <https://doi.org/10.1002/chem.201102888>

12. Pospech, J., Fleischer, I., Franke, R., & Kragl, U. (2013). Alternative metals for homogeneous catalyzed hydroformylation reactions. *Angewandte Chemie International Edition*. Wiley. <https://doi.org/10.1002/anie.201208330>
13. Riener, K., Haslinger, S., Raba, A., Högerl, M. P., & Puchberger, M. (2014). Chemistry of iron N-heterocyclic carbene complexes: Syntheses, structures, reactivities and catalytic applications. *Chemical Reviews*. ACS Publications. <https://doi.org/10.1021/cr4006439>
14. Rosati, F., & Roelfes, G. (2010). Artificial metalloenzymes. *ChemCatChem*. Wiley. <https://doi.org/10.1002/cctc.201000011>
15. Searles, K., Tran, B. L., Pink, M., Chen, C. H., & Mindiola, D. J. (2013). 3d early transition metal complexes supported by a new sterically demanding aryloxy ligand. *Inorganic Chemistry*. ACS Publications. <https://doi.org/10.1021/ic401363p>
16. Spokoiny, A. M., Machan, C. W., Clingerman, D. J., & Rosen, M. S. (2011). A coordination chemistry dichotomy for icosahedral carborane-based ligands. *Nature Chemistry*. Nature. <https://www.nature.com/articles/nchem.1088>
17. Villanneau, R., Marzouk, A., Wang, Y., Djamaa, A. B., & Proust, A. (2013). Covalent grafting of organic-inorganic polyoxometalates hybrids onto mesoporous SBA-15: A key step for new anchored homogeneous catalysts. *Inorganic Chemistry*. ACS Publications. <https://doi.org/10.1021/ic302374v>
18. Bellemin-Laponnaz, S., & Dagorne, S. (2014). Group 1 and 2 and early transition metal complexes bearing N-heterocyclic carbene ligands: Coordination chemistry, reactivity and applications. *Chemical Reviews*. ACS Publications. <https://doi.org/10.1021/cr500227y>
19. Bryliakov, K. P., & Talsi, E. P. (2012). Frontiers of mechanistic studies of coordination polymerization and oligomerization of  $\alpha$ -olefins. *Coordination Chemistry Reviews*. Elsevier. <https://www.sciencedirect.com/science/article/pii/S0010854512001737>
20. Trifonov, A. A. (2010). Guanidinate and amidopyridinate rare-earth complexes: Towards highly reactive alkyl and hydrido species. *Coordination Chemistry Reviews*. Elsevier. <https://www.sciencedirect.com/science/article/pii/S0010854510000147>
21. Hao, X., Zhu, N., Gschneidner, T., Jonsson, E. Ö., & others. (2013). Direct measurement and modulation of single-molecule coordinative bonding forces in a transition metal complex. *Nature Communications*. Nature. <https://www.nature.com/articles/ncomms3121>
22. Magano, J., & Dunetz, J. R. (2011). Large-scale applications of transition metal-catalyzed couplings for the synthesis of pharmaceuticals. *Chemical Reviews*. ACS Publications. <https://doi.org/10.1021/cr100346g>
23. Poyatos, M., Mata, J. A., & Peris, E. (2009). Complexes with poly(N-heterocyclic carbene) ligands: Structural features and catalytic applications. *Chemical Reviews*. ACS Publications. <https://doi.org/10.1021/cr800501s>
24. Marr, A. C., & Marr, P. C. (2011). Entrapping homogeneous catalysts by sol-gel methods: The bottom-up synthesis of catalysts that recycle and cascade. *Dalton Transactions*. RSC. <https://pubs.rsc.org/en/content/articlehtml/2011/dt/c0dt00888e>