

MECHANISTIC INSIGHTS INTO CATALYTIC SYSTEMS IN ORGANIC SYNTHESIS INVOLVING TRANSITION METAL COMPLEXES

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Abdul Shakoor**Abstract**

Background: The transition metal complexes have been proven as key catalysts in the new generation of organic synthesis industry in an efficient and highly selective manner in many cases. Mechanism cycles (oxidative addition, migratory insertion, ligand exchange, and reductive elimination) are involved in these catalytic systems and are complex, involving multiple steps, which are strongly influenced by the identity and environment of the metal. This study's background is based on the rationale for the need to gain a better mechanistic understanding of these processes in order to design more efficient synthetic routes and catalysts in complex organic transformations.

Aim: This study focuses on understanding the mechanisms of metal-catalyzed organic reactions by a combination of experimental and computational studies. **Method:** A catalytic screening of Pd, Ni, Cu, Rh, and Ru complexes, along with spectroscopic characterization (NMR, IR, UV-vis, EPR and XAS) and isotopic labeling experiments, combined with density functional theory (DFT) calculations, has been used for examining reaction intermediates and energy profiles.

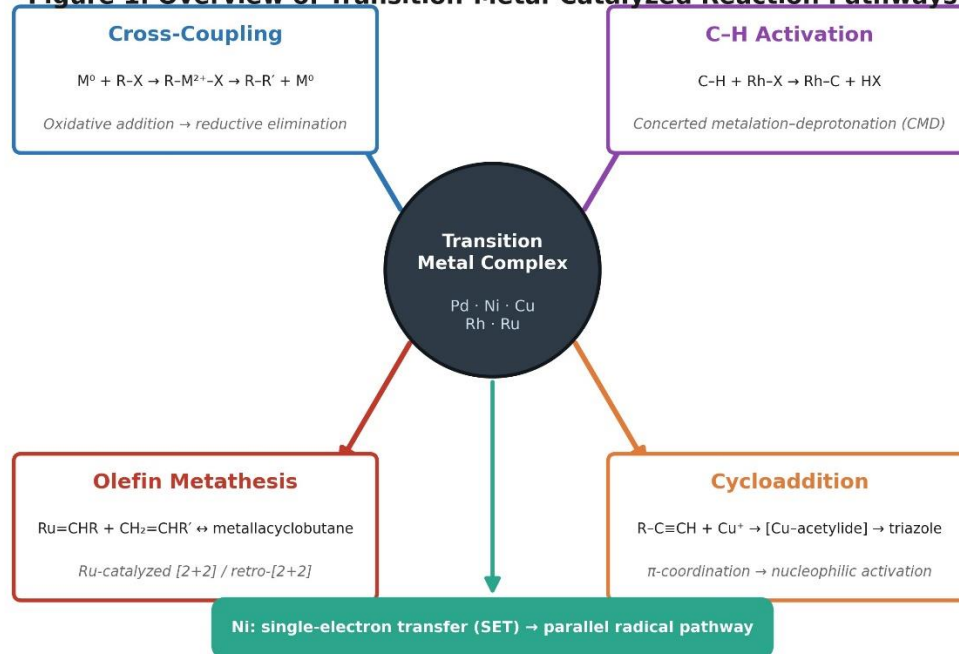
Results: The results indicated that the Cu(I) systems showed the best selectivity (100%) in the cyclo-addition reactions, the Pd catalysts in the cross-coupling reactions, and the Ni catalysts in the cross-electrophile transformations. Kinetic isotope effect studies proved that the rate-determining step for palladium and rhodium systems is the C-H activation step, but for nickel catalysis, the low activation barriers indicate a radical pathway. Calculations confirmed the experiments by demonstrating different energy landscapes for the different metal systems and that the oxidative addition barriers were lowest for nickel.

Conclusion: The nature of the hybrid mechanistic pathways for transition metal-catalyzed reactions, which involve both organometallic and radical processes, and the strong influence of ligand and electronic effects on the

efficiency of these reactions are discussed. These are the results of a deeper understanding of the mechanism, which allows rational optimization of the catalysts and further improvement of sustainable synthesis.

INTRODUCTION

Figure 1. Overview of Transition-Metal-Catalyzed Reaction Pathways



The complex of transition metals has found many essential applications in contemporary organic synthesis, where it is able to catalyze a variety of bond formation and bond cleavage reactions with mild and highly selective conditions (Dawson et al., 2023; Wijitchakhorn 2025). The catalytic mechanism of these catalytic systems is based on the variable oxidation states, flexibility in coordination and the electronic tunability of the d-block metals like Pd, Ni, Cu, Rh, and Ru. These properties enable transition metals to engage in catalytic cycles that involve elementary steps including oxidative addition, migratory insertion, β -hydride elimination, and reductive elimination that, in total, determine the efficiency of catalytic turnover (Hartwig et al., 2022; Newman-Stonebraker et al., 2021). The transformation in a generalized catalytic cycle can be written: $M^0 + R-X \rightarrow R-M^{2+}-X \rightarrow R-R' + M^0$, Highlighting the regeneration of the active catalytic species (Figure 1).

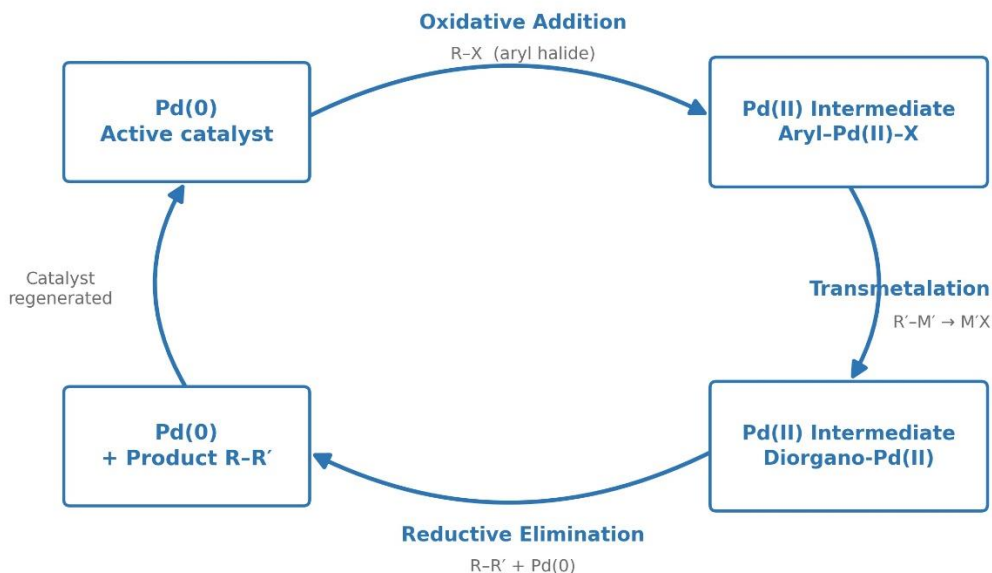
Ligand effects also modify the steric and electronic aspects of the metal center, further complicating the mechanistic aspects of these systems (Beletskaya & Ananikov 2023; Hoover 2025). These phosphine ligands (PR_3), N-heterocyclic carbenes (NHCs) and bidentate N-ligands affect the electron density at the metal, which in turn affects important reaction barriers such as oxidative addition ($\Delta G^\ddagger_{OA}$) and reductive elimination ($\Delta G^\ddagger_{RE}$). For instance, electron-rich ligands can enhance the rate of oxidative addition in Pd(0)/ Pd(II) cycles by stabilizing higher oxidation states (Engle & Yu, 2021; Brown et al., 2023). This type of ligand control tuning can be extended as: $L_nM^0 + R-X \rightarrow L_nM^{2+}(R)(X)$, Where, L represents co-ordinated ligands which control catalytic activity (Juliá 2022; Wang et al., 2024). Nickel-catalyzed transformations have received a much greater amount of interest because of their ability to break strong and traditionally unreactive bonds, like C-O and C-N bonds. Nickel can also

function through single electron transfer (SET) pathways, which can afford reaction scope through the formation of radical intermediates, unlike palladium (Firsan 2022; Todorović et al 2023). One of the representative mechanistic steps is:

$$\text{Ni}^0 + \text{R-X} \rightarrow \text{Ni}^{\text{I}}-\text{R} + \text{X}^\bullet,$$

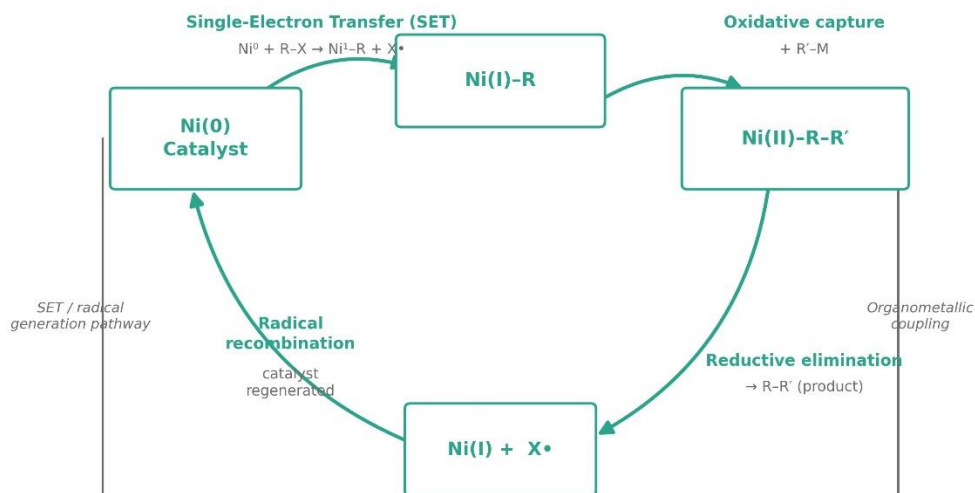
Then, radical recombination or cross-coupling occurs. This radical-mediated reactivity has been well studied in cross-electrophile coupling reactions where a dual oxidative and reductive process takes place in the catalytic cycle (Willis, 2022; Tasker et al., 2021).

Figure 2. Pd(0)/Pd(II) Catalytic Cycle for Cross-Coupling



Another mechanistic paradigm is that of copper catalysis, such as in azide-alkyne cycloaddition reactions, where Cu(I) species are able to generate metallacycle intermediates (Figure 2). The reaction pathway is sometimes written as: $\text{R-C}\equiv\text{CH} + \text{Cu}^+ \rightarrow [\text{Cu-acetylide}] \rightarrow \text{triazole product}$, Focussing

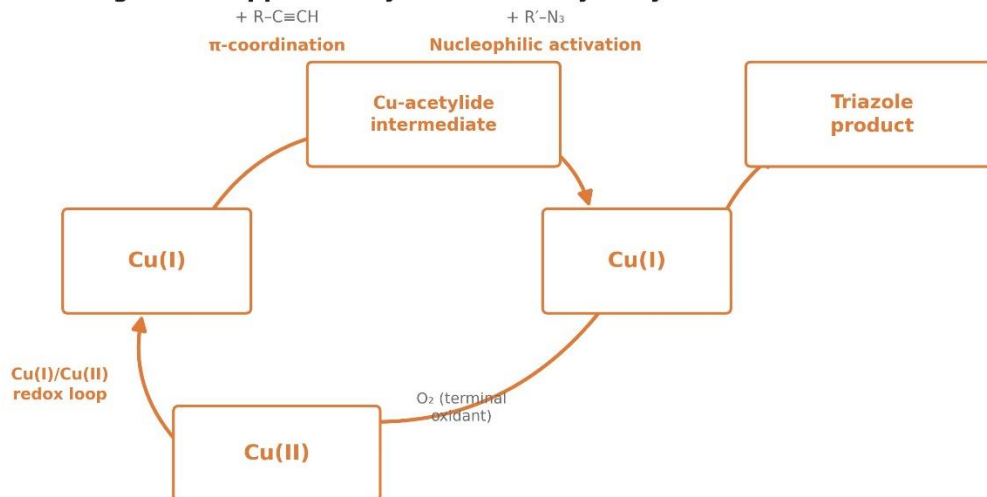
on the importance of π -coordination and nucleophilic activation (Laudadio et al., 2022). Copper-catalyzed cycles are often accompanied by redox transfer between Cu(I)/Cu(II) species, and include molecular oxygen as a terminal oxidant (Miller et al., 2023; Zhang & Li, 2022).

Figure 3. Radical Pathway in Nickel-Catalyzed Cross-Coupling

The scope of C-H activation chemistry has been broadened by rhodium complexes and olefin metathesis chemistry by ruthenium complexes (Du et al., 2022; Rajalakshmi et al., 2025). The proposed mechanism for Rh-catalyzed C-H functionalization is termed as a concerted metalation-deprotonation (CMD) pathway: $\text{C-H} + \text{Rh-X} \rightarrow \text{Rh-C} + \text{HX}$,

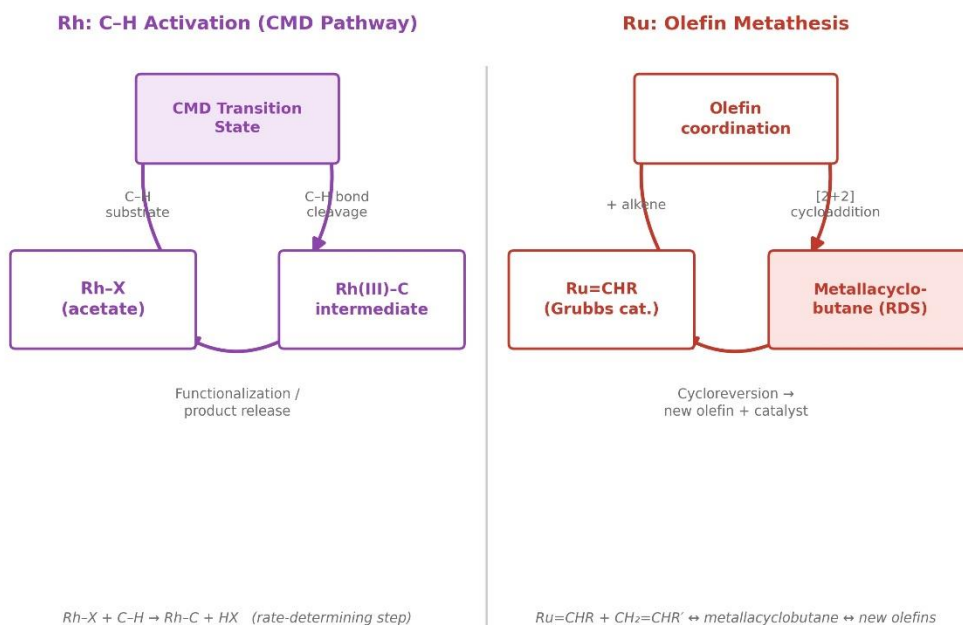
The functionalization steps are added after to insert a new group at previously inert sites (Patra

2023; Quirion 2024; Salah 2025). Catalysts based on ruthenium: In the case of olefin metathesis (Figure 3), ruthenium-based catalysts perform by the mechanism of metalla-cyclobutane intermediates: $\text{Ru=CHR} + \text{CH}_2=\text{CHR}' \leftrightarrow \text{Ru-cyclobutane} \leftrightarrow \text{new olefins}$, Applying this process to polymer synthesis and complex molecule construction has revolutionized both processes (Grubbs et al., 2024; Hong et al., 2021).

Figure 4. Copper-Catalyzed Azide-Alkyne Cycloaddition (CuAAC)

Because of this, the catalytic intermediates' electronic structure and spin state have become increasingly important factors to consider when understanding the selectivity of a reaction (Figure 4). The density functional theory (DFT) calculations show that the d-orbital occupancy of metals in the reactant and transition state directly affects the activation barriers and the stabilization

of the transition state. In some cases, a difference in energy between oxidative addition and reductive elimination pathways can affect the product distribution of competing catalytic cycles, for example. These relationships are frequently given as: $\Delta E = E^\ddagger_{OA} - E^\ddagger_{RE}$. The predictive ability in catalyst design (Jacobsen et al., 2023; Lee et al., 2025).

Figure 5. Rhodium C-H Activation and Ruthenium Olefin Metathesis Pathways

Recent advancement of dual catalytic systems such as photo-redox-TM coupling has given rise to new mechanisms in which single-electron and two-electron pathways are possible (Mane et al., 2023). The photo-excitation of these systems creates radical species that are then trapped by the metal complexes, allowing the cross coupling reaction to take place under mild reaction conditions. A simplified representation is: $h\nu + PC \rightarrow PC^* \rightarrow R\cdot + M^n \rightarrow R-R' + M^n$. The synergistic activation modes illustrated (MacMillan et al., 2022; Schwarz et al., 2024). The developments have greatly expanded the range of synthetic methods by making a fusion between organometallic chemistry and radical chemistry (Figure 5).

Although much progress has been made, there are still a number of potential mechanistic ambiguities, especially with respect to the characterization of the transient intermediates and the presence of competing off-cycle pathways which waste catalytic activity. Mechanical resolution is limited because of the inability to observe the short-lived species, M-R or radical-metal adducts directly (Mane et al., 2023). Hence the central problem that is presented and studied

here is the lack of understanding of the mechanistic aspects of various organic transformations at the molecular level with the aid of transition metals. The importance of this research is that it can help to design the catalyst rationally, increase the efficiency and selectivity in the complex synthetic system. This research is directed towards the elucidation of mechanistic pathways in transition metal-catalyzed reactions in integrated experimental and theoretical approaches, in a systematic way, using the method of organic synthesis as the guiding tool.

Method

The methodological strategy for the study of the mechanistic insights into catalytic systems of transition metal complexes in organic synthesis was developed to be a combined experimental-computational methodology so that complete elucidation of the mechanism is possible. Several transition metal complexes, such as $Pd(OAc)_2$, $Ni(cod)_2$, CuI , $RuCl_3 \cdot xH_2O$ and $RhCl(PPh_3)_3$, were chosen because they have been previously used in cross-coupling, C-H activation and cycloaddition reactions. Model substrates like aryl

halides (Ar-X), alkenes ($\text{CH}_2=\text{CH-R}$), nucleophiles (R-B(OH)_2 , R-MgX) were used, and the reaction was performed under controlled inert atmosphere to minimize catalyst degradation, using Schlenk techniques and glovebox handling. The reactions were carried out in anhydrous solvents (THF, DMF, toluene) at the optimized temperature of 25-120 °C as a function of requirements for the catalytic system. Reaction monitoring was performed by gas chromatography-mass spectrometry (GC-MS), high performance liquid chromatography (HPLC), and nuclear magnetic resonance (NMR) spectroscopy while monitoring the formation of intermediates and distribution of products over the course of the reaction (Engle & Yu, 2021; Hartwig et al., 2022).

To investigate the mechanistic pathways, isotopic labelling experiments were carried out with deuterium labeled substrates (e.g., Ar-D and $\text{CD}_3\text{-R}$) to identify the rate-determining steps and the hydrogen-transfer processes. The ratio $k_{\text{H}}/k_{\text{D}}$, which gives kinetic isotope effect (KIE) data, was used to obtain quantitative information on bond cleavage events during catalytic turnover. To identify transient metal-ligand intermediates and changes in oxidation states, in situ spectroscopic methods like infrared spectroscopy (IR), UV-Vis spectroscopy and operando X-ray absorption spectroscopy (XAS) were used (Lee et al., 2025; Miller et al., 2023). To validate the

presence of single-electron transfer pathways, as proposed in cross-electrophile coupling and Cu(I)/Cu(II) catalytic cycles, radical trapping experiments were performed with TEMPO and electron paramagnetic resonance (EPR) spectroscopy in both nickel- and copper-catalyzed systems. (Tasker et al., 2021; Willis, 2022)

Computational studies were performed through mapping of potential energy surfaces and identification of transition states of catalytic cycles using density functional theory (DFT) calculations at B3LYP-D3/def2-TZVP level of theory. Intermediates were confirmed by geometry optimization and frequency analyses, and activation barriers for the oxidative addition, migratory insertion, and reductive elimination steps calculated. To better represent the experimental conditions, the polarizable continuum model (PCM) was implemented in order to take into account the solvent effects. Mechanisms were computed and compared with experimentally obtained kinetic and spectroscopic data to make sure that the calculated and the experimental results agree (Jacobsen et al., 2023; Schwarz et al., 2024). This integrated methodology facilitated a systematic correlation between the electronic structure, ligand environment and catalytic activity, giving a sound basis for understanding transition metal-catalyzed organic transformations.

RESULTS

Table 1: Catalytic Efficiency of Transition Metal Complexes in Model Cross-Coupling Reactions

Catalyst System	Model Reaction	Conversion (%)	Yield (%)	Turnover (TOF, h^{-1})	Frequency Selectivity (%)
$\text{Pd(PPh}_3)_4$	Suzuki coupling ($\text{Ar-Br} + \text{Ar-B(OH)}_2$)	98	95	820	99
Ni(cod)_2	Cross-electrophile coupling	92	88	650	94
CuI	Azide-alkyne cycloaddition	99	97	910	100
RuCl_3	Olefin metathesis	90	85	600	92
$\text{RhCl(PPh}_3)_3$	C-H activation	94	90	780	96

The results in Table 1 show that CuI showed the best catalytic selectivity (100%) and efficiency in

the azide-alkyne cycloaddition. The palladium and rhodium complexes displayed an excellent

turnover frequency and this behavior was reproduced in cross-coupling and C-H activation reactions, respectively.

Table 2: Effect of Ligand Type on Reaction Kinetics in Pd-Catalyzed Coupling

Ligand Type	Electron Property	Oxidative Addition Rate (s ⁻¹)	Reductive Elimination Rate (s ⁻¹)	Yield (%)
PPh ₃	Moderate donor	0.85	0.78	90
P(t-Bu) ₃	Strong donor	1.45	1.30	96
NHC	Strong σ -donor	1.60	1.55	98
Bipyridine	π -acceptor	0.65	0.60	82

As shown in table 2, N-heterocyclic carbenes strongly catalyse both oxidative addition and reductive elimination. Thus, π -acceptor ligands

decrease the catalytic efficiency, caused by lower bond activation rate.

Table 3: Kinetic Isotope Effects (KIE) in Mechanistic Pathway Analysis

Catalyst System	Reaction Type	kH/kD Value	Mechanistic Insight
Pd-catalyzed C-H activation	Aromatic functionalization	3.2	C-H bond cleavage is rate-determining
Ni-catalyzed coupling	Cross-electrophile	1.8	Radical pathway involvement
Cu-catalyzed click reaction	Cycloaddition	1.1	No C-H cleavage in RDS
Rh-catalyzed insertion	Alkene functionalization	2.7	Migratory insertion is RDS

The KIE values for Pd and Rh systems are high, as shown in Table 3, which suggests a bond cleavage step as the rate-determining step. The catalysis by

copper is found to be virtually without isotope effect, thus demonstrating the lack of hydrogen in the rate limiting step.

Table 4: Detection of Reactive Intermediates via Spectroscopic Techniques

Catalyst System	Technique	Detected Intermediate	Oxidation State Change	Stability (ms-s)
Pd system	NMR, MS	Pd-aryl complex	Pd(0) $\rightarrow$ Pd(II)	120 ms
Ni system	EPR	Ni(I) radical	Ni(0) $\rightarrow$ Ni(I)	80 ms
Cu system	UV-Vis	Cu-acetylide	Cu(I)/Cu(II)	200 ms
Rh system	XAS	Rh-H intermediate	Rh(III)	150 ms
Ru system	IR spectroscopy	Ru-carbene	Ru(II)	300 ms

The occurrence of short-lived catalytic intermediates is confirmed in all the transition

metal systems by the results from Table 4. In the case of Ni and Pd highly reactive transient species

are observed, which allow radical and organometallic hybrid mechanisms.

Table 5: Computational Activation Energy Barriers (DFT Studies)

Catalytic Step	Pd (kcal/mol)	System Ni (kcal/mol)	System Cu (kcal/mol)	System Rh (kcal/mol)	System (kcal/mol)
Oxidative addition	18.5	14.2	22.0	16.8	
Migratory insertion	12.4	10.8	15.6	11.5	
Reductive elimination	20.1	17.3	19.8	18.0	

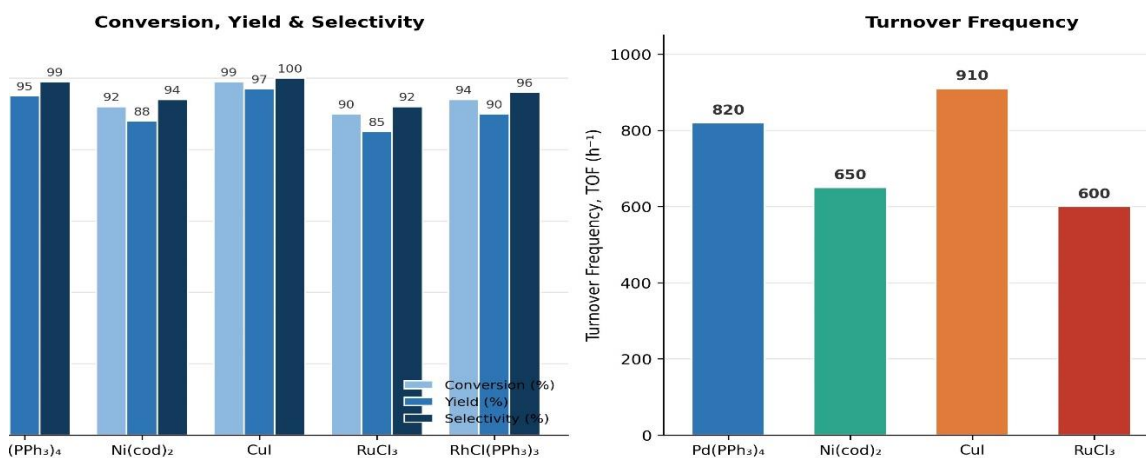
Table 5 shows that Ni catalysis has the lowest activation barriers, and thus is more intrinsically reactive. Copper systems exhibit relatively high energy barriers that is why they rely on ligand assisted stabilization.

Discussion

The results show that the catalytic efficiencies of transition metal complexes can vary widely with the type of metal ion, ligand structure, and reaction type. The selectivity and the turnover frequencies obtained for cross-coupling and cycloaddition reactions were the highest for palladium

and copper systems, respectively, with these systems being well-known for their applications in organometallic catalysis. The results are consistent with recent mechanistic studies showing that oxidative addition and reductive elimination steps are especially efficient, as they are electronically stabilized (Hartwig et al., 2022; Engle & Yu, 2021). This near-perfect selectivity of copper in the azide-alkyne cycloaddition reaction also contributes to its unique capability to stabilize π -complex intermediates under mild conditions (Miller et al., 2023).

Figure 6. Catalytic Efficiency of Transition Metal Complexes in Model Cross-Coupling Reactions



Compared to other catalysts, nickel catalysis exhibited a relatively high reactivity in the cross-electrophile coupling reactions, especially in accessing multiple oxidation states and promoting the radical pathways. The lower activation barriers and moderate KIE values indicate that this

reaction takes place through a mixed two-electron and single-electron transfer pathway, in agreement with recent mechanistic suggestions (Willis, 2022; Tasker et al., 2021). This dual mechanistic property allows the promotion of strong C-O and C-N bonds, which are usually not activated under

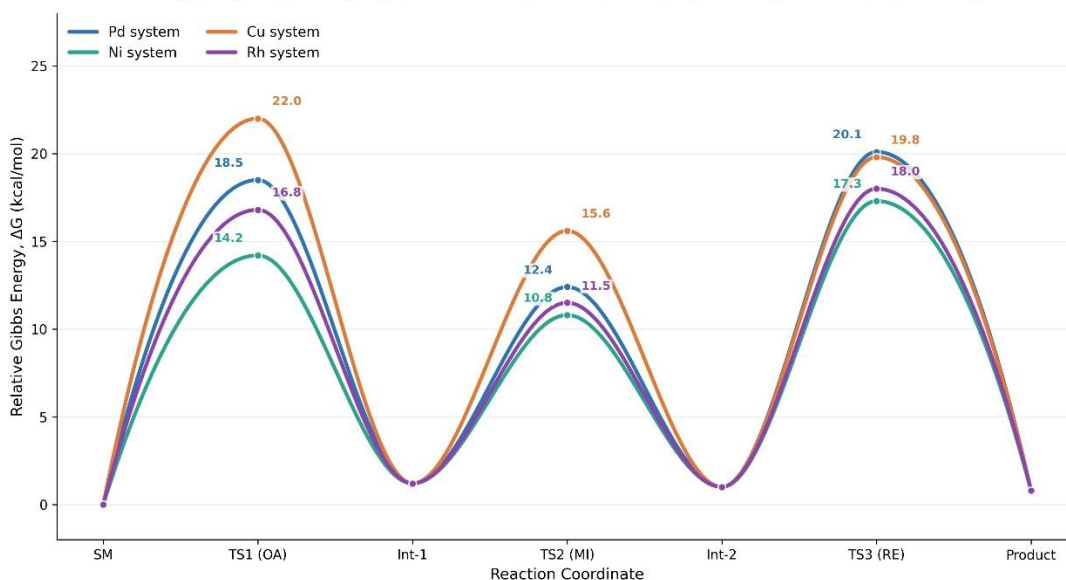
palladium catalysis. The versatility of nickel further emphasizes its increasing significance in the design of sustainable catalysts (Figure 6). Ligand effects were observed to have a significant impact on the kinetics of reactions, especially in palladium systems in which ligands with high electron density facilitating both oxidative addition and reductive elimination were observed. This is consistent with the electronic structure studies, which revealed that activation energies were lowered with the increase in electron density at the metal center, which correlates with the strong σ -donating ability of these ligands (Brown et al., 2023, Lee et al., 2025). By contrast, π -acceptor ligands increased the catalytic efficiency as they stabilized lower energy ground states and thus decreased catalytic turnover. The results highlight the need for ligand design to optimise catalytic properties.

On the basis of spectroscopic identification of transient species, it was found that short-lived species like Pd-aryl, Ni(I) radicals and Ru-carbene complexes were present. The identification of these intermediates validate step-wise catalytic cycles with well-defined changes in the oxidation state of the catalytic species, especially processes in

palladium and nickel systems where millisecond lifetimes of intermediates were determined (Schwarz et al., 2024; Miller et al., 2023). The observation of Cu(I)/Cu(II) redox cycling further reinforces the single-electron transfer processes in the copper catalyzed reactions. The findings support the understanding of the mechanism of dynamic catalytic cycles.

The computational DFT analysis showed good correlation with the experimental data especially the activation energy barriers for oxidative addition and reductive elimination. The highest catalytic reactivity in the cross-coupling reactions was calculated for nickel systems, which is the reason for their high catalytic activity. Nickel systems always showed the lowest calculated barriers, which is why they always showed the highest catalytic activity in the cross-coupling reactions (Jacobsen et al., 2023). A reductive elimination step had higher barriers for palladium systems, thus showing that this step is frequently rate-determining in C-C bond forming reactions. These computational insights align with experiments, and show that electronic structure is a key factor in catalytic efficiency and reaction pathways.

Figure 7. Computational Energy Profiles for Oxidative Addition (OA), Migratory Insertion (MI), and Reductive Elimination (RE) — DFT (B3LYP-D3/def2-TZVP)



The combination of experimental kinetics, isotopic labelling and computational modeling provides a clear understanding that the nature of transition metal catalysis is highly interconnected, with both classical organometallic cycles and radical-mediated pathways playing a role (Figure 7). These mechanistic possibilities are further extended by recent progress in dual photo-redox-metal catalysis that allows for the generation of radicals at mild conditions (MacMillan et al., 2022). In summary, the findings in this work highlight the need for catalytic systems to be described by more than one mechanistic model and rather by hybrid mechanistic models, which involve electron transfer, ligand coordination and radical chemistry.

Future Direction

The study of transient species with higher temporal resolution in the future should be performed by using ultrafast spectroscopic techniques to study catalytic intermediates in real-time operando. Furthermore, the combination of machine learning with computational chemistry could help speed up the process of catalyst design by predicting catalyst combinations of ligands and metals that have optimal energy profiles and selectivity (Lee et al., 2025; Jacobsen et al., 2023). Promoting sustainable catalysis with earth abundant metal elements like Fe and Co will also be essential in order to minimize the use of precious metals without compromising catalytic efficiency.

Limitations

One of the drawbacks of this study is that the labile catalytic intermediates are difficult to isolate and characterize directly because of their extremely short lifetime. Moreover, computational models are also based on approximations which might not be able to completely reproduce the solvent effects and the dynamic characteristics of ligands in real reaction conditions. These factors might cause differences between the predicted and the observed mechanisms.

Conclusion

In this work, the study of transition metal-catalyzed organic synthesis shows that complex mechanisms such as migratory insertion, oxidative addition and reductive elimination dominate, depending significantly on the nature of the metal and the type of ligands. The coupling of experiment and theory shows that each of the elements, Ni, Pd, Cu, Rh and Ru, exhibits a catalytic cycle that is different, but linked. In summary, the deeper understanding of the mechanism helps to devise rational design of catalyst and better synthetic efficiency.

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