

Synthesis and spectral investigation of mixed Schiff base derived from-trimethoprim and L-valine complexes and their biological activity

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ABSTRACT

In this manuscript, mixed-ligand metal(II) complexes were synthesized using a Schiff base (L) derived from trimethoprim and N,N-dimethylaminobenzaldehyde as the primary ligand, with L-valinate as the secondary ligand. The bonding mode of the Schiff base was confirmed using infrared, UV-visible, ¹H, and ¹³C NMR spectroscopy, mass spectrometry, and elemental analysis. All complexes were characterized by elemental analysis, conductivity measurements, magnetic moment evaluations, and spectroscopic techniques, including UV-Vis and FT-IR. A thorough discussion is provided of the structural and bonding features of the mixed-ligand complexes formed from the Schiff base (L) and L-valine with ions [Fe(II), Co(II), Ni(II), Cu(II), Zn(II), Cd(II), and Hg(II)], based on results from various research studies. In addition, the complexes were assessed for biological activity against specific microbial strains. Antimicrobial effectiveness was tested against two Gram-positive and Gram-negative bacterial strains. Furthermore, antifungal activity against *Candida* was evaluated, using tetracycline as a reference and DMSO as a control and solvent.

Keywords: *Biological evaluation, Metal ions, Schiff base, Spectral analysis, Trimethoprim*

1 INTRODUCTION

Metal complexes with mixed ligands have attracted researchers' interest because of their wide range of applications in a variety of fields, including catalysis, medicine, and materials science [1–5]. In medicinal chemistry, incorporating pharmacologically active molecules into metal complexes in the form of ligands can enhance their properties, thereby allowing them to act as new therapeutic agents [1]. Complexation can also lead to improved bioavailability, selectivity, solubility, and overall higher efficacy in comparison to the free ligand [6, 7].

Paracetamol (Para), also known as acetaminophen, is considered one of the most widely used analgesics and antipyretic drugs, with a high safety profile [8, 9]. Its mechanism of action includes inhibition of cyclooxygenase (COX) enzymes, which are responsible for producing inflammatory mediators [8]. However, the antibacterial and antifungal activities of this drug are very limited and low [10]. In contrast, 1,10-phenanthroline (Phen) is a bidentate N,N-chelating ligand that can form coordination complexes with metals and has potential biological activity [2]. Many studies have reported the efficacy of this compound as an antibacterial agent after incorporation into complexes, specifically against *Pseudomonas aeruginosa* and its biofilms [2, 11]. Moreover, other studies have suggested using Phen and its complexes as insecticidal and antiparasitic agents [3, 5, 12]. These activities can be attributed to potential interactions of this compound and its complexes with cellular components, as well as to the disruption of related biological processes [4, 13].

Although various studies have synthesized metal com-

plexes involving 1,10-phenanthroline and paracetamol, such as the work by Jamil et al. (2018) with Co(II), Ni(II), and Cu(II) in a 1:1:1 molar ratio [14], the biological potential of these systems remains insufficiently explored. In particular, the activity of bivalent metal complexes formed with Para and Phen ligands has not been thoroughly investigated across a broader range of metal ions and stoichiometries. In this study, we report the synthesis and characterization of a novel series of bivalent metal complexes involving Mn(II), Fe(II), Co(II), Ni(II), Cu(II), Zn(II), and Cd(II) ions in a 1:2:1 stoichiometric ratio of [M(Para)(Phen)₂]Cl₂. Chelation of paracetamol to metal ions is anticipated to improve target specificity and enhance cellular uptake, whereas complexation with 1,10-phenanthroline may broaden biological activity due to its known interactions with biomolecular targets [15]. The aim of the present work is to investigate the structural, spectroscopic, and electronic properties of these complexes, to evaluate their antimicrobial activities, and to employ density functional theory (DFT) calculations to model their optimized geometries and to explore associated electronic parameters.

2 MATERIALS AND METHODS

2.1 Chemicals and materials

The chemicals were obtained from BDH or Sigma and used without further purification. 3-Hydroxybenzaldehyde, DMSO, and CH₃OH were of Analar grade (BDH).

2.2 Characterization methods

FT-IR spectra were recorded using an A224160-Shimadzu spectrophotometer in the 400-4000 cm⁻¹ region. Metal determination was performed using a spectrophotometer (A.A-160). Magnetic moment measurements of the complexes were carried out using a Johnson balance by the Gouy method. Effective magnetic moments were calculated after applying diamagnetic corrections for the ligand components using Pascal's constants [12]. An MS Model 5973 spectrometer was employed to record mass spectra, and elemental microanalysis was performed using a C.H.N.-2400 elemental analyzer. The ¹H and ¹³C NMR spectra for (HL) were recorded in DMSO using an INOVA-500 MHz instrument and are reported as δ (ppm). An Ino Lab.720 digital conductivity meter was used to measure molar conductivity (Λ m) for 10⁻³ mol/L solutions in ethanol. UV spectra (10⁻³ M) were recorded using a Shimadzu UV-A1800 spectrophotometer. The

¹H and ¹³C NMR spectra of (L) were recorded in DMSO (INOVA-500 MHz) and are reported as δ (ppm).

2.3 Synthesis of schiff base

The Schiff base ligand (L) was prepared through a condensation reaction between N,N-dimethylaminobenzaldehyde (3 mmol) and trimethoprim (3 mmol) in ethanol (30 mL), with the addition of four drops of CH₃COOH. The resulting mixture was refluxed for 10 h. The mixture volume was reduced by gradual evaporation at room temperature, and the solution was left to settle overnight. The resulting yellow precipitate was washed several times with absolute ethanol, dried at room temperature, and recrystallized from ethanol to obtain a pure sample, which was finally stored in a desiccator. Yield: 87%. Anal. Calc. for C₂₃H₂₇N₅O₃ (formula weight 421.501 g/mol): C, 62.54%; H, 6.46%; N, 16.62%; Found: C, 57.29%; H, 6.38%; N, 14.44% [9]. The schematic representation of the reaction is depicted in Figure 1.

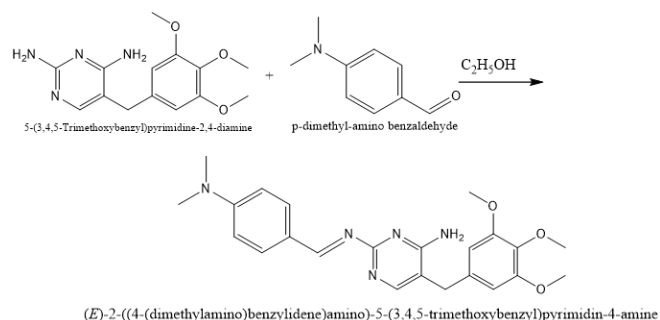


Fig. 1 Synthetic route for ligand (L)

2.4 Preparation of the schiff base complexes

Potassium L-valinate (K⁺L-Val) was prepared by neutralizing 2 mmol of L-valinic acid with 2 mmol of potassium hydroxide in a flask, which was then stirred at room temperature in accordance with the method described in Figures 2 and 3.

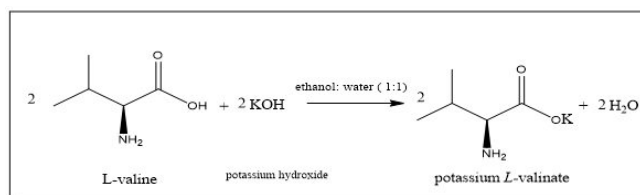


Fig. 2 synthesis diagram of Potassium-L-Valinate

The mixed-ligand complexes of Schiff base (L) with L-valinate (L-Val) were formed with the formula $[M(L)(L-Val)_2]$, where M represents Co(II), Ni(II), Cu(II), Fe(II), Zn(II), Hg(II), and Cd(II). These complexes were prepared by combining alcoholic solutions in a 1:1:2 molar ratio with an aqueous solution of the corresponding metal chloride. The entire mixture was refluxed for eight hours, yielding the desired product. The product was recrystallized multiple times from an alcoholic solution, dried, and finally stored in a desiccator.

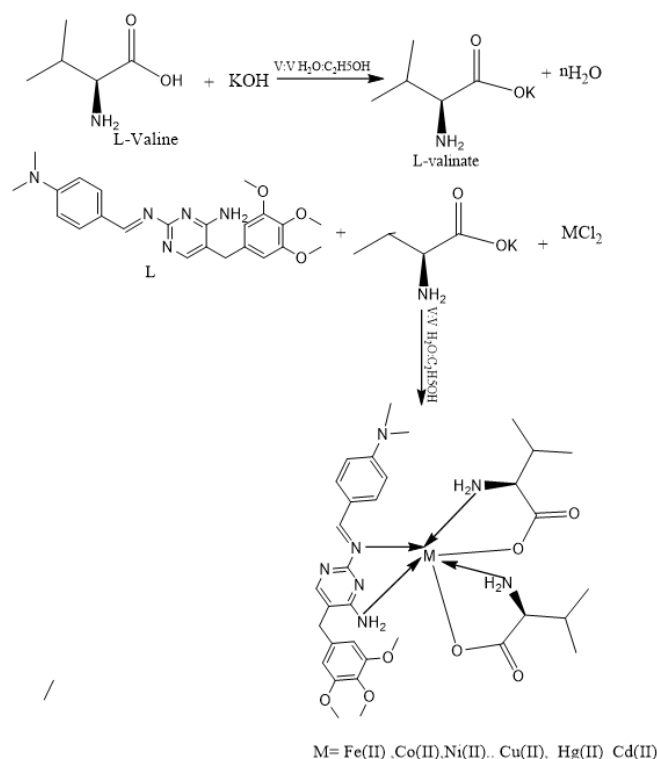


Fig. 3 A synthesis diagram of metal complexes

2.5 Antimicrobial activity

The disc diffusion method was used to evaluate the compounds' in vitro biological activity against the fungus *Candida albicans* and the bacteria *Staphylococcus aureus*, *Pseudomonas aureginosa*, *Bacillus subtilis*, and *Escherichia coli*. To create a 1×10^6 M solution, these chemicals were dissolved in DMSO. After being dipped in this solution, sterile discs were dried and placed on a nutrient agar plate, inoculated with bacteria. The inhibitory zone diameters were measured in millimeters after incubation for 24 to 48 h at 37 °C. Tetracycline also functioned as the positive control.

3 RESULT AND DISCUSSION

3.1 Characterization of the schiff base (I)

Spectroscopic analysis: The NMR spectral data obtained in deuterated DMSO-d₆ indicate that all proton and carbon atoms in the molecular structure occur within their expected regions [11].

The ^1H NMR spectrum (δ , ppm; DMSO-d₆; 400 MHz) of ligand L (Figure 4) showed singlet and doublet signals at 9.67 ppm δ (s, 1H, Ca) for the proton of the (-CH-N) group, 7.7 ppm δ (d, 2H, Cb), 7.5 ppm δ (s, 1H, Cc), 6.79 ppm δ (d, 2H, Cd), 6.57 ppm δ (s, 2H, Ce), 3.73 ppm δ (s, 9H, Cf), 3.54 ppm δ (s, 2H, NH₂), and 3.04 ppm δ (s, 6H, Cn). In addition to the above peaks, a signal at 1.9 ppm δ (s, 2H, Ck) was observed [15, 16].

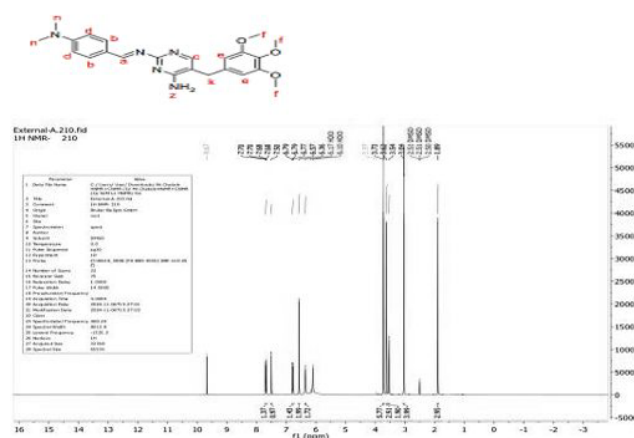


Fig. 4 The ^1H NMR spectrum of the ligand (L)

The ^{13}C NMR (δ , ppm; DMSO-d₆; 400 MHz) spectrum of L showed chemical shifts for carbon atoms at 190.35 ppm δ (Ca) for the carbon of the (-CH-N) group, 106.24–173.26 ppm δ (CAr) for aromatic carbon signals, 60.41 ppm δ (Cb) for the (O-CH₃) group, 56.22 ppm δ (Cc) for N(CH₃)₂ groups, and 33.37 ppm δ (Cd). In addition to the above peaks, a signal at 21.96 ppm δ (Ce) for (CH₂) was observed. The chemical shift due to DMSO-d₆ was observed at 40.1 ppm δ [8, 14, 17], as shown in Figure 5.

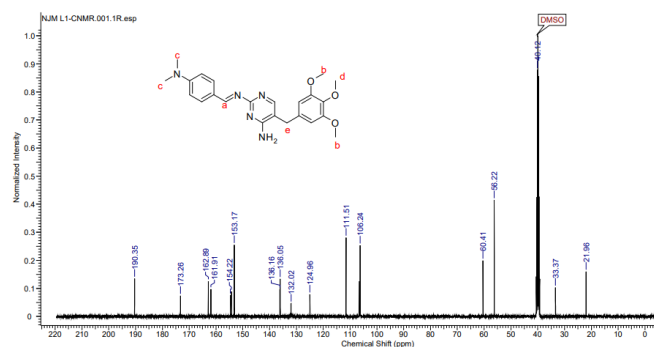


Fig. 5 The ^{13}C NMR spectrum of the ligand (L)

The mass spectrum of L was recorded to determine its molecular weight and fragmentation pattern (Figure 6). The suggested structure formula is located as follows: Mass]: m/z Spectrum (Calc.), 421.50, 421.00 (Found). The relatively low abundance indicates that condensation between trimethoprim and aldehyde has taken place, resulting in the formation of this Schiff base at a (1:1) rate; this consistency supports the proposed formula for ligand L (Figure 6), based on the findings mentioned in Table 1.

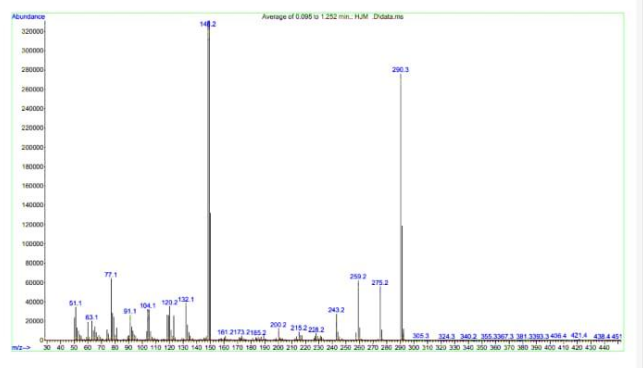


Fig. 6 ESI-MS of the ligand (L)

FT-IR spectra of the compounds: The identification of distinct bands for the compounds is documented in Table 2. The FT-IR spectrum of the original compound (TMA) gave prominent bands at (3465 and 3316) cmv, which are related to the $\nu(\text{NH}_2)$ group (asymmetrical and symmetrical). In addition, the peak at 1120 cmv corresponds to $\nu(\text{OCH}_3)$ aromatic groups), while the bands at 1264 and 1229 cmv relate to $\nu(\text{C}-\text{O}-\text{C})$ vibrations (asymmetrical and symmetrical, respectively). Furthermore, intense bands observed at 1558 and 1637 cmv are associated with the $\nu(\text{C}=\text{N})$ pyrimidine nitrogen

group [18]. The FT-IR spectrum of the initial material 2,4-dimethoxybenzaldehyde ((CH_3O) $_2\text{C}_6\text{H}_3\text{CHO}$) shows a strong absorption indicative of $\nu(\text{C}=\text{O})$ located at 1655 cmv. The bands at 2902 and 2795 cmv are related to $\nu(\text{C}-\text{H})$ for both aromatic and aliphatic groups. A band at 1310 cmv arises from stretching of $\nu(\text{C}-\text{N})$, while the 1159 cmv band corresponds to $\nu(\text{C}-\text{O})$ stretching [16,17,19,20]. The bands at (1334 and 1229) cmv are assigned to $\nu(\text{C}-\text{O}-\text{C})$ (asymmetrical) and $\nu(\text{C}-\text{O}-\text{C})$ (symmetrical), respectively [21–23].

Table 1 ESI-MS fragmentation data of the ligand (L)

M.wt	Format
421.50	$[\text{C}_{23}\text{H}_{27}\text{N}_5\text{O}_3]^+{}^+$
406	$[\text{C}_{22}\text{H}_{24}\text{N}_5\text{O}_3]^+$
104	$[\text{C}_5\text{H}_2]^+$
148	$[\text{C}_9\text{H}_{12}\text{N}_2]^+$
77	$[\text{C}_6\text{H}_5]^+$
259	$[\text{C}_{14}\text{H}_{15}\text{N}_2\text{O}^3]^+$
120	$[\text{C}_8\text{H}_8]^+$

The FT-IR spectrum of ligand (L), illustrated in Figure 7, shows sharp bands near 3448 and 3422 cmv related to the stretching vibrations of asymmetric and symmetric primary amines $\nu(\text{NH}_2)$. The bands at 3118 and 2960 cmv correspond to asymmetrical and symmetrical $\nu(\text{CH}_3)$, respectively. This spectrum also highlights a strong band at 1657 cmv, attributed to $\nu(\text{C}=\text{N}-)$ stretching, which differs from the bands observed in the TMA spectrum. In addition, a strong band at 1589 cmv is associated with the $\nu(\text{C}=\text{O})$ group [24]. The peaks at (1333, 2831) cmv, (1235) cmv, and (1506) cmv are assigned to $\nu(\text{C}-\text{H})$ -aliphatic, $\nu(\text{C}-\text{H})$ -aromatic, $\nu(\text{C}-\text{C})$ -aliphatic, and $\nu(\text{C}=\text{C})$ -aromatic, respectively [1, 7]. The band at (1211) cmv corresponds to $\nu(\text{C}-\text{N})$. The band at (1126) cmv is related to $\nu(\text{C}-\text{O})$ [17, 18]. The bands at (1333 and 1235) cmv represent $\nu(\text{C}-\text{O}-\text{C})$ stretching vibrations (asymmetric and symmetric) [9].

The thermal characteristics of the synthesized ligand led to different decomposition patterns. TG/DTG analysis was conducted in a nitrogen atmosphere within a temperature range of 0 °C to 700 °C. The TG/DTG curve for the ligand, as depicted in Figure 8 and Table 2, illustrates three distinct phases with midpoint temperatures of 150 °C, 300 °C, and 500 °C, respectively.

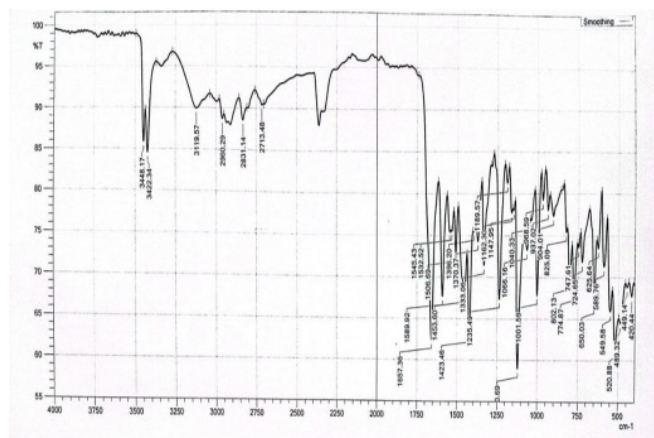


Fig. 7 FT-IR spectrum of the ligand (L)

Table 2 Comparison of Classification Results.

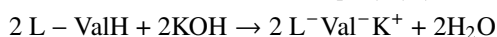
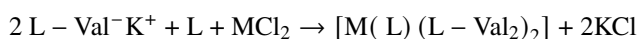
Stage	Decomposition Temp. [°C]	Molar mass loss	Assignments
1	150	30	-2CH ₃
2	300	116	
3	500	240	
			C ₁₃ H ₈ O ₃ N ₂



Fig. 8 TGA-DTGA curves of the ligand (L)

3.2 Characterization of [I- metal-I-valine]

All complexes were designed to react with metal chlorides $MCl_2 \cdot nH_2O$, while the ligands were applied using a 1:2:1 mole ratio (metal: two moles of L-valinate: L). The formation of $[M(L)(L-valine)_2]$ complexes can be illustrated by the general equation provided below.



Where, primary ligand L = Schiff base (C₂₇H₂₅NO₆) accrued from the condensation of N, N-dimethyl amino-benzaldehyde and Trimethoprim.

The chemical formulas and compositions for metal complexes 1-7, melting point, color, molar conductivity values (Ω) in DMSO (10^{-3} M), and analytical data are depicted in Table 3.

Table 3 Elemental analysis and physical properties of the ligand (L) and its metal complexes

Comp.	Color	Molecular weight	m.p. (°C)	$\Omega^{-1} \text{ cm}^2 \text{ mol}^{-1}$	C% (Theo.)	H% (Theo.)	N% (Theo.)	M% (Exp.)
[Fe (L) (L-Val) ₂]	brown	708.62	176180	11.1	55.86 (55.00)	6.68 (6.89)	13.82 (14.1)	7.87 (7.75)
[Co (L) (L-Val) ₂]	brown-red	712.71	234240	18.5	55.61 (55.99)	6.65 (7.10)	13.76 (12.16)	8.27 (7.38)
[Ni (L) (L-Val) ₂]	Pale Blue	712.47	126130	16.6	55.63 (55.99)	6.65 (6.99)	13.76 (14.02)	8.24 (8.94)
[Cu (L) (L-Val) ₂]	blue	2	215220	19.2	55.0 (55.70)	6.60 (6.66)	13.67 (13.00)	8.86 (8.06)
[Zn (L) (L-Val) ₂]	Yellow	719.16	180188	13.5	55.11 (55.00)	6.59 (6.89)	13.63 (14.54)	9.09 (9.89)
[Cd (L) (L-Val) ₂]	Off-White	766.19	190196	16.8	51.0 (51.76)	5.90 (6.50)	14.9 (14.19)	13.05 (13.97)
[Hg (L) (L-Val) ₂]	Yellow	854.37	201209	14.11	46.39	5.55 (-)	11.48 (-)	23.48 (-)

Note. Chemical Formula of (L) is C₃₃H₄₇MN₇O₇

Elemental analysis results indicated that all complexes were synthesized in a 1:1:2 (2Valinat:M:L) stoichiometry. Molar conductivity values (Ω) = 4.0-11.0 $\Omega^{-1} \text{ cm}^2 \text{ mol}^{-1}$; these results showed that all complexes are non-electrolytic in nature [22, 25]. To determine the metal ion percentage in the complexes, AAS analysis was performed using the direct method, yielding a percentage of metal ions. The calculated and measured metal percentages for each complex displayed reasonable consistency [22, 24]. The AgNO₃ solution tested negative for chloride ions (0%), indicating that no chloride ions were present outside the central metal coordination sphere. The FTIR spectra of the metal complexes are summarized in Table 4, and the detailed spectra are shown in Figure 5.

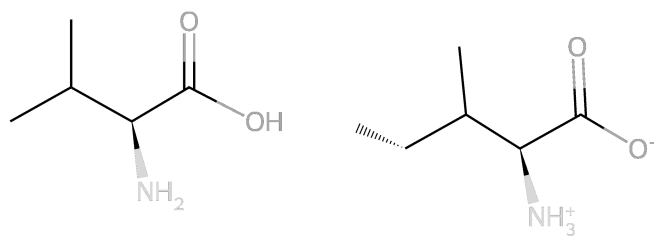
Ligand L features a total of eight potential donor sites: two nitrogen atoms in the pyrimidine ring, one amine group (NH₂) in the pyrimidine ring, one nitrogen atom in the azomethine (imine) group (-RC=N-), three methoxy groups (C-O-C), and one nitrogen atom in the benzene ring. The FT-IR spectrum of L-valine indicated.

The vibrational frequency of the methoxy C-O-C group remained unchanged in the ligand and complexes 1-7, suggesting that there was no coordination involving the C-O-C group [22-24]. The FT-IR spectrum of the free amino acid (L-valine) in the ν NH₃⁺ and ν COO⁻ regions shows the zwitterion form (Figure 9).

Table 4 Infrared spectral data (wave number ν' cm^{-1} of the prepared complexes

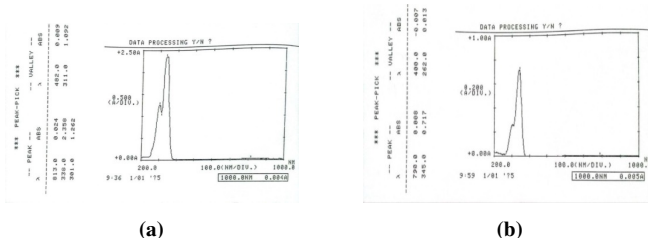
Complex	ν (M-O)	ν (M-N)	ν (C-N)	ν sym	(-COO) sym	(C=C) arom.	(C=N)	(C=O) a	(C-H) aliph	ν (-OCH ₃)	ν (CH ₃)	(NH ₂)
[Fe(L)(L-Val) ₂]	470 409	591 482	1236	231	1391	1503	1584	1532	2933, 2821	1123	3145 2933	,3442 2423
[Co(L)(L-Val) ₂]	470 426	625 424	1202	221	1317	1508	1587	1532	2933, 2872	1126	3155 2964	,5403 3317
[Ni(L)(L-Val) ₂]	507 424	651 535	1202	224	1360	1508	1677	1584	2958, 2870	1112	3168, 2957	3327, 3255
[Cu(L)(L-Val) ₂]	459 420	605 576	1236	204	1378	1504	1668	1582	2956, 2668	1196	3156	,3405 3287
[Zn(L)(L-Val) ₂]	510 469	591 539	1032	235	1330	1504	1565	1565	2956, 2870	1139	3151 3005	,3330 3258
[Cd(L)(L-Val) ₂]	474 424	591 540	1234	249	1328	1508	1654	1587	2934 2829	1120	3162	,3455 3331
[Hg(L)(L-Val) ₂]	510 431	583 550	1238	219	1332	1505	1624	1542	2035, 2822	1122	3222 2954	,3442 3345

A band at 3382 cm^{-1} corresponding to the stretching vibration of $\nu(\text{N-H}) + \nu(\text{O-H})$, another band at 1745 cm^{-1} asymmetrically assigned to $\nu(\text{COO})$, and symmetric $\nu(\text{COO})$ observed at 1300 cm^{-1} [17, 26]. The spectra of the complexes show that the $\nu(\text{N-H})$ band originally located between 3370 and 3300 cm^{-1} shifts to a lower frequency, indicating that the ligand (L-Val) may be coordinated through the nitrogen atom in the amine group [17–19]. The absorption of $\nu(\text{OCO})$ sym is in the range of 1422–1382 cm^{-1} and shifts to a higher position, while the absorption band of $\nu(\text{OCO})$ asym is observed between (1612–1532) cm^{-1} and is shifted by (210–130) cm^{-1} , indicating coordination of the carboxyl group to the central metal ion [17–20].

**Fig. 9** Zwitter ion of L-Valine

The bands around (650–450) cm^{-1} and (570–400) cm^{-1} confirm the presence of metal-nitrogen bonds (M–O) and metal-nitrogen bonds (M–N) [15, 16]. The carboxylic acid group (COO^-) is monodentate, as shown by the values of $\Delta\nu = [\nu(\text{COO}^-)] \text{ asym} - [\nu(\text{COO}^-)] \text{ sym}$, which lie between (201–294) cm^{-1} . Therefore, (L-Val) acts as a bidentate monobasic ligand via the primary nitrogen amine group (NH_2) and oxygen group (COO^-). These binding sites are the nitrogen atom (amine NH_2) and the oxygen atom (ν COO^- -carboxyl). L-valine acts as a mono-negative bidentate ligand by forming M–N and M–O bonds [20]. According to the magnetic moment values, as shown in Table 5, all prepared complexes are paramagnetic, except Zn, Cd, and Hg complexes, which are diamagnetic because these ions occupy the (d10) orbital.

The ultraviolet-visible (UV-Vis) spectrum for L-valinate L in DMSO solvent shows an absorption peak at 279 nm (36900 cm^{-1}) and a strong peak at 342 nm (3250 cm^{-1}), Figure 10. These peaks relate to ($\pi \rightarrow \pi$) and $n \rightarrow \pi$ transitions, respectively [20, 22, 24]. In the UV-Vis analysis of (L) in DMSO solvent, a significant absorption band appears at 346 nm (28901 cm^{-1}). This band is linked to the overlap of ($\pi \rightarrow \pi$)/($n \rightarrow \pi$) from the two peaks, as well as transitions involving the aromatic ring and the pyrimidine group [21, 22]. The UV-Vis spectrum for [Fe(L)(L-Val)₂] revealed four absorption bands: charge-transfer transitions are responsible for the two high-intensity peaks at (232 nm) (43103 cm^{-1}) and (345 nm) (28985) cm^{-1} , and the ($d \rightarrow d$) transitions are responsible for one absorption band at (994 nm) (10060 cm^{-1}), which is determined to be $4T_1g \rightarrow 4A_2g(f) v_3$ with a magnetic moment of 6.22 B.M. Based on these findings, an octahedral geometry around the Fe(II) ion can be proposed. Its magnetic moment μ_{eff} 2.83 BM.

**Fig. 10** UV-Vis spectra of (a) Cd(II) and (b) Ni(II) metal complexes

In the UV-Vis analysis of the [Co(L)(L-Val)₂] complex. The charge transfer transitions are responsible for the two high intensity peaks at (277 nm) (36101 cm^{-1}) and (346 nm) (28901 cm^{-1}) in the V-Vis spectrum, while the ($d \rightarrow d$) transitions at (553 nm) (18083 cm^{-1}) and (771 nm) (12970 cm^{-1}) are responsible for two absorption bands, which are regarded for $4T_1g \rightarrow T_1g(p) v_3$ and $T_1g \rightarrow 4A_2g(f) v_2$. [10, 26] respectively, which are allotted to the distorted octahedral geometry for the Co(II) ion [27–29]. The transition B, β , and Dq are calculated theoretical

limits; by using the data energy level diagram (Tanabe-Sugano):

$$\nu_2 = 18Dq, \nu_2 = 18Dq \therefore Dq = \frac{12970}{18} = 720 \text{ cm}^{-1},$$

$$\nu_3 = 6Dq + 15 B$$

$$18083 = 6 \times 720 + 15 B$$

$$18083 = 4320 + 15 B$$

$$15 B = 13703$$

$$B_{\text{complex}} = \frac{13703}{15} = 913.533$$

This reveals the Oh geometry for this complex and shows a 49% decrease in the Racah and Lees parameters, indicating an impressive nephelauxetic effect. The [Ni(L)(L-Val)₂] complex (UV-Vis) spectrum showed two bands at 345 nm caused by charge transfer and one at 790 nm caused by the [d-d] transition for 3A₂g→3T₂g (Figure 6b). These shifts indicate octahedral geometry in the vicinity of nickel(II) [30,31]. Its magnetic moment μ_{eff} 5.33 BM.

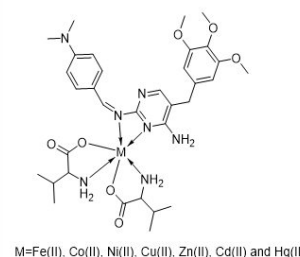
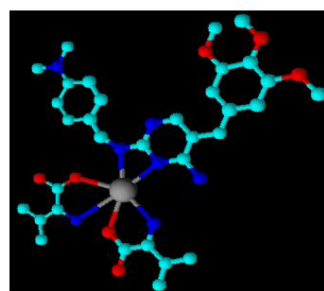
The spectrum of [Cu(L)(L-Val)₂] complex (Table 5) exhibited four bands at (272 nm) 36764 cm⁻¹, (339 nm) 29498 cm⁻¹, (598 nm) 16722 cm⁻¹, and (715 nm) 13986 cm⁻¹, respectively. The high-energy bands in the (29498–36764) cm⁻¹ range are owing to ligand field and ligand-to-metal charge-transfer (LMCT) transitions. Two bands were observed at 16722 and 13986 cm⁻¹ and were attributed to spin-allowed transitions 2B₁g→2B₂g (v₂) and 2B₁g→2E_g (v₃), respectively, for Jahn-Teller-distorted octahedral Cu(II) complexes [1,32]. Its magnetic moment μ_{eff} 1.74 BM. The UV-Vis spectra for the [Zn(II), Hg(II), and Cd(II)] (d₁₀) diamagnetic complexes (Figure 9a) revealed no peaks in the visible range [32]. The bands that appeared in the spectra of the three complexes could be attributed to charge-transfer transitions induced by the conjugated π system.

3.3 Proposed molecular structure for the studied complexes

Considering the complexes based on their examination, perceptions propose octahedral geometry for all synthesized complexes, which displayed a coordination number of six and may be defined as [(L-Val)M(II)(L)] and [(L-Val)M(III)(L)]Cl. The proposed structures are shown in Figure 11.

Table 5 (UV-Vis) Spectral data of the prepared complexes

Complex	nm λ	ν' cm ⁻¹	Assignment	eff. B.M.
[Fe(L)(L-Val) ₂]	2.83	Charge transfer	43103	232
		Charge transfer	28985	345
		5 T ₂ g → 5 A ₁ g	10060	994
[Co(L)(L-Val) ₂]	4.59	Ligand .Field	36101	277
		charge transfer	28901	346
		⁴ T ₁ g → ⁴ T ₁ g ^(p) v ₃	18083	553
		T ₁ g → ⁴ A ₂ g ^(f) v ₂	12970	771
[Ni(L)(L-Val) ₂]	5.33	charge transfer	28985	345
		³ A ₂ g(F) → ³ T ₁ g ^(p)	12658	790
[Cu(L)(L-Val) ₂]	1.74	Ligand field	36764	272
		LMCT	29498	339
		² B ₁ g → ² E _g (v ₃)	16722	598
		² B ₁ g → ² B ₂ g (v ₂)	13986	715
[Zn(L)(L-Val) ₂]	diam	charge transfer	33670	297
		charge transfer	28985	345
[Cd(L)(L-Val) ₂]	diam	charge transfer	33222	301
		charge transfer	29585	338
[Hg(L)(L-Val) ₂]	diam	charge transfer	34246	292
		charge transfer	29069	344



M=Fe(II), Co(II), Ni(II), Cu(II), Zn(II), Cd(II) and Hg(II)

Fig. 11 3D molecular modeling proposed of the complexes

3.4 Antimicrobial screening

The antimicrobial activity results shown in Figure 12 and Table 6 indicate that the Fe(II), Co(II), and Ni(II) complexes have low effectiveness against *Proteus mirabilis* when compared to negative and gram-positive cells. Overall, the metal complexes and the Schiff base ligand exhibited better performance than L-valine as a standalone ligand, likely due to increased lipophilicity and enhanced coordination [1,33]. This can be understood through the concept of Tweedy's chelation theory [5].

The fungicidal activity results exposed that the Tetra (anti) and [Co(L)(L-Val)₂] shows weak activity while Zinc(II), Cadmium(II), and mercury(II) complexes shows good activity may be effect d₁₀, and the toxicity of these complexes can be related to the strength of the metal-ligands bonds and system-donation formed during coordination π bond [33].

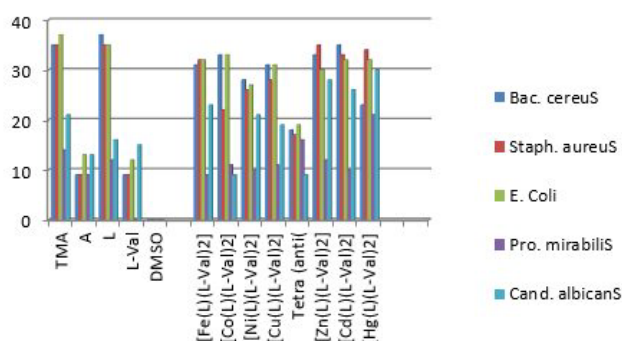


Fig. 12 Comparison of the sensitivity test of complexes against microbial strains

Table 6 Biological activity of the compounds inhibition (mm) against the tested organisms

Compound	Bacillus subtilis (G+)	Staphylococcus aureus (G+)	Escherichia Coli (G-)	Proteus mirabilis	Cand. albicans S
TMA	35		37	14	21
A	9	9	13	9	13
L	37	35	35	12	16
L-Val	9	9	12	0	15
DMSO	0	0	0	0	0
Tetra (anti)	18	17	19	16	9
Fe	31	32	32	9	23
Co	33	22	33	11	9
Ni	28	26	27	10	21
Cu	31	28	31	11	19
Tetra (anti)	18	17	19	16	9
Zn	33	35	30	12	28
Cd	35	33	32	10	26
Hg	23	34	32	21	30

4 CONCLUSION

In this study, we discussed how amino N,N dimethylbenzaldehyd reacts with trimethoprim to produce Schiff base (L). Complexes 1–7 were created by reacting metal chlorides with the Schiff base ligand and L-potassium valinate and were then characterized using spectroscopic, magnetic, and analytical techniques. Regarding the metal ions, Schiff and L-valinate exhibit bidentate behavior. The metal bonding through the N- and O-donor atoms of both ligands is visible in the IR spectra. Octahedral geometries were proposed for the complexes.

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N/A

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