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Synthesis, characterization, thermal, theoretical and antimicrobial studies of Schiff base ligand and its Co(II) and Cu(II) complexes

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Abstract: A Schiff base ligand **L** have been synthesized by condensation of 1,2-diaminoethane with creatinine. The reaction of the ligand with metal chloride salt gives Co(II) and Cu(II) complexes. The synthesized ligand and its metal complexes were characterized by elemental analysis, FT-IR, NMR, UV-Visible, conductivity and magnetic susceptibility measurements as well as thermal analyses. Based on spectral data a tetrahedral geometry have been proposed for Co(II) and Cu(II) complexes. The molar conductivity data shows that the complexes are non-electrolytic in nature. In DFT studies the geometry of the Schiff base ligand and its Co(II) and Cu(II) complexes were fully optimized using B3LYP functional together with 6-31g(d,p) and LANL2DZ basis sets. The ligand and its metal complexes were tested against four bacterial species and two fungal species. The results revealed that the metal complexes are more potent against the microbes than the parent ligand.

Keywords: Schiff base; Co(II), Cu(II); DFT; biological

INTRODUCTION

Transition metal complexes with organic ligands have been the premise of concentrated research due to their role as contrasting agents, radiopharmaceutical and chemotherapeutics in the treatment of metal toxicity¹. Schiff bases are interesting class of compounds in coordination chemistry² and are called as privileged ligands due to their facile synthetic approaches by condensing an aldehyde or ketone with amines. These ligands easily stabilize different metals in various oxidation states³. Schiff bases and their transition metal complexes show a wide range of applications in industrial⁴, pharmaceutical^{5,6} and chemical fields^{7,8}. They also exhibit biological activities such as antitumor, anti-bacterial, fungicidal, anticarcinogenic⁹⁻¹³ and antioxidant activities^{14,15}.

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A number of substituted imidazoles act as interesting drug targets in inflammation, neurodegenerative diseases and tumors of the nervous system^{16,17}. Synthetic imidazoles are present in many fungicides and antifungal, antiprotozoal and anti hypertensive medications. In view of the above findings we incorporated imidazole pharmacophore in the synthesis of Schiff base ligand. Herein we report the synthesis of a Schiff base ligand and its Co(II) and Cu(II) complexes. The prepared ligand was characterized by FT-IR, ¹H NMR, ¹³C NMR, UV-Vis, in addition to elemental analysis and the complexes were characterized by FT-IR, UV-Vis, elemental analysis, molar conductivity and magnetic susceptibility. The structure of the ligand and its metal complexes were optimized by DFT methods. The antimicrobial activity of the ligand and the complexes were tested against various microorganisms.

EXPERIMENTAL

Materials and methods

All the chemicals and the solvents were purchased from Sigma-Aldrich and Hi media Ltd and used without further purification. FT IR spectra were recorded in the range 4000 – 400 cm⁻¹ on Shimadzu IR affinity 1 spectrophotometer. Electronic spectra of the ligand and the complexes were recorded in the range 200 – 800 nm at room temperature in solid state using Shimadzu model UV-1601 spectrophotometer. Micro analysis (C, H and N) of the ligand and their complexes were carried out on an elementar vario EL III CHN analyser. Melting points of the compounds were determined in open capillaries in electrical melting point apparatus. NMR spectra of the ligand was recorded in DMSO-d₆ using Bruker Avance III 400 MHz FT-digital NMR spectrometer. The magnetic moments of the complexes were determined on a Guoy balance and the diamagnetic corrections of the complexes were calculated using Pascal's constants. Molar conductivities of the complexes were measured in DMSO solution with 10⁻³ concentration. Metal content were estimated with standard Ethylenediaminetetraacetic acid solution. Thermogravimetric analysis of the complexes was carried out from room temperature to 800°C using a Perkin Elemer STA 6000 thermal analyser.

Synthesis of ligand

A mixture of hot ethanolic solution of 1,2-diaminoethane (1 mmol) and creatinine (2-imino-1-methyl-imidazolidin-4-one) (2 mmol) was refluxed with stirring for 6h. The reaction mass was degassed on a rotary evaporator, over a water bath. The Schiff base obtained was filtered, washed with cold ethanol, dried and recrystallised from ethanol.

Yield: 82 %, m.pt: 215°C, Anal. Calcd (%) for C₁₀H₁₈N₈: C, 47.98; H, 7.25; N, 44.77; found (%): C, 47.76; H, 9.17; N, 44.62. IR (ν_{max} in cm⁻¹): 1690 (ν_{C=N}), 1560 (ν_{C=NH}), 3277 ring(ν_{NH}). ¹H – NMR (DMSO – d₆): δ 2.9 (s, 3H, methyl); δ 3.3, δ 3.6 (2s, 6H, methylene); δ 9.8 (s, 1H, NH); UV-Vis (DMSO) λ_{max} nm: 235, 350.

Synthesis of metal complexes

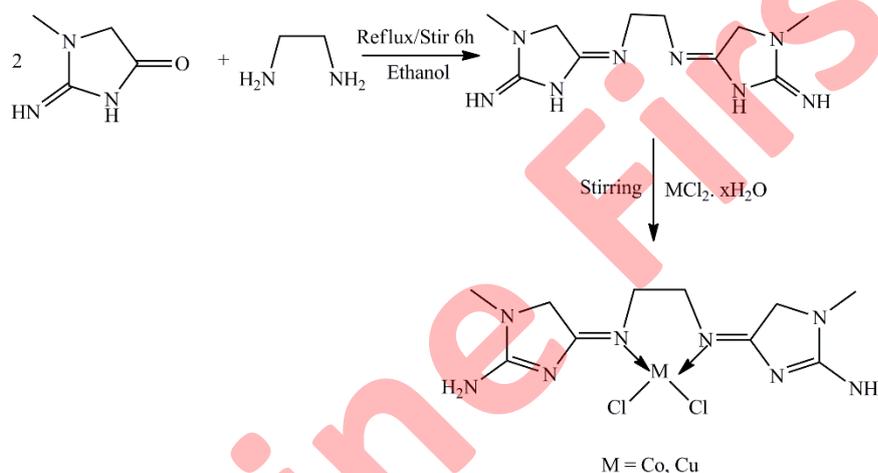
The methanolic solution of metal chlorides CoCl₂.6H₂O and CuCl₂.2H₂O (1 mmol) was added dropwise to a magnetically stirred solution of ligand (1 mmol) dissolved in 15 ml of methanol. The stirring was continued for 2h. The solid complexes separated out was filtered, washed with methanol and dried in vacuum. The synthetic procedure for Schiff base and their metal complexes are shown in (Scheme 1).

[Co(L)Cl₂]

Yield:77%, m.pt: >250°C , Anal. Calcd (%): C,31.60; H, 4.77; N, 29.48; Co, 15.5; found (%):C,31.47; H, 4.89; N, 29.35; Co, 15.28. IR (ν_{\max} in cm^{-1}): 1641 ($\nu_{\text{C=N}}$), 3347, 3186 (ν_{NH_2}), 418 ($\nu_{\text{M-N}}$), 369 ($\nu_{\text{M-Cl}}$).UV-Vis (DMSO) λ_{\max} nm: 620, 581. μ_{eff} (BM): 4.25.

[Cu(L)Cl₂]

Yield:76%, m.pt: >250°C , Anal. Calcd (%): C,31.22; H, 4.71; N, 29.12; Cu, 16.52; found (%):C,31.09; H, 4.59; N, 29.25; Cu, 16.38. IR (ν_{\max} in cm^{-1}): 1628 ($\nu_{\text{C=N}}$), 3362, 3156 (ν_{NH_2}), 434 ($\nu_{\text{M-N}}$), 371 ($\nu_{\text{M-Cl}}$). UV-Vis (DMSO) λ_{\max} nm: 850-950. μ_{eff} (BM): 1.93.



Scheme 1. Synthesis of Schiff base ligand and their metal

DFT studies

Theoretical calculations of the ligand and complexes were conducted using Density Function Theory (DFT)^{18,19} using B3LYP functional together with 6-31G(d,p) and LANL2DZ basis sets^{20,21}. Geometry optimization, molecular energy, dipole moments, the Natural Bond Orbital (NBO), NLO properties, Molecular electrostatic potential calculations was calculated at the same level with 6-31G (d,p) basis setas incorporated in Gaussian 09 program^{22,23}.

Antimicrobial activity

The newly synthesized Schiff base ligand and its metal complexes were screened for their antimicrobial activities by well dilution method²⁴. The *in vitro* antibacterial activity of the test compounds was tested against two Gram positive bacterial strains *Staphylococcus aureus* and *Bacillus subtilis* and two Gram negative bacterial strains *Escherichia coli* and *Pseudomonas aeruginosa*. The *in vitro* antifungal activities were carried out against two fungal strains *Aspergillus niger* and *Candida albicans*.

RESULTS AND DISCUSSION

The newly synthesized Schiff base ligand and its metal complexes are colored solids and stable at room temperature. The complexes possess high melting point (> 250°C).The Schiff base ligand is soluble in common organic solvents like

methanol, ethanol etc., whereas the complexes are soluble in DMF and DMSO. The elemental analysis and analytical data suggest that the metal to ligand ratio of the complexes is 1:1 stoichiometry of the type $[ML(Cl)_2]$.

FT IR spectroscopy

The prominent mode of bonding in Schiff base ligand **L** and their complexes has been investigated by the comparative study of the FT-IR spectral data (Table S1). The IR spectrum of the Schiff base ligand **L** (Fig. S1) shows a strong band at 1690 cm^{-1} which was assigned to azomethine $\nu(>C=N)$ group. The FT-IR spectra of the complexes **1** and **2** showed bands around 1641 and 1628 cm^{-1} exhibiting a downward shift, which is in accordance with the coordination of azomethine nitrogen to the metal ions²⁵. This is further confirmed by the appearance of bands around 418 and 434 cm^{-1} corresponding to $\nu(M-N)$ stretching vibration²⁶. The ligand exhibits medium intensity bands around 1560 and 3277 cm^{-1} corresponding to $\nu(C=NH)$ and ring $>NH$ groups. The metal complexes showed bands around 3347 , 3186 cm^{-1} and 3362 , 3156 cm^{-1} corresponding to NH_2 group. The disappearance of bands corresponding to $\nu(C=NH)$ and ring $>NH$ vibrations and appearance of bands corresponding to NH_2 vibrations in the metal complexes indicates the existence of amino-imino tautomerism. The appearance of bands around 369 and 371 cm^{-1} can be attributed to $\nu(M-Cl)$ stretching of the complexes⁹.

Molar conductance

The molar conductance of the newly synthesized complexes was measured at room temperature. The Co(II) and Cu(II) complexes have molar conductivity values of 15 and $22\ \Omega^{-1}\text{cm}^2\text{mol}^{-1}$ respectively. These data suggest that the complexes are non electrolytic in nature²⁷.

¹H NMR spectrum

The ¹H NMR spectrum of the Schiff base ligand **L** (Fig. S3) shows signals at $\delta 3.3$ ppm and $\delta 3.6$ ppm corresponding to CH_2 protons of five membered ring and ethane. The signal at $\delta 2.9$ ppm was assigned to CH_3 protons. The singlet at $\delta 9.8$ ppm corresponds to NH proton of the creatinine moiety.

¹³C NMR spectrum

The signal corresponding to imine carbon atom ($C = N$) of the ligand **L** is observed at $\delta 172.01$ ppm. The signals corresponding to methyl carbon of the heterocyclic ring is observed at $\delta 39.99$ ppm and the CH_2 carbon of the heterocyclic ring at $\delta 56.66$ ppm. The signal observed at $\delta 185.27$ ppm correspond to $(C = NH)$ carbon. The signal at $\delta 31.17$ ppm correspond to CH_2 carbon of ethane. The ¹³C NMR spectrum of the ligand **L** is shown in (Fig S4).

UV-Vis spectra and magnetic moment

The electronic spectral data and the magnetic moments reveal the information regarding the geometry of the metal complexes. The UV-Vis spectra of the ligand

and the metal complexes (Fig. S2a) were recorded in solid state at room temperature and the data are shown in Table S2. The electronic spectra of the ligand exhibited two characteristic bands at 235 and 350 nm corresponding to $\pi \rightarrow \pi^*$ and $n \rightarrow \pi^*$ transitions respectively²⁸. The Co(II) complex **1** showed two bands at 620 and 581 nm which may be assigned to ${}^4T_1(F) \leftarrow {}^4A_2$ and ${}^4T_1(P) \leftarrow {}^4A_2$ transitions indicating tetrahedral geometry^{29,30}. The magnetic moment value 4.25 BM also confirms the tetrahedral geometry³⁰ of Co(II) complex **1**. The Cu(II) complex **2** showed a broad band around 850-950 nm corresponding to d-d transition indicating the tetrahedral geometry^{32,33}. The magnetic moment value of 1.93 BM also supports the tetrahedral geometry³⁴ of Cu(II) complex **2**.

Thermogravimetric analysis

The thermogravimetric and differential thermal analysis of Co(II) and Cu(II) complexes were carried out from room temperature to 800 °C to study the thermal stability of the complexes. The stepwise thermal degradation of the complexes is depicted in Table 1.

The thermogram of Co(II) complex **1** (Fig. S5) shows three decomposition steps. The first two decomposition steps within the temperature range 200 - 485 °C corresponds to loss of chlorine atoms and organic moiety of the ligand with mass loss 32.49% (calcd.33.38%). The last decomposition within the temperature range 485 - 760 °C corresponds to loss of creatinine moiety with weight loss of 46.33 (calcd. 51.02) leaving behind CoO as the product of decomposition.

The thermogram of Cu(II) complex **2** (Fig. S6) represents decomposition in two steps. The decomposition step within the range 160 - 300 °C corresponds to loss of chlorine atoms with the mass loss of 17.54% (calcd. 18.43%). The second decomposition step within the range 300 - 658 °C with an estimated mass loss of 58.26% (calcd.65.75%) may be attributed to loss of organic moieties of the ligand leaving behind CuO as the product of decomposition.

Table 1. Thermogravimetric data of the complexes

Complexes	Decomposition temperature, °C	Weight loss, %		Content of metal oxide, %		Inference
		Obsd.	Calcd.	Obsd.	alcd.	
[Co(L)Cl ₂] (1)	262	32.49	33.4	-	-	Loss due to Cl ₂ + C ₂ H ₄ N ₂
	357	46.33	48.02	-	-	Loss due to C ₈ N ₆ H ₁₄
	717			21.18	19.71	Loss due to remaining organic moiety.
[Cu(L)Cl ₂] (2)	299	17.54	18.43	-	-	Loss of Cl ₂
	605	58.26	59.75	-	-	Loss due to C ₁₀ N ₈ H ₁₈
				21.2	20.67	Loss due to remaining organic moiety.

Computational studies

Geometry optimization and electronic structure

The ground state geometry optimization for the ligand **L** and its Co(II) and Cu(II) complexes were performed in gas phase using B3LYP functional together with LANL2DZ and 6-31G(d,p) basis sets as incorporated in the Gaussian 09W programme. The optimized geometry of the ligand and its Co(II) and Cu(II) complexes are shown in Fig. 1. The C₆–N₄, C₃–N₃ bond lengths of Schiff base ligand **L**, Co(II) complex **1** and Cu(II) complex **2** was found to be 1.273, 1.274 Å and 1.303, 1.303 Å and 1.304, 1.304 Å respectively. The slight increase in bond length of the complexes confirms the coordination of ligand to the metal ion through azomethine nitrogen. The slight elongation of C₂–N₈ and C₈–N₇ bonds of the complexes from 1.278 Å to 1.359 Å corresponds to the change of double to single bond in both the complexes. A decrease in bond length was observed for C₂–N₂ and C₈–N₆ bonds from 1.403 Å to 1.341 Å in the complex compared with ligand confirms the amino-imino tautomerism of the creatinine moiety. The ligand shows absorption band around 235 nm corresponding to $\pi \rightarrow \pi^*$ transition. This assignment was supported by TDDFT calculations. The Co(II) complex shows two bands around 620 and 581 nm corresponding to ${}^4T_1(F) \leftarrow {}^4A_2$ and ${}^4T_1(P) \leftarrow {}^4A_2$ transitions. The TDDFT calculations also show two bands for 830 and 596 nm supporting the experimental data. The Cu(II) complex shows a broad d-d transition around 850-950 nm. The TDDFT calculations also show a band around 996 nm supporting the experimental data (Fig. S2b).

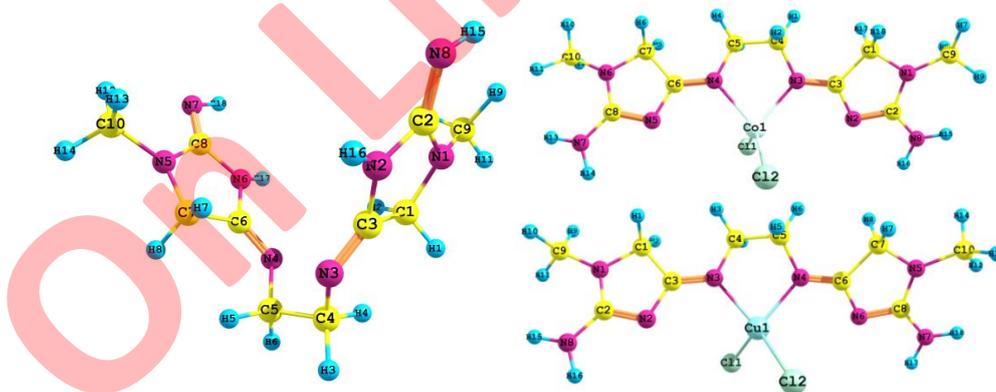


Fig. 1 Optimized geometry of the ligand **L**, Co(II) and Cu(II) complex

Frontier molecular orbitals

The frontier molecular orbitals (HOMO and LUMO) contribute to the stability or reactivity of the compounds. The activity, stability and excitability of the compounds can be studied with the energy difference of HOMO and LUMO³⁵.

Higher the energy difference greater is the stability of the compounds. The HOMO of the ligand is located on one of the imidazoline moiety whereas the LUMO is located on the two azomethine groups and imidazoline moieties. The HOMO and LUMO energy difference of the ligand **L** was found to be 6.1775eV indicating good stability of the ligand. The Koopmans theorem³⁶ was used to calculate various chemical reactivity parameters and is tabulated in Table S3.

Molecular electrostatic potential

The molecular electrostatic potential can be used for describing the structural properties of the molecule such as chemical reactivity and dipole moment. The MEP map of the ligand **L** was calculated by the same level of theory and shown in Fig. 2. The negative regions shown by red colour were located on the azomethine nitrogen atoms. The electron deficient regions (positive region) indicated by blue colour were located on the hydrogen atoms. According to the figure nitrogen atoms are electrophilic sites while hydrogen atoms have positive charge. Hence the azomethine nitrogen atom can coordinate to the metal atoms in complex formation.

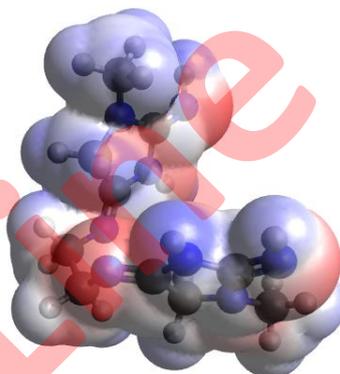


Fig. 2 Molecular electrostatic potential of the Schiff base ligand **L**

Nonlinear optical properties

The dipole moment, linear polarizability and first-order hyperpolarizability of the ligand was calculated at B3LYP functional with 6-31G(d,p) basis set using Gaussian 09W program. The polarizability and hyperpolarizability tensors are obtained by job output file of Gaussian. The mean polarizability (α_{tot}), anisotropy of polarizability ($\Delta\alpha$) and average of the first order hyperpolarizability (β_{tot}) were calculated. The calculated values are listed in Table S4. The values of α_{tot} and β_{tot} for the ligand are -107.78 a.u and 7.17026×10^{-31} esu which is greater than urea (α_{tot} and β_{tot} of urea are -21.5925a.u and 1.3729×10^{-31} esu calculated at the same level). The β_{tot} value of the ligand is 5 times larger than that of urea. These results reveal that the Schiff base ligand can be a candidate of NLO material.

Biological studies

The synthesized Schiff base ligand **L** and their Co(II) and Cu(II) complexes **1** and **2** were screened for their antimicrobial activity against two Gram positive bacteria, *Staphylococcus aureus* and *Bacillus subtilis*, two Gram negative bacteria, *Escherichia coli* and *Pseudomonas aeruginosa*, two fungi, *Aspergillus niger* and *Candida albicans*. The diameter of the zone of inhibition (mm) was used to compare the antimicrobial activity with the standards Ciprofloxacin and Clotrimazole and is presented in Table S5 and Figs.S7 and S8.

The results revealed that the metal complexes exhibit enhanced activity against all the microbes compared to the ligand. The metal complex **1** showed sound activity against *E. coli* and *P.aeruginosa* with zone diameter 33 mm and 37 mm, respectively which is close to that of the standards, whereas complex **2** showed better activity with zone diameter 25 mm and 17 mm against the same microbes. The metal complexes **1** and **2** exhibited potential inhibition with zone diameter of 26 mm, 28 mm and 27 mm, 9 mm respectively against *C.albicans* and *A.niger* higher than the standards. The metal complexes **1** and **2** showed influential zone of inhibition against *S. aureus* and *B. subtilis* with zone diameter 29 mm, 29mm and 20 mm, 18mm respectively.

The MIC's of Co(II) complex **1** against *B.subtilis*, *E.coli* and *C.albicans* are given in Table 2. It is clear from the data that the complex **1** (MIC 31.25 µg/ml) exhibits good activity against *C.albicans* compared to (MIC 125 µg/ml) against *B.subtilis* and *E.coli*. From these data it can be concluded that the metal complexes exhibit good activity against the microorganisms than the ligand.

Table 2. Minimum inhibitory concentration (MIC) of [Co LCl₂] (1)

S. No	Organism	MIC, µg/ml						
		1000	500	250	125	62.5	31.25	15.625
1.	<i>B.subtilis</i>	-	-	-	-	+	+	+
2.	<i>E.coli</i>	-	-	-	-	+	+	+
3.	<i>C.albicans</i>	-	-	-	-	-	-	+

The enhanced activity of the metal complexes can be explained on the basis of Tweedy's chelation theory³⁷. The chelation reduces the polarity of metal ions due to partial sharing of its positive charge with hetero atoms of the ligand. The reduction in polarity enhances the lipophilic nature of the chelates forming an interface between the lipid and metal ion which subsequently breakdown the permeability barrier of the cell. This leads to blockage of metal binding sites in the enzymes of the microorganisms. The metal chelators perturb the respiration of the cell and reduce the synthesis of proteins which inhibits the growth of microorganisms. Apart from chelation various other factors such as size, solubility, dipole moment, concentration and hydrophobicity have substantial influence on the antimicrobial

activity. Thus the results reveal that enhanced antimicrobial of the metal complexes may not only due to chelation but also due various other factors as well³⁸⁻⁴¹.

CONCLUSIONS

A novel Schiff base ligand and its Co(II) and Cu(II) complexes were synthesized and characterized by various spectroscopic and analytical techniques. These data suggested a tetrahedral geometry for Co(II) and Cu(II) complexes with 1:1 (metal:ligand) stoichiometry. The thermal stability of the complexes was studied by TGA/DTA analysis. The structures of the ligand and its metal complexes were optimized by DFT methods. In addition in-vitro antimicrobial activities of the ligand and the metal complexes were carried out which revealed that the metal complexes were more potent against the microorganisms.

Acknowledgements: It is a pleasure to dedicate this article to Prof. em. Miljenko Perić (University of Belgrade) on the occasion of his 70th birthday. C.M.M. would like to thank him for his longstanding friendship and fruitful scientific collaborations.

ИЗВОД

СИНТЕЗА, КАРАКТЕРИЗАЦИЈА, ТЕРМАЛНА И АНТИМИКРОБНА ИСПИТИВАЊА КОМПЛЕКСА КОБАЛТА(II) И БАКРА(II) СА ШИФОВОМ БАЗОМ КАО ЛИГАНДОМ

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Кондензационом реакцијом између 1,2-диаминоетана и креатинина синтетисан је лиганд (L) типа Шифове базе. Полазећи од CuCl₂ и CoCl₂ и лиганда (L) синтетисани су одговарајући комплекси ових јона метала. Синтетисани комплекси су окарактерисани на основу резултата елементалне микроанализе, FT-IR, NMR и UV-Vis спектроскопије, термалне анализе и магнетних мерења. На основу спектроскопских мерења закључено је да комплекси Co(II) и Cu(II) имају тетраедарску геометрију. Резултати кондуктометријских испитивања су показали да су синтетисани комплекси неелектролити. Оптимизација геометрије лиганда и одговарајућих комплекса извршена је DFT методом применом B3LYP функционала, као и 6-31g(d,p) и LANL2DZ базних сетова. Антимикробна својства лиганда и комплекса Co(II) и Cu(II) испитивана су на различитим сојевима бактерија и гљива. Резултати ових испитивања су показали да су наведени комплекси значајно активнији у односу на одговарајући лиганд.

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On Line First

SUPPLEMENTARY MATERIAL TO
**Synthesis, characterization, thermal, theoretical and
 antimicrobial studies of Schiff base ligand and its
 Co(II) and Cu(II) complexes**

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Table S1. IR stretching frequencies of the ligand and their metal complexes

Compound	ν / cm^{-1}					
	C=N	C=NH	Ring NH	NH ₂	M-N	M-Cl
C ₁₀ H ₁₈ N ₈ L	1690	1560	3277	-	-	-
[Co(L)Cl ₂] (1)	1641	-	-	3347, 3186	418	369
[Cu(L)Cl ₂] (2)	1628	-	-	3362, 3156	434	371

Table S2. Electronic spectral data and magnetic moment values

Compounds	$\lambda_{\text{max}} / \text{nm}$	Band assignments	μ_{eff} BM
C ₁₀ H ₁₈ N ₈ L	235, 350	$\pi \rightarrow \pi^* \pi^*$	-
[Co(L)Cl ₂] (1)	620, 581	${}^4A_2 \rightarrow {}^4T_1$ (F); $A_2 \rightarrow {}^4T_1$ (P)	4.25
[Cu(L)Cl ₂] (2)	850-950	d-d envelope	1.93

Table S3. Chemical reactivity parameters of the ligand L

E_{total} (Hartree)	-829.9286
$\Delta E_{\text{HOMO-LUMO}}$ / eV	6.17757
Ionisation potential, eV	5.88260
Electron affinity, eV	-0.29497
Chemical hardness, eV	3.08878
Electronegativity, eV	2.7938
Chemical potential, eV	-2.7938
Global softness, eV ⁻¹	0.16187
Electrophilicity index, eV	1.26349
Dipole moment, Debye	3.3672

Table S4. The polarizability (α), the first – order hyperpolarizability (β_{tot}) and their components for the ligand and urea.

	$\langle\alpha\rangle$ (a.u)	$\Delta\alpha$ / a. u.	β_{tot} / a. u.	β_{tot} / esu	$\beta_{tot} / \beta_{tot(urea)}$
Ligand	-107.78	31.36	82.99	7.17026×10^{-31}	5.223
Urea	-21.5925	8.375	15.892	1.3729×10^{-31}	1

Table S5. The zone of inhibition of ligands and their metal complexes

Compounds	Zone of inhibition, mm					
	Bacterial species Std (Ciprofloxacin)				Fungal species Std (Clotrimazole)	
	Gram + ve		Gram - ve		<i>C.albicans</i>	<i>A. niger</i>
	<i>S. aureus</i>	<i>B. subtilus</i>	<i>E. coli</i>	<i>P. aeruginosa</i>		
L	11	13	10	12	20	10
[Co LCl ₂]	29	29	33	37	26	28
[CuLCl ₂]	20	18	25	17	27	09
Standard	38	34	36	40	16	11

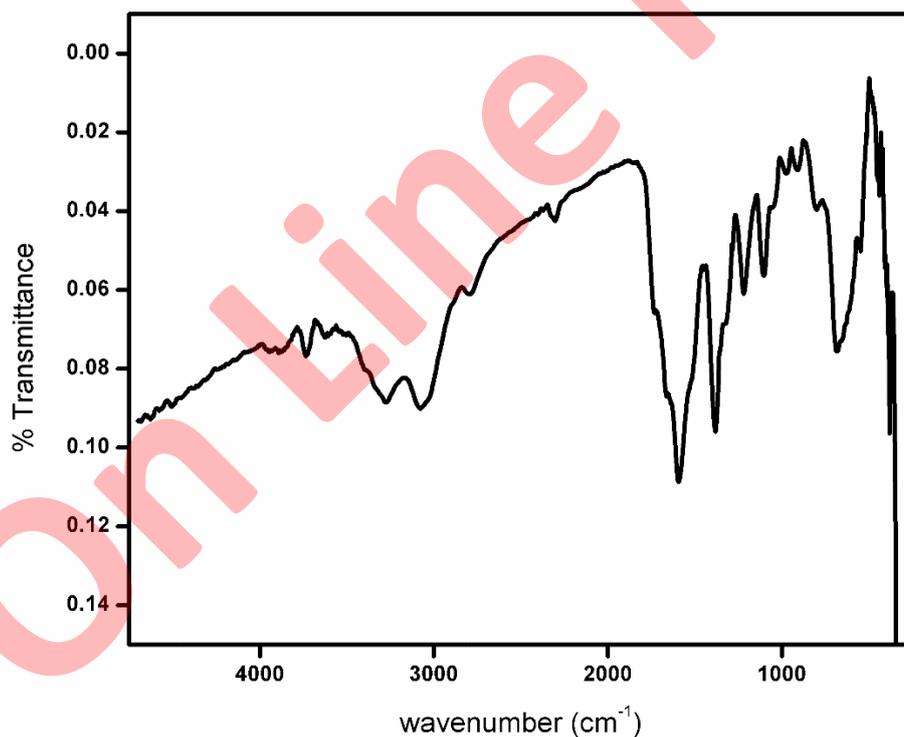


Fig. S1. FT IR spectrum of Schiff base ligand L

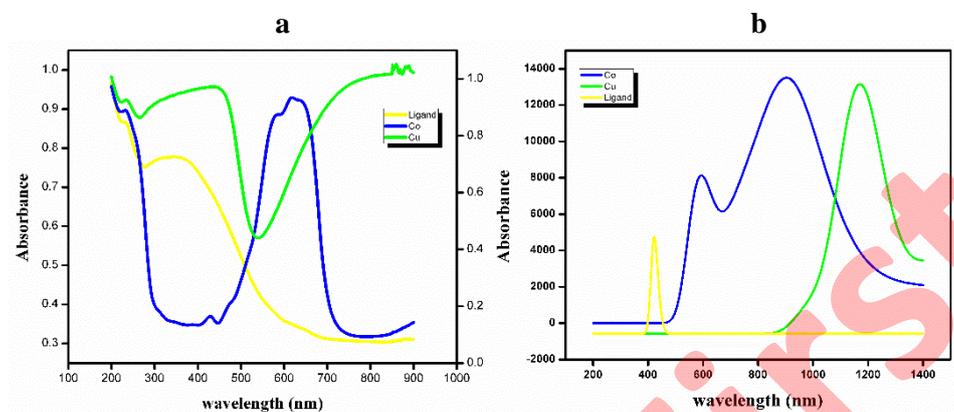


Fig. S2. Electronic spectrum of Schiff base ligand L and its Co(II) and Cu(II) complexes: a – experimental; b - calculated

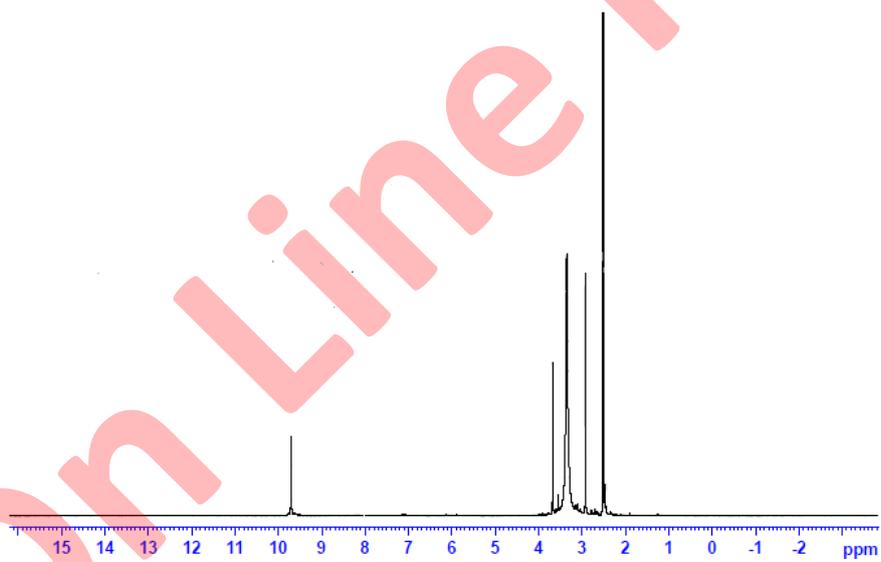


Fig. S3. ^1H NMR spectrum of Schiff base ligand L

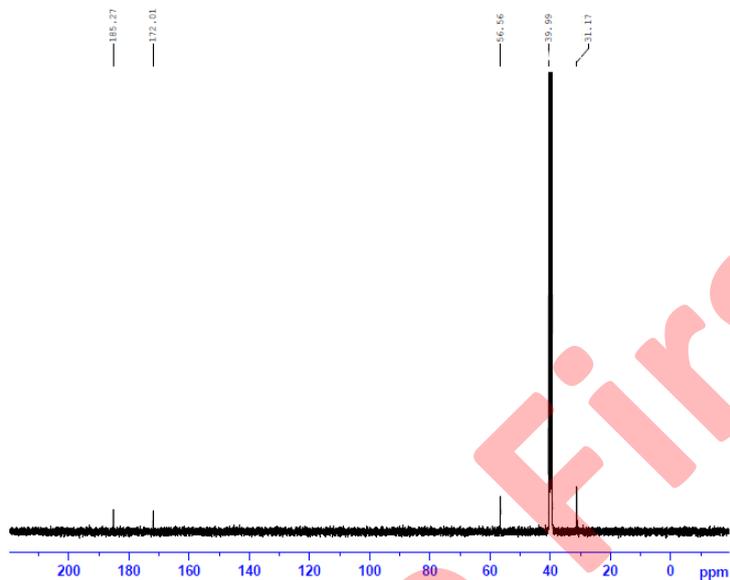
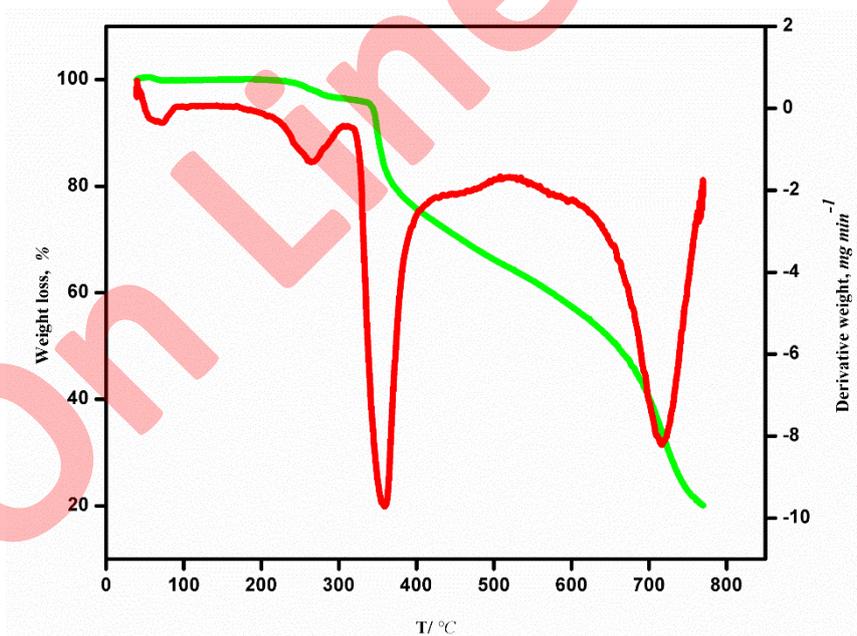
Fig. S4 ^{13}C NMR spectrum of Schiff base ligand L

Fig. S5. Thermogram of Co(II) complex 1

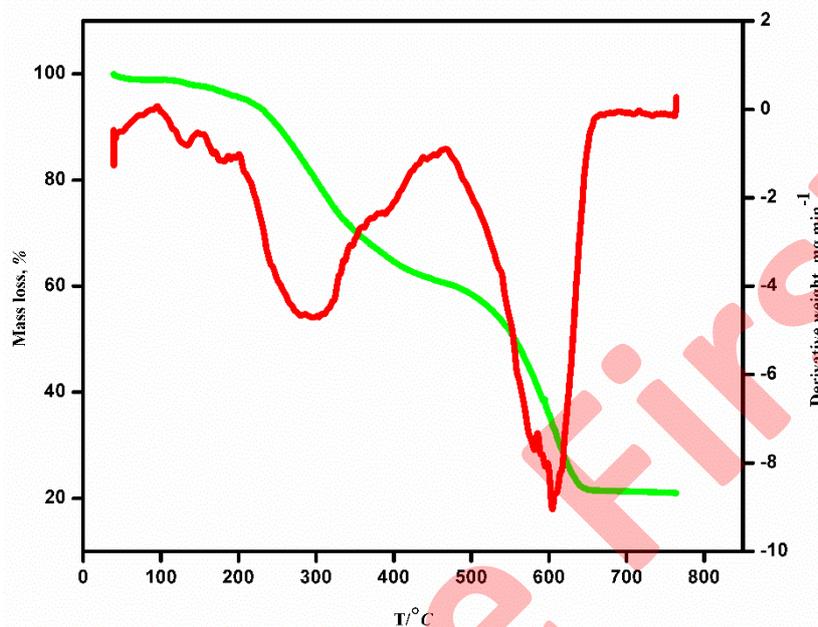


Fig. S6. Thermogram of Cu(II) complex

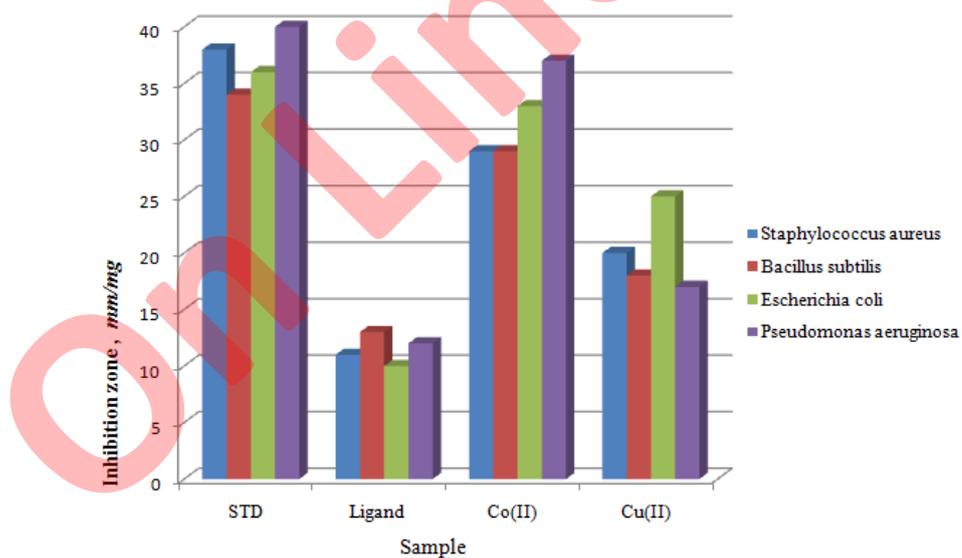


Fig. S7. Antibacterial activity of the Schiff base ligand and their metal complexes

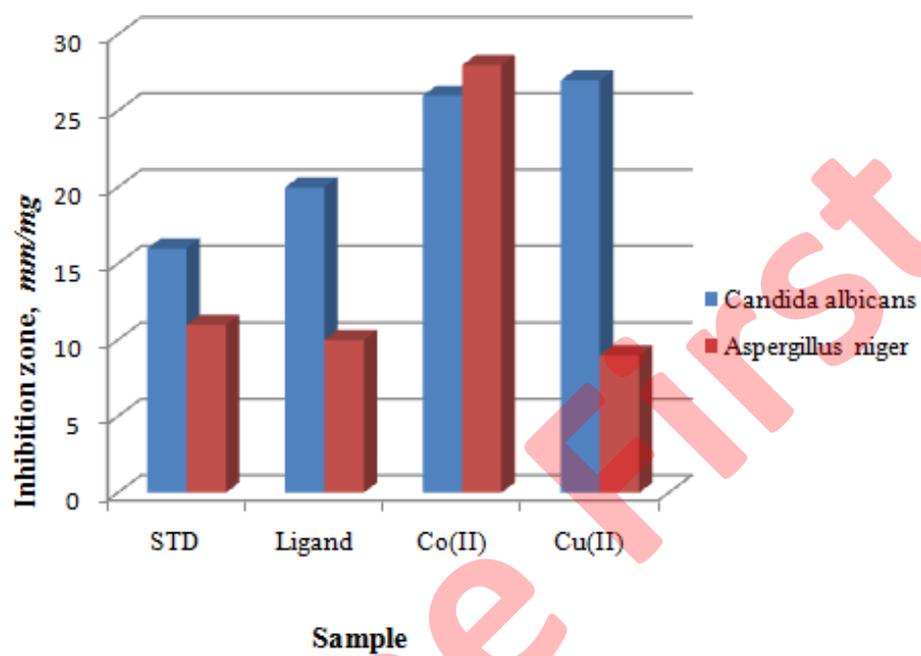


Fig. S8. Antifungal activity of the Schiff base ligand and their metal complexes