Solvent effects on the electronic and optical properties of Ni(II), Zn(II), and Fe(II) complexes of a Schiff base derived from 5-bromo-2-hydroxybenzaldehyde

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Abstract
In this article, the electronic, optical, and charge transfer properties of a Schiff base ligand prepared using 5-bromo-2-hydroxybenzaldehyde and ethyl 6-acetyl-2-amino-4,5,6,7-tetrahydrothieno[2,3-c]pyridine-3-carboxylate (C19H19BrN2O4S) and its Fe(II) (C19H30BrN2O10SClFe), Ni(II) (C19H28BrN2O9SClNi), and Zn(II) (C19H28BrN2O9SClZn) complexes are described based on different solvents environments and supported by theoretical calculations. Theoretical calculations are carried out using density functional theory (DFT/UB3LYP/LANL2DZ). The optical densities, optical band gaps, and refractive indices of the ligand and its Fe(II), Ni(II), and Zn(II) complexes in different solvent environments are obtained. The reorganization energies are calculated to determine the charge transfer rate of the studied compounds using both experimental and theoretical data. These experimental and theoretical results show that the ligand and its metal complexes can be used for optoelectronic applications and charge transfer materials in organic light-emitting diode applications.

Keywords
charge transfer properties, metal complexes, nonlinear optical properties, optical parameters, Schiff base

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Introduction
Schiff base ligands have interesting electrochemical properties since they possess electron-donor or electron-attracting groups. In recent years, Schiff base metal complexes have received significant attention. Transition-metal complexes, especially Schiff base complexes, have emerged as promising candidates for the design and development of nonlinear optical (NLO) materials because of their efficient charge transfer behavior and ability to tailor metal-organic-ligand interactions.1,2 Transition-metal complexes are used as organic light-emitting diodes (OLEDs) because of their optoelectronic properties.3–7 Schiff bases and their transition metal complexes are also used as photometric materials in optical computers and display systems.8 In particular, Ni(II), Pt(II), and Zn(II) complexes of Schiff bases have found widespread use in organic optoelectronics because of their NLO properties.9,10 In addition, metal complexes are used as hole-transport materials in solar cells.11–13 Both optical and hole-transport properties are important factors in OLEDs because the formation and propagation of light is directly influenced by the movement of electrons and holes in the material.14

In recent studies, materials with high charge transfer rates have been designed for better OLED performance in the visible region.15–18 Also, theoretical calculations have become important in terms of the electronic, optical, and structural properties of complexes in comparison with experimental results.19–22

The ligand and its metal complexes that we use in this study have not been reported in the literature. In this study, the electronic and optical properties of the newly

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synthesized ligand and its metal complexes, which are organic semiconductors in various solvent environments (dichloromethane (DCM), dimethylformamide (DMF), chloroform and ethanol), have been investigated along with their suitability for optoelectronic applications. Both experimental techniques and theoretical methods such as density functional theory (DFT) are used to obtain the results. First, the theoretically most stable structure of the ligand and its Fe(II), Ni(II), and Zn(II) complexes was identified. The ultraviolet-visible (UV-Vis) spectra, frontier molecular orbitals (HOMO and LUMO), and the energy difference between these orbitals ($E_g$) in different solvents were calculated using the TD-DFT/B3LYP method. Calculated $E_g$ values were compared with the experimental values obtained in different solvents. Also, the reorganization energies and NLO properties are calculated and discussed in detail. The refractive indices of the ligand and its metal complexes in DCM, DMF, chloroform, and ethanol were obtained using reflectance and extinction coefficient ($k$) data. Solvent effects were investigated for the properties mentioned above. The experimental results were compared with these obtained from theoretical calculations.

**Results and discussion**

**UV spectra analysis in different solvents**

UV-Vis spectroscopy is an important technique in terms of determining electronic, optical, solvatochromic, and charge transfer properties of compounds dissolved in various solvent environments. For the ligand, Fe(II), Ni(II), and Zn(II) complexes (Scheme 1), electronic absorption spectra were obtained in different solvent environments and are presented in Figure 1. The ligand and its metal complexes exhibited small and large peaks in the near ultraviolet (NUV), UV-A, UV-B, and visible regions in different solvents. The ligand exhibited maximum peaks in DCM and chloroform at 403 nm. In Figure 1, it can be seen that the Fe(II) complex exhibited maximum peaks at 403 nm in DCM and chloroform. Also, the Fe(II) complex did not show strong absorbance peaks in DMF and ethanol. The Ni(II) complex in DCM and chloroform gave maximum peaks at 404 nm, and in ethanol and DMF gave maximum peaks at 501 nm. The Zn(II) complex gave maximum peaks at 402 and 404 nm in DCM and chloroform, respectively, and in DMF gave a maximum peak at 339 nm. The Zn(II) complex did not exhibit strong absorbance peaks in ethanol. A solvent with a large dielectric constant leads to a greater stabilization energy for polar species. The stabilizing effects of DMF ($\varepsilon = 36.7$) and ethanol ($\varepsilon = 24.5$) were greater than those of DCM ($\varepsilon = 8.93$) and chloroform ($\varepsilon = 4.81$). As a result, the absorbance values in DMF and ethanol were higher than those in DCM and chloroform. As can be seen from Figure 1, the wavelengths greater than 500–600 nm remained constant at the lowest values and in the visible region of the strongest peaks. In addition, the title compounds gave the same wavelength peaks in DCM and chloroform, while in DMF and ethanol, they gave different wavelength peaks.

The experimental absorbance values of the ligand and complexes in chloroform gave peaks at almost the same maxima (see Figure 1). Theoretical absorbance calculations for all solvents used in the experimental measurements were made using the TD-DFT method and are presented in Figure 2. It can be seen that the absorbance values of the studied compounds did not change much with the solvent, similar to the experimental results. The ligand produced the maximum absorbance peak at approximately 411 nm, the Fe(II) complex at 535 and 541 nm, the Ni(II) complex at 393 and 493 nm, and the Zn(II) complex at 470 nm. In addition, it is seen from theoretical results that the ligand and its metal complexes give many peaks in the UV-Vis region.

**The optical parameters of the ligand and its complexes in different solvents**

We next investigated optical parameters such as the optical band gap ($E_g$) and the refractive indices ($n$) of the ligand and its metal complexes in DCM, DMF, chloroform, and ethanol.

The correlation between the $E_g$ band gap of a sample and its photon energy ($h\nu$) and absorbance is given by $(\alpha h\nu) = \beta(h\nu - E_g)^m$, and is known as the Tauc model, where $\alpha$ is the absorption coefficient, $\beta$ is a constant, $E_g$ is the optical band gap, $h\nu$ is the photon energy, and $m$ is a parameter. The parameter $m$ defining the optical transitions was found to be 1/2 as the sign of the direct allowed band gap for the title compounds.

![Scheme 1. Suggested structure of the ligand and its Fe(II), Ni(II), and Zn(II) complexes.](image-url)
Figure 3 gives the experimental Tauc plots of the ligand and its metal complexes in DCM, DMF, chloroform, and ethanol. The $E_g$ band gap of the sample was found by extrapolating the straight-line portion of the Tauc curve to $h\nu = 0$, with the measured $E_g$ values of the studied compounds being in the range of 2.10–2.82 eV. The results obtained suggest that the compounds examined are materials with an optical gap spacing suitable for the production and application as optical and optoelectronic devices.

The molecular orbitals (HOMO, LUMO) that play an important role in the transfer of electrical, optical, and molecular charge of a molecule were calculated using the TD-DFT/UB3LYP/LANL2DZ basis set for all the studied solvents and the results are presented in Table 1. The electrical band gap values shown in Table 1 define the energy difference between the HOMO and LUMO levels, and the optical band gap describes the excitation energy for transitions between vertical bands.26 HOMO’s high energy value indicates that it is prone to donating electrons. Likewise, the low value of LUMO indicates its greater interest in accepting electrons.27,28 Therefore, the Ni(II) complex has the highest potential for electron donation in DCM and chloroform. The electrical band gap having values greater than the optical band gap is an expected result in charge transfer materials.29 In addition, the LUMO energy level of the Ni(II) complex has the greatest value compared to the ligand and other complexes (see Table 1). This showed that Ni(II) had better electron-transfer properties. Similarly, Table 1 shows that the Fe(II) complex had the highest HOMO energy level indicating that the Fe(II) complex is the best transporting of holes.

We calculated the refractive indices of the ligand and its metal complexes using equation 1 with the reflectance ($R$) and extinction coefficient ($k$) data23 obtained from the experimental absorbance values in DCM, DMF, chloroform, and ethanol. The results are given in Table 2. Although the reflection indices for the compounds investigated in DCM and chloroform gave similar results, it generally varied on changing the solvent.

\[
n = \left( \frac{4R}{(R-1)} - k^2 \right)^{1/2} \frac{R + 1}{R - 1}
\]  

(1)

**NLO analysis**

NLO materials are widely utilized in areas such as laser technology, optical switching, photonic devices, optical sensors, screens, and data storage.30–32 Useful and reliable results are obtained in the search of new nonlinear materials through quantum computing approaches. In this respect, DFT-based methods are the best in terms of computation time and accuracy.33 To investigate the electrical and optical responses of the ligand and its metal complexes, electrical dipole moment ($\mu$), hyperpolarizability ($\beta$), and polarizability ($\alpha$) values from NLO properties were investigated using DFT/B3LYP theory. The values of mean polarizability ($\alpha$), anisotropy of polarizability ($\Delta\alpha$), and mean molecular hyperpolarizability ($\beta$) and total dipole moment were calculated using the equations below:
Figure 2. The theoretical absorbance spectra of the ligand and its Fe(II), Ni(II), and Zn(II) complexes in ethanol.

Figure 3. The \((a\nu v)^2\) graphs of the ligand and its Fe(II), Ni(II), and Zn(II) complexes in DCM, DMF, chloroform, and ethanol.
The calculated values are tabulated as Supplementary Information in Tables SI 3–6. For a molecule to be considered a good NLO material, the $\beta$, $\alpha$, $\Delta \alpha$, and dipole moment values must be sufficiently large. This sufficient magnitude is interpreted by comparing with the values of the urea molecule.\(^{34}\) In this study, the $\beta_{\text{tot}}$ and $\Delta \alpha$ values were calculated for the ligand and its metal complexes. The values for urea are $\beta_{\text{tot}} = 194.7 \times 10^{-33}$ esu and $\Delta \alpha = 3.8312 \times 10^{-24}$ esu. It is understood that the values of the hyperpolarizability and the mean polarization in the first order of the studied compounds were many times higher than those of urea. These results show that the ligand and its metal complexes can potentially be used as efficient NLO materials for future applications.

**Charge transport properties and reorganization energy values ($\lambda$)**

The calculated reorganization energies ($\lambda$) using the adiabatic potential energy surface method are listed in Table 3. Lower reorganization energy values mean higher charge transfer rates.\(^{35,36}\) The reorganization energies for hole transfer ($\lambda_h$) of the ligand and the Fe(II) complex were both much smaller than that the electron transfers the ($\lambda_e$), so we proposed that the ligand and the Fe(II) complex were more likely to be $p$-type organic semiconductors. For the Ni(II) and Zn(II) complexes, the reorganization energy for hole transfer ($\lambda_h$) was larger than the electron transfers ($\lambda_e$), which indicates that the Ni(II) and Zn(II) complexes are more likely to be $n$-type organic semiconductor rather than $p$-type organic semiconductors. Furthermore, the difference between the $\lambda_h$ and $\lambda_e$ values for the Ni(II) complex was 0.0545 eV. This shows that the Ni(II) complex had better equilibrium properties for electron and hole transport.

**Conclusion**

In this work, the electronic, optical, and charge transfer properties of the synthesized compounds were explored using theoretical methods and compared with experimental data. The UV spectra of the ligand and the Fe(II), Ni(II), and Zn(II) complexes were studied in DCM, DMF, chloroform, and ethanol. The effects of these different solvents on the

### Table 1. The calculated energies values of the ligand and its Fe(II), Ni(II), and Zn(II) complexes.

| Compound      | Solvent      | $E_{\text{HOMO}}$ (eV) | $E_{\text{LUMO}}$ (eV) | Optical band gap (eV) | Electrical band gap (eV) |
|---------------|--------------|------------------------|------------------------|-----------------------|-------------------------|
| Ligand        | DCM          | 5.94                   | 2.27                   | 3.02                  | 3.67                    |
|               | DMF          | 5.96                   | 2.28                   | 3.03                  | 3.68                    |
|               | Chloroform   | 5.92                   | 2.26                   | 3.00                  | 3.66                    |
|               | Ethanol      | 5.96                   | 2.27                   | 3.04                  | 3.69                    |
| Fe(II) complex| DCM          | 5.67                   | 2.76                   | 2.29                  | 2.91                    |
|               | DMF          | 6.13                   | 2.75                   | 2.31                  | 3.38                    |
|               | Chloroform   | 5.66                   | 2.77                   | 2.47                  | 2.89                    |
|               | Ethanol      | 5.68                   | 2.75                   | 2.31                  | 2.92                    |
| Ni(II) complex| DCM          | 6.12                   | 3.13                   | 2.51                  | 2.99                    |
|               | DMF          | 6.11                   | 3.12                   | 2.30                  | 2.98                    |
|               | Chloroform   | 6.12                   | 3.14                   | 2.50                  | 2.97                    |
|               | Ethanol      | 6.11                   | 3.12                   | 2.32                  | 2.98                    |
| Zn(II) complex| DCM          | 5.81                   | 2.73                   | 2.63                  | 3.07                    |
|               | DMF          | 5.82                   | 2.73                   | 2.64                  | 3.08                    |
|               | Chloroform   | 5.80                   | 2.74                   | 2.61                  | 3.05                    |
|               | Ethanol      | 5.82                   | 2.73                   | 2.64                  | 3.08                    |

DCM: dichloromethane; DMF: dimethylformamide.

### Table 2. Refractive indices ($n$) of the ligand and its Fe(II), Ni(II), and Zn(II) complexes in different solvents.

| Solvents     | Ligand  | Fe(II) complex | Ni(II) complex | Zn(II) complex |
|--------------|---------|----------------|----------------|----------------|
| DCM          | 1.78    | 1.95           | 1.89           | 1.98           |
| DMF          | 1.90    | 1.90           | 1.81           | 1.97           |
| Chloroform   | 1.78    | 1.97           | 1.89           | 1.98           |
| Ethanol      | 1.80    | 1.99           | 1.80           | 1.89           |

DCM: dichloromethane; DMF: dimethylformamide.
optical properties of the ligand and its Fe(II), Ni(II), and Zn(II) complexes have been studied in detail. From their optical band gap values and NLO properties in all the solvents used, it is apparent that the compounds studied herein are potential candidate compounds for OLEDs and NLO materials. Moreover, from the calculated reorganization energy, it can be seen that the ligand and Fe(II) complex are hole-transfer materials, while the Ni(II) and Zn(II) complexes are electron-transfer materials.

**Experimental and theoretical details**

All chemicals and solvents used for the synthesis and the measurements were of analytical reagent grade. The optical measurements were recorded using a Shimadzu UV-1800 Spectrophotometer in different solvents (DCM, DMF, chloroform, and ethanol) and at different molarities using the solution technique. Fourier transform infrared spectra were recorded on a Perkin Elmer 65 Spectrum One spectrometer in the range 400–4000 cm\(^{-1}\) as KBr disks. The Schiff base ligand and its metal complexes were prepared according to the method described in the literature.\(^{28}\)

All calculations were performed using the Gaussian 09 program\(^{37}\) by employing DFT calculations based on the B3LYP change correlation, which is functional on the mixed basis of 6-311++G(d,p)+LanL2DZ.\(^{38}\) The molecular structures of the Fe(II), Ni(II), and Zn(II) complexes were confirmed by elemental analysis. The complexes exist in octahedral geometry. The structures of the ligand and its metal complexes were optimized [DFT/B3LYP/6-311++G(d,p)] and are presented in Figure 4. The electronic, molecular orbital energies (HOMO and LUMO), \(E_g\) (energy gap), and NLO properties were calculated for the different solvents and compared with those observed. The solvent effect was studied using the polarizable continuum model (PCM).\(^{31}\) PCM models have also been particularly useful in simulating the reactivity and spectroscopy of different solvents.

The reorganization energy consists of two parts: internal and outer contributions. The internal reorganization energy results from molecular geometric relaxation, while the outer reorganization energy is caused by the polarization of the surrounding compounds.\(^{32}\) External organization energy is neglected by researchers because it is calculated as being too small for semiconductors.\(^{33,35}\) Here, we took into account the internal energy using the adiabatic potential energy surface method.\(^{33–36}\) The reorganization energy for holes (\(\lambda_h\)) and electrons (\(\lambda_e\)) of the studied compounds was calculated from the single-point energies of the optimized (DFT/B3LYP/6-311++G(d,p)+LanL2DZ) anionic, cationic, and neutral geometries\(^{39}\)

\[
\lambda_h = E_{h \text{, calc}} - E_{0 \text{, calc}}
\]

\[
\lambda_e = E_{e \text{, calc}} - E_{0 \text{, calc}}
\]

where \(E_{0 \text{, calc}}\) is the energy of the anion (cation) calculated with the optimized structure of the neutral molecule. Similarly, \(E_{h \text{, calc}}\) is the energy of the anion (cation) calculated with the optimized anion (cation) structure.

| Compound | \(\lambda_h\) (eV) | \(\lambda_e\) (eV) |
|----------|------------------|------------------|
| Ligand   | 0.4112           | 0.5236           |
| Fe(II)   | 0.4089           | 0.5174           |
| Ni(II)   | 0.5410           | 0.4865           |
| Zn(II)   | 0.5233           | 0.4498           |

![Figure 4. The optimized ground state structures of the ligand and the Fe(II), Ni(II), and Zn(II) complexes.](image)
$E^0_0$ ($E^0_{\pm}$) is the energy of the neutral molecule calculated in an anionic (cationic) state. $E^0_{\pm}$ is the energy of the neutral molecule in the ground state.

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Supplemental material
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