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A Review on N-Ortho-Hydroxymethyl Benzyl Valine and Its 4d Metal Complexes; and Their Biological and Spectroscopic Properties

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ABSTRACT

This review paper focuses on the development and applications of metal-based coordination compounds, particularly those involving N-ortho-hydroxymethyl benzyl valine (N-OHMBV) as a ligand. The ability of N-OHMBV to coordinate with transition metals such as ruthenium (Ru), rhodium (Rh), palladium (Pd), silver (Ag), and cadmium (Cd) results in the formation of complexes with notable biological activities, including anticancer, antibacterial, antioxidant, and enzyme-inhibitory effects. These complexes exhibit promising therapeutic potential, and their mechanisms of action are primarily influenced by the coordination environment and the interaction between the metal center and N-OHMBV's functional groups. Spectroscopic techniques, including infrared (IR) and nuclear magnetic resonance (NMR) spectroscopy, provide crucial insights into the structural features of these metal-ligand complexes, which is important for understanding their biological efficacy. The paper reviews the synthesis, coordination properties, biological activities, and spectroscopic characterization of N-OHMBV-metal complexes, underscoring their potential in drug design and therapeutic applications.

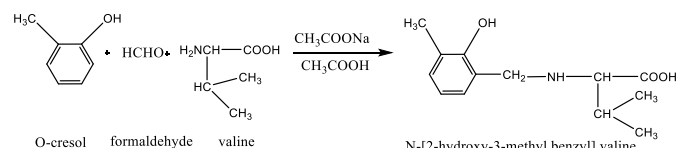
1. Introduction

The development of metal-based coordination compounds has gained significant attention in medicinal chemistry due to their unique biological activities, such as anticancer, antibacterial, and enzyme-inhibiting effects [1]. N-Ortho-hydroxymethyl benzyl valine is an important ligand with both hydroxyl and amine functional groups, making it capable of forming stable complexes with 4d transition metals like ruthenium (Ru), rhodium (Rh), palladium (Pd), and silver (Ag) and cadmium (Cd) [2]. These metal complexes exhibit a range of promising biological activities due to the coordination [3]. Between the metal ion and the ligand's functional groups, influencing their ability to interact with biomolecules such as DNA and proteins [4]. N-OHMBV-4d metal complexes have been found to exhibit notable anticancer and antibacterial properties, along with antioxidant effects and enzyme inhibition [5]. The coordination of metal ions enhances the ligand's stability and reactivity, facilitating targeted biological interactions [6]. Spectroscopic techniques like Infrared (IR) and Nuclear Magnetic Resonance (NMR) spectroscopy are crucial for characterizing the metal-ligand bonding and understanding the structural features that govern their biological activity [7]. This review focuses on the synthesis, coordination chemistry [8]. Biological activities, and spectroscopic characterization of N-OHMBV based metal complexes, providing insight into their potential as therapeutic agents [9]. Further research into these complexes could lead to the development of more effective metal-based drugs for treating diseases like cancer and bacterial infections [10].

2. Synthesis of Ligand N-Ortho-Hydroxymethyl Benzyl Valine

N-OHMBV is synthesized by reacting benzyl alcohol derivatives with formaldehyde and the amino acid valine. The ligand's structure includes an N-ortho-hydroxy group that can engage in hydrogen bonding and coordination to the metal, while the methyl group enhances the stability of the complex [10]. The amine group on the valine portion of the ligand is another crucial donor site for coordination. The synthesis involves simple condensation reactions, making N-OHMBV a versatile ligand for coordination chemistry. To prepare the ligand, we begin with N-[2-hydroxy-3-methyl benzyl] valine. This process involved the utilization of

ortho-cresol valine sodium acetate trihydrate, formalin, and glacial acetic acid. We initiated the synthesis by simultaneously mixing 0.5 moles of each component: ortho-cresol (54 g), valine (37 g), and sodium acetate trihydrate (68 g), along with 250 mL of formalin and glacial acetic acid until a homogeneous solution was achieved. Following this, authors introduced 40% of the formalin solution dropwise into the mixture on a water bath while maintaining a temperature range of 60 to 80 degrees Celsius for a duration of 2 to 3 hours. Subsequently, the entire solution was heated on a water bath for an additional 12 to 14 hours, with periodic stirring. Upon cooling, a yellowish viscous solution resembling wax was obtained (shown in Scheme 1). This wax, constituting the ligand, was then transferred into distilled water and subjected to filtration. A portion of the filtrate underwent recrystallization by treatment with NaOH and 50% HCl solution. The resulting precipitate was dried in an oven for 2 to 3 days at temperatures ranging from 20 to 30 degrees Celsius, yielding the pure form of our desired ligand [11].



Scheme 1 General synthesis of ligand N-OHMBV preparation

3. Coordination Chemistry of 4d Metal Complexes with N-OHMBV

The coordination chemistry of 4d metal complexes with the bidentate ligand N-OHMBV (O-hydroxy- α -methylbenzylamine) involves the formation of stable complexes through the coordination of the metal center to the ligand's nitrogen and oxygen donor atoms [12]. The metal ions in question Ru (Ruthenium), Rh (Rhodium), Pd (Palladium), Ag (Silver), and Cd (Cadmium) each exhibit distinct behaviors when complexed with OHMBV [13].

3.1 Ru (Ruthenium) Complexes

In Ru (Ruthenium) complexes, the metal typically adopts an octahedral geometry [14]. The bonding involves both electrostatic interactions and π -back donation from the metal's d-orbitals. This results in strong metal-ligand bonding, especially in the +2 oxidation state [15].

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3.2 Rh (Rhodium) Complexes

For Rh (Rhodium), complexes usually adopt square planar or octahedral geometries, depending on the oxidation state [16]. Rhodium exhibits stronger metal-ligand π -back donation, especially in its +3 oxidation state, which enhances the stability of the complex and influences its electronic properties [17].

3.3 Pd (Palladium) Complexes

For Pd (Palladium) complexes, typically in the +2 oxidation state, tend to form octahedral structures with N-OHMBV. Similar to rhodium, the metal-ligand interactions are influenced by d-orbital overlap, leading to stable complexes with distinct spectroscopic properties [18].

3.4 Ag (Silver) Complexes

For Ag (Silver) complexes, the metal typically adopts a linear or tetrahedral geometry due to the weaker metal-ligand interactions [19]. The bonding is mainly electrostatic, as silver does not effectively engage in π -back donation, resulting in less stable complexes compared to those of other 4d metals [20].

3.5 Cd (Cadmium) Complexes

For Cd (Cadmium), which is a d10 metal in the +2 oxidation state, the coordination geometry is typically octahedral [21]. The bonding in these complexes is primarily electrostatic and covalent, as cadmium does not participate in π -back donation, making these complexes relatively stable but less electronically rich compared to other 4d metal complexes [22].

4. Biological Importance of N-Ortho-Hydroxymethyl Benzyl Valine

The biological importance of N-ortho-hydroxymethyl benzyl valine stems from its unique structure, which combines a hydroxyl group and an aromatic ring [23]. These modifications enhance its ability to interact with enzymes and receptors, potentially influencing metabolic pathways where valine plays a role [24]. The hydroxyl group may contribute antioxidant properties, protecting cells from oxidative stress, while the aromatic functionality can aid in stabilizing protein structures and facilitating molecular recognition [25].

This compound holds promise in drug development, particularly for creating enzyme inhibitors or therapeutic peptides, and in biotechnology as a precursor for bioactive molecules. Its role in improving protein stability and metabolic modulation highlights its significance in biochemical and pharmaceutical research. The compound you refer to, N-ortho-hydroxymethyl benzyl valine, appears to describe a derivative of valine, an essential amino acid, potentially with an aromatic ring and hydroxymethyl group substitution. The biological importance of such a compound can be understood in several contexts [26].

4.1 Role in Biochemical Processes

4.1.1 Precursor in Metabolic Pathways

Valine, a branched-chain amino acid (BCAA), is essential for protein synthesis, tissue repair, and energy production. Derivatives like N-ortho-hydroxymethyl benzyl valine, with modifications such as the hydroxymethyl group, may have altered biochemical roles, influencing these processes [27].

4.1.2 Hydroxy Substitution

The hydroxyl group (-OH) increases the compound's hydrophilicity, which can affect its solubility and interactions within biological systems. This change could lead to different behaviors compared to the unmodified amino acid [28].

4.1.3 Aromatic Functionality

The presence of an aromatic ring with N-ortho-hydroxymethyl substitution enhances the ability to form π - π interactions or hydrogen bonds. These interactions could influence protein-ligand binding, enzyme activity, and overall molecular stability [29].

4.2 Potential Antioxidant Properties

Hydroxyl groups on aromatic systems are well-known for their antioxidant activity. The compound may act as a free radical scavenger, reducing oxidative stress and potentially protecting cells from damage. This antioxidant property is crucial in preventing cellular degeneration and may have implications in cancer prevention and aging [30].

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4.3 Pharmaceutical Relevance

4.3.1 Drug Development

Modifying amino acids, such as valine, is a common strategy in drug design. The modifications in N-ortho-hydroxymethyl benzyl valine could enhance pharmacokinetic properties and increase specificity for certain biological targets, making it a promising candidate in drug development [31].

4.3.2 Enzyme Inhibitors

The compound might mimic natural substrates or act as an enzyme inhibitor, making it valuable in treating conditions where enzyme activity is dysregulated, such as metabolic disorders or certain cancers. Its structural similarity to valine allows it to influence enzyme function by competing for binding sites [32].

4.4 Antioxidant Properties

The hydroxyl group in N-Ortho-hydroxymethyl benzyl valine imparts strong antioxidant capabilities by scavenging free radicals and mitigating oxidative stress. This activity plays a critical role in protecting healthy cells from oxidative damage, a process closely linked to the initiation and progression of cancer [33].

4.5 Anticancer-Potential

The aromatic ring in the compound enhances its interaction with cancer-specific molecular targets, enabling it to disrupt pathways involved in tumor metabolism and proliferation. This unique structural feature positions it as a potential modulator of cancer-related mechanisms, targeting cellular processes essential for tumor growth [33].

4.6 Therapeutic-Relevance

Combining antioxidant and anticancer activities, N-ortho-hydroxymethyl benzyl valine shows significant promise in drug development. Its dual functionality could be leveraged in therapies addressing oxidative stress-induced oncogenesis and metabolic dysregulation in cancer cells, paving the way for novel treatment strategies [34].

4.7 Biochemical-Significance

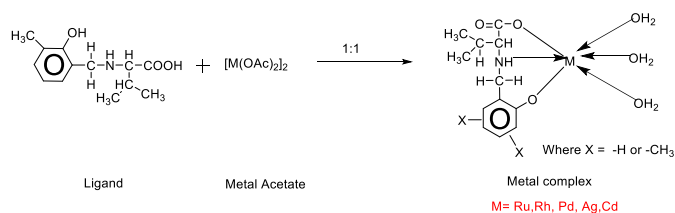
The compound's ability to stabilize proteins and enhance molecular recognition makes it an attractive candidate for the synthesis of bioactive molecules. These properties further underscore its potential as a versatile agent in both antioxidant defense and anticancer therapy [35].

5. Metal Complexes of N-Ortho-Hydroxymethyl Benzyl Valine

The synthesis of metal complexes of N-ortho-hydroxymethyl benzyl valine involves reacting the ligand, which contains both an amino group (-NH₂) and a hydroxyl group (-OH), with metal salts like [Ru(OAc)₂], [Rh(OAc)₂], [Pd(OAc)₂], [Ag(OAc)], or [Cd(OAc)₂] in a 1:1 molar ratio [35]. The reaction is carried out in solvents such as ethanol, acetonitrile, or water, where the ligand coordinates to the metal ion through its nitrogen and oxygen donor atoms, forming a stable bidentate chelate complex. The reaction mixture is stirred or heated gently to facilitate complexation, and the product is isolated by evaporating the solvent or filtration. Further purification, if needed, can be done by recrystallization or chromatography. These metal-ligand complexes are of interest for applications in bioinorganic chemistry, catalysis, and drug development due to their enhanced stability and reactivity [36].

6. Bidentate Metal Complexes of N-Ortho-Hydroxymethyl Benzyl Valine

The ligand (which contains an amino group and a hydroxyl group) to a metal ion, such as Ru²⁺, Rh³⁺, Pd²⁺, Ag⁺, or Cd²⁺. The ligand binds to the metal at two sites, forming a stable chelated complex. The synthesis involves mixing the ligand with a metal acetate salt (e.g., [M(OAc)₂]) in a 1:1 molar ratio, typically in a solvent like ethanol or acetonitrile, and heating or stirring to promote complexation. The result is a bidentate metal-ligand complex, which can be purified by filtration or recrystallization. These complexes have applications in catalysis, bioinorganic chemistry, and drug development [37]. The synthesis of bidentate metal complexes of N-ortho-hydroxymethyl benzyl valine can vary depending on the metal ion used. Each metal interacts with the ligand differently based on its electronic configuration and coordination preferences.



Scheme 2 General synthesis of 4d metal complexes with N-OHMBV

6.1 Ruthenium (Ru) Complexes

Ruthenium complexes with N-ortho-hydroxymethyl benzyl valine are typically synthesized by reacting the ligand with $[\text{Ru}(\text{OAc})_2]$ in a 1:1 molar ratio. The ligand coordinates through the amino ($-\text{NH}_2$) and hydroxyl ($-\text{OH}$) groups, forming a stable bidentate chelate. The Ru ion is often chosen for its versatility in catalysis and its ability to form stable complexes with a wide range of ligands [38].

6.2 Rhodium (Rh) Complexes

In the case of Rhodium complexes, $[\text{Rh}(\text{OAc})_2]$ reacts with the ligand, facilitating coordination through the nitrogen and oxygen donor atoms. Rhodium's strong affinity for ligands with soft donor atoms makes it an ideal candidate for these types of bidentate complexes. The resulting complex is particularly useful in catalytic applications, such as hydrogenation reactions [38].

6.3 Palladium (Pd) Complexes

Palladium, $[\text{Pd}(\text{OAc})_2]$ is commonly used to form bidentate metal-ligand complexes with N-ortho-hydroxymethyl benzyl valine. Palladium's ability to coordinate with the ligand through both the amino and hydroxyl groups enhances the stability of the complex, making it suitable for applications in cross-coupling reactions and catalysis in organic synthesis [39].

6.4 Silver (Ag) Complexes

When reacting with Silver salts such as $[\text{Ag}(\text{OAc})]$, N-ortho-hydroxymethyl benzyl valine forms bidentate complexes by coordinating with the silver ion through the nitrogen and oxygen donor atoms. Silver complexes are often used in antimicrobial and catalytic processes, where the unique coordination chemistry with the ligand is beneficial [40].

6.5 Cadmium (Cd) Complexes

Cadmium complexes, typically formed with $[\text{Cd}(\text{OAc})_2]$, coordinate with the ligand through the nitrogen and oxygen atoms to create a stable bidentate chelate. Cd complexes with N-ortho-hydroxymethyl benzyl valine can be useful in various fields, including environmental chemistry and the development of new materials [41].

7. DFT and Molecular Modeling of Metal Complex of N-Ortho-Hydroxymethyl Benzyl Valine

The N-ortho-hydroxymethyl benzyl valine ligand analyzed using DFT. This compound consists of a benzene ring (as indicated by the carbon atoms in the aromatic ring) attached to a hydroxy group ($-\text{OH}$) at the ortho position, a methyl group ($-\text{CH}_3$), and a valine residue (Fig. 1).

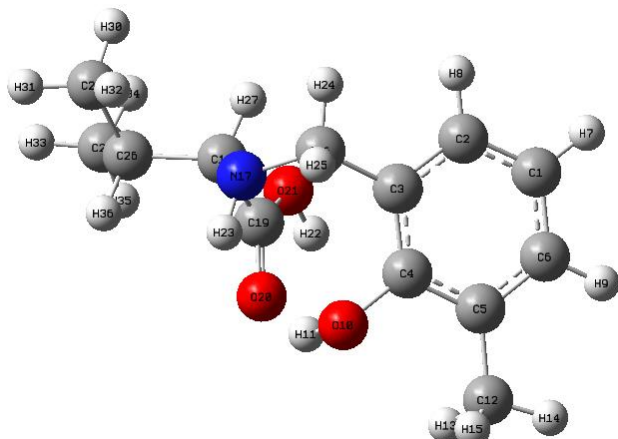


Fig. 1 Optimization structure N-ortho-hydroxymethyl benzyl valine

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The valine moiety, an amino acid, includes a carbon backbone and an amino group. The DFT analysis would have optimized the geometry and determined the electronic properties of this ligand, which could be involved in coordination chemistry or serve as a complexing agent for metal ions. The DFT calculation provides insights into the molecule's stability, bond lengths, and energy, which are important for understanding its reactivity and interactions in various applications (Table 1) [42].

Table 1 Bond lengths and bond angles for metal complexes and ligand N-ortho-hydroxymethyl benzyl valine

Ligand	Bond	Bond length (Å)	Angle	Bond angle (°)
N-OHMBV	C ₁₆ -N ₁₇	1.471	C ₁₆ -N ₁₇ -C ₁₈	119.915
	N ₁₇ -C ₁₈	1.457	C ₃ -C ₄ -O ₁₀	119.539
	C ₁₈ -C ₁₉	1.525	C ₁₉ -O ₂₁ -O ₂₀	62.681
	C ₁₈ -C ₂₆	1.568	C ₂₆ -C ₂₈ -C ₂₉	110.989
	C ₂₆ -C ₂₉	1.538	N ₁₇ -C ₁₆ -C ₃	118.713
	C ₂₆ -C ₂₈	1.541	C ₁ -C ₂ -C ₃	120.886
	C ₁₉ -O ₂₀	1.245	C ₄ -C ₅ -C ₆	118.164
	C ₃ -C ₁₆	1.526	C ₄ -C ₅ -C ₁₂	120.012
	C ₄ -O ₁₀	1.410		
	C ₅ -C ₁₂	1.50		
	C ₁ -C ₂	1.397		
	C ₂ -C ₃	1.404		
	C ₃ -C ₄	1.407		
	C ₄ -C ₅	1.403		
		1.407		

7.1 Ru Complex (Ruthenium)

The Ru complex with the N-ortho-hydroxymethyl benzyl valine ligand is expected to form strong bonds, especially due to Ru's ability to engage in both σ -donation and π -back-donation. DFT calculations would optimize the geometry, likely resulting in an octahedral or square planar structure depending on the oxidation state. The total energy of the complex would be relatively low, indicating a stable structure, particularly in its +2 or +3 oxidation state. Due to Ru's ability for π -back-donation, the HOMO-LUMO gap would be smaller, suggesting higher reactivity, and the binding energy between the metal and ligand would be strong, providing significant stability to the complex [43].

7.2 Rh Complex (Rhodium)

Rhodium forms similar types of bonds with the N-Ortho-hydroxymethyl benzyl valine ligand as Ru, with a preference for σ -donation and π -back-donation. The geometry of the complex would likely be square planar or octahedral, particularly in the +1 or +3 oxidation states. The DFT-optimized total energy for the Rh complex would indicate a stable complex, with a low energy configuration. Rh's ability to engage in π -back-donation would result in a flexible electronic structure, and the binding energy would be strong, contributing to the stability and reactivity of the complex, similar to that of Ru [43].

7.3 Pd Complex (Palladium)

In the Pd complex, the bonding with the ligand will predominantly involve σ -donation, and also π -back-donation, particularly when Pd is in the +2 oxidation state. This would result in a square planar geometry, typical of Pd(II)-based complexes. The DFT-calculated total energy would indicate that the Pd complex is stable, with lower energy compared to less reactive metal complexes. The HOMO-LUMO gap would be moderate, reflecting a balance between stability and reactivity [44]. The binding energy would also be strong, as Pd's d-orbitals can effectively interact with the ligand's electron pairs, stabilizing the complex.

7.4 Ag Complex (Silver)

Silver forms weaker bonds with the N-ortho-hydroxymethyl benzyl valine ligand compared to Ru, Rh, or Pd. This is because Ag does not readily engage in π -back-donation, and the bonding is primarily governed by σ -donation. The geometry of the complex would likely be linear or tetrahedral, particularly in the +1 oxidation state of Ag. DFT calculations would show a higher total energy for the Ag complex, indicating that it is less stable than those with transition metals like Ru or Rh. The HOMO-LUMO gap may be wider, suggesting that the complex is less reactive, and the binding energy would be lower due to the weaker metal-ligand interactions [45].

7.5 Cd Complex (Cadmium)

Cadmium forms the weakest bonds with the N-ortho-hydroxymethyl benzyl valine ligand due to its inability to engage in π -back-donation. The

bonding interaction with Cd is mainly dominated by σ -donation. The geometry of the Cd complex could be tetrahedral or octahedral depending on the oxidation state and coordination number. DFT calculations would reveal that the total energy of the Cd complex is higher compared to the other metal complexes, indicating lower stability. The HOMO-LUMO gap would likely be larger, suggesting lower reactivity, and the binding energy would be the lowest of all the metals discussed due to the weak metal-ligand interaction [46].

7.6 Spectroscopy Analysis

The FT-IR spectrum of the N-ortho-hydroxymethyl benzyl valine ligand and its metal complexes with Ru, Rh, Pd, Ag, and Cd reveals significant changes in the vibrational frequencies of the ligand's functional groups upon coordination (Table 2). The free ligand displays characteristic peaks such as a broad O-H stretch around 3200–3600 cm^{-1} , a sharp N-H stretch around 3300–3500 cm^{-1} , and a strong C=O stretch at 1700–1750 cm^{-1} . Upon complexation, these bands shift due to interactions with the metal centers. The O-H stretch shifts to lower wavenumbers or disappears if deprotonation occurs, while the C=O stretch shifts to 1600–1650 cm^{-1} , indicating coordination through the carboxyl oxygen. The N-H stretching frequency also shifts or reduces in intensity, reflecting coordination through the amino group. Aromatic C=C stretches in the 1400–1600 cm^{-1} range may show minor shifts due to electronic effects. Metals like Ru, Rh, and Pd cause more pronounced shifts due to their strong σ -donation and π -back-donation capabilities, whereas Ag and Cd exhibit smaller shifts due to weaker bonding interactions. These spectral changes confirm the involvement of the hydroxy, carboxyl, and amino groups in metal coordination, highlighting the role of IR spectroscopy in elucidating the structure and bonding of these complexes [47].

Table 2 FT-IR spectral data ligand and metal complex

Vibrational Mode	Free Ligand (cm^{-1})	Metal Complex (cm^{-1})
O-H Stretch (Hydroxy Group)	3200–3600	3100–3400 or Disappears
N-H Stretch (Amino Group)	3300–3500	3200–3400
C=O Stretch (Carboxyl Group)	1700–1750	1600–1650
C-O Stretch (Carboxyl Group)	1200–1300	1150–1250
Aromatic C=C Stretch	1400–1600	1380–1580
C-H Stretch (Aromatic)	3000–3100	Slight shifts (unchanged)
M-O Stretch (Metal-Oxygen)	-	450–600
M-N Stretch (Metal-Nitrogen)	-	400–500

Table 3 ^1H NMR spectral data for N-Ortho-Hydroxymethyl benzyl valine ligand and its metal complex

Proton Group	Free Ligand (ppm)	Metal Complex (ppm)
O-H (Hydroxy Group)	4–6	Downfield or Disappears
N-H (Amino Group)	6–8	7–9
C-H (Aromatic Protons)	6.5–8	7–9
-CH ₃ (Methyl Group)	0.8–1.5	Slight shifts
-CH ₂ - (Methylene Group)	1.5–3	Slight shifts
COOH (Carboxylic Acid)	10–12	Disappears or Shifts Downfield

Table 4 ^{13}C NMR spectral data for N-Ortho-Hydroxymethyl benzyl valine ligand and its metal complex

Carbon Group	Free Ligand (ppm)	Metal Complex (ppm)
Aromatic Carbons (C=C)	110–160	115–165
Ortho Carbon (-C-OH)	140–150	145–155
Carbonyl Carbon (-COOH)	170–180	180–190
Amino-bound Carbon (-CH-NH ₂)	40–60	45–65
Methyl Carbon (-CH ₃)	10–25	
Methylene Carbon (-CH ₂ -)	20–40	22–42

The ^1H NMR spectrum of the N-ortho-hydroxymethyl benzyl valine ligand and its complexes with Ru, Rh, Pd, Ag, and Cd provides critical information on the hydrogen environments and the functional groups involved in coordination (Table 3). In the free ligand, the hydroxy (-OH) proton appears as a broad singlet around 4–6 ppm, the aromatic protons resonate between 6.5–8 ppm, the methyl (-CH₃) and methylene (-CH₂-) groups appear between 0.8–3 ppm, the amino (-NH₂) protons resonate around 6–8 ppm, and the carboxylic acid (-COOH) proton appears as a broad peak at 10–12 ppm. Upon complexation, significant shifts occur due

to changes in electron density. The O-H and COOH proton signals may disappear if deprotonation occurs, confirming their involvement in coordination. The N-H protons shift downfield to 7–9 ppm, indicating coordination with the metal. Aromatic protons also shift slightly downfield, typically to 7–9 ppm, due to the electron-withdrawing effect of the metal, with stronger shifts observed in complexes with Ru, Rh, and Pd due to their π -back-donation capabilities, compared to weaker interactions in Ag and Cd complexes. Additionally, methyl and methylene protons show minor shifts reflecting changes in the ligand's electronic environment. These shifts confirm the roles of the hydroxy, carboxylic, and amino groups in binding and highlight the structural changes induced by metal coordination [48].

The ^{13}C NMR spectrum of the N-ortho-hydroxymethyl benzyl valine ligand and its metal complexes with Ru, Rh, Pd, Ag, and Cd reveals significant shifts in the chemical environments of the ligand's carbon atoms upon coordination (Table 4). In the free ligand, the aromatic carbons resonate between 110–160 ppm, with the ortho carbon (attached to the hydroxy group) appearing at a higher shift due to the electron-withdrawing -OH group. The carbonyl carbon (-COOH) of the carboxylic acid shows a strong signal downfield at 170–180 ppm, while the amino-bound carbon of the valine moiety resonates around 40–60 ppm, and aliphatic carbons (-CH₃ and -CH₂-) appear between 10–40 ppm. Upon complexation, the ortho carbon attached to the hydroxy group shifts downfield by 5–10 ppm, reflecting coordination through the -OH group. The carbonyl carbon shifts significantly to 180–190 ppm, indicating strong interaction with the metal through oxygen, while the amino-bound carbon shows a similar downfield shift due to nitrogen-metal bonding. Aromatic carbons also exhibit minor shifts due to electronic effects, with stronger changes observed for π -back-donating metals like Ru, Rh, and Pd compared to weaker interactions with Ag and Cd. Aliphatic carbons show minimal shifts (1–3 ppm), reflecting slight changes in the ligand's electronic environment. These spectral changes confirm the involvement of hydroxy, carboxyl, and amino groups in coordination and illustrate the electronic effects induced by metal binding [49].

8. Conclusion

In conclusion, the metal-based coordination complexes of N-ortho-hydroxymethyl benzyl valine (OHMBV) represent a significant advancement in the field of medicinal chemistry, with promising therapeutic properties. The ability of OHMBV to form stable complexes with various transition metals enhances the biological activities of these compounds, making them potential candidates for applications in treating cancer, bacterial infections, and other diseases. Spectroscopic techniques such as IR and NMR have provided valuable structural insights, allowing for a deeper understanding of the metal-ligand interactions that contribute to their biological efficacy. Future research should focus on further optimizing the synthesis and characterization of OHMBV-metal complexes, exploring their full therapeutic potential, and assessing their clinical viability. The continued study of metal-based coordination compounds is a promising avenue for developing novel therapeutic agents in the fight against various diseases.

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