

Original Article: Computational Investigation of Infrared Vibrational Frequency Shift Modes in Schiff Base-Transition Metal Complexes



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ABSTRACT

The computational investigation of change in the infrared vibrational frequency of some Schiff base-transition metal complexes relative to that observed in the Schiff base ligand was performed using density functional theory (DFT) based on the hybrid functional of three parameters Becke-3-Lee-Yang-Parr (B3LYP) with 6-31G(d,p) basis set. All the calculations were carried out using the Gaussian 09 program package, and the data obtained from the frontier molecular orbitals of the optimized ligand and its complexes showed that the complexes were less stable and more reactive than the ligand. The infrared vibrational frequencies of the Schiff base functional group had lower stretching vibrations in the complexes than the ligand, with the appearance of the new vibrational frequencies therein not observed in the ligand spectrum. These observations can be used to confirm a bond formation between a Schiff base and a transition metal in chemical synthesis.

Introduction

Infrared spectroscopy is one of the most common and widely used spectroscopic techniques for determining the type of functional groups within a molecule since different functional groups absorb different

frequencies of radiation. Schiff bases are those compounds formed by the condensation of the primary amines with carbonyl compounds. They carry the imine or azomethine nitrogen ($-C=N-$), an important pharmacophore in binding drugs to the biological targets [1].

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Many researchers have explored the medicinal properties of many Schiff bases and their coordination compounds in the past and the recent times, and further their findings have been promising [2, 3]. Likewise, they have been reported to reveal catalytic activity [4] and corrosion inhibitory properties [5]. Their derivatives have also been used to design the novel heterocyclic compounds for green technological applications [6].

Metals or metal ions can bond with several other molecules to form metal complexes. A metal complex is made up of a central metal atom or an ion bonded to one or more ions or molecules called ligands. These ligands contain one or more pairs of electrons which can be shared with the central metal [7]. The unique properties of transition metal complexes have been applied in science, engineering, and medicine. They have played a remarkable role in catalysis, photochemistry, drug design, and materials synthesis. Schiff bases can form the stable complexes with transition metal ions for both theoretical and practical applications. Schiff base complexes are synthesized by the combination of an imine-containing ligand with various types of transition metal compounds to form the transition metal-imine complex. The reaction is usually carried out under anhydrous conditions to avoid the hydrolysis of the starting transition metal compound, the intermediates, and the desired final complex [8]. Many imine-metal complexes have been synthesized and reported extensively in literature [9-11]. The biological activity of Schiff bases has further been indicated to be enhanced by its coordination with some transition metal complexes [12].

The shift in the absorption frequencies of functional groups in Schiff base-metal complexes, and other ligand-metal complexes in the infra-red spectrum have generally served as confirmation of a bond formation between

the metal and ligand in many studies [13-20]. In addition, the appearance of the new absorption peaks in the ligand-metal infra-red absorption spectrum which was not in the initial spectrum of the ligand has been attributed to the interaction between the metal and electronegative elements in the complexes [21-23]. However, the extent and mode of the shift in the infrared absorption frequencies of functional groups in the ligand-metal complexes have not been illustrated using theoretical models. Density functional theory (DFT) is used to obtain an approximate solution to the Schrodinger equation of a many-electron system. DFT computational codes can be used to investigate the electronic, magnetic, and structural properties of molecules. In this study, a molecule with an imine of a Schiff base and its iron, cobalt, nickel, copper, and zinc complexes were modeled without any external constraints. The changes and trends followed in the shift in the vibrational frequencies of the imine functional group in the Schiff base complexes vis-a-vis the Schiff base ligand were deduced.

Theoretical Framework

Frontier orbital energies (E_{HOMO} and E_{LUMO})

The Highest Occupied Molecular Orbital energy (E_{HOMO}) and the Lowest Unoccupied Molecular Orbital energy (E_{LUMO}), also called the frontier molecular orbitals, are used to determine the interaction of molecules with other species. The HOMO is the outermost orbital and acts as an electron donor, while the LUMO is the electron acceptor located in the innermost orbital. The energy gap (ΔE) is the variation in energy between the HOMO and LUMO levels.

$$\Delta E = E_{LUMO} - E_{HOMO} \quad (1)$$

The ionization potential (I) is the magnitude of energy required to separate an electron from an isolated atom or molecule. The electron

affinity (EA) is the energy released when an electron is attached to a neutral atom or molecule in the gaseous state to form a negative ion. The HOMO and LUMO energies can be applied to calculate I and EA in the framework of Koopmans theorem as follows [24]:

$$I = -E_{HOMO} \quad (2)$$

$$EA = -E_{LUMO} \quad (3)$$

The changes in the electron density of a chemical system in quantum theory result from the mixing of excited-state wave functions with the ground-state wave function. The chemical hardness (η) is the resistance to change in the electron cloud density or electron distribution of a chemical system [25]. Chemical softness (σ) is the converse of this definition. A hard molecule has a large HOMO-LUMO gap (energy gap), while a soft molecule has a small one. Chemical hardness is given by [26]:

$$\eta = \frac{I-EA}{2} \quad (4)$$

$$\sigma = \frac{1}{\eta} \quad (5)$$

Computational details

Molecular modeling uses theoretical and computational methods to mimic the behavior of molecules [27]. Density Functional Theory (DFT) method is used for the quantum mechanical simulation of periodic systems [28-29]. The electronic structure of ethylmethanolamine (EMA) was studied using density functional theory. The optimization and frequency calculations were carried out on this molecule and its iron(II) [Ar 4s⁰ 3d⁶], cobalt (II) [Ar 4s⁰ 3d⁷], nickel (II) [Ar 4s⁰ 3d⁸], copper (II) [Ar 4s⁰ 3d⁹], and zinc (II) [Ar 4s⁰ 3d¹⁰] complexes using Gaussian 09 program in the framework of three parameters Becke-3-Lee-Yang-Parr (B3LYP) [30], with 6-31G(d,p) basis set, which gives a high correlation with the experimental spectra [31]. The full EMA geometry and its complexes were drawn on

Gauss View 6.0.16. The geometry optimization was initially performed to remove any constraints on molecular symmetry. The optimized structures were then applied for the frequency calculations. All the molecules obtained in the frequency calculations were local minima and had no imaginary frequencies.

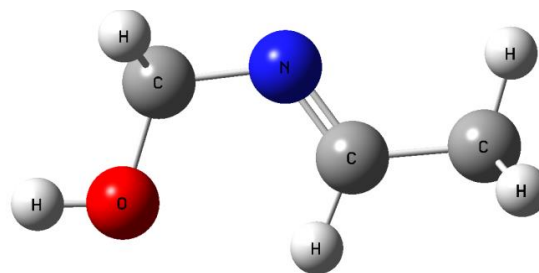


Figure 1. Theoretical optimized geometric structure of EMA

The frontier orbital energies (E_{LUMO} and E_{HOMO}), energy gaps, chemical hardness, ligand-metal bond length, and infra-red frequencies of EMA and its metal complexes were computed in vacuum and the data analyzed. The vibrational animations of the optimized molecules were used for the accurate assignment of frequencies to functional groups on the molecules.

Results and Discussion

The electrostatic potential mapping on the surface of EMA molecule in vacuum is displayed in Figure 2. Metal-ligand interactions in ligands with multiple functional groups occur at the points of the highest electron density [32]. Based on Figure 2, the electron density increased in the order blue < green < yellow < orange < red. The electron density was highest around the azomethine nitrogen of the EMA molecule and located at the orange region of the spectrum. This position was used to form coordination bonds between EMA and the studied transition metals.

The calculated energy of the lowest unoccupied molecular orbital (LUMO), energy of the highest occupied molecular orbital (HOMO), energy gap, chemical hardness, and

ligand-metal bond length (L – M) of EMA and its transition metal complexes in vacuum are presented in Table 1.

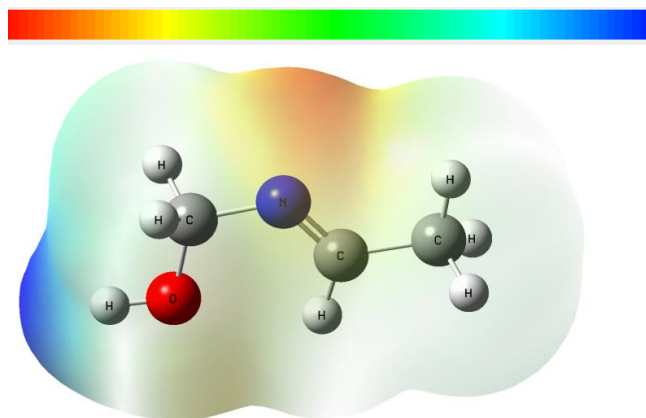


Figure 2. Molecular electrostatic potential (MEP) surface mapping of EMA

Table 1. Energy of LUMO, energy of HOMO, energy gap, chemical hardness, chemical softness, and L – M bond lengths of EMA

Molecule	E_{LUMO} (eV)	E_{HOMO} (eV)	ΔE (eV)	η (eV)	σ (eV)	L – M (Å)
EMA	0.013	-0.250	0.263	0.132	7.56	–
EMA – $_{26}\text{Fe}$	-0.054	-0.157	0.103	0.052	19.23	1.81
EMA – $_{27}\text{Co}$	-0.022	-0.174	0.152	0.076	13.16	1.83
EMA – $_{28}\text{Ni}$	-0.033	-0.132	0.099	0.050	20.00	1.80
EMA – $_{29}\text{Cu}$	-0.022	-0.212	0.190	0.095	10.53	1.82
EMA – $_{30}\text{Zn}$	-0.036	-0.144	0.108	0.054	18.52	2.30

The HOMO and LUMO energy states in a molecule are concerned with its molecular orbital regarding the electron transition. They play a prominent role in governing chemical reactions because the separation between them called the energy gap is a vital stability index. A large energy gap implies the high stability and low chemical reactivity, while a small energy gap implies the low stability and high chemical reactivity [33]. The energy gap is related directly to chemical hardness and inversely with chemical softness. The energy gaps of all the metal complexes were much lower than that of the ligand, suggesting that these complexes were more reactive than the ligand. A plot of the chemical hardness of EMA transition metal complexes as a function of the atomic number of the transition metals is

indicated in Figure 3. The EMA chemical hardness reduced significantly after the formation of complexes with the transition metals. This is due to the decrease in the energy gap of the complexes formed and revealed that the complexes are less stable and more reactive than the ligand.

The metal-ligand bond lengths of Fe, Co, Ni, and Cu were very close (1.80 – 1.83 Å) compared to Zn (2.30 Å). The atomic radii of these metals are 1.26, 1.25, 1.25, 1.28, and 1.37 Å for Fe, Co, Ni, Cu, and Zn, respectively. This observation is an indication that the bond length of these complexes is directly related to the atomic radius of the participating metal. Therefore the larger covalent radius between Zn and the azomethine nitrogen in the Schiff base is due to the longer atomic radius of Zn.

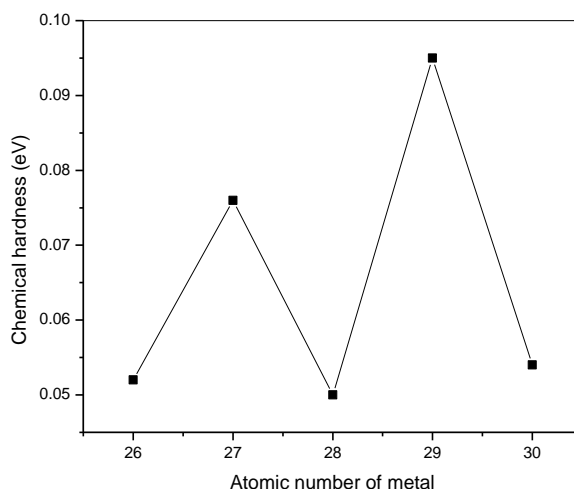


Figure 3. Plot of the chemical hardness of EMA complexes

Against atomic number

The chemical hardness of the complexes alternated periodically with the increase in the atomic number of the transition metals. Complexes with metals whose atomic numbers were odd were chemically harder than the even ones. The EMA nickel complex had the shortest ligand-metal bond length and the highest chemical softness value, followed by its complexes with iron and zinc. These observations indicated that the imine complexes of nickel, iron, and zinc are less stable coordination compounds of EMA.

The infrared spectra of EMA and its complexes with the studied transition metals are provided in Figure 4.

The superimposed spectra of EMA and its transition metal complexes are demonstrated in Figure 5.

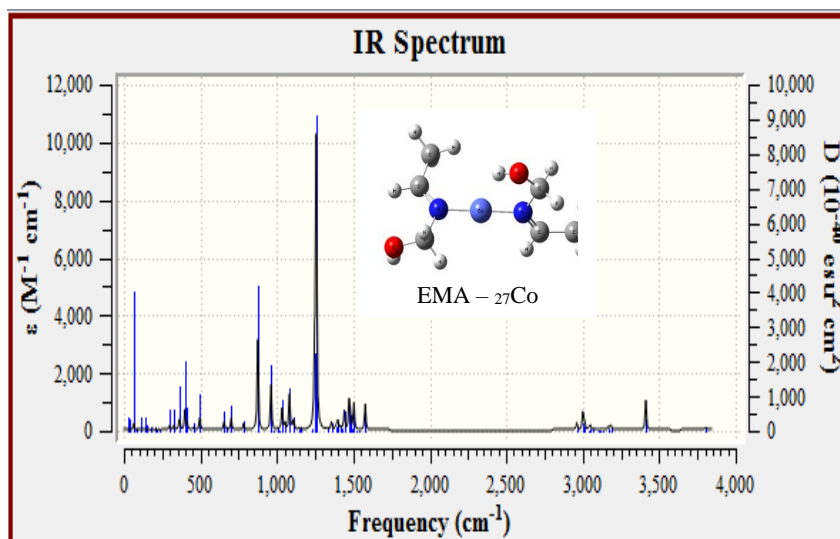
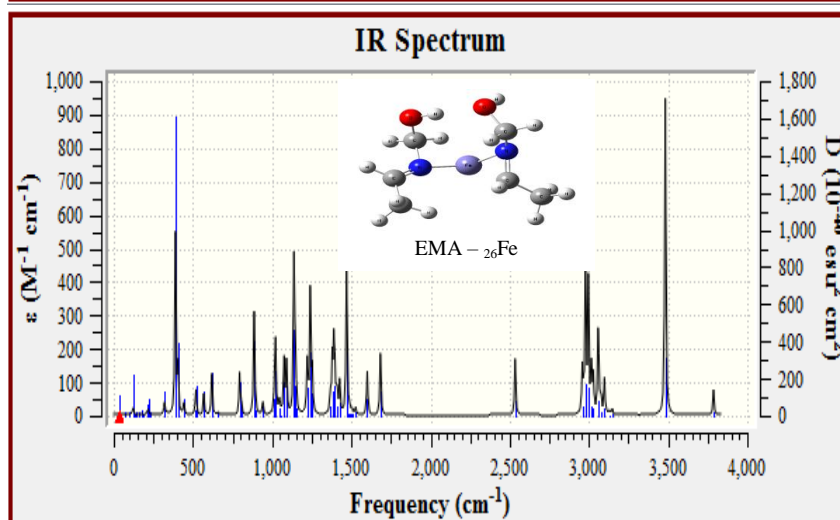
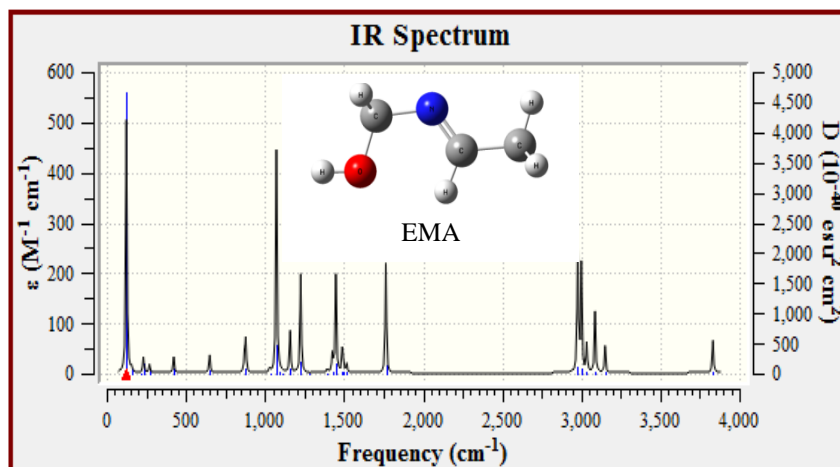
The chemical hardness measures the resistance of a chemical substance to change its electronic configuration and is an indicator of chemical reactivity and stability [34]. The absorption intensities of the functional groups in EMA-Co and EMA-Cu were very sharp and

prominent. The chemical hardness values of these two complexes were further the highest in the metal series studied. This observation indicated that the intensity of absorption peaks in these complexes increased with an increase in their stability and hardness.

The vibrational frequency (ν_m) of a mechanical oscillator which is dependent on the force constant of the spring and the mass of the attached body and independent of energy impinging on the system, is given by Eq.6 [35]:

$$\nu_m = \frac{1}{2\pi} \sqrt{\frac{k}{\mu}} \quad (6)$$

Where k is the force constant (N/cm) and μ is the reduced mass (kg). The heavier the masses of the attached atoms, the lower the vibrational frequency of the moiety formed. These relationships imply that the bonding of large atoms to a molecule would reduce the IR stretching vibrations of functional groups close to the point of coordination in the molecule. The IR frequency of the azomethine nitrogen in EMA and its coordinate bond vibrational frequencies with the transition metals are depicted in Table 2.



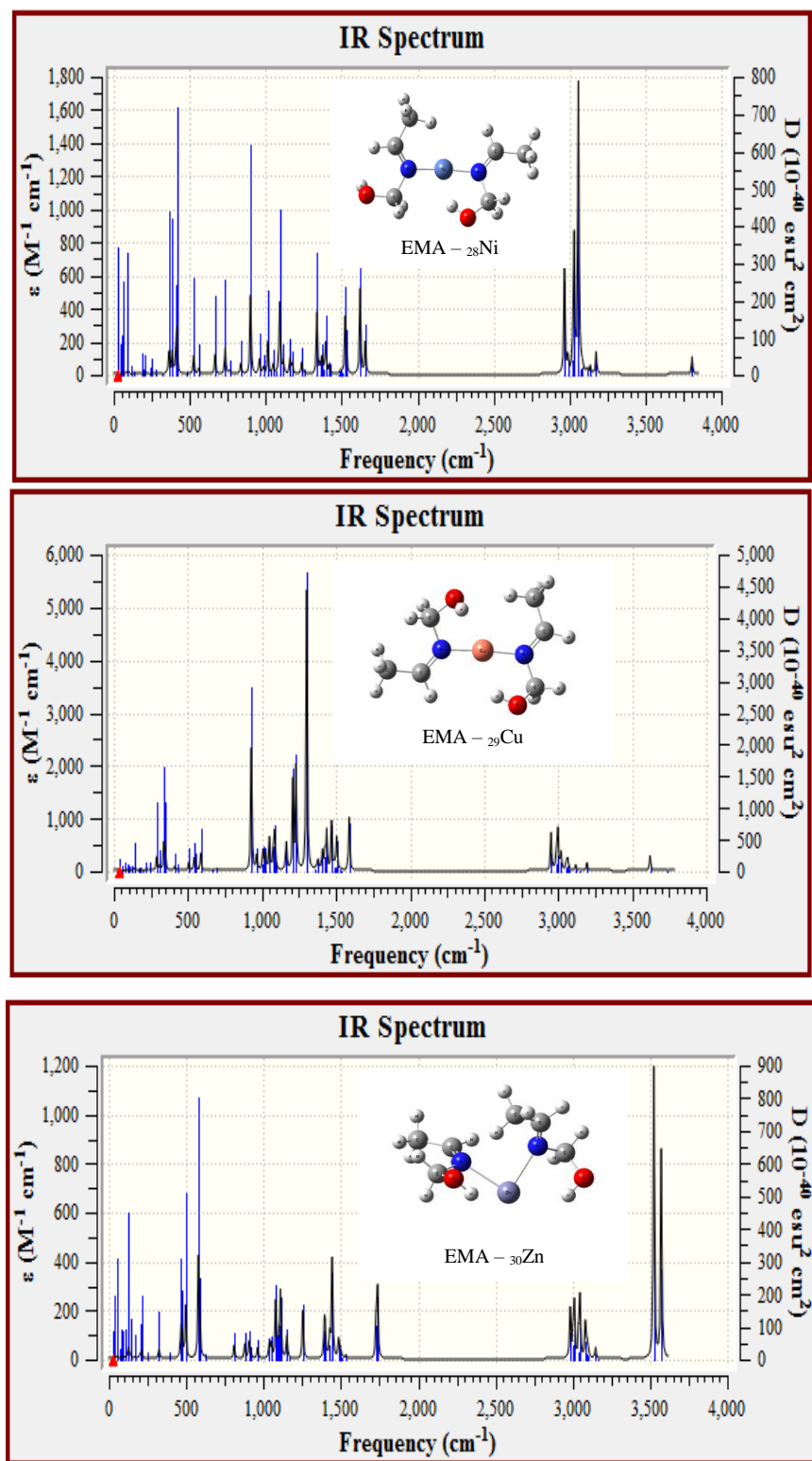


Figure 4. The optimized structures and infra-red spectra of EMA and its complexes

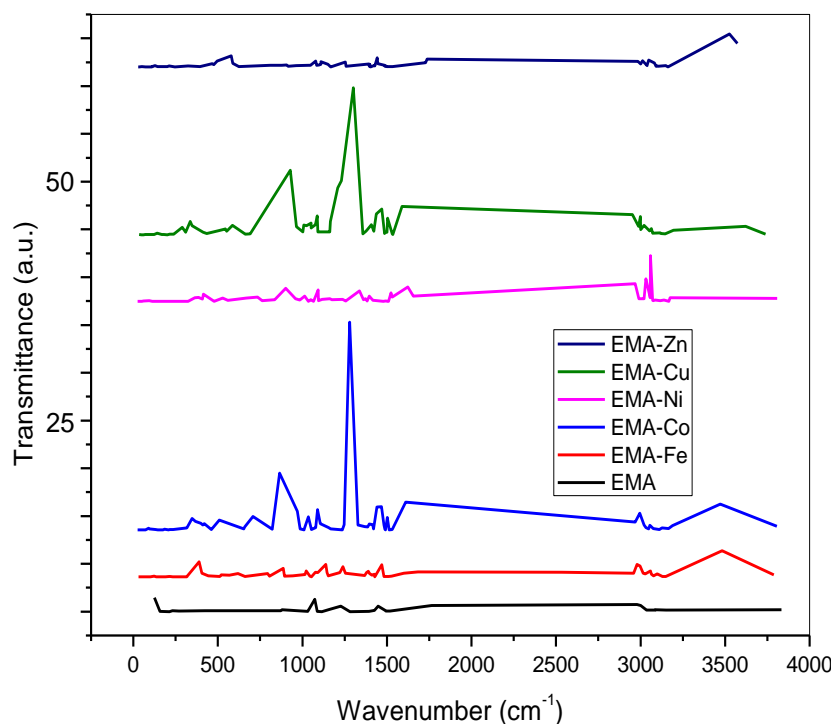


Figure 5. The superimposed IR spectra of EMA and its complexes

Table 2. IR frequency at metal-ligand and imine functional groups in EMA and its complexes

Molecule	M – N stretching	C=N stretching
EMA	–	1764.84
EMA – ₂₆ Fe	659.76	1683.47
EMA – ₂₇ Co	654.63	1578.63
EMA – ₂₈ Ni	666.84	1622.75
EMA – ₂₉ Cu	662.24	1589.09
EMA – ₃₀ Zn	624.66	1728.43

The IR vibrational frequencies of C=N were observed at 1764.84 cm⁻¹. When compared with the free ligand, the stretching frequency of the azomethine linkage with all the metal complexes shifted to lower frequencies by 36–186 cm⁻¹. The reduction in the vibrational frequency of this functional group confirms that it is linked to another atom by a chemical bond. The M–N vibrations appeared in all the complexes and were observed in the range 625–667 cm⁻¹. This vibration was not present in the spectrum of EMA, and therefore

confirmed that its appearance is a characteristic of ligand-metal bond formation. These deductions were compared with data obtained from some empirical works reported in literature.

Sevgi *et al.* [36] reported the zinc (II), copper (II), nickel (II), cobalt (II), and iron (III) complexes of Schiff bases derived from 2-hydroxynaphthaldehyde with glycine. They observed the C=N vibration at 1641 cm⁻¹. The stretching frequency of azomethine linkage in the metal complexes shifted to lower

frequencies in all the metals by 11–36 cm^{-1} . Al-Sree Devi and SudhaKumari [37] studied Schiff base ligand from amino acid L-arginine and its nickel (II), cobalt (II), and copper (II) complexes. They reported the C=N vibration at 1638 cm^{-1} . The stretching frequency of azomethine linkage in metal complexes shifted to lower frequencies in all the metals by 8–12 cm^{-1} . They observed the M–N vibration within 461–485 cm^{-1} . In the study of bacterial activity of Schiff bases from the selective amino acid and their complexes [38], the C=N vibration was observed at 1645 cm^{-1} . The stretching frequency of azomethine linkage in the metal complexes shifted to lower frequencies in all the metals by 29–59 cm^{-1} . The report by Al-Zaidi *et al.* [39] on new bidentate chelated Schiff base complexes of cobalt (II), nickel (II), and copper (II) revealed the vibrational frequencies of C=N at 1616 cm^{-1} . When compared with the free ligand, the stretching frequency of azomethine linkage in the metal complexes shifted to lower frequencies by 4–10 cm^{-1} . The new vibration bands were noticed in the spectra of the prepared complexes at wavenumbers ranging from 432–440 cm^{-1} and assigned to M–N vibration. Kareem *et al.* [40] prepared new Schiff base complexes of cobalt (II), nickel (II), and copper (II). They reported the C=N vibration at 1616 cm^{-1} and M–N vibration was 428–455 cm^{-1} . The stretching frequency of azomethine linkage in the metal complexes shifted to lower frequencies by 21–28 cm^{-1} .

However, some researchers have published reports claiming the complex formation between a transition metal and Schiff base ligand with an increase in the vibrational frequency of C=N or the absence of the M–N vibration. Mohamed *et al.*, [41], in their study of Schiff base complexes of iron (II), cobalt (II), nickel (II), copper (II), and zinc (II), observed the C=N vibration at 1659 cm^{-1} . The stretching frequency of azomethine linkage in metal

complexes shifted to lower frequencies in all the metals by 4–55 cm^{-1} except zinc, where the value was 1662 cm^{-1} , which is an increase by 3 cm^{-1} . They concluded that the zinc complex was formed with this observation, which does not agree with the mathematical theory (Eq. 6) and results from the model. Echekwube *et al.* [42] studied Schiff base derivatives of cobalt (II) and nickel (II) complexes. They observed the C=N vibration of one of the three ligands studied (Lp) at 1610 cm^{-1} . The azomethine linkage in the metal complexes shifted to higher frequencies in the two metals by 5 cm^{-1} . Likewise, they reported M–N vibration at 450 cm^{-1} for cobalt and none for the nickel complex. Their report indicated no coordination between the ligand and either cobalt or nickel with shifts in the C=N band to the higher frequencies after coordination. Furthermore, the non-existence of an M–N vibration for nickel indicated that ligand-metal coordination did not occur. In the study of the biological activity of copper (II), cobalt (II), and nickel (II) complexes of Schiff base derived from O-phenylenediamine and 5-bromosalicylaldehyde, Fasina *et al.*, [43] reported the C=N vibration at 1602 cm^{-1} . They concluded that the nitrogen of the azomethine participated in bond formation as a result of the shift in the C=N vibration to lower frequencies with values 1580 cm^{-1} , 1593 cm^{-1} , and 1603 cm^{-1} for cobalt, nickel, and copper, respectively. However, the vibrational frequency of the C=N in the copper complex was higher than the value obtained in the free ligand by 1 cm^{-1} . As such, the ligand could not have coordinated with copper against their earlier claim.

Conclusions

The shift in the infrared vibrational frequencies of imine and ligand-metal functional groups in Schiff base after coordination with iron (II), cobalt (II), nickel (II), copper (II), and zinc (II) was studied using density functional theory

method. Data from the frontier orbital energies indicated that the metal complexes were more reactive and less stable than the ligand whose energy gap was much higher than its complexes. The stretch vibrational frequencies of the azomethine functional group in the complexes shifted to values lower than what was obtained in the original ligand, and new vibrational frequencies between 625 and 667 cm^{-1} appeared in the spectra of all the complexes confirming metal-ligand interaction. These observations can be used to verify the coordinate bond formation between the azomethine nitrogen of a Schiff base and a transition metal in the IR spectra results of synthesized complexes.

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Conflicts of Interest/Competing Interest

The authors have no conflicts of interest to declare that are relevant to the content of this article.

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