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Synthesis, characterizations, and DFT studies of some vanillin Schiff base derivatives

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ABSTRACT

The increase in bacterial infections has necessitated the need for the design of new drugs that can fight against multidrug-resistant bacteria. Schiff bases, especially those of vanillin, have shown promising activity against some bacterial infections. In this article, six new vanillin Schiff bases (L1–L6) were prepared by condensation of vanillin with various substituted anilines for possible medicinal applications. The compounds were characterized by infrared spectra, UV/visible spectra, and melting point measurements. Infrared spectra confirmed the formation of the compounds by the newly emerged azomethine (C=N) bands observed at 1676–1620 cm⁻¹ for the synthesized compounds. The UV/visible spectra showed the expected π - π^* transition of the azomethine group at 38000–34000 cm⁻¹, and the n- π^* transition at 32000–25000 cm⁻¹, which are characteristics of the molecules. The Schiff bases, L5 and L6, were obtained as thick viscous liquids, while L1–L4 came out as crystals of different colors characterized by sharp melting points. The molecules were modeled and optimized using DFT at the 6-31G(d) level of theory. The computational study shows that the compounds could effectively accept and donate protons, which is a remarkable characteristic for medicinal and other applications. The characterization results reveal that the compounds were successfully prepared. Spectroscopic and computational studies suggested that the compounds may have some medicinal and electronic applications.

Highlights

- New Schiff bases obtained via the reaction of vanillin and substituted anilines
- FTIR, UV/Vis spectra and melting point measurement confirmed the formation of the compounds
- Compounds are colored and crystalline in nature
- Compounds were modeled and optimized using DFT at 6-31G(d) level of theory
- Computational studies and spectroscopic analysis suggest electronic and medicinal properties

1. Introduction

Schiff bases are compounds defined by azomethine groups, which are commonly prepared by the reaction of carbonyl compounds (aromatic or aliphatic) and primary amines. Stability is an important factor usually considered when new compounds are prepared for various applications, and for this reason, Schiff bases obtained from the condensation of aryl

carbonyl compounds are considered more important than those obtained from aliphatic carbonyl compounds because the latter are relatively unstable and easily polymerizable (Boulechfar et al., 2023; Jain et al., 2022).

Schiff bases are versatile coordinating multifunctional ligands with structural varieties, preparative accessibilities, and easily tunable electronic and steric effects. They are capable of coordinating with a wide

variety of metal ions in different oxidation states and geometries (Mahmoud et al., 2024; Venkatesh et al., 2024). Consequently, these classes of compounds are considered important in the field of medicine, biochemistry, supra-molecular chemistry, optics, and pharmaceutical chemistry (Keypour et al., 2009; Boghaei et al., 2000; Uddin et al., 2020; Osowole, 2008). Furthermore, their applications as fluorescent sensors, photovoltaic materials, antioxidants, antibacterial, antifungal, anti-inflammatory, antiviral, and anticancer agents cannot be overemphasized (Boulechfar et al., 2023; Sinicropi et al., 2022).

Since metal coordination enhances the applications of organic ligands, many metal(II) Schiff base complexes have been synthesized in the last few decades (Lacopetta et al., 2023; Xie et al., 2005; Di-Bella et al., 1997; Ahmed et al., 2013). Moreover, many Schiff bases and their metal complexes have also been prepared because of their vast applications in luminescence, agrochemicals, optics, medicine, etc (Tufa et al., 2018; Chan et al., 2008; Yadav et al., 2012; Osowole, 2011). They have also been used as catalysts in polymerization, carbonylation, and coupling reactions like Suzuki/Heck (Wiedermann et al., 2006). This emphasizes their versatility in the field of medicine, bioinorganic chemistry, and material science.

Vanillin is a versatile organic compound that exhibits different pharmacological activities, including but not limited to anti-inflammatory, anticancer, and antioxidant properties. Its applications further extend to flavoring agents in fragrance enhancement and confectionery, especially in perfumes and cosmetics (Hassan & Said, 2021; Karthika et al., 2025). It has been well established that Vanillin Schiff bases and their metal complexes also possess diverse pharmacological applications such as antifungal, antibacterial, antitumor, antipyretic, and anti-proliferative properties (Jain et al., 2022; Amin et al., 2012; Chigurupati, 2015; Fugu et al., 2013; Song et al., 2013; Liang et al., 2014; Karthika et al., 2025). Consequently, they have gained wider attention among other derivatives of compounds.

In recent times, there has been an increase in occurrences of bacterial infections and drug-resistant pathogenic organisms, which necessitates the development of compounds that can fight against multidrug-resistant bacteria. Therefore, in search of the development of new therapeutic agents, there is motivation for the synthesis, characterization, and study of antibacterial activity of some vanillin Schiff bases derived from structurally and electronically diversified 4-((phenylimino)methyl) phenols. In this research, a new series of six Vanillin Schiff bases were prepared (L1 to L6) and structurally characterized by spectroscopic studies (Scheme 1). Also, their physicochemical properties were investigated by Density Functional Theory.

2. Materials and Methods

Without undergoing additional purification, the analytical grade reagents and all of the starting ingredients were purchased commercially from British Drug Houses (BDH) Chemicals Limited and Sigma-Aldrich. The Schiff bases were prepared in compliance with the guidelines outlined in published procedures (Osowole, 2011; Fugu et al., 2013). A Shimadzu 8740 FT-IR spectrometer was used to record IR spectra with KBr discs within the 4000–400 cm^{-1} range. UV/Visible spectra were captured using a UV/Visible Spectrophotometer. Melting points were measured using an uncorrected Gallenkamp melting point instrument.

2.1 Syntheses of the compounds

2.2 Typical synthetic procedure

2.2.1 Synthesis of L1 (Schiff base derived from vanillin and 2,4-dinitrophenylhydrazine)

3.0430 g (20 mmol) of ethanolic vanillin solution (10 mL) was dropwise added to a 30 mL hot ethanolic solution of 3.9628 g (20 mmol) of 2,4-dinitrophenylhydrazine while stirring in a 250 mL round-bottomed flask. An immediate reaction was observed by the formation of a red suspension. To this suspension was added 70 mL of ethanol, and the mixture was refluxed in an oil bath at 60–70 °C for 6 hrs. The red product was then filtered and washed with ethanol. Yield = 6.540 g, 98%, M.P. = 234–236 °C, Colour = red.

IR(cm⁻¹): $\nu_{\text{OH}} = 3387$; $\nu_{\text{Ph/C-H}} = 3111$; $\nu(\text{C=N}) + \nu(\text{C=C}) = 1620, 1589, 1514$; $\nu_{\text{Ph/C-O}} = 1280$, UV/(cm^{-1}) = 47569, 45244, 36345, 30278. This method was similarly used for other compounds.

2.2.2 L2 (Schiff base derived from vanillin and 2,5-dichloroaniline)

Vanillin, 3.0430 g (20 mmol) and 3.2404 g (20mmol) of 2,5-dichloroaniline were reacted in ethanol. After being filtered, the crystals that emerged from the solution were cleaned using ethanol and n-hexane. Yield = 2.699 g, 46%, M.P. = 53–56 °C, Colour = light yellow. IR(cm⁻¹): $\nu_{\text{OH}} = 3373$; $\nu_{\text{Ph/C-H}} = 3180$; $\nu(\text{C=N}) + \nu(\text{C=C}) = 1662, 1589, 1510$; $\nu_{\text{Ph/C-O}} = 1300$, UV/(cm^{-1}) = 47147, 43531, 37075, 30228.

2.2.3 L3 (Schiff base derived from vanillin and p-phenylenediamine)

3.0430g (20 mmol) vanillin and 1.0814 g (10 mmol) p-phenylenediamine were reacted in ethanol. The product was washed with ethanol and n-hexane. Yield = 3.8185 g, 97%, M.P. = 144–146 °C, Colour = brown.

IR(cm⁻¹): $\nu_{\text{OH}} = 3338$; $\nu_{\text{Ph/C-H}} = 3084$; $\nu(\text{C=N}) + \nu(\text{C=C}) = 1674, 1593, 1514$; $\nu_{\text{Ph/C-O}} = 1288$, UV/(cm^{-1}) = 43698, 36417, 32894, 30988, 25717.

2.2.4 L4 (Schiff base derived from vanillin and o-toluidine)

2.14 mL (20 mmol) of o-Toluidine and 3.0430g (20 mmol) vanillin were reacted in ethanol. After the evaporation of the solvent, the compound came out as light brown crystals. Colour = light brown; M.P. = 156–158 °C; Yield = 71%. IR (cm^{-1}): $\nu_{\text{Ph/C-H}} = 3012$; $\nu(\text{C=N}) + \nu(\text{C=C}) = 1624, 1589$; $\nu_{\text{Ph/C-O}} = 1274$, UV/(cm^{-1}) = 42027, 36231, 31543, 29418.

2.2.5 L5 (Schiff base derived from vanillin and m-anisidine)

3.043 g (20 mmol) of vanillin and 2.23 mL (20 mmol) m-Anisidine were reacted in ethanol. The compound came out as a brown, thick liquid. Yield = 3.5 g 63 %, Colour = brown.

IR(cm⁻¹): $\nu_{\text{OH}} = 3379$; $\nu_{\text{Ph/C-H}} = 3068$; $\nu(\text{C=N}) + \nu(\text{C=C}) = 1674, 1589, 1512$; $\nu_{\text{Ph/C-O}} = 1289$, UV/(cm^{-1}) = 43898, 42238, 30936.

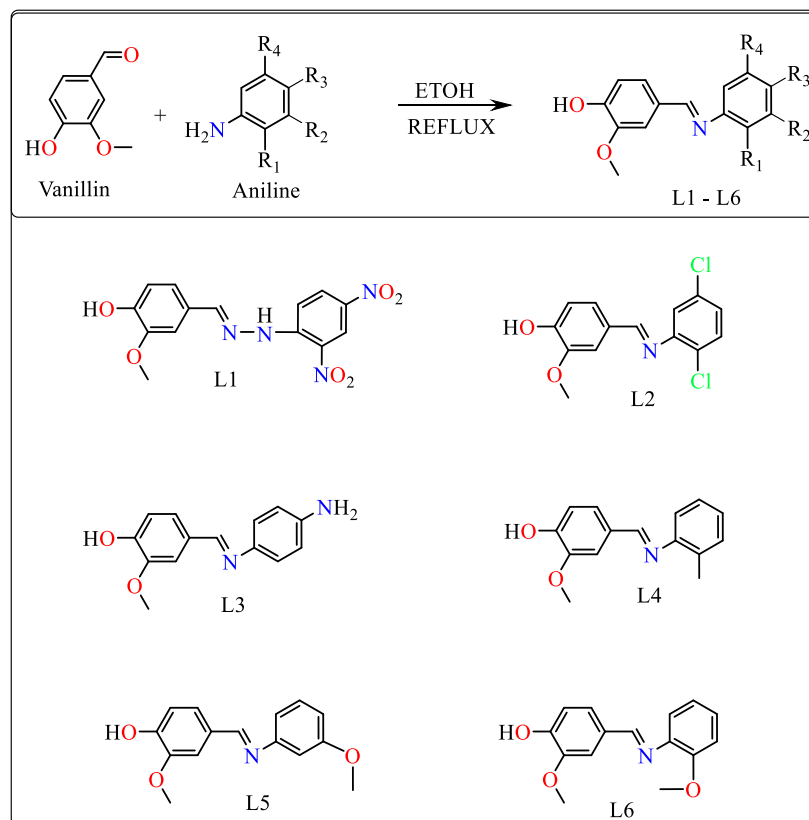
2.2.6 L6 (Schiff base derived from vanillin and *o*-anisidine)

3.043 g (20 mmol) of vanillin and 2.25 mL (20 mmol) of *o*-Anisidine in a 200 mL round-bottomed flask were reacted. The compound came out as a brown, viscous liquid. Yield = 3.2 g, 59% , Colour = brown

IR(cm⁻¹): νOH = 3379; νPh/C-H = 2935; ν(C=N) + ν(C=C) = 1676, 1585, 1510; νPh/C-O = 1290, UV/(cm⁻¹) = 45367, 42238, 40985, 35132.

2.3 Computational details

The molecules (L1-L6) were modeled and optimized using DFT at the 6-31G(d) level of theory. This level of theory has been reported to be consistent with experimental trends. The molecular descriptors calculated include the frontier molecular orbitals energies (EHOMO and ELUMO), energy band gap, chemical hardness and softness, as described earlier (Ogunyemi et al., 2020), all on Spartan 14 (Irvine, 2014).



Scheme 1: Synthetic route and compositions of the obtained compounds.

3. Results and Discussions

3.1. Synthesis of the compounds

Vanillin reacts with the different anilines to give the different products. The synthetic procedure and the compositions of the compound are presented in Scheme 1. The products came in two different forms: liquid syrup (L5 and L6) or solid crystalline compound (L1–L4). The compounds display a range of colors, from deep brown to red. All of the solid products melted sharply, with the lowest melting point recorded for L2. The high purity of the synthesized compounds is indicated by the sharp melting points.

3.2. Infrared spectra

The IR spectra of the synthesized compounds are discussed by comparing the notable and important IR features of the parent starting material, vanillin, to those of the new compounds. (Osowole, 2011; Liang et al., 2014; Lacopetta et al., 2023). The νOH of phenol was found as a broad band at 3178 cm⁻¹ in the infrared spectrum of vanillin, and the

νC=O carbonyl functional group was found at 1666 cm⁻¹. These are two very noticeable, significant, and important IR bands. The wide band of phenolic νO-H has covered up the νC-H (aromatics). The benzene ring's νC=C was observed at 1589 and 1510 cm⁻¹. The phenolic/methoxy, νC-O bands at 1300 cm⁻¹ and 1267 cm⁻¹ are other noteworthy bands.

Nevertheless, the band at 1666 cm⁻¹ in the spectra of the synthesized compounds, which is caused by vanillin's νC=O, is either completely absent or vanished. This verified that the azomethine, C=N group has taken the place of the C=O, carbonyl functional group, as indicated by newly emerged bands observed at 1676–1620 cm⁻¹ for all the synthesized compounds (Osowole, 2008; Osowole, 2011). This further supports the formation of the Schiff bases. Other noteworthy bands showed a distinct bathochromic/hypsochromic shift in the synthesized compounds. Bands observed in the range 3387 to 3338 cm⁻¹ are due to phenolic νOH. Similarly, the phenolic νC-O band for the Schiff bases was observed in the range 1300–1274 cm⁻¹, and the νC-H (aromatics/imine) was observed at 3111–3012 cm⁻¹. Figures 1 and 2 show the FTIR spectra of L1 and L2, respectively. Other FTIR spectra are contained in the supporting Information file (Figures S1 – S6).

3.3. Ultraviolet spectra

The UV spectra of aromatic Schiff bases typically contain important and notable features or transitions. These include the $\pi - \pi^*$ transition linked to the benzene ring at 48000–43000 cm^{-1} , the $\pi - \pi^*$ transition of the azomethine group at 38000–34000 cm^{-1} , and the $n - \pi^*$ transition of the azomethine chromophore, which is typically found between 32000–25000 cm^{-1} (Osowole, 2011). All of these transitions were seen in the UV spectra of the compounds that were prepared (Figures 3 and 4). The

benzene ring's $\pi - \pi^*$ transition was detected between 47569 cm^{-1} and 40985 cm^{-1} . Bands seen between 37075 cm^{-1} and 32894 cm^{-1} are attributed to $\pi - \pi^*$ transition of the azomethine groups. At 31543–25717 cm^{-1} , the azomethine chromophore's $n - \pi^*$ transitions were detected. The tailing of the UV band of the azomethine chromophore L4 into the visible suggested that the compound may have luminescence properties. Figures 3 and 4 show the UV spectra of L2 and L3, while others are in the supporting information file (Figures S7 – S12).

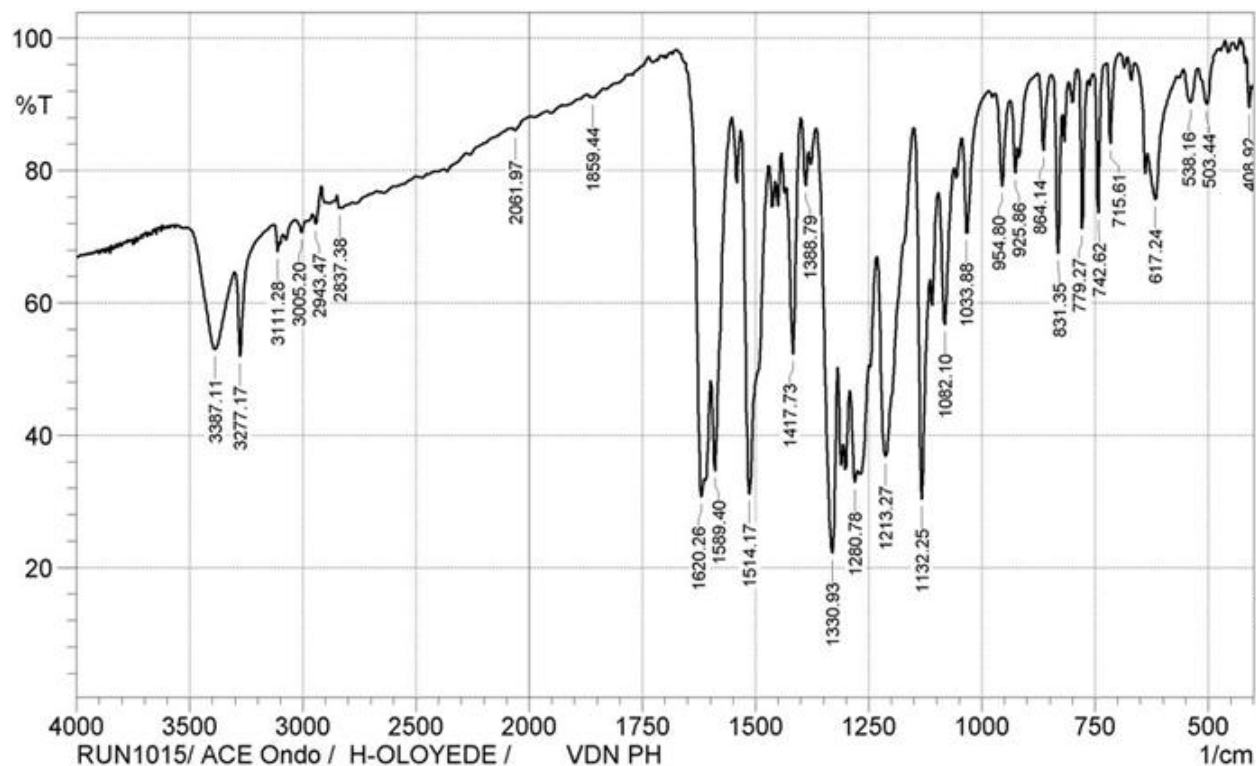


Figure 1: Infrared spectrum of L1.

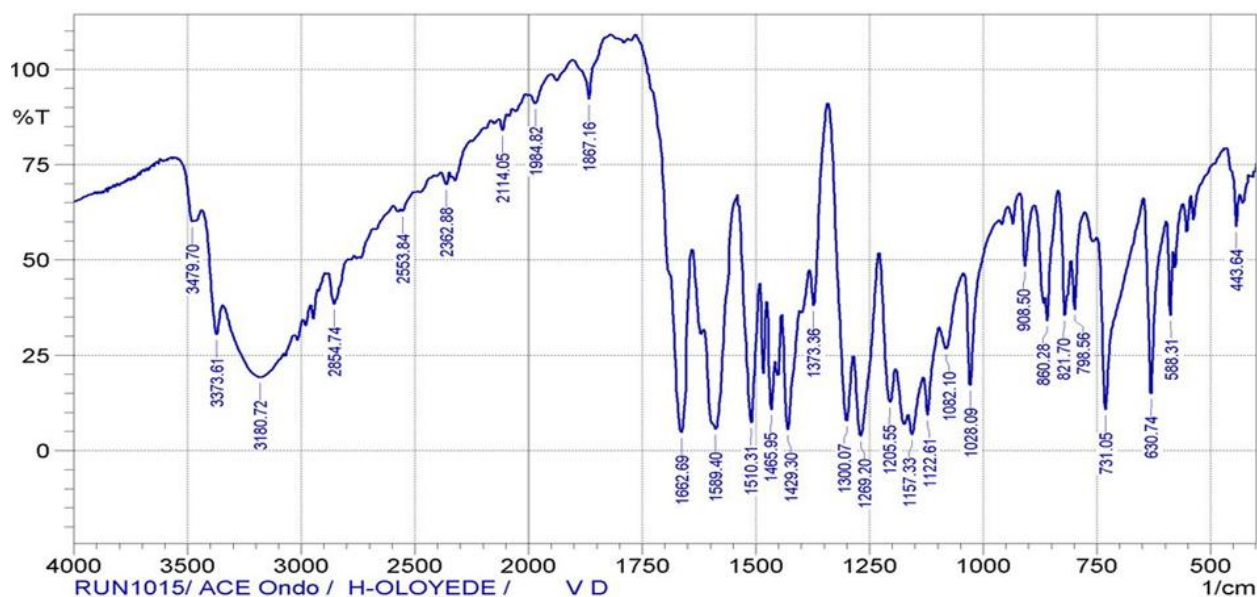


Figure 2: Infrared spectrum of L2.

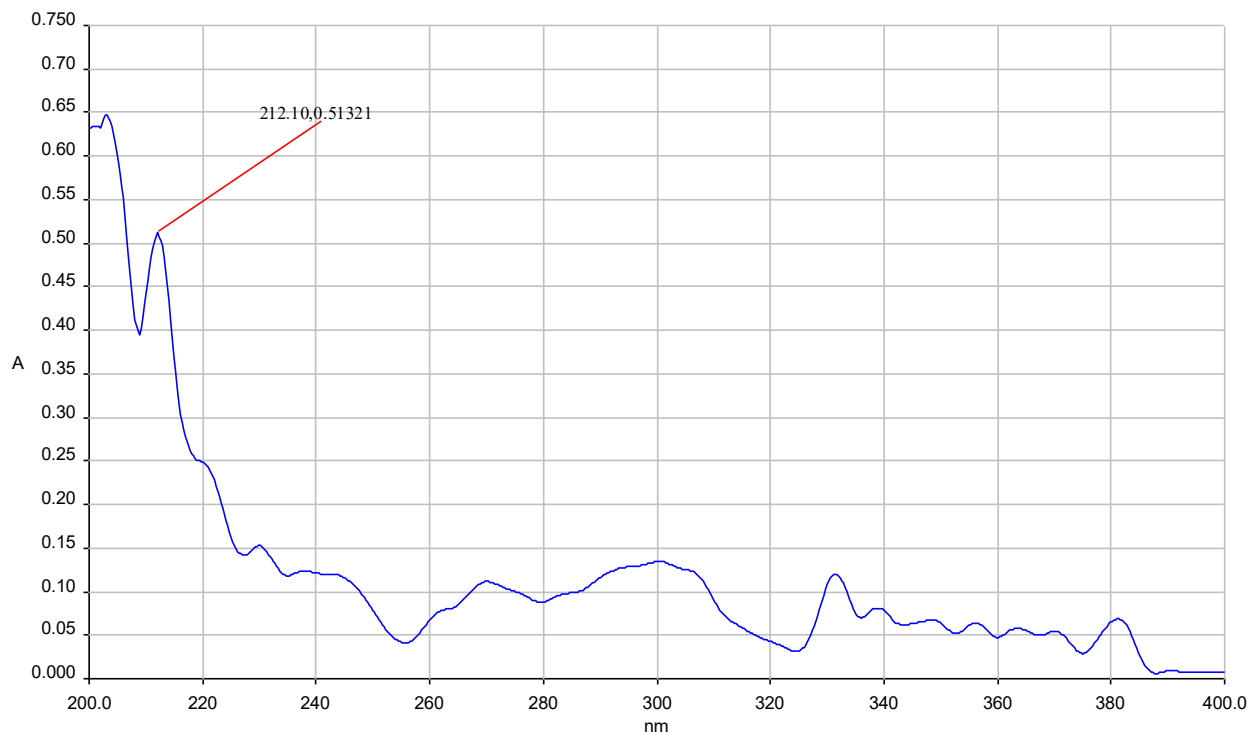


Figure 3: UV spectrum of L2.

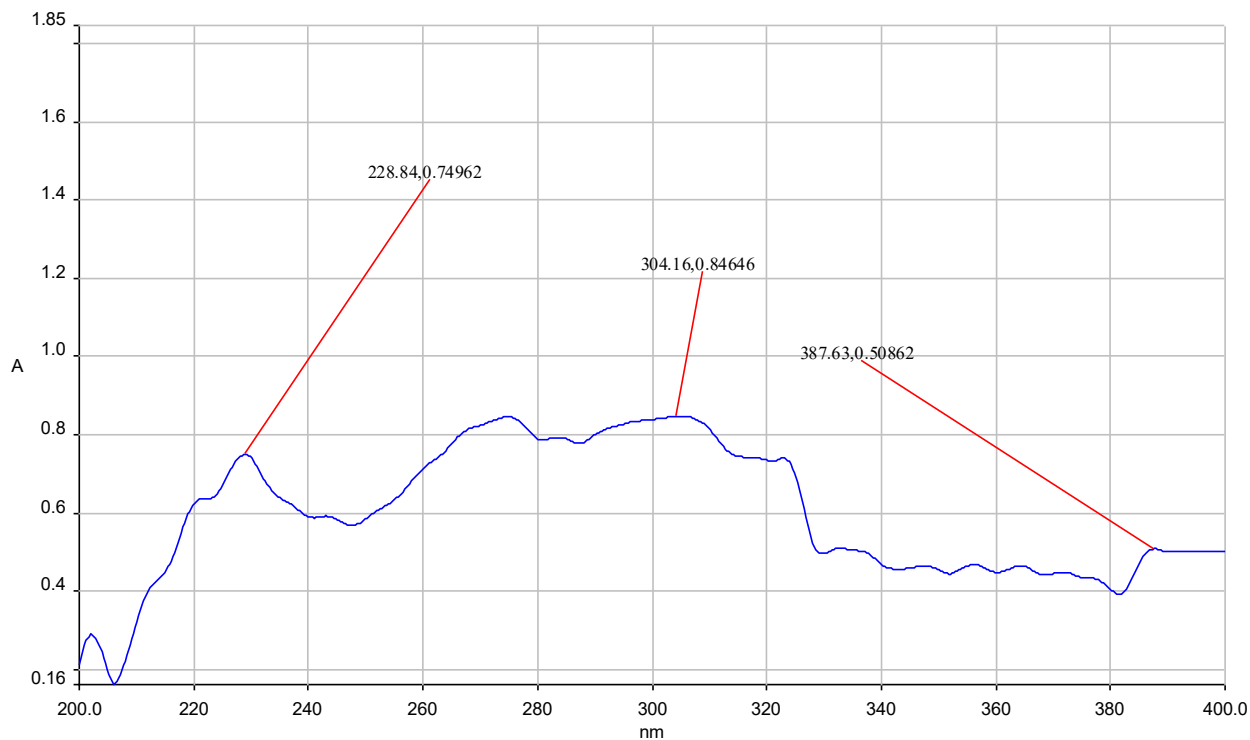


Figure 4: UV spectrum of L3.

3.4. Molecular descriptor/physicochemical properties

The frontier molecular orbital energies (EHOMO and ELUMO), which are measures of ionization potential and electron affinity of the molecules, respectively, are displayed in Table 1. A high HOMO value

indicates more readiness to donate an electron. The lower the LUMO energy of a molecule, the better its electron-accepting ability. L3 has the highest HOMO energy; its ability to donate electrons is the highest. The HOMO energies of the molecules follow the order, L3 > L5 > L4 > L6 > L1 > L2. L1 has the lowest LUMO energy, indicating that it has the

highest electron-accepting ability. The LUMO energies of the molecules follow the order, $L3 > L5 > L4 = L6 > L2 > L1$. The energy band gap, E_g , describes the gap between the EHOMO and ELUMO, and measures the reactivity and stability of molecules. L1 has the lowest E_g value (3.45 eV), indicating the highest chemical reactivity and lowest stability. The energy band gap follows the order, $L2 > L6 > L4 > L5 > L3 > L1$. The chemical hardness (η) is directly proportional to the energy band gap, so it follows the same order as E_g , $L2 > L6 > L4 > L5 > L3 > L1$, while softness (δ) follows the reverse trend ($L1 > L3 > L5 > L4 > L6 > L2$) as the chemical hardness, since chemical softness is inversely proportional to the chemical hardness. Despite the low HOMO energy value of L1, it is the most reactive of all the molecules because of its low E_g value, which is a result of its very low ELUMO value when compared to others (Oyeneyin et al., 2022; Oyeneyin, 2023).

The optimized structures, HOMO, LUMO, and electrostatic potential maps of the molecules are displayed in Figures 5, 6, S13–22. The HOMO map of L1 is spread over almost all parts of the molecule, except for the methyl on the methoxy group, while the LUMO is located on one side of the molecule, starting from the imine through the azo bonds and the dinitrophenyl ring (Figure 5). The electrostatic potential map of L1 (Figure 6) revealed the parts susceptible to nucleophilic (blue and green regions on the phenyl carbons, azo hydrogen, and methoxy group) and electrophilic (red and orange regions on the nitro and hydroxyl oxygen and the azo nitrogen) attacks (Oyeneyin et al., 2022; Oyeneyin, 2023). The HOMO map of L2, just like L1, is spread over almost all parts of the molecule, with the exception of the methyl on the methoxy group, while the LUMO is located on one side of the molecule, starting from the imine bond to the hydroxyphenyl ring (Figure S13). In the electrostatic potential map of L2 (Figure S14), the nucleophilic attack would be on (blue and green regions on the hydroxyl, methoxy, and phenyl carbons) while electrophilic attacks would be on (red, orange regions on the imine nitrogen, chlorine close to the imine group, and hydrogens on the hydroxyphenyl ring). The HOMO map of L3 spreads from the imine

group to the entire aminophenyl ring, while the LUMO covers from the imine group through the hydroxyphenyl ring, except the methoxy group (Figure S15). In the electrostatic potential map of L3 (Figure S16), the nucleophilic attack would be on (blue and green regions on the amino, methoxy, and some phenyl carbons) while electrophilic attacks would be on red and orange regions on the imine nitrogen and some phenyl carbons. The HOMO map of L4 spreads from the imine group to all of the methylphenyl ring, while the LUMO, like in L3, covers from the imine group through the hydroxyphenyl ring, with the exception of the methoxy group (Figure S17). In the electrostatic potential map of L4 (Figure S18), the nucleophilic attack would be on (blue and green regions on the basically almost all the hydrogen atoms, save for the methyl hydrogen atoms on the methylphenyl ring and its neighboring hydrogen atom) while electrophilic attacks would be on (red, orange regions) the imine nitrogen, methyl hydrogen atoms on the methylphenyl, oxygen atoms and some phenyl carbons. The HOMO map of L5 spreads from the imine group to all of the methoxyphenyl ring, while the LUMO covers from the imine group through the entire hydroxyphenyl ring, except for the methoxy group (Figure S19). In the electrostatic potential map of L5 (Figure S20), the nucleophilic attack would be on (blue and green regions on basically almost all the hydrogen atoms) while electrophilic attacks would be on (red, orange regions on the imine nitrogen, methoxy oxygen on the methoxyphenyl ring, and almost all the carbon atoms in the rings). The HOMO map of L6, like in L5, spreads from the imine group to all of the methoxyphenyl ring, while the LUMO covers from the imine group through the entire hydroxyphenyl ring, except the methoxy group (Figure S21). In the electrostatic potential map of L6 (Figure S22), the nucleophilic attack would be on (blue and green regions on basically almost all the hydrogen atoms) while electrophilic attacks would be on (red, orange regions on the imine nitrogen, methoxy oxygen on the methoxyphenyl ring, and almost all the carbon atoms in the rings). These maps would help in investigating the effectiveness of these molecules as drugs, corrosion inhibitors, and in other possible applications.

Table 1: Physicochemical properties of L1–L6.

Compounds	EHOMO (eV)	ELUMO (eV)	E_g (eV)	η (eV)	δ (eV ⁻¹)
L1	-5.99	-2.54	3.45	1.725	0.579
L2	-6.02	-1.52	4.50	2.25	0.40
L3	-4.93	-1.06	3.87	1.935	0.516
L4	-5.55	-1.20	4.35	2.175	0.459
L5	-5.48	-1.18	4.30	2.15	0.465
L6	-5.59	-1.20	4.39	2.195	0.455

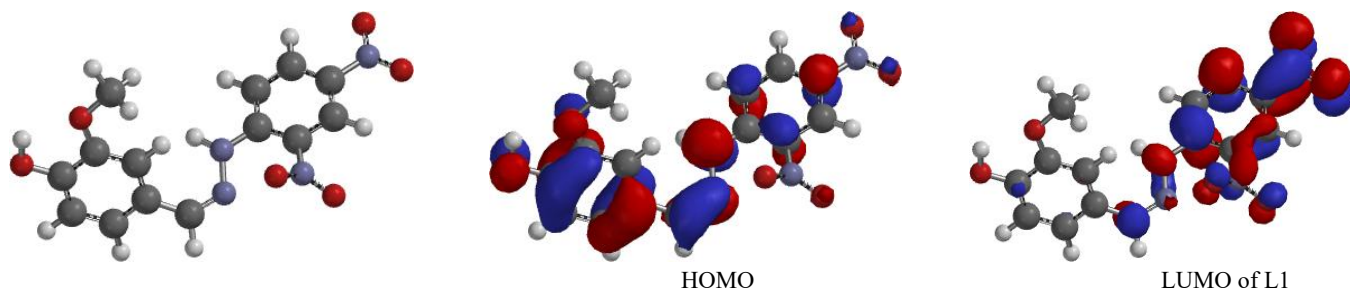


Figure 5: Optimized structure.

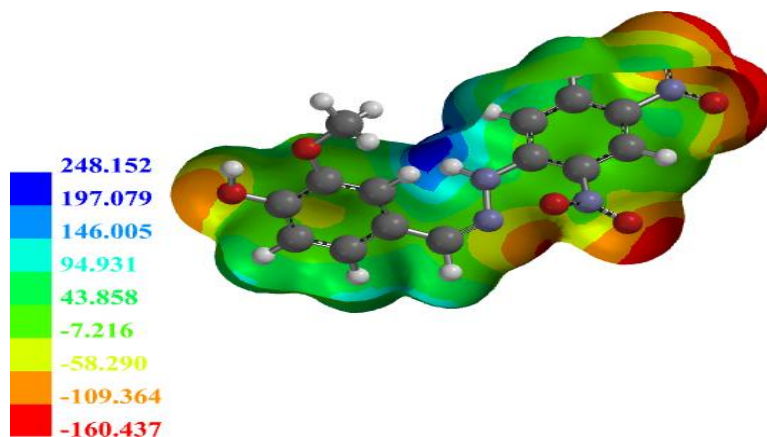


Figure 6: Electrostatic potential map of L1.

4. Conclusion

New derivatives of vanillin Schiff bases (L1-L6) were successfully synthesized and characterized. The compounds were prepared through the condensation of different aniline derivatives and vanillin. Compounds L1-L4 were obtained as crystals, while L5-L6 were prepared as semi-solids. Characterization of the compound was carried out by melting point determination, UV/visible, and IR spectral measurements. Sharp melting points of the compounds revealed the purity of the compounds. Some notable transitions in the spectra of the compounds, together with the results of the computational studies, suggest that the compounds may have potential medicinal and electronic properties.

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Competing Interest

The author affirms that there are no identifiable conflicts of interest, either financial or personal, that could be perceived as influencing the work presented in this paper.

Data Availability Statement

All data generated or analyzed during this study are included in this published article.

Ethics Approval

This study did not involve human participants or animals and therefore did not require ethics approval.

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