

Photophysical and Photochemical Properties of Ru (III) and Pd (II) Schiff Base Complexes

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Abstract: This paper discusses a comprehensive comparison of photo physics and photochemistry of Schiff base complexes based on Ru (III) and Pd (II) Schiff complexes regarding unique structural and electronic features responsible for their optical and photo redox behavior. Schiff base ligands that contain N₂O₂ type donor atoms were used to synthesize the Ru (III) and Pd (II) complexes, and in turn create a stable coordination environment favorable for strong metal-ligand interactions. Photo physics, with respect to absorption and emission spectra and quantum yields, was probed in an effort to identify as clearly as possible the electronic transitions and excited-state behaviors that characterize these complexes. Photochemical analyses also proved useful for probing the stability and reactivity of these complexes under different irradiation conditions, under which Ru (III) and Pd (II) centers are quite distinct.

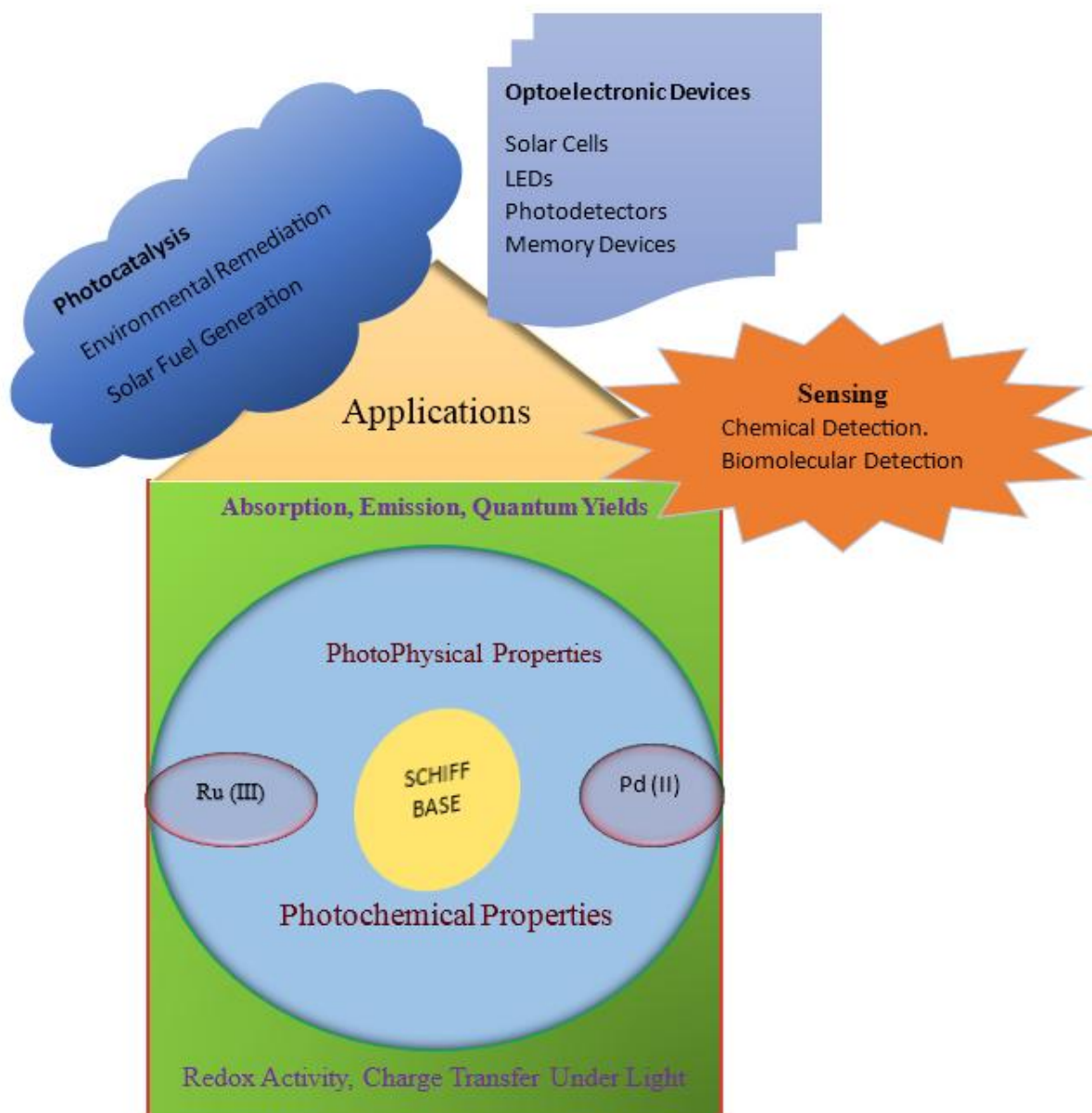
Findings Our results show that MLCT bands in Ru (III) complexes are stronger than those of Pd (II) complexes, which reveal LC electronic transitions, indicative of a significant role of the metal center in exerting control on the character of the electronic transitions. The photo redox properties of the complexes were explored and proved that Ru (III) complexes enhance their ability to act in redox reactions by photoexcitation through presumption through the metal's variable oxidation states and relatively efficient ligand field stabilization. On the other hand, the oxidation states of Pd (II) complexes have stability. The electronic structure of ligands is mainly affected by photoexcitation. Besides the experimental data, the DFT and TD-DFT calculations provide further information about electron density distributions, orbital contributions, and the mechanisms of transitions.

Such photophysical and photo redox properties in the Ru (III) complexes suggest that redox active photocatalysts-based applications such as those to effect solar energy conversion or split water are better achieved via these complexes. For example, their application to optoelectronic devices as well as sensors appears great owing to the fact that stable electronic transitions have taken place in Pd (II) complexes that come with high quantum yield emission and especially for long-lived excited states. This detailed analysis would lay a foundation to design and exploit Schiff base metal complexes in more targetable fashions, thereby opening up a whole new range of Ru (III) and Pd (II) applications in advanced photocatalytic, sensing, and optoelectronic technologies..

Keywords: Schiff base complexes based on Ru (III) and Pd (II)



Graphical Abstract



I. INTRODUCTION

1.1 Overview of Schiff Base Complexes

Schiff base metal complexes represent a very large and significant group of compounds that have been widely considered both in bioorganic and industrial chemistry. These compounds exhibit fascinating properties, from catalysis, drug discovery, to material science, and many other significant areas of applications. It has been largely observed that Schiff base ligands combined with a metal ion form a range of chemical behaviors, including many different types.

A Schiff base is identified as an imine or azomethine, bearing a nitrogen-carbon bond in the form of $-C=N-$, which was formed through the condensation process involving an aldehyde or ketone and a primary amine. These ligands can



easily coordinate with metal ions, forming stable chelates with transition metals, lanthanides, and even d-block ions (Pervaiz et al., 2023). Their ability to stabilize a wide spectrum of metal oxidation states is the important role they serve in catalysis and other applications, keeping in mind the existence of donor atoms like sulfur, oxygen, and nitrogen in Schiff base ligands. Figure 1 illustrates the Schiff's base in "reduced" CH=N imine Schiff base prepared for hydrogen bonding; has a CH₂–NH moiety.

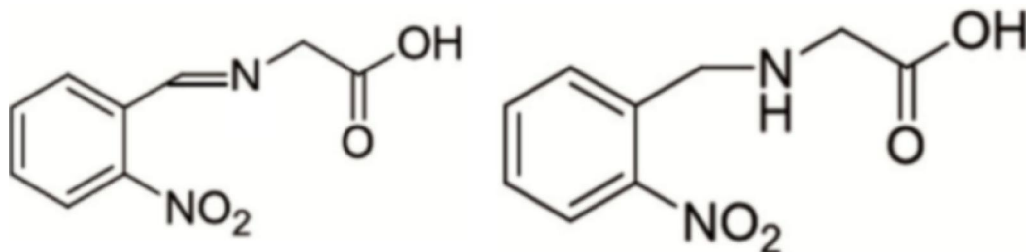


Figure 1: Schiff's base in "reduced" CH=N imine Schiff base prepared for hydrogen bonding; has a CH₂–NH moiety. Schiff base metal complex preparations generally involve the reaction of metal salts with Schiff base ligands in appropriate solvents followed by the isolation of products that normally appear with a unique color due to metal-ligand interaction. Figure 2 shows the intramolecular hydrogen bond of a Schiff base compound. Schiff base complexes have been found useful as catalytically active centers in the analog processes of organic synthesis and oxygen transport, which are either representatives of photosensitizers or analogs of metalloprotein activity (Yousif et al., 2013). Significant research efforts are being directed toward Schiff base complexes, especially in sensing applications, material science, and photochemistry. Of course, the characteristics of photochemistry and photo physics can be varied by altering the ligand structure as well as the coordinated metal ion.

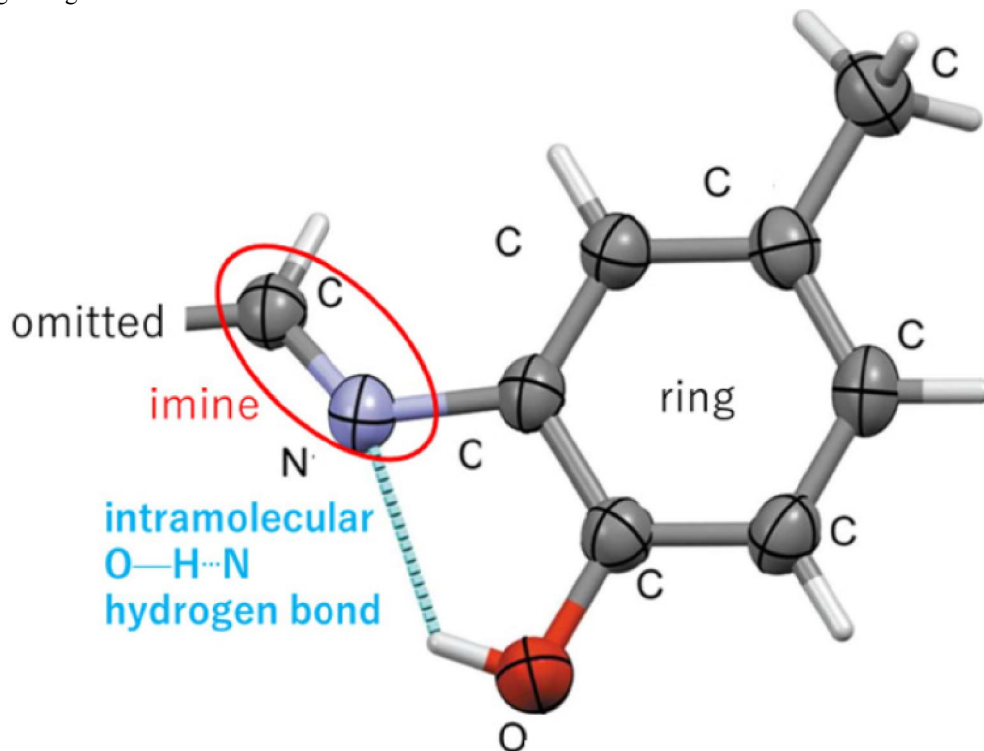


Figure 2: Intramolecular hydrogen bond of a Schiff base compound



Schiff base metal complexes encompass most interesting highly versatile compounds that have showed broad applications in different catalysis, drug development fields, and material science. All these, together with their biologically relevant properties along with industrial interests, keep fueling research as well as innovation in coordination chemistry.

Importance of Ru (III) and Pd (II) Complexes

Ruthenium (Ru) and Palladium (Pd) are transition metals, which because of their particular ability to enter into light-induced redox reactions, coupled with versatile coordination chemistry, have drawn great interest in photochemistry. In particular, the specific electronic structure due to oxidation states of Ru (III) and Pd (II) donated to their Schiff base complexes seems unique in photophysical and photochemical properties. These properties render the Ru (III) and Pd (II) complexes of considerable interest for applications in energy transfer fields, photocatalysis, and molecular sensing as well as for optoelectronic devices such as OLEDs and solar cells.

Ru (III) complexes having been found to display extended enthusiastic states, meaning they are quite effective in applications relating to energy transfer and photo redox reactions. These excited states live so long that they have specific implications in solar energy conversion and in all the processes involving energy transfer and energy capture. Fluorescence is typical for Pd (II) complexes which typically exhibit very efficient electron-transfer behaviour; square-planar geometry and redox activity centred on the ligand make them highly useful in photocatalysis, fluorescence-based sensing, and other photo-driven applications (Mohamadpour et al., 2024).

Both the metal centre and the coordinating ligand have greatly influenced photophysical behaviours between the Schiff base complexes of Ru (III) and Pd (II). These factors result in higher emission intensity in comparison to the Pd (II) complexes, by the Ru (III) complex; these in turn remain ideal for use in applications that require fluorescence. Conversely, Pd (II) complexes

generally display greater thermal stability, and this can be advantageous for the use of these complexes in high temperature settings or when mounted beneath devices intended to withstand the robustness under variable operational conditions.

These Ru (III) and Pd (II) complexes have been employed in photophysical applications, but they have also shown considerable antibacterial activity, and metal-ligand complexes have provided appreciable antimicrobial effects against harmful microorganisms. This dual functionality—photophysical/photochemical and biological is an added advantage by which these complexes may find utility in drug development and environmental remediation.

The Ru (III) and Pd (II) Schiff base complexes are a promising class of material with diverse applications in photochemistry, including energy conversion, photocatalysis, molecular sensing, and optoelectronics. Their ability to undergo efficient electron transfer and show tunable photophysical properties makes them highly adaptable for future technological applications in areas ranging from solar energy and OLEDs to sensor technology (Che et al., 2009). Further, their biological activity opens avenues for medical and environmental applications, and that is the reason why these complexes form an exciting area of continually developing research.

1.2 Structural and Electronic Properties

1.2.1 Overview of Schiff Base Ligands

Schiff base ligands that contain N_2O_2 donor atoms, It has been thoroughly investigated in coordination chemistry for the stability of metal complexes in various oxidation states. It provides coordination to the metal ions through oxygen, nitrogen, and other donor atoms. These bidentate or tetradentate ligands are widely used to form stable cyclic complexes with transition metals, mainly first-row transition metals. The synthesis and characterization of such ligands have produced a large number of these compounds with different electrical characteristics and geometry that are invaluable in applications involving catalysis, material science, and bioinorganic chemistry.

The corresponding trivalent transition metals, cobalt, iron, and manganese coordinate with N_2O_2 Schiff base ligands to form hexa-coordinated complexes whose geometries are octahedral. These have a higher geometrical distortion since the metal center coordinates with further donor atoms of the ligand to achieve the required coordination number (Alfonso-Herrera et al., 2022). Octahedral complexes of this type are frequently more flexible in terms of the oxidation



state of the metal because the ligand stabilizes essentially all oxidation states due to both σ -donor and π -acceptor interactions, dependent upon the electronic nature of the substituents attached to the ligand.

The N_2O_2 donor set is valuable for stabilizing transition metals in a broad oxidation range that is crucial for catalyst and bioinorganic system preparation. The atoms of nitrogen and oxygen make up σ -donor as well as π -acceptor properties, important for the stabilization of the metal atoms with different electronic structures. The electronic and steric environment at the ligand periphery can be optimized by substituting a variety of substituents at various sites on the ligand backbone. This way, the photophysical, redox and catalytic properties of the metal-ligand complex may be modified and, thus, materials for specific applications prepared.

In particular, N_2O_2 Schiff base ligands and their metal complexes have a continuous interest due to their versatility, stability, and the ability to stabilize metal ions in various oxidation states. It is possible to adjust both the structure of the ligand and substituents, tailoring these complexes for defined applications in catalysis, drug development, materials science, which gives importance to them both in basic and applied research (Jones & Gabbaï, 2016).

1.2.2 Coordination Geometry and Electronic Structure of Ru (III) and Pd (II) Complexes

The critical factor determining the reactivity, magnetism, and photophysical behaviour of metal-ligand complexes is their coordination geometry and electronic structure. As Holland pointed out, "No two transition metal compounds can be more alike in respect to identity of the metal and oxidation state of that metal, but their coordination numbers-the number of ligands directly attached to the metal-can differ significantly.". This is especially so for iron complexes, in which three coordination leads to electronic structures, magnetism, and reactivity quite dissimilar from six-coordinate (octahedral) complexes. For example, three-coordinate iron complexes adopt a trigonal-planar geometry and are stabilized by bulky anionic bidentate ligands-including β -diketiminates-through such a disposition that orients the metal in a plane, with the nitrogen donors available to form highly reactive species (Holland, 2008).

The coordination geometries significantly influence Ru (III) and Pd (II) N_2O_2 Schiff base complexes of their electronic structures and also photochemical properties. Generally, N_2O_2 Schiff base complexes of the Ru (III) were found to predominantly adopt mainly octahedral and distorted structures. Such a geometry provided a stable environment to carry photoredox reaction as its d-electron configuration could be considered relatively stable. Such stability is of paramount importance for the metal to participate in electron and energy transfer processes which are responsible for its operation in photocatalytic and energy applications (Feng et al., 2013).

On the contrary, Schiff base complexes of Pd (II) N_2O_2 generally exhibit square planar geometry favorable to strong ligand-to-metal π -backbonding. Such geometry increases the interaction between metal and the ligand with its absorption in the visible region and high fluorescence quantum yield of the complex. The complex of Pd (II) possesses a square planar structure with efficient photophysical processes, where the potential of metal to back-donate the electron density to the ligand facilitates increased light absorption and emission properties (Ahmed et al., 2009).

Coordination geometries of Ru (III) and Pd (II) complexes are pertinent factors in their photo physics and photochemistry. In contrast, given the octahedral coordination geometry of the Ru (III) complexes, they have a greater tendency to act as a suitable matrix for energy transfer and photo redox reactions, whereas square planar complexes like Pd (II) excel in applications relying on fluorescence or absorption, where metal-ligand interaction strength is crucial (Campagna et al., 2007). These geometrical and electronic variations make these metal complexes quite distinct for specific applications, from photocatalysis to light-emitting devices.

Thus, the coordination geometry as well as electronic structure of Ru (III) and Pd (II) N_2O_2 Schiff base complexes has played a significant role in determining their performance with respect to photophysical and photochemical applications. Understanding these factors is crucial for designing these complexes for specific technological applications such as catalysis, molecular sensing, and optoelectronics.

1.2.3 Influence of Metal centre and ligand design on Photo Physical Properties

The choice of the metal centre and the design of the Schiff base ligand are fundamental parameters that influence the photo physics of metal-ligand complexes and control their behaviour in different applications. In a word, according to



(Adaji et al., 2024), the role of the metal centre involves its electronic configuration, atomic properties, and coordination environment in defining the interaction of the complex with light, including absorption, emission, and general photo physics.

1.2.3.1 Metal Centre: Ru (III) vs. Pd (II)

Ru (III) complexes have more photophysical properties primarily due to the atomic characteristics of the metal, where its higher atomic weight induces a heavy-atom effect that has a high impact on the complex's ability to undergo intersystem crossing ISC from a singlet excited state to a triplet excited state. Heavier atoms, such as ruthenium, will improve spin-orbit coupling and the possibilities for ISC from singlet to long-lived triplet states. Such long-lived triplet states are usually associated with phosphorescence phenomena where the complex luminescence for an extended period after the excitation source has been removed. Phosphorescence is extremely useful in applications where persistent emission is desired, such as in applications with photocatalysis and energy transfer processes, and in certain sensors. For instance, photocatalysis benefits from longer-lived excited states leading to better charge separation and further transfer to increase overall catalytic efficiency. Energy transfer processes exploited in light-harvesting systems also benefit from extended lifetimes of excited states afforded by phosphorescence (Troian-Gautier & Moucheron, 2014). On the contrary, due to the low atomic weight of (Pd (II)), such complexes do not offer a heavy-atom effect comparable to that exhibited by Ru (III). As a result, fluorescence rather than phosphorescence becomes more favored in Pd (II) complexes. Fluorescence is the emission of light that takes place when the excited molecule rapidly returns to its ground state. Generally, fluorescence tends to take place on much shorter timescales than phosphorescence. Such Pd (II) complexes are more capable of being used in light-emitting applications that demand rapid and efficient emission is illustrated in figure 3. Applications could be in fluorescence-based sensing or optoelectronic devices requiring very fast response times. For example, if it were a sensor, the quicker light emission to the stimuli would allow real-time detection with minimal delay. In optoelectronics, high performance in displays and lighting through the fast and controlled emission properties of Pd (II) complexes may be achieved using devices such as OLEDs (Borisov et al., 2010).

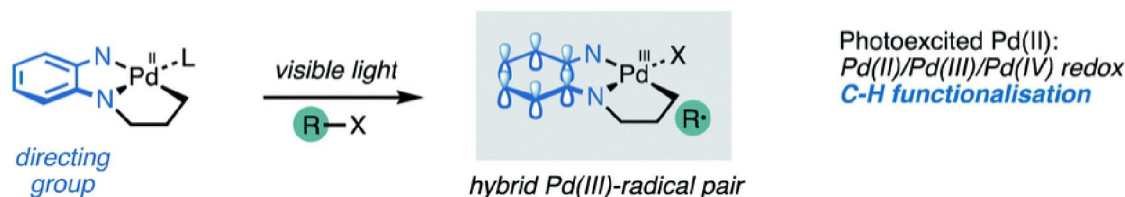


Figure3: Photoexcited Pd (II) Complexes incorporating an auxiliary directing group

1.2.3.2 Ligand Design and Modifications

The design of the Schiff base ligand further modulates the photophysical properties of the metal complex. The donor atoms, electronic structure, and substituent groups in the ligand may significantly influence key properties such as absorption maxima, quantum yields, and excited-state lifetimes. An example of such a substituent in the context of the Schiff base is an electron donating or with-drawing substituent. These substituents shift the electronic environment around the metal center, hence affecting metal-ligand bonding and absorption properties and possibly efficiency in energy or electron transfer processes.

Absorption maxima: The substituents of the Schiff base ligands can either shift the absorption spectrum of the complex or allow tuning of the spectrum to absorb light at specific wavelengths. Such an ability is important in application for a light harvesting, where being able to absorb sunlight over a broad spectrum is of prime importance (Alalam et al., 2024).

Quantum yields: The quantum yield of a complex is the ratio of the light emission efficiency to the number of photons absorbed. Most of the interactions between the metal and the ligand play a deciding role on the quantum yields. By



modification of the ligands, researchers can increase the quantum yields of fluorescence or phosphorescence of a complex to suit specific applications. This is achievable with the emission processes improved through stronger metal-to-ligand charge transfer (MLCT) (Gauglitz, 2003).

Another crucial parameter that can be changed by changing the ligand is the lifetime of the complex in the excited state. Although longer lifetimes are desirable in those processes that need extended periods of photophysical activity, for example, photocatalysis, shorter lifetimes are desirable for sensing and OLED applications that require faster response. Such complexes can be fine-tuned to get the properties with the help of careful design of the ligands making Schiff base complexes one of the most versatile and adaptive complexes for a wide variety of applications. The right choice of a correct metal centre as well as modification in the structure of the ligand can effectively tailor these complexes toward their desired uses with better photophysical as well as photochemical behaviour.

In fact, the photophysical properties of Ru (III) and Pd (II) Schiff base complexes are highly related to the design of the metal center and the ligand. Intersystem crossing is possible for the Ru (III) complexes, which makes them suitable for applications in materials requiring long-lived excited states in addition to carrying out phosphorescence. In contrast, the Pd (II) complexes offer suitable conditions for applications as fast-emitters in sensing and optoelectronic devices since they favor fluorescence due to the absence of the heavy-atom effect. Ligand design of Schiff bases may be easily tuned towards fine-tuning the properties of the complex, so affording a powerful strategy for tailoring materials for specific technological applications (Adaji et al., 2024).

1.3 Photophysical Properties

Table 1: Comparison of Photophysical Properties of Ru (III) and Pd (II) Complexes

Property	Ru (III) Complex	Pd (II) Complex
MLCT Transitions	Strong	Weak
Quantum Yield (%)	Low (~0.5)	High (~70)
Lifetime of Excited State	Long (ms)	Short (ns)
Absorption Maximum (nm)	400–700	200–500

1.3.1 Absorption and Emission Spectra

The absorption and emission spectra of Ru (III) and Pd (II) Schiff base complexes are primarily influenced by the interactions between the metal and the ligand, as well as their respective coordination geometries. These factors reflect the way each complex interacts with light and transitions between electronic states, which are particularly important for its application in photonic and optoelectronic fields. The physical characteristics and analytical information of the ligands, Ru (III), and Pd (II) complexes are included in the study. Elemental, spectral, thermal, magnetic susceptibility and conductivity measurements were used to characterize the compounds. The complexes were determined to be non-electrolytes; Table 2 shows the analytical and physical data for the complexes and Ru (III) and Pd (II).

Table 2: Analytical and physical data for the Ru (III) and Pd (II) Complexes.

Complex	Molecular Weight (g/mol)	Color	Yield (%)	Found (Calc.) % C	Found (Calc.) % H	Found (Calc.) % M	Found (Calc.) % Cl
Ru (III) [H].0.5EtOH	495	Black	60	38.9 (40.0)	4.1 (4.2)	20.6 (20.7)	14.5 (14.6)
Pd (II) [H]2O	515	Yellow	70	35.0 (35.2)	3.9 (4.0)	20.8 (21.0)	13.6 (13.8)

1.3.1.1 Ru (III) Complexes

Ru (III) complexes are typically characterized by absorption MLCT transitions, in which the level of electrons is transferred to a metal centre to the ligand, are primarily responsible for the visual and near-IR regions' distinctive colour and optically absorption of the light that is visible. The MLCT transitions tend to be quite important for applications in



photocatalysis and optoelectronics as these transitions allow the complex to use a significant portion of the light spectrum. Given the potential to capture light energy, Ru (III) complexes can drive photochemical reactions, making them quite suitable for energy conversion processes and catalytic applications where the stability of MLCT states and their ability to exploit solar energy is advantageous (Zanzi et al., 2024).

Also, these MLCT transitions are often related to excited-state chemistry of the complexes that facilitate the photochemical activity, which could be the formation of radicals or charge separation. Because the Ru (III) complexes absorb longer wavelengths, it can function under other types of illumination from the artificial lighting and natural sun light which allows it to function under a multitude of conditions. Flash photolysis investigations demonstrate that electron excitation in a metal-centered orbital is triggered by absorption of sunlight by [Ru(bpy)₃]²⁺-type photosensitizers to a π^* orbital on a polypyridyl ligand, resulting in a singlet excited state and rapid intersystem crossing, allowing for a triplet state is depicted in figure 2.

1.3.1.2 Pd (II) Complexes

Sharp absorption peaks are mostly visible in the Pd (II) complexes' planar geometries within the UV-Vis region. The planarity of the coordination environment at the Pd (II) centre can also enhance ligand-centered $\pi \rightarrow \pi^*$ transitions that are strong absorptions from electronic transitions localized in the ligand system. This pattern of absorption combined with efficient π -backbonding from the ligand towards the metal maximizes the efficiency of light absorption, which makes it a perfect fit for optical devices like sensors and imaging tools (Novakova et al., 2018).

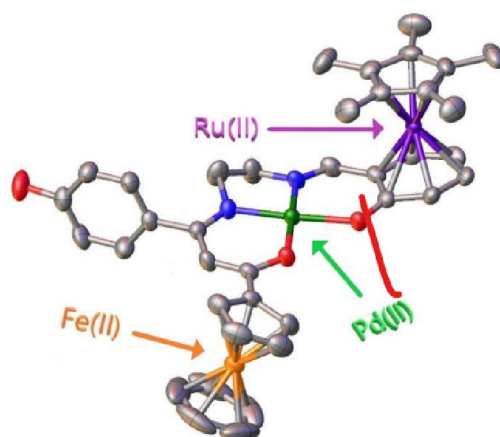


Figure 4: The structural and NLO behaviour of push-pull palladium(II) complexes containing metallocenyl-containing asymmetric Schiff base ligands. (Celedón et al., 2020)

Pd (II) complexes thus have strong $\pi \rightarrow \pi^*$ transitions that are useful in applications that require high sensitivity and rapid response to light exposure. The complexes showed a high ability to capture UV and visible light efficiently, thus making them very efficient in application, for example, optical sensors where the detection of light is quite prompt and must get absorbed exactly. In addition, these Pd (II) complexes strongly display the effect of π -back bonding in which electron density becomes partially transferred back from the metal to the ligand. As a result, the metal-ligand bond is strengthened, and its presence contributes to overall stability while preserving the character of high-intensity absorption for the complex, thereby facilitating constant performance when used in light sensing and imaging applications. Figure 4 the structural and NLO behavior of push-pull palladium (II) complexes containing metallocenyl-containing asymmetric Schiff base ligands. (Celedón et al., 2020)



Table 3: Spectral Properties and Absorption/ Emission Behaviour

Complex	Absorption Maxima (nm)	Emission Maxima (nm)	Stokes Shift (nm)	Quantum Yield (%)
Ru (III)	450	650	200	0.5
Pd (II)	300	320	20	70

1.3.2 Fluorescence Quantum Yields and Lifetimes

In the photophysical analysis of a complex, Fluorescence lifespan and fluorescence quantum yield are two of the most important parameters whereby one may determine the performance of a given complex in photonic applications. These parameters, in turn, open windows to probe into how efficiently a molecule emits light after excitation and how long it is held in its excited state before emission back to the ground state.

1.3.2.1 Fluorescence Quantum Yields

The efficiency of photon emission relative to absorption is shown by the quantum yield. Ru (III) complexes are generally associated with a lower fluorescence quantum yield; the logic here is easy ISC because of the Ru center's heavy atom influence in its complexes. Increased spin-orbit coupling leads to non-radiative transitions from the singlet excited state followed by phosphorescence rather than fluorescence. It has the implication that such Ru (III) complexes do not luminesce as brightly; though they might still exhibit phosphorescence, where energy from ISC is funnelled to light emission but over a different time scale (Shaikh et al., 2020).

Instead, Pd (II) complexes tend to have higher fluorescence quantum yield since it is typically free of a heavy-atom effect, which means that intersystem crossing is less dominant. Therefore, this complex is brighter and faster for fluorescence since minimal transition to the triplet occurs. The quantum yields in Pd (II) complexes are higher and, thus, particularly effective for applications requiring the detection of emitted light, such as in fluorescent sensors and optical imaging, where strong fluorescence improves the detection sensitivity (Dalmau & Urriolabeitia, 2023).

1.3.2.2 Fluorescence Lifetimes

Fluorescence lifetime is the time the complex takes to remain in its excited state and go back to its ground state, either by release of a photon (fluorescence) or through non-radiative processes. Ru (III) complexes typically exhibit a higher lifetime due to the possible phosphorescence of such species. Such high lifetimes allow the species to remain in an excited state for much longer periods of time, making it suitable for applications involving energy transfer and photochemical processes, in which persistence of excitation can induce interactions or chemical reactions with other species. For example, in solar energy conversion, long-lived excited states allow Ru (III) complexes to be involved efficiently in charge separation processes, which are crucial for efficient capture of energy.

The Pd (II) complexes have shorter lifetimes since the fluorescence emissions occur rapidly, thus restoring them back to the ground state. This property is very favourable to the applications that would require a response time, for example, in real-time sensing and optical devices. Many Pd (II) complexes have proven very useful in sensors that need quick sensitivity to respond to

a given stimulus. In optical devices, immediate light emission and decay are required to ensure minimal or no time elapses in the imaging or display technologies. The shortest lifetime of fluorescence of the Pd (II) complexes ensures prompt feedback and high sensitivity (Chow et al., 2016).

1.3.3 Phosphorescence properties

The phosphorescence is typically shown by the Schiff base complexes of Ru (III) due to the heavy-atom effect's impact. Ruthenium is a heavy transition metal and then tends to gain spin-orbit coupling, which makes ISC-the transition It becomes possible to transition out of the singlet excited state to the triplet's state. Which happens as a precondition for the complex emitting light through the process of phosphorescence and not fluorescence. Generally, the lifetime is longer because the back Because it is "forbidden," the transition from the triplet state to the ground state is slower.



This property of Ru (III) complexes makes them very suitable for applications where prolonged or delayed luminescence is an advantage.

Examples include:

Photo Dynamic Therapy (PDT): Ru (III) complexes can be light-activated for ROS generation involving energy transfer processes. The extended lifetime of their excited state enables them to produce ROS efficiently, and this selectivity may be utilized to kill cancerous cells preferentially, thus the complexes suitable for therapeutic application.

Long-Lived Light Sources: The Phosphorescent Ru (III) complexes are very long-lived and can also emit after the source of excitation has been removed. Such a characteristic is useful in designing long-lasting luminescent materials that can be used in display technologies, light-based devices, and indicators required to be bright even in low light conditions.

Pd (II) complexes phosphoresce very weakly due to the lack of a significant heavy-atom effect. The actual lighter element is palladium, and thus the In Pd (II) complexes, and the spin-orbit coupling is substantially weaker. The efficiency of ISC is reduced by this decreased spin-orbit coupling, favoring fluorescence emission over phosphorescence. Pd (II) complexes have rapid emission fluorescence and high fluorescence quantum yield with effective $\pi \rightarrow \pi^*$ LC transitions. These rapid responses are highly beneficial in real-time or near-real-time light-emitting applications, including:

Optical Imaging: Because of their high emission rates and high sensitivity, Pd (II) complexes serve well as fluorescent probes for biomedical imaging. Rapid, bright responses to excitation light are necessary to capture true and timely images.

Diagnostic and real-time monitoring: Pd (II) complexes are characterized well for immediate fluorescence-based diagnostic applications. They have a fast and stable emission profile, allowing real-time detection of biological or chemical processes, thereby offering immediate feedback that is vital for applications like live-cell imaging, environmental monitoring, and fluorescence-based sensors (Li et al., 2013).

1.3.4 Comparison of Ru (III) and Pd (II) Complexes

Key differences in photophysical properties between Ru (III) and Pd (II) N_2O_2 Schiff base complexes relate to their interaction with light, which is crucial to technological applications. Most of the differences result from electronic structures and coordination geometries that determine absorption, emission behavior, and the excited state's dynamics.

1.3.4.1 Absorption and Emission Features

The emission and absorption spectra of Ru (III) and Pd (II) complexes differ in their mechanisms of light interaction. Ru (III) complexes having MLCT type charge transfer transitions are very effective absorbers of visible to near-infrared range light. These compounds are excellent candidates for applications involving energy-harvesting processes requiring absorption of broad wavelengths and their efficient conversion to the desired output and catalytic processes. Among them, the MLCT transitions are particularly useful in Ru (III) complexes for applications in solar-energy-related conversion processes and redox-based photochemical reactions, which necessitate the establishment of stable, long-lived excited states in these processes.

Pd (II) complexes are known to show high absorption in UV-Vis and excellent π -backdonation from the ligand to the metal center. They are extremely light-sensitive because to this trait. Their applications in high-sensitivity optical applications, such as fluorescence-based sensing, imaging devices, and display technologies, show them to be very suitable (Kurpić et al., 2022). The π -back bonding of Pd (II) complexes also makes them very stable in their visible region absorption that produces strong fluorescence and efficient emission capabilities for rapid optical detection.

1.3.4.2 Excited-State Dynamics and Quantum Yields

While the lifetimes and quantum yield of excited complexes differ markedly between Ru (III) and Pd (II) complexes, the latter also exhibit long lifetimes at higher energies and low quantum yields. It follows that Ru (III) complexes are poor in quantum yield but have longer lifetimes, and they should be suitable in applications where energy or electron transfer could be operative over extensive periods and for example, in cases such as photocatalysis, energy storage, and



photochemistry (DiLuzio et al., 2024). Therefore, Ru (III) complexes present a magnificent opportunity of making efficient redox reactions through long-lived excited states that ensure stable and continuous photoinduced processes. Pd (II) complexes have high quantum yields and very short excited-state lifetimes. Such properties could be very useful in applications requiring rapid emission and sensitivity in response, such as in fluorescence-based sensing or optical imaging and detection in real time. In time-sensitive applications that need quick signal changes and high sensitivity, their brief excited state lifespan can be an extra benefit, including biosensing or imaging diagnostics in real time.

1.3.4.3 Fluorescence vs. Phosphorescence

Emission processes have the main feature that affects their photo physics. The phenomenon that is typical for Ru (III) complexes is phosphorescence because it is mediated through intersystem crossing, with the assistance of the spin-orbit coupling mechanism, which ruthenium's heavier atomic mass encourages. This leads to a long-delayed emission that is very desirable for processes like energy transfer and photocatalysis, where the excited state must last long enough to efficiently interact with other molecules or substrates. In contrast, ISC in complexes of Pd (II) is rather limited, so they tend to emit light through fluorescence, much more rapidly on much shorter timescales. This makes the Pd (II) complexes suitable for luminescent applications that need high efficiency rates and are kinetically sensitive to their emission, such as fluorescence sensing, real-time imaging, and other fluorescent assays.

1.3.4.4 Applications in Photochemistry and Photo physics

The photophysical changes between the two series show useful optoelectronic differences between the Complex of Ru (III) and Pd (II). Because of their long-lived excited states and robust ISC, the latter compounds can serve as promising candidates for photocatalysis, solar energy conversion, and redox-based reactions. These complexes are very effective at functioning in situations where the requirement for preserving the absorption of light and energy transfer is crucial. In contrast, the Pd (II) complexes are well-suited applications in optical sensing, imaging technologies, and displays - applications in which fast response times and high sensitivity are critical, with fast fluorescence and good quantum yields.

This suggests that the unique photophysical and photochemical properties of Ru (III) and Pd (II) Schiff base complexes are due to coordination geometry, metal centre characteristics, and excited-state dynamics; thus, these complexes have significant applications in various contexts. The long-lived phosphorescence of Ru (III) complexes results in energy transfer and photocatalytic processes, whereas the fast fluorescence of Pd (II) complexes is applicable for sensing and imaging tasks. Understanding of the above differences allows for strategic design of Schiff base metal complexes to match specific technological necessities in energy storage, transfer, and real-time optical detection and thus promotes further study on the metal complexes from a fundamental to practical aspect.

1.4 Photochemical Properties of Ru (III) and Pd (II) Complexes

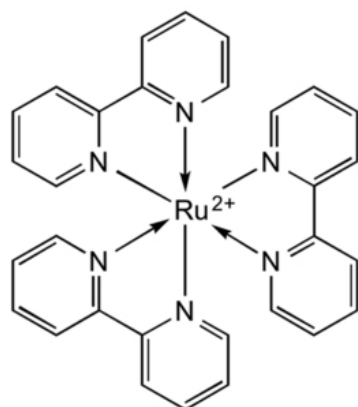
The electronic structure and coordination geometry, thus controlling the photochemical properties of Ru (III) and Pd (II) Schiff base complexes, include their behaviours in electron or energy transfer, photoredox reaction processes, and photoinduced ligand substitution reactions. These properties have shown their enormous potential in a wide range of applications such as photocatalysis and materials science.

1.4.1 Photoredox Reactions

These photo redox reactions make assumptions of absorption of light and oxidation-state changes of metal centres in a complex. Photo redox reactions are available both in Ru (III) and Pd (II) complexes, and their distinct electronic configuration and specific metal-ligand interactions lead to differences in reactivity.

Ru (III) Complexes: Ru (III) complexes are excellent candidates for photo redox catalysis because the oxidizing ability of light-induced photochemical electron transfer can lead to Ru (III)/Ru (II) or even Ru (III)/Ru (IV) processes; this has been useful in several synthesis schemes that result in Ru (III) complexes. In Ru (III) complexes, MLCT transitions are strong enough, meaning electron transfer occurs very efficiently upon photoexcitation.





Photochemical Properties

Absorption λ_{\max} : 454 nm

$\epsilon = 14,600 \text{ M}^{-1} \text{ cm}^{-1}$

Excited State: $^3\text{MLCT}$

Triplet Energy: 2.12 eV

τ_0 (MeCN): 1100 ns

Emission λ_{\max} : 605 nm

Redox Properties

$E_{1/2} (\text{Ru}^{2+}/\text{Ru}^{3+}) = +1.29 \text{ V vs. SCE}$

$E_{1/2} (\text{Ru}^{2+}/\text{Ru}^+) = -1.33 \text{ V vs. SCE}$

$E_{1/2} (\text{Ru}^{3+}/^*\text{Ru}^{2+}) = -0.81 \text{ V vs. SCE}$

$E_{1/2} (^*\text{Ru}^{2+}/\text{Ru}^+) = +0.77 \text{ V vs. SCE}$

Figure 5: Photochemical properties of a Ruthenium complex

In addition, it has outstanding advantages in applying photocatalysis and solar fuel, wherein its ability to switch between the two oxidation states reversibly leads to effective charge separation and energy storage in such application. The photochemical characteristics of a Ruthenium complex are depicted in the figure 5.

Pd (II) complexes: The Pd (II) complexes are much less tolerant to structural change to the oxidation state under photoredox conditions due to the fact that the +2-oxidation state is inherently favoured for the palladium centre. However, they are useful in reactions where the sufficient electron transfer is from ligands and not the centre of the metal. This includes applications such as organic transformations or sensing. In this process, through ligand-centred excitations, Pd (II) complexes can participate in electron transfer processes without requiring modifications to the metal centre's oxidation state., making them useful in catalytic applications that do not require important redox cycles.

Photochemical Property	Ru (III) Complex	Pd (II) Complex
Oxidation States	+2, +3, +4	Predominantly +2
Electron Transfer	Efficient via MLCT	Ligand-centered transitions
Stability Under Irradiation	High	Moderate
Applications	Photocatalysis, Solar Energy	Fluorescent Sensing, Imaging

Table 4 ; Photochemical properties of Ru(III) and Pd (II)

1.4.2 Electron Transfer and Energy Transfer Processes

Both Ru (III) and Pd (II) complexes have the ability to facilitate electron and energy transfer events, however the nature of these processes differs based on the ligand environment and the metal centre's electronic structure.

Ru (III) Complexes: Ru (III) complexes are excellent energy transfer agents, largely because of the stabilization of their long-lived excited state triplets. The high atomic weight of the metal Favors intersystem crossing and makes it possible for the Ru (III) complex to reach the triplet state, favourable for energy transfer. Such ability can play a crucial role in the application of light harvesting and artificial photosynthesis, wherein the Ru (III) complex's energy transmission to nearby molecules either absorbs energy or promote chemical processes. Because the excited state lasts a long time and permits extended charge separation, it also encourages the phenomena of electron transfer in redox processes.

Pd (II) complexes: Pd (II) complexes are well suited to fast electron-transfer schemes based on immediate-response-to-light-excitation properties as they exhibit fluorescence that occurs very quickly with a high quantum yield. The Pd (II) complexes' square planar geometry favors easy electron transport centred on ligands, such that it can be returned to its ground state without delay after excitation (Smucker et al., 2003). Such properties are especially convenient in real-time



applications, such as sensing technologies and catalytic transformations in organic chemistry. Here fast electron transfer sensitivity is required for detecting small environmental changes or for initiating rapid reactions.

1.4.3 Photoinduced Ligand Substitution Reactions

Photoinduced ligand substitution is the reaction where another ligand replaces the ligand occupying the position in the metal complex, triggered by the presence of light. Such reactions in Ru (III) and Pd (II) complexes have different tendencies, because their metal-ligand bonding and photochemical stability are different.

Ru (III) Complexes: The stronger metal-ligand bonds and the very high binding energy attached to the ruthenium center make ruthenium (III) complexes generally more stable and less susceptible to irradiation-induced ligand substitution. However, certain conditions provide for the possibility of photoinduced ligand exchange in Ru (III) complexes when irradiated with the suitable wavelength of light. This property is useful in photocatalysis, where controlled release or exchange of ligands can influence the catalytic activity and provide routes to multi-step reactions. Ru (III) complexes can also be used in drug delivery systems where, upon irradiation, light-induced substitution reactions trigger the release of therapeutic agents in a controlled fashion within biological environments.

Pd (II) complexes: Their metal-ligand interactions are generally weaker, with the binding energies at the Pd center being substantially lower than those within the Ru (III) compounds. Hence, Pd (II) complexes are quite reactive towards ligand substitution. Their light sensitivity enables Pd (II) complexes to undergo ligand exchange by photolysis; this property is utilized in photochemical synthesis as well as catalytic processes. The Pd (II) complexes are quite easily susceptible to ligand exchange,

and the rate of ligand exchange can be fine-tuned for any particular reactions or products desired. Pd (II) complexes are thus found to be valuable in dynamic photocatalytic cycles (Vogler et al., 2000).

1.4.4 Photo reactivity of Ru (III) and Pd (II) complexes towards Photochemical Applications

Complex of Ru (III) and Pd (II) are photoreactive and thus have different photochemical applications because of the diversity in their respective metal-ligand interactions and photo reactivity.

Ru (III) Complexes: With the Ru (III) complexes, long-lived excited states could be sustained and passed through efficient energy and electron transfer processes, promising potential applications in solar energy conversion, artificial photosynthesis, and photocatalysis. The complexes can absorb and retain light energy for a long period, which fosters charge separation and allows redox processes necessary to facilitate energy storage and catalytic reactions.

Pd (II) complexes: The main advantage of Pd (II) complexes is their rapid fluorescence emission, as well as a trend towards ligand-centred electron transfer, that makes them applicable for sensing, optical imaging applications, and even real-time diagnostics. Due to high fluorescence quantum yields, Pd (II) complexes can respond immediately to light as their fast emission allows, making them highly effective in applications with requirements for rapid feedback. In addition, the Pd (II) complex reactivity through ligand substitution reactions under light makes them particularly valuable in synthetic and catalytic applications requiring rapid ligand exchange.

1.4.4 Comparison of Ru (III) and Pd (II) Complexes

The photochemical properties of each of the Ru (III) and Pd (II) complexes thus offer something unique with potential advantages by different electron configurations, lifetime excitation states, and behaviour in reactivity.

1.4.4.1 Ru (III) Stability, Long-lived excited States, and robust Redox Activity

The Ru (III) complexes are ideal for applications requiring stable, long-lived excited states, which would allow the efficient storage and transfer of energy. These complexes have the following characteristics:

Long-Lived Excited States: When ruthenium undergoes the heavy-atom effect, the Ru (III) complexes greater crossover of ISC from singlet to triplet states due to increased spin-orbit coupling. This conversion results in long-lived triplet states that can store and transfer energy over time periods. This feature is particularly useful in photocatalysis, where the reaction can be maintained constantly for extended periods of time as long as there is light illumination. When it



comes to water splitting, the long-lived excited state generated by the Ru (III) complex improves charge separation, which makes it easier for water molecules to divide into hydrogen and oxygen.

High Redox Activity: The Ru (III) complexes exhibit high activity in redox; in this case, the metal centre can readily gain or lose electrons, such as moving from the Ru (III) to the Ru(II) or Ru(IV). It is therefore possible for the Ru (III) complex to capture the light energy to drive redox in applications for photo redox catalysis and the production of solar fuels. The ability of Ru (III) complexes to change oxidation states further enhances their application in energy storage devices, wherein they can sustain charge and act in cycles of controlled redox, making it possible for the proper storage and release of energy.

Applications in Energy Conversion and Catalysis: The long-lived excited states and the redox abilities of the Ru (III) complexes place these compounds in interesting applications, such as artificial photosynthesis-mimicry of the energy-conversion processes that occur in plants. The Ru (III) complexes have applications in solar energy devices and environmental remediation through photocatalytic degradation of pollutants, whereby persistence in energy states allows for a photochemical activity that lasts longer and effective degradation of the pollutant.

1.4.4.2 Pd (II) Complexes: Fast Electron Transfer with Immediate Photochemical Activity

Therefore, for scenarios that require rapid responding electron transfer phenomena combined with the immediacy of photoactivity of compounds, Pd (II) complexes are preferred. Some of the main photochemical properties of the Pd (II) complexes include:

Fast Transfer Rates for Electrons: In square planar geometries, such as those of Pd (II) , it is LC transitions like $\pi \rightarrow \pi^*$ end. Unlike the cases of Ru (III) complexes, the fluorescence of Pd (II) complexes is not related to the long-lived triplet states. It has been observed that these complexes fluoresce very rapidly with very high quantum yields. Fast electron transfer is desirable for a real-time sensor and a molecular probe, as one can get immediate feedback in the case of a Pd (II) complex interaction with light, so that target molecules or changes in the environment can be identified rapidly.

Sensing and diagnostic application: Such Pd (II) complexes are excellent for applications where a strong photochemical response is required immediately due to their high fluorescence yield and fast emission nature. The electronic transitions ligand-centred in nature quickly return to the ground state, making them suitable for high-speed sensing and diagnostics. This makes Pd (II) complexes useful in optical imaging and biosensing where they act as fluorescent probes that respond in real time to changes in biological or chemical environments. For example, a Pd (II) complex may be applied for live-cell imaging to observe dynamic cellular processes in real-time.

Applications in diagnostics and rapid-response systems: Rapid photochemical reactivity of Pd (II) complexes applies to medical diagnostics, fluorescence-based sensors, and display technologies. Optical sensors may be devised from Pd (II) complexes to detect biological markers or environmental pollutants rapidly with high sensitivity. The fast fluorescence of Pd (II) complexes makes them highly suited for use in devices requiring high efficiency with quick refresh rates, such as OLEDs and other light-emitting components.

Ru (III) and Pd (II) complexes will be chosen on the basis of their photochemical properties. For the applications that need an extended energy transfer along with steady redox cycling, energy-intensive reactions, and long-lasting photochemical processes, Ru (III) complexes work efficiently. In fact, they play a crucial role in energy conversion, photocatalysis, and storage systems. High speed transfer and immediate photochemical reactivity make Pd (II) complexes suited to the applications requiring fast reaction. They are suitable for real-time sensing, diagnostics, and imaging applications with fast response times, and good sensitivity, owing to their quantum yields and fast fluorescence emission (Alam et al., 2019).

Thus Pd (II) complexes are best suited to fluorescence-based applications that require fast responses, whereas Ru (III) complexes are well matched to applications that involve energy and electron transfer.

1.5 Applications

Ru (III) complexes are stable photochemical reactions that utilize light as the energy source for catalysis. Pd (II) complexes must be applied to low-energy, high-speed applications such as molecular sensing, organic synthesis, biosensors, and environmental monitoring. Ru (III) complexes may take advantage of phosphorescence to facilitate



efficient energy transfer and long-lived excited states. Multipurpose systems that combine catalysis, light emission, and sensing can be realized.

Table 5: Comparison of Application of Ru (III) and Pd (II) Complexes

Application	Ru (III) Complex	Pd (II) Complex
Photocatalysis	Excellent	Moderate
Optoelectronics (OLEDs)	Good	Excellent
Sensing (Chemical Detection)	Limited	Excellent
Solar Energy Conversion	Excellent	Limited

1.5.1 Photocatalysis

Photocatalysis is an application of light energy to catalyse a chemical reaction. It has been used extensively in environmental applications, such as splitting water to generate hydrogen or reduction of CO₂ to provide useful chemicals or fuels.

Ru (III) Schiff Base Complexes:

Stability: Ru (III) complexes are very stable, and this is particularly crucial for photocatalytic applications where light must be employed for extended periods without degrading the catalyst. These complexes can absorb light to reach a long-lived excited state; therefore, Ru (III) complexes are promising candidates for photocatalytic reactions. This is since it allows such a complex to act as an electron reservoir, which is a fundamental aspect in water splitting, by allowing it to transfer with a higher efficiency.

Electron transfer: Ru (III) complexes transfer electrons into these reactions-well, they are good electron shuttles in these kinds of reactions and so support chemical reactions wherein electron movement is required, an important basis of applications like CO₂ reduction and water splitting.

Pd (II) Complexes:

Greater Fluorescence: Pd (II) complexes generally exhibit greater fluorescence than Ru (II)-an important consideration for organic transformations requiring input of light energy to induce chemical change.

Shorter excited-state lifetimes: This makes Pd (II) complexes more suitable for applications requiring faster, lower energy reactions, such as organic synthesis. In these applications, Pd (II) complexes provide efficient catalysis at relatively small amounts of inputted energy.

Organic transformations: Pd (II) is used in various applications, which include C-C coupling reactions or functional group transformations where its fluorescence and faster excited-state relaxation can be used to catalyse those applications efficiently.

1.5.2 Sensing and Detection

Molecular Sensing: The detection of single molecules, ions, or other analytes through the monitoring of changes in the properties of a sensing material, such as its optical response, for instance, fluorescence.

Pd (II) Complexes:

High fluorescence and fast electron transfer: due to their strong fluorescence and fast electron-transfer characters, Pd (II) complexes have great potential in molecular sensing. Upon the interaction of Pd (II) complexes with analytes, the often-resulting effect appears to be photophysical property changes, such as fluorescence quenching or fluorescence enhancement caused by a reduction in emission or emission enhancement.

Selective Sensitivity: This sensitivity toward the analytes comes with many advantages for the detection of ions, small molecules, or biological analytes in a solution and makes Pd (II) complexes good prospects for such applications as biosensors and environmental monitoring. The detection of these substances with high selectivity by the Pd (II) complexes makes them invaluable tools in diagnostic systems and pollutant detection.



Ru (III) Complexes:

Long-lived excited states: The lifetimes for excited states of Ru (III) complexes are more prolonged. It proves to be useful in sensing applications where time-resolved fluorescence assays with measurements of emission are taken after a delayed time. This is one reason this system will be able to detect more sensitively when interference from background scatter might be a problem.

Sensitive and tuneable photo physics: Ru (III) complexes are characterized by extremely stable photo physics that could be very finely modulated for a variety of sensing purposes and hence provide highly selective and sensitive sensors. Due to the stability of these materials, they could be used in those environments where other materials would degrade or lose their sensitivity

These complexes find applications in environmental monitoring, biological assays, and detection of harmful substances as their photophysical properties remain reliable under various conditions.

1.5.3 Optoelectronic Devices

Optoelectronics is the branch of electronics dealing with devices which source, detect, and control light, e.g. LEDs, solar cells, and display technologies.

Ru (III) Complexes:

These Ru (III) complexes were determined to be phosphorescent, such that it emits light for an enormously longer duration than any other element following excitation. For an OLED, the light-emitting efficiency has to be stable for a longer duration.

Energy Transfer: Long-lived excited states in Ru (III) complexes enable effective energy transfer, which is essential for solar cell and other device applications. Long-term stability is necessary for the constant conversion of light into power.

Charge Transfer: In OLEDs and solar cells, Ru (III) complexes help in efficient charge transfer, which is the essential process for device efficiency in devices that convert electrical energy to light and vice versa, in the case of solar cells.

Pd (II) Complexes:

High Fluorescence Efficiency: Pd (II) complexes emit efficiently enough to be perfectly applicable in situations requiring rapid light emission. For instance, some Pd (II) complexes have been used in displays as well as fluorescent markers for bio-imaging or diagnostics because they emit within the shortest time after excitation.

Quick Emission: The short lifetimes of the excited state of Pd (II) complexes make it appropriate for applications that demand fast response times, such as display technologies, which require light states to switch quickly.

These kinds of complexes can also be used in high-performance optical devices where visible light emission plays a crucial role in how display systems operate, lighting, and fluorescent marking.

1.5.4 Comparison of Ru (III) and Pd (II) Complexes in Applications

Photophysical properties between Ru (III) and Pd (II) complexes are complementary to one another. The major applications of Ru (III) complexes lie in processes that require the long-lived excited state and sustained energy transfer - photocatalysis, solar cells, and OLEDs. Such properties rendered Ru (III) complexes to be the best choices for those processes requiring stability and prolonged electron transfer.

On the other hand, the Pd (II) complexes are better suited for applications where high fluorescence efficiency and rapid response are demanded along with rapid electron transfer. This is owing to these properties that make the Pd (II) complexes more applicable in sensing, organic transformations, and real-time optoelectronics applications like displays, where fast reaction kinetics are mandatory.

Further the complementary nature of Ru (III) and Pd (II) complexes allows them to be used in tandem in multifunctional systems. For example, the device may co-embed the photocatalytic nature of the Ru (III) complexes with the fast-response properties of the Pd (II) complexes into a chemical sensor or a light-emitting-catalytic device that detects analytes and catalyzes reactions in parallel. This synergy opens rather exciting avenues toward multifunctional devices combining sensing, light emission, and catalysis into one system (Beil et al., 2024).



In conclusion Ru (III) and Pd (II) complexes hold a high value in an exceptionally wide range of applications, where the photo physics vary significantly. Ru (III) complexes are well suited to stable, long-lived reactions like photocatalysis and solar cells, whereas Pd (II) complexes are perfect for applications that necessitate the ability to respond very quickly, like sensing or real-time optoelectronics. Together, they offer complementary capabilities for multifunctional devices that can serve in diverse applications such as biosensing, displays, catalysis, and energy conversion.

1.6 Conclusion and Future Directions

1.6.1 Summary of Key Findings

This study draws attention to some special characteristics of Ru (III) and Pd (II) Schiff base complexes, along with their vast applications across different disciplines. Ru (III) complexes are characterized by strong MLCT transitions and the long-lived excited state properties, and also have relatively high redox activity, ensuring that the complexes are well suited for energy-intensive applications, such as photocatalysis and solar energy conversion, in various fields. Such long-lived excited states afford the possibility for persistent charge transfer and energy retention - special benefits where an application shows natural photosynthesis, such as solar energy harvesting. The photo-redox reactions of Ru (III) complexes, which are well-controlled, also make them plausible candidates for the water splitting process, which is essentially involved in the generation of renewable energy. Thus, Ru (III) complexes excel in a process that requires stability and robustness under continuous or even high-energy irradiation.

The Pd (II) complexes have demonstrated high fluorescent efficiency coupled with rapid response to excitation due to square-planar geometry combined with ligand-centred π -back bonding. Such features in these complexes make them very potent in applications requiring fast emission and high sensitivity, such as in real-time sensing and molecular imaging. Pd (II) complexes are different from the Ru (III) analogs as they do not show a heavy-atom effect, which leads to a decrease in intersystem crossing and Favors quick fluorescence, so they become applicable for high sensitivity and fast diagnostics.

Though structurally stable, Pd (II) complexes are generally less thermally stable than their Ru (III) counterparts and, thus, limited usage at elevated temperatures is expected. However, their rapid fluorescence sensitivity places them ideally as candidates for fluorescence-based sensing as well as optoelectronic devices. In general, while Ru (III) complexes appear to be suitable for stable, energy-intensive applications, Pd (II) complexes appear to be ideal for applications requiring immediate photonic response and precision in detection.

1.6.2 Challenges and Opportunities in the Field

The major challenge with Ru (III) and Pd (II) Schiff base complexes relates to the balance of the strengths of these complexes for reactivity on the one hand and stability in different applications on the other. Ru (III) complexes are excellent for applications that require excited-state lifetimes and by definition are highly stable, but such complexes are not so good in an environment requiring the rapid response needed for applications such as real-time sensing. While the optical properties of the Pd (II) complexes are outstanding in applications where a fast response is needed, such as diagnostics, fluorescence being instantaneous, stability toward higher temperatures or intense energy exposure was limited. Such a compromise between stability and response time constitutes an important challenge for trying to extend applications toward a larger range.

However, a very promising opportunity still exists in the making of hybrid or mixed-metal systems, which might both include Ru (III) and Pd (II), and therefore combine the stability and the long duration of energy transfer of Ru (III) with the sensitivity and the fast response of Pd(II). Hybrid systems may give birth to a new generation of multifunctional devices, capable not only of operating under energy conversion conditions but also of real-time sensing.

The last challenge in this area is the rather complex synthesis required to synthesize complexes of the desired properties. Such minute structural changes in Schiff base ligands, such as the attachment of substituent groups or changing the coordination geometry, are assumed to make a big difference in the photophysical behavior of the resulting complex, and this aspect leads to extensive trial and error in the experimental synthesis. This can be time-consuming, and delays the development process; thus, the properties cannot be finely controlled according to the



desired application criteria. Advances in the computational technique can overcome these problems. Predicting the impact of structural variation on photophysical properties with computational models allows synthesis attempts to be directed toward obtaining complexes with optimized characteristics without having to test experimentally all possibilities. This could lead to much faster design of Ru (III) and Pd (II) complexes, whose target absorption and emission properties should be aimed at applications in renewable energy and real-time diagnostics as discussed above. A third challenge is improving the thermal and photochemical stability of these complexes, especially of Pd (II), to expand their application areas in different environments. The Pd (II) complexes, although perfect for very fast fluorescence applications, are more sensitive to thermal degradation or degrade by photolysis in prolonged light exposure and therefore cannot be used at high-energy operations. Strategies to stabilize these complexes under more demanding conditions could thus open applications into areas that demand stability, such as industrial sensing or environmental monitoring outdoors. Some of the possible solutions are ligand modification for stabilizing or synthesis of a composite material that can encapsulate Pd (II) complex in harsh environments. Overcoming this stability barrier would extend the scope of uses of Pd (II) complexes from low-temperature to high-temperature applications.

1.6.3 Future Research Directions

Developments of Mixed-Metal and Hybrid Complexes: one direction of further research is the development of hybrid complexes, including Ru(III) and Pd(II) in the same structure. These may take advantage of the stability and redox activity of Ru(III) and the high speed of fluorescence of Pd(II) in one and the same multifunctional devices. Such complexes can support long-term energy storage, as well as fast optical sensing, for example, environmental monitoring, artificial photosynthesis, and dual-function sensors. For the hybrid materials composed of Schiff base ligands, the photophysical characteristics would require precise control of the coordination geometry as well as the electronic structure.

The other area to be explored relates to the development of Schiff base ligands in such a way that the photo physics of Ru(III) and Pd(II) complexes could be further modulated. For instance, one might design modifications within these ligands in ways that the features such as absorption maxima, quantum yield, and lifetime of the excited states may be altered. For instance, electron donation may improve the thermal stability of Ru(III) complexes, while electron-rich ligands may yield more fluorescent Pd(II) complexes. In such optimized properties, these materials could be employed in applications of energy conversion, catalysis, and biosensing, providing a great potential for further optimization.

Mechanistic investigations on photocatalytic processes: Elaborate investigations on the photocatalytic mechanism of Ru(III) complexes, particularly concerning the processes driven by solar light such as water splitting and CO₂ reduction, shall be important. These studies might also reveal means by which their energy and electron transfer efficiency can be improved for renewable energy application. Investigations of Pd(II) complexes in low-energy organic transformations can also offer insights into the function that Pd(II) complexes play in efficient catalysis. Investigations in this direction might include the expansion of these kinds of complex applications in sustainable energy and green chemistry, and that would eventually uncover new paths toward eco-friendly energy and industrial processes.

Development in Computational Modelling and Simulation: To understand the properties of Ru(III) and Pd(II) complexes, computations such as Density Functional Theory (DFT) and Time-Dependent DFT (TD-DFT) are fundamental. The modelling of electronic transitions and charge distributions may better predict which changes in ligands or metals would have significant effects on photophysical behaviour, thus making synthesis more aimed. Pre-synthetic computation can inhibit several trial and error experiments that might be required in the experimental synthesis for such applications as light harvesting, biosensing, and optoelectronics.

The complementary properties of Ru (III) and Pd(II) complexes open up an exciting opportunity to form multifunctional devices. The association of the energy transfer ability of Ru(III) with the Pd(II) fluorescence quickly turned off can offer promise as a method in devices storing energy and sensing real-time. The devices would thus be sensitive detectors of pollutants, monitors for cellular processes or phototherapeutic agents capturing solar energy. This combines Ru(III) and Pd(II) in single devices, upholding novel avenues of technological application that the world will be challenged with, answering energy, health, and environmental challenges more ingeniously.



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