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Preparation and Characterization of Novel Mixed-Ligand Compounds of Mn(II), Fe(II), Co(II), Cu(II), and Zn(II) Derived from Schiff Bases and Nitrogenous Bases with Biological Activity Evaluation

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تحضير وتشخيص معقدات جديدة مختلطة الليكند من المنغنيز(II)، الحديد(II)، الكوبلت(II)، النحاس(II) والخارصين(II) مشتقة من قواعد شف وقواعد نيتروجينية مع تقييم الفعالية البيولوجية

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الملخص:

تم تحضير ليكند قاعدة شف (**ScB**) عن طريق تفاعل تكثيف (2-هيدروكسي بنزالدهيد) مع (**O**-توليدين). وتم تحضير معقدات التناسق لقواعد شف والقواعد النيتروجينية عن طريق تفاعل قاعدة شف والقواعد النيتروجينية مع كلوريدات الفلزات (**II**)، نتج عن التفاعل خمس معقدات مخلبية جديدة مع أيونات المنغنيز والحديد والكوبلت والنحاس والزنك باستخدام الإيثانول كمذيب. تم تشخيص الليكند المُحضر ومعقداته باستخدام طرق كيميائية وفيزيائية مختلفة، تضمنت تحديد درجة الانصهار، والتحليل الدقيق للعناصر (**C.H.N**)، طيف الامتصاص الذري، والتحليل الحراري الوزني (**TGA**)، والرنين المغناطيسي النووي للبروتون (**H-NMR**، **^{13}C-NMR**)، طيف الكتلة، طيف الأشعة فوق البنفسجية والمرئية (**UV-Vis**)، طيف الأشعة تحت الحمراء (**FT-IR**)، وقياس الحساسية المغناطيسية، والتوصيل الكهربائي المولي. وقد أثبتت الدراسة أن المعقدات (1-5) الناتجة غير موصلة والمعقدات (6-15) موصلة بنسبة 1:2. أشارت النتائج إلى هندسة ثمانية السطوح للمعقدات. بالإضافة إلى ذلك، تم قياس النشاط البيولوجي لليكند المُحضر ومعقداته ضد نوعين من البكتيريا، وهما الإشريكية القولونية (***E.coli***) سالبة الغرام، والمكورات العنقودية الذهبية (***Staphylococcus aureus***) موجبة الغرام. تم اختيار هاتين البكتيريتين لأهميتهما في المجال الطبي، وأكدت النتائج أن معظم المعقدات المُحضرة تتمتع بنشاط تثبيطي عالٍ ضد البكتيريا المستخدمة.

الكلمات الدالة: الفعالية البيولوجي، معقدات العناصر الانتقالية، ليكند قواعدة شف، المكورات العنقودية الذهبية، الزائفة الزنجارية.

Abstract

This Schiff base ligand (ScB) was synthesized by the condensation reaction of (2-hydroxybenzaldehyde) with (O-tolidine). Coordination complexes of Schiff bases and Nitrogenous bases were prepared by reacting the Schiff base and Nitrogenous bases with metal(II) chlorides, yielding five new chelating complexes with manganese, iron, cobalt, copper, and zinc ions using ethanol as the solvent. The prepared ligand and its complexes were characterized by various chemical and physical methods, including melting point determination, elemental analysis (C.H.N), atomic absorption spectroscopy, thermogravimetric analysis (TGA), proton nuclear magnetic resonance (H-NMR,^{13}C-NMR), mass spectrometry, UV-visible spectroscopy (UV-Vis), infrared spectroscopy (FT-IR), measuring magnetic sensitivity, and molar electrical conductivity, where the study proved that (1-5) the resulting complexes are non-conductive and (6-15) complexes are conductive in ratio 1:2. The results suggested an octahedral geometry for the complexes. In addition, the biological activity of the prepared ligand and its complexes were measured against two types of bacteria, namely (*E.coli*) negative gram and (*Staphylococcus aureus*) positive gram. These bacteria were chosen due to their importance in the medical field, and the results confirmed that most of the prepared compounds have high inhibitory activity against the bacteria used.

Keywords: Global climate change. Climate change indicators. Climate change induced stress in olive trees.

Introduction

SChiff bases are widely distributed organic compounds containing the azomethine group (CH=N-). They were first prepared by the German scientist Hugo Schiff in 1864 by condensing aliphatic or aromatic aldehydes or ketones with aliphatic or aromatic primary amines(Al-khyaat, 2020). Alphatic Schiff bases are less stable and follow a pathway leading to polymerization(Pinheiro Pires et al., 2019). while aromatic Schiff bases are more stable due to the presence of resonant pairs of electrons on the nitrogen atom and double bonds in the aromatic ring. Schiff bases have the general formula (R1R2C=NR3), and their names depend on the nature of the groups (R1, R2, R3). They can also be named after the aldehyde, ketone, or amine (Mene & Kale, 2016). Schiff bases are important in coordination chemistry because they can form stable and diverse coordination complexes with different shapes and properties, especially with various transition metal ions, with which they can coordinate via nitrogen and oxygen atoms(Derafa et al., 2024; Raj et al., 2023) Schiff bases and their complexes are of great importance in the medical and biological fields, as the type of metal ion and the type of Schiff base have a significant impact on biological activity. Coordination complexes of Schiff bases also give drugs greater efficacy compared to other organic compounds due to the presence of the highly biologically active azomethine group. Schiff bases facilitate better bond formation in coordination complexes, as the azomethine group contains an electron-poor carbon atom and an electron-rich nitrogen atom, which enhances the possibility of electrophilic and nucleophilic reactions at the relevant sites(Timofeeva et al., 2019; Tyagi et al., 2023) The topic of coordination complexes derived from Schiff bases has attracted the attention of researchers due to their biological activity, and the main objective has been. This involves the discovery of direct therapeutic agents for treating various bacterial diseases. Over the past few years, from 2015 to the present, coordination complexes derived from Schiff bases have gained significant importance due to their biological properties(Soroceanu & Bargan, 2022) Coordination complexes of Schiff bases exhibit far superior antibacterial activity compared to their free ligands(Reena et al., 2023; Tsacheva et al., 2023) Furthermore, Schiff bases act as antifungal, antitumor, antioxidant, and antiviral agents in biological applications(Chohan et al., 2010; Jayaseelan et al., 2016) Many aspects of Schiff bases, including the most applicable complexes by Abu-Dief et al.(Mohamed & Abu-Dief, 2015) have been discussed. A detailed analysis of the anticancer properties of quinoline derivatives has also been presented. This information is valuable for chemists, aiding in the development of effective anticancer drugs It has been shown that quinoline hydrazone derivatives can serve as a starting point for the production of anti-tuberculosis and anticancer drugs(Nainwal et al., 2019). In addition, to other applications. Schiff bases have been used in analytical chemistry because of their ability to form colored complexes with many metal ions, which facilitates the estimation of these ions using sensitive selective methods. They are used in qualitative analytical chemistry.(Abd El-Razek et al., 2020) and also in the field of industrial chemistry, where they are used as polymer inhibitors, plasticizers, antioxidants, and polymerization initiators. They are also used in the production of dyes, printing inks, and pigments used in aircraft paints, which help them not to be detected by radar(Wahba et al., 2017). The ligand and its compounds were characterized using various physical and chemical methods. Based on the results, hexagonal mononuclear compounds. Finally, the biological activity of the ligand and its compounds was evaluated, demonstrating excellent antibacterial activity against selected bacterial strains.(Okpechi et al., 2024)

2- EXPERIMENTAL PART

2.1- Materials and Equipment

All materials used were supplied by (Merak, BDH, Fluka) known for their high purity. Including (2-hydroxybenzaldehyde and O-Tolidine) The solvents used were absolute ethanol, diethyl Ether, and distilled water, and the mineral salts were $MnCl_2.4H_2O$, $FeCl_2.4H_2O$, $CoCl_2.6H_2O$, $CuCl_2.2H_2O$, and $ZnCl_2$.

The following instruments were used for the analytical, spectroscopic, and physical measurements of the prepared ligand and its complexes: Thin-layer chromatography (TLC) was performed on the ligand and complexes using the solvent (Et_2O:n-Hexane) (2:1). The completion of the reaction and the formation of the product were confirmed. The melting points of the prepared ligand and complexes were measured at the University of Mosul, College of Education for Pure Sciences, using an Aparatues-Stuart-SMP instrument. The molar conductivity of the prepared complexes was measured using an Eutech PC700 Instrument, and the magnetization of the prepared complexes was measured using the (curie method) and a PG Instruments. Both measurements were performed at the University of Mosul, College of Education for Pure Sciences. Electron spectra were measured using an instrument in the range of (200-1100 nm) and quartz cells at the University of Mosul, College of Education for Pure Sciences. Infrared spectra were measured for the ligand and complexes using a Shimadzu-type spectrometer in the (200-4000 cm^{-1}) region and cesium iodide (CsI) discs at Tikrit University, College of Education for Pure Sciences. Proton (^1H-NMR) and carbon-13 (^{13}C-NMR) nuclear magnetic resonance spectroscopy was performed on the prepared ligand using a Varian Agilant USA device (400 MHz) by dissolving the sample in (DMSO-D6) and using tetramethylsilane (TMS) at the University of Basra. Thermal analysis (TGA) was performed on the complexes at Tehran University. The amount of each element in the prepared complexes was measured using atomic absorption spectroscopy (Analytik Jena Nova A350) at Mosul University, College of Agriculture. Elemental analysis (C.H.N) was performed on the ligand and complexes using elemental analysis. At Tehran University

2.2- Synthesis of ligand (ScB)

Schiff base ligand was prepared using conventional methods (Abood & Hussein, 2014) by reacting (0.002 mol, 0.24 gm) 2-hydroxybenzaldehyde dissolved in (20 ml) of absolute ethanol. (0.001 mol, 1.06 gm) of O-Tolidin dissolved in (20 ml) of absolute ethanol was then added. During the reaction, (3-5) drops of glacial acetic acid were added. The reaction mixture was heated refluxed with stirring on a water bath at (70 °C) for (3 h). the reaction was tracked by TLC (Et_2o:n-hexane) (2:1) showed that the reaction was completed. The mixture was then allowed to cool down to room temperature. A yellow powder was formed, which was washed with diethyl Ether and ethanol, dried, and then recrystallized with ethanol. Its melting point was (200 °C).

2.3- Preparation of complexes of the ligand with the for mula $[M(ScB)_2Cl_2]$

The complexes were prepared in a ratio of [1:2][M:ScB] by reacting (0.002 mol, 0.84 gm) of the ligand dissolved in (20 mL) absolute ethanol with (0.001 mol, 0.19 gm) of ($MnCl_2.4H_2O$) dissolved in (10 mL) distilled water using The reaction mixture was heated refluxed with stirring on a water bath at (70 °C) for (3 h). The mixture was then left to cool to room temperature, where the reaction product precipitated as a precipitate. This precipitate was separated by filtration, washed with cold ethanol and ether, dried, and then recrystallized with ethanol.

The (2,3,4,5) complexes were prepared in the same way, using the same weights of the (ScB) along with the weights of the metal salts for each metal.(0.001 mol, 0.19 gm of $FeCl_2.4H_2O$) (0.001 mol, 0.23 gm of $CoCl_2.6H_2O$).(0.001 mol, 0.17 gm of $CuCl_2.2H_2O$) and (0.001 mol, 0.13 g of $ZnCl_2$).

2.4-Preparation of complexes of the ligand with the formula $[M(ScB)_2(en)]$

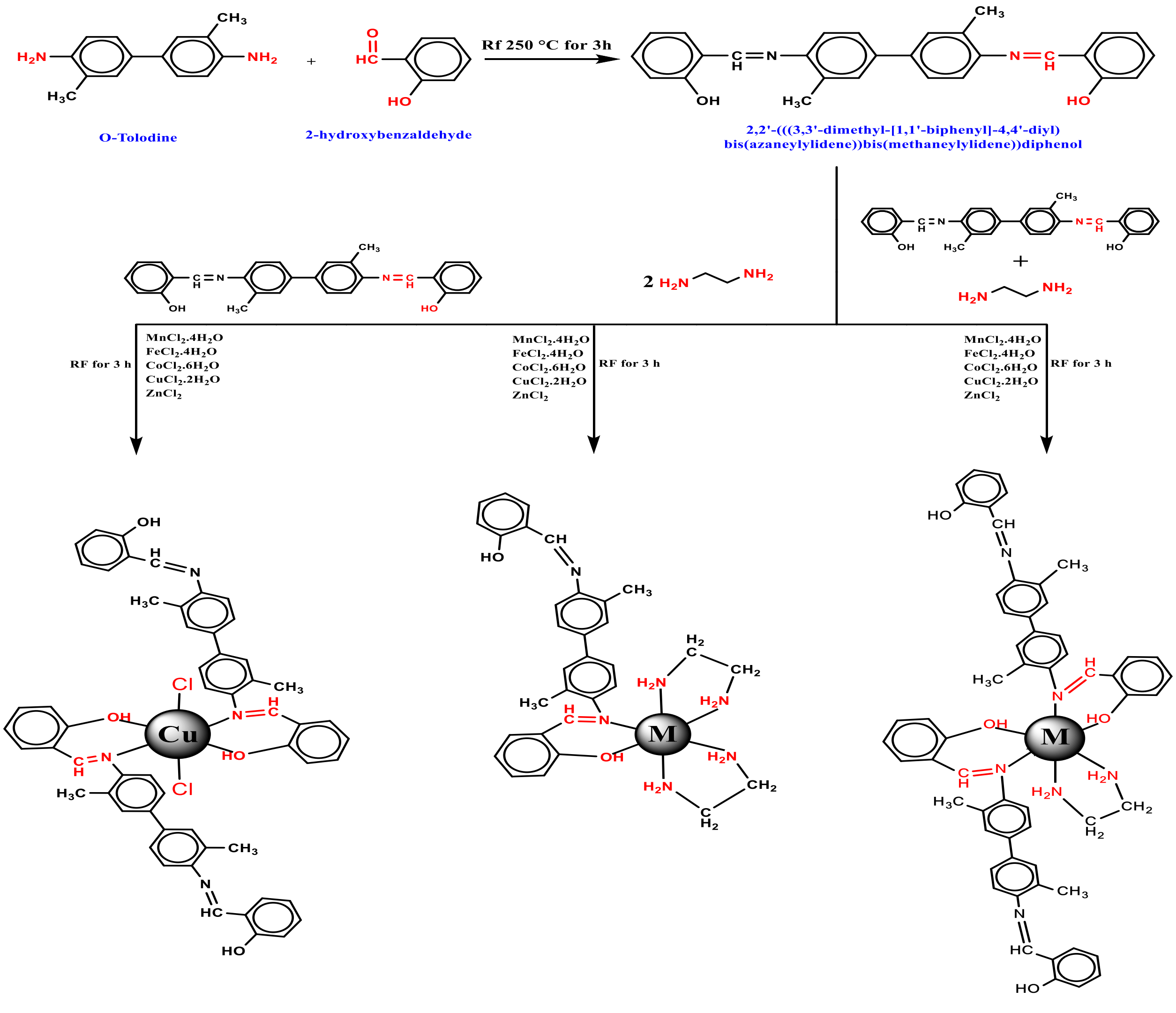
The complexes were prepared in a ratio of [1:2:1][M:ScB:1] by reacting (0.001 mol, 0.19 gm) of ($MnCl_2.4H_2O$) dissolved in (10 mL) distilled water with reacting (0.002 mol, 0.84 gm) of the ligand dissolved in (20 mL) absolute ethanol The mixture was heated refluxed with stirring on a water bath at (70 °C) for half an hour, followed by the addition of (0.001 mol,0.06 gm) ethyl enediamine dissolved in (15 mL) absolute ethanol The reaction mixture was heated refluxed with stirring on a water bath at (70 °C) for (3 h). The mixture was then left to cool to room temperature, where the reaction product precipitated as a precipitate. This precipitate was separated by filtration, washed with cold ethanol and ether, dried, and then recrystallized with ethanol.

The (2,3,4,5) complexes were prepared in the same way, using the same weights of the (ScB) and ligand (en) along with the weights of the metal salts for each metal.(0.001 mol, 0.19 gm of $FeCl_2.4H_2O$) (0.001 mol, 0.23 gm of $CoCl_{2.}6H_2O$).(0.001 mol, 0.17 gm of $CuCl_2.2H_2O$) and (0.001 mol, 0.13 gm of $ZnCl_2$).

2.5-Preparation of complexes of the ligand with the formula [M(L1(ScB)(en)$_2$]

The complexes were prepared in a ratio of [1:1:2][M:ScB:en] by reacting (0.001 mol, 0.19 gm) of ($MnCl_2.4H_2O$) dissolved in (10 mL) distilled water with reacting (0.001 mol, 0.42 g) of the ligand dissolved in (20 mL) absolute ethanol The mixture was heated refluxed with stirring on a water bath at (70 °C) for half an hour followed by the addition of (0.002 mol,0.12 gm) ethylenediamine dissolved in (15 mL) absolute ethanol The reaction mixture was heated refluxed with stirring on a water bath at (70 °C) for (3 h). The mixture was then left to cool to room temperature, where the reaction product precipitated as a precipitate. This precipitate was separated by filtration, washed with cold ethanol and ether, dried, and then recrystallized with ethanol.

The (2,3,4,5) complexes were prepared in the same way, using the same weights of the (ScB) and ligand (en) along with the weights of the metal salts for each metal.(0.001 mol, 0.19 gm of $FeCl_2.4H_2O$) (0.001 mol, 0.23 gm of $CoCl_{2.}6H_2O$).(0.001 mol, 0.17 g of $CuCl_2.2H_2O$) and (0.001 mol, 0.13 gm of $ZnCl_2$).



Scheme 1: for preparing the Schiff base and its complexes

3-RESULT AND DISCUSSION

3.1-Micro Elemental Analysi(C.H.N)

The elemental ratios (C.H.N) of the prepared coordination complexes were determined and the obtained result are presented in table (1) the experimental values showed good agreement with theoretically calculate ones indicating high degree ot consistency and supporting the validity of the proposed molecular formulas.(Raoof et al., 2022)

3.2-Atomic absorption

The concentrations of manganese, iron, cobalt, copper, and zinc in the prepared complexes were determined. The results were analyzed and compared with calculated theoretical values. The concentrations of these compounds were found to be within the standard range .The values are shown in Table1(1) (Abed et al., 2021)

Table 1: The table presents the expected formulas, analytical results, and various physical properties of the bond and the prepared compounds.

No.	**Molcular Formula**	**Molcular Wight**	**M.p℃**	**Yelid%**	**Colour**	**Elemental analysis theoretical (Practical)**			
						C% (Exp.)	H% (Exp.)	N% (Exp.)	M% (Exp.)
ScB	$C_{28}H_{24}O_2N_2$	420.51	200	85	Yellow	79.98 (79.63)	5.75 (5.32)	6.66 (6.05)	-----
1	$[Mn(ScB)_2(Cl)_2]$ $C_{56}H_{48}Cl_2MnN_4O_4$	966.86	230	88	Brown	69.57 (69.50)	5.00 (4.65)	5.81 (5.11)	5.68 (5.32)
2	$[Fe(ScB)_2(Cl)_2]$ $C_{56}H_{48}Cl_2FeN_4O_4$	967.77	180	83	Dark green	69.50 (68.98)	4.80 (4.21)	5.79 (5.21)	5.78 (5.21)
3	$[Co(ScB)_2(Cl)_2]$ $C_{56}H_{48}Cl_2CoN_4O_4$	970.86	280	78	Light orange	69.28 (68.00)	4.98 (4.44)	5.77 (5.34)	6.07 (5.98)
4	$[Cu(ScB)_2(Cl)_2]$ $C_{56}H_{48}Cl_2CuN_4O_4$	975.47	265	88	Light brown	68.95 (67.99)	4.96 (4.31)	5.74 (5.22)	6.51 (6.01)
5	$[Zn(ScB)_2(Cl)_2]$ $C_{56}H_{48}Cl_2ZnN_4O_4$	977.30	173	89	Yellow	68.82 (68.01)	4.95 (4.43)	5.73 (5.42)	6.69 (6.43)
6	$[Mn(ScB)_2(en)]Cl_2$ $C_{58}H_{56}Cl_2MnN_6O_4$	956.06	190	77	Dark brown	72.87 (71.89)	5.90 (5.00)	8.79 (8.01)	5.75 (5.00)
7	$[Fe(ScB)_2(en)]Cl_2$ $C_{58}H_{56}Cl_2FeN_6O_4$	956.97	186	78	Dark brown	72.80 (72.09)	5.90 (5.12)	8.78 (8.56)	5.84 (5.65)
8	$[Co(ScB)_2(en)]Cl_2$ $C_{58}H_{56}Cl_2CoN_6O_4$	960.06	98	83	Light brown	72.56 (72.00)	5.88 (5.22)	8.75 (8.00)	6.14 (5.98)
9	$[Cu(ScB)_2(en)]Cl_2$ $C_{58}H_{56}Cl_2CuN_6O_4$	964.67	72	85	Dark green	72.22 (70.55)	5.85 (4.76)	8.71 (7.98)	6.59 (6.33)
10	$[Zn(ScB)_2(en)]Cl_2$ $C_{58}H_{56}Cl_2ZnN_6O_4$	966.50	74	84	Yellow	72.08 (70.43)	5.84 (5.11)	8.70 (8.22)	6.76 (6.43)

11	[Mn(ScB)(en)$_2$]Cl$_2$ $C_{32}H_{40}Cl_2MnN_6O_2$	595.65	180	79	Brown	64.53 (64.12)	6.77 (6.76)	14.11 (13.90)	9.22 (9.00)
12	[Fe(ScB)(en)$_2$]Cl$_2$ $C_{32}H_{40}Cl_2FeN_6O_2$	596.56	87	78	Orange	64.43 (62.87)	6.76 (6.00)	14.09 (13.87)	9.36 (9.02)
13	[Co(ScB)(en)$_2$]Cl$_2$ $C_{32}H_{40}Cl_2CoN_6O_2$	599.25	130	85	Light brown	64.10 (63.75)	6.72 (6.32)	14.02 (13.87)	9.83 (9.66)
14	[Cu(ScB)(en)$_2$]Cl$_2$ $C_{32}H_{40}Cl_2CuN_6O_2$	604.26	115	86	Dark brown	63.61 (62.11)	6.67 (6.32)	13.91 (13.01)	10.52 (10.01)
15	[Zn(ScB)(en)$_2$]Cl$_2$ $C_{32}H_{40}Cl_2ZnN_6O_2$	606.09	132	89	Yellow	63.41 (61.99)	6.65 (6.00)	13.87 (13.23)	10.79 (10.31)

3.3-Electronic spectra

In this study, the electronic spectra of the ligand and the prepared complexes were measured using dimethylformamide as solvent at a concentration of (10^{-3} mol.L^{-1}) and using two cells with a diameter of (1 cm) . The prepared complexes gave bands for the (d–d) transitions except for manganese (II), and zinc (II) complexes as well as the charge transfer bands The complexes of manganese(II) showed absorption bands associated with charge transfer within the (35543-34329 cm^{-1}) range, while no (d→d) transitions were observed in the visible region. This confirms that the complexes have highly spin-hexagonal shapes, as these transitions are not allowed (Laporte-forbidden). The electronic spectra of the iron(II) complexes exhibit one absorption band within the (12449-11275 cm^{-1}) range, associated with the ($^5T_2g \rightarrow {}^5Eg$) transition in the visible and near-infrared regions. Absorption bands within the (35674-34352 cm^{-1}) range were associated with charge transfer bands. This confirms that the iron(II) complexes have a highly spin-hexagonal shape. The electronic spectra of the cobalt(II) complexes showed absorption bands within the (12167-11456 cm^{-1}) range associated with the ($^4T_1g \rightarrow {}^4T_2g$) transition and absorption bands within the (18663-16386 cm^{-1}) range associated with the transition. The ($^4T_1g \rightarrow {}^4A_2g$) and absorption bands within the (24365-21766 cm^{-1}) range are attributed to the ($^4T_1g \rightarrow {}^4T_1g(p)$) transition, and the appearance of absorption bands within the (34426-32631 cm^{-1}) range is attributed to charge transfer. This proves that the cobalt complexes have taken on highly spin-hexagonal symmetric geometries. As for the copper(II) complexes, they showed a single transition band within the (11705-13847 cm^{-1}) range attributed to the ($^2T_2g \rightarrow {}^2Eg$) transition, and also the appearance of an absorption band within the (34226-32155 cm^{-1}) range. This confirms that the copper complexes have taken on highly spin-hexagonal symmetric geometries attributed to charge transfer. As for the zinc(II) complexes, their outer shell is filled with electrons, and therefore no bands for (d→d) electron transitions appear because they are not allowed spin-orbitally (Laporte-forbidden). However, they showed bands attributed to the electron transitions within the (34574-31973 cm^{-1}) rang due to ($n \rightarrow \pi^*$)($\pi \rightarrow \pi^*$) ligand, which have undergone a change in position from what they were in the ligand spectrum, indicating the formation of comphexes.(Ameen & Ahmed, 2023; Shukla et al., 2021)

3.4- Molar electrical conductivity

The molar electrical conductivity measurements showed that the chemical formulas correspond to the proposed structures of the prepared complexes which have the formula [M(ScB)$_2$Cl$_2$], [M(ScB)$_2$(en)]Cl$_2$, and [M(ScB)(en)$_2$]Cl$_2$, the electrical conductivity measurments were performed in tow solvents dimethylformamide (DMF) and dimethylsulfoxide (DMSO) because they are inert towards the complex and the electrical insulation is stable and has low in viscosity measurements have shown that the complexes with the formula [M(ScB)$_2$Cl$_2$] were non-conductive,while the complexes with the formula [M(ScB)$_2$(en)] and [M(ScB)(en)$_2$] are conductive at [1:2] ratio.(Ahmed, 2025; Mohan et al., 2020)

3.5-Magnetic measurements

Measurements of the magnetic susceptibility of manganese(II), iron(II), cobalt(II), and copper(II) complexes showed paramagnetic behavior and relatively high magnetic moment values, indicating the presence of unpaired electrons, which supports high spin hexagonal coordination. Zinc complexes, on the other hand, exhibited diamagnetic behavior due to their d^{10} electron configuration**.(Elkanzi et al., 2023)**

Table 2: Data on the electronic spectra and effective magnetic moment of the ligand and prepared complexes.

No	**Molcular Formula**	**Molar Conductivity $Cm^2.\Omega^{-1}.mol^{-1}$**		**μeff B.M**	**UV-Vis. Bands (cm^{-1})**	**Charge transfer**
		DMF	**DMSO**			
ScB	$C_{28}H_{24}O_2N_2$	-----	-----	-----	-----	-----
1	$[Mn(ScB)_2(Cl)_2]$	7	9	5.97	-----	34329
2	$[Fe(ScB)_2(Cl)_2]$	15	5	5.21	11275	34352
3	$[Co(ScB)_2(Cl)_2]$	5	13	4.60	11456,18663,23958	34426
4	$[Cu(ScB)_2(Cl)_2]$	17	12	1.72	11895	33455
5	$[Zn(ScB)_2(Cl)_2]$	15	8	0	-----	34574
6	$[Mn(ScB)_2(en)]Cl_2$	135	70	5.92	-----	35167
7	$[Fe(ScB)_2(en)]Cl_2$	132	74	5.00	12036	35674
8	$[Co(ScB)_2(en)]Cl_2$	132	72	4.69	11674,16386,21766	32631
9	$[Cu(ScB)_2(en)]Cl_2$	140	74	1.73	13847	32155
10	$[Zn(ScB)_2(en)]Cl_2$	134	75	0	-----	32441
11	$[Mn(ScB)(en)_2]Cl_2$	133	73	5.94	-----	35543
12	$[Fe(ScB)(en)_2]Cl_2$	142	74	5.14	12449	35572
13	$[Co(ScB)(en)_2]Cl_2$	140	71	4.65	12167,16934,24365	33548
14	$[Cu(ScB)(en)_2]Cl_2$	135	74	1.71	11705	34226
15	$[Zn(ScB)(en)_2]Cl_2$	136	72	0	-----	31973

3.6-Infrared spectrum

Infrared spectra (IR), indicate that the coordination in the complexes is mediated by the nitrogen atom in the (C=N) groups, while the nitrogen atom in the second azomethine group remains inconsistent, as evidenced by the shift of the (C=N) vibrational bands towards lower values compared to the free bond. A shift of the vibrational bands of the (C-O)phenolic, (OH) alcohol groups towards lower values were also observed. Based on these spectral results, we conclude that coordination is mediated by the nitrogen and oxygen atoms, i.e., the bond is doubly coordinated. Furthermore, the appearance of new bands associated with (M-Cl, M-N, M-O) in the bands (293–298 cm^{-1}, 482–464 cm^{-1}, and 557–533 cm^{-1}) confirms the presence of coordination. (Mannaa et al., 2025)

Table 3: IR bands (cm^{-1}) data of the ligand and prepared complexes.

No.	**Formula of complexes**	**ν (C=N)**	**ν (C-O)**	**ν (M-O)**	**ν (M-N)**	**ν (M-Cl)**
ScB	$C_{28}H_{24}O_2N_2$	1614	1279	-----	-----	-----
1	$[Mn(ScB)_2(Cl)_2]$	1579	1250	556	475	293
2	$[Fe (ScB)_2(Cl)_2]$	1577	1252	555	469	298
3	$[Co (ScB)_2(Cl)_2]$	1574	1249	557	473	298

4	[Cu (ScB)$_2$(Cl)$_2$]	1576	1254	555	478	295
5	[Zn (ScB)$_2$(Cl)$_2$]	1588	1255	510	466	293
6	[Mn(ScB)$_2$(en)]	1578	1250	549	473	----
7	[Fe(ScB)$_2$(en)]	1579	1256	557	482	----
8	[Co(ScB)$_2$(en)]	1577	1254	557	471	----
9	[Cu(ScB)$_2$(en)]	1579	1252	535	466	----
10	[Zn(ScB)$_2$(en)]	1578	1250	555	473	----
11	[Mn(ScB)(en)$_2$]	1577	1255	549	469	----
12	[Fe(ScB)(en)$_2$]	1576	1250	545	473	----
13	[Co(ScB)(en)$_2$]	1578	1249	557	479	----
14	[Cu(ScB)(en)$_2$]	1577	1251	556	473	----
15	[Zn(ScB)(en)$_2$]	1579	1252	533	482	----

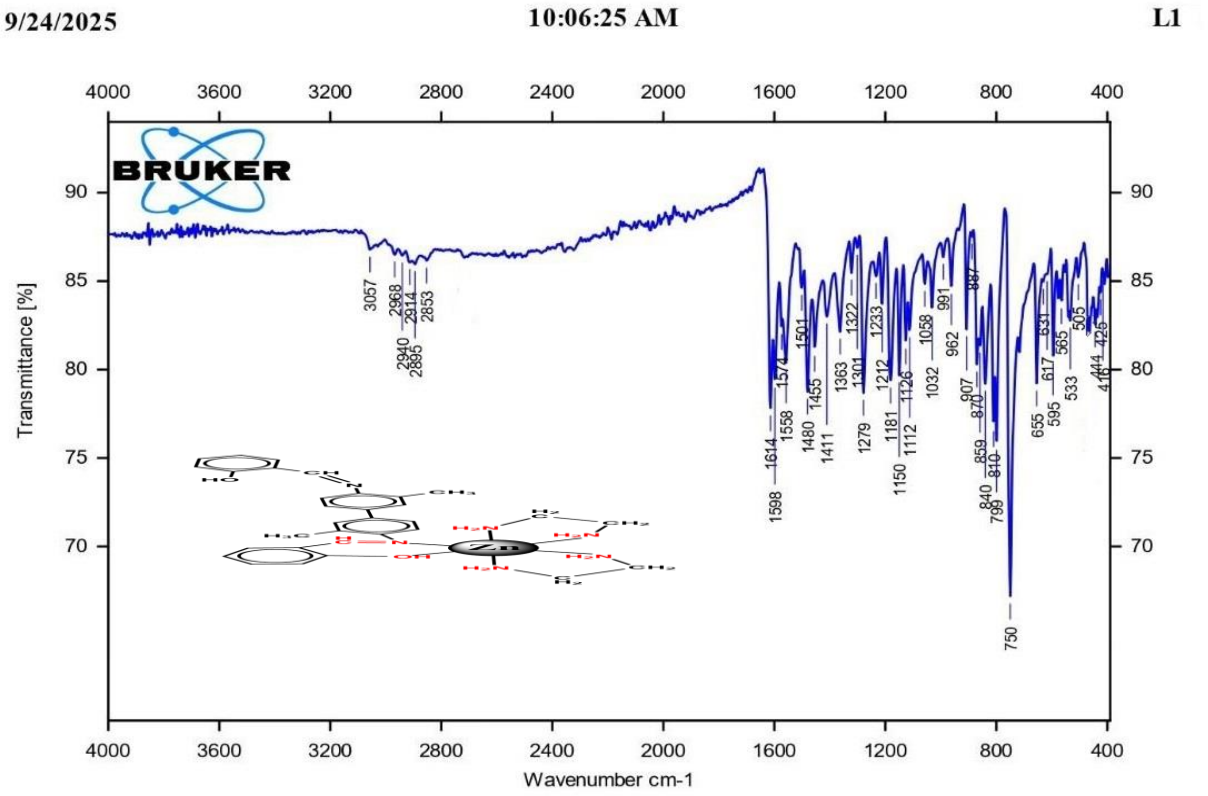


Figure 1: Infrared spectrum of the Ligand (ScB).

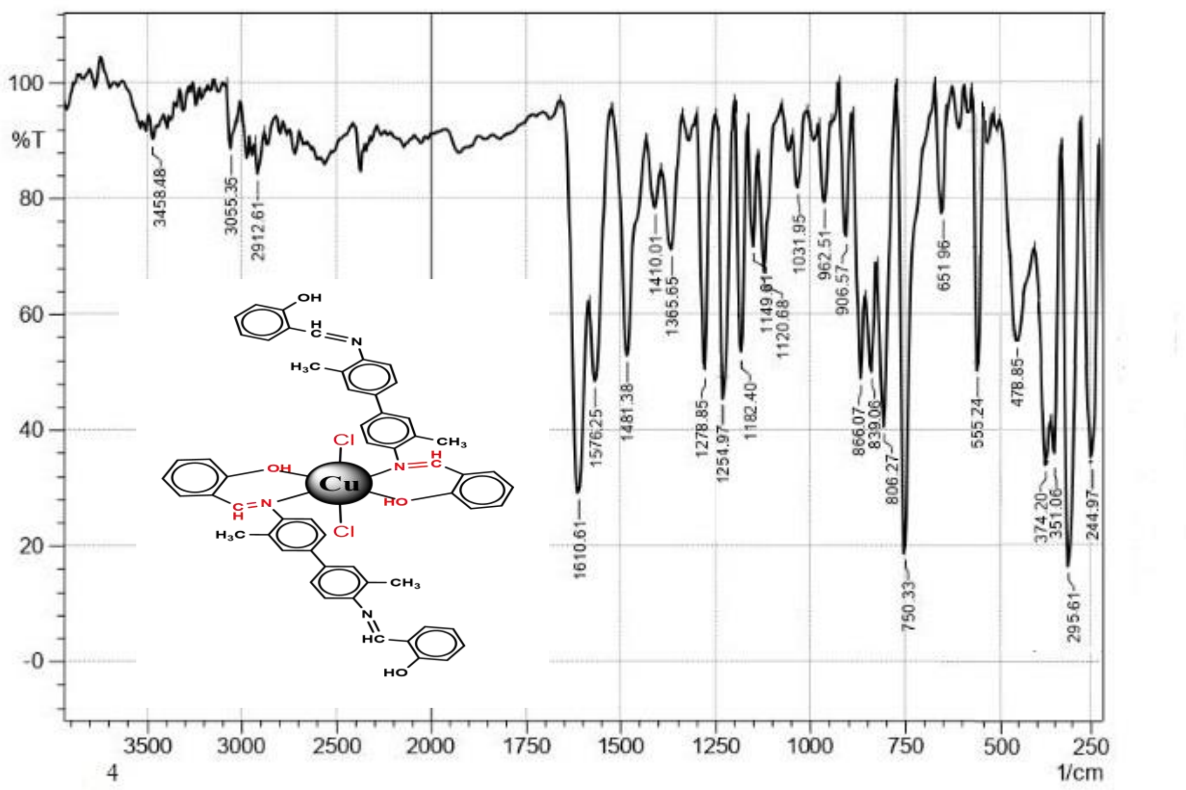


Figure 2: Infrared spectrum of the complex (4).

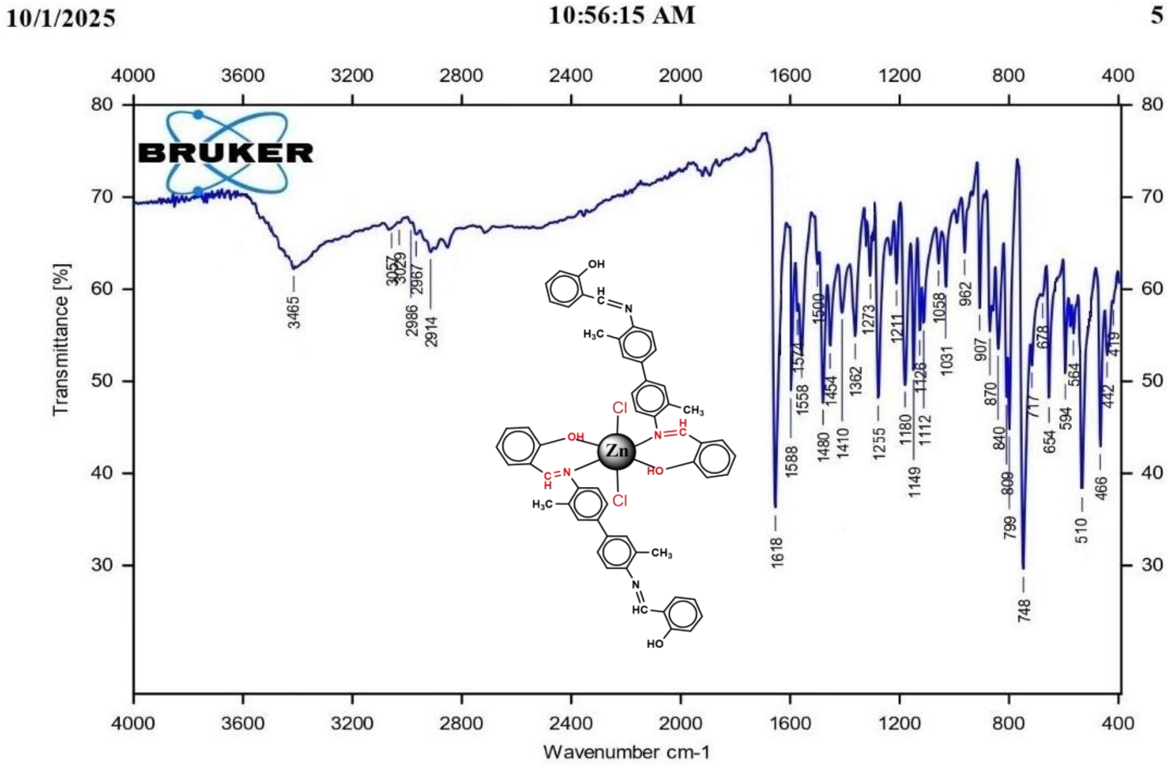


Figure 3: Infrared spectrum of the complex (5).

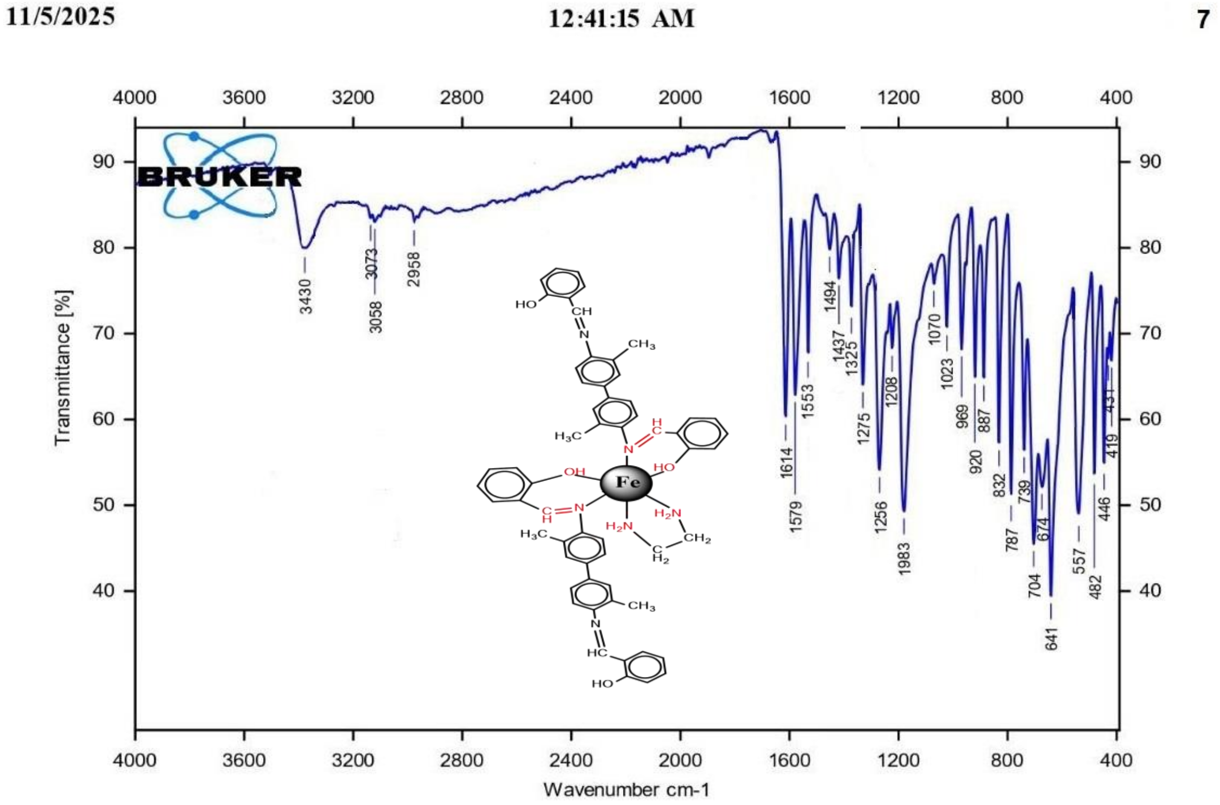


Figure 4: Infrared spectrum of the complex (7).

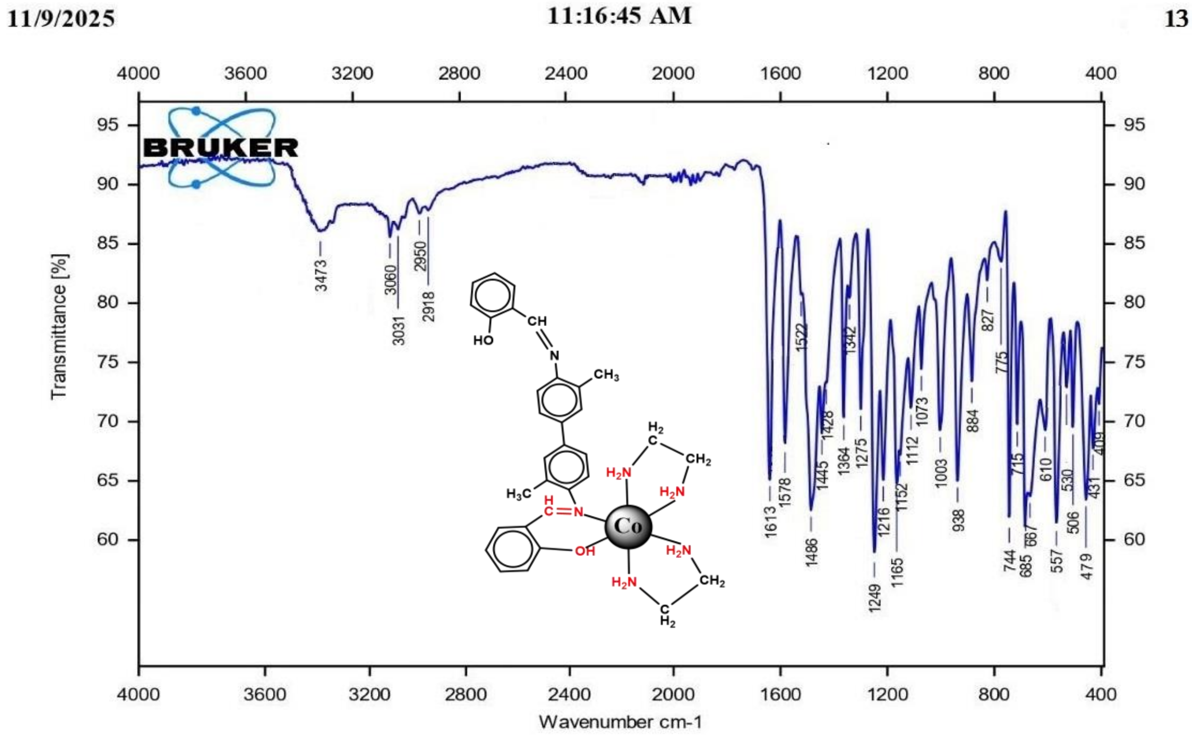


Figure 5: Infrared spectrum of the complex (13).

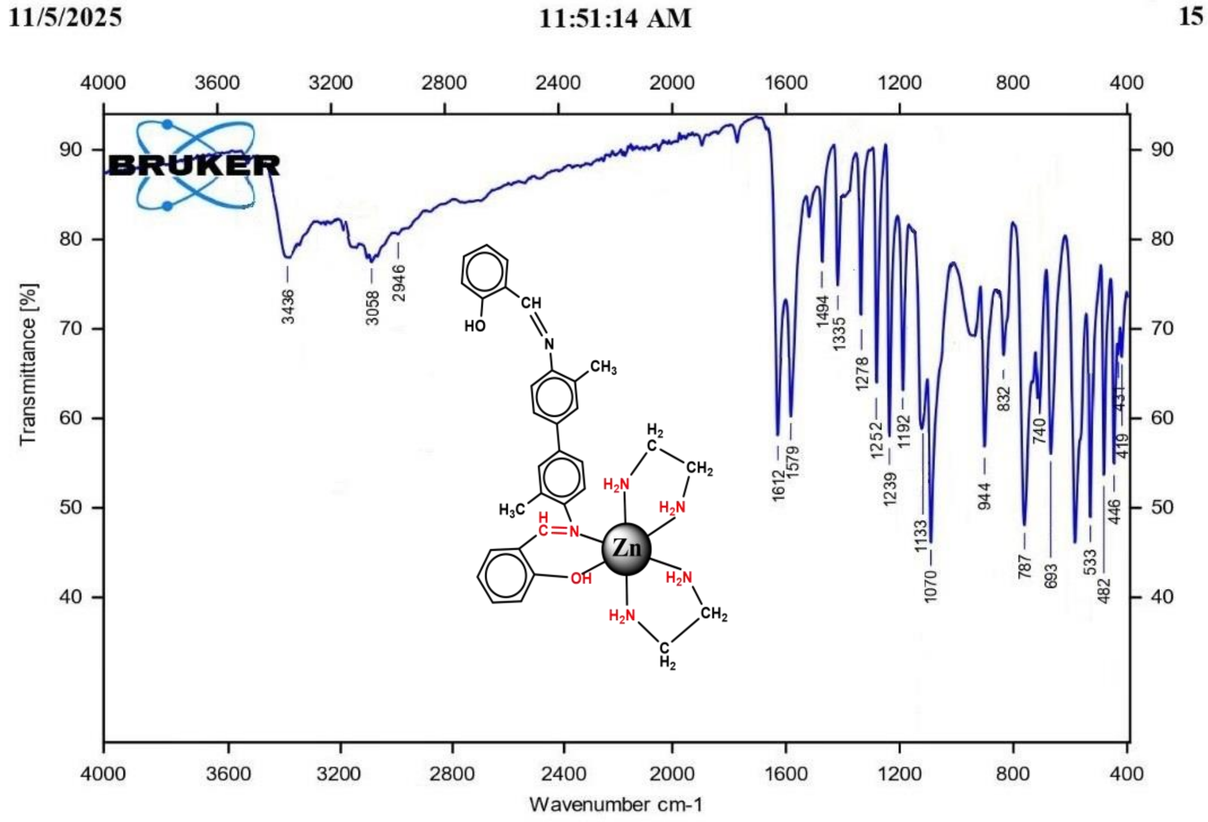


Figure 6: Infrared spectrum of the complex (15).

3.7- Mass spectrum

The mass spectrum of ligand (ScB) and complexes (5,12) were measured. The mass spectrum of the ligand (ScB) shows a prominent molecular ion peak at 420m/z, corresponding to the molecular weight of the ligand. This confirms the successful synthesis and purity of the ligand. For the zinc complex [Zn(ScB)$_2$Cl$_2$], the molecular ion peak appears at 977m/z, which matches the expected molecular weight of the complex, while the iron complex [Fe(ScB)(en)$_2$], the molecular ion peak appears at 596m/z, which matches the expected molecular weight of the complex. Fragmentation pathways likely involve the sequential cleavage of the ligand moieties or loss of small neutral molecules (e.g.CH_3, H_2O, Cl), leading to characteristic fragment ions. These fragmentation patterns support the proposed structure of both the ligand and its zinc complex. Through the fragmentation peaks, we observe bands at (330-345m/z) indicating the loss of a small molecule such as H_2O, bands at (280-330m/z) indicating the loss of an organic part of the ligand, and bands at (200-260m/zindicating ligand residues related to an aromatic part.As well as, lower peaks 200> indicating organic fragments. This fragmentation pattern supports the formation of Schiff complexes.(Ahmed, 2025)

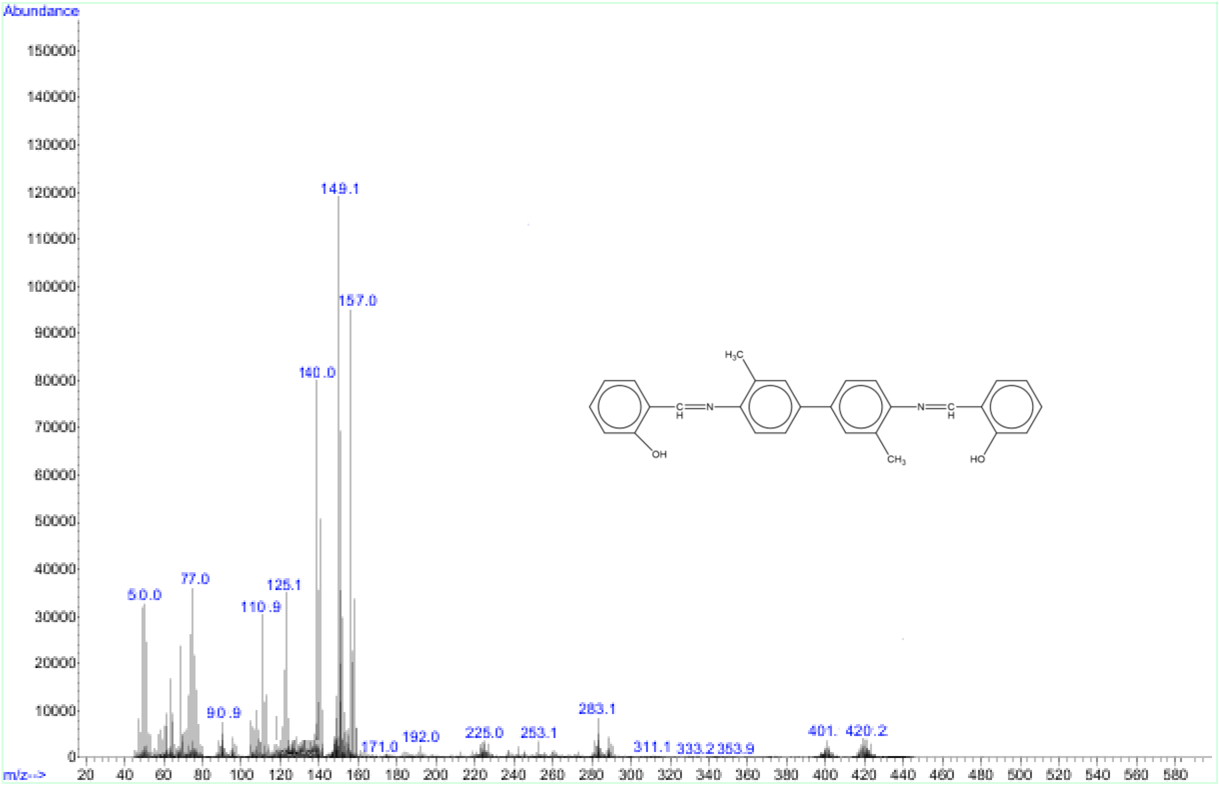


Figure 7. Mass spectrum of the ligand.

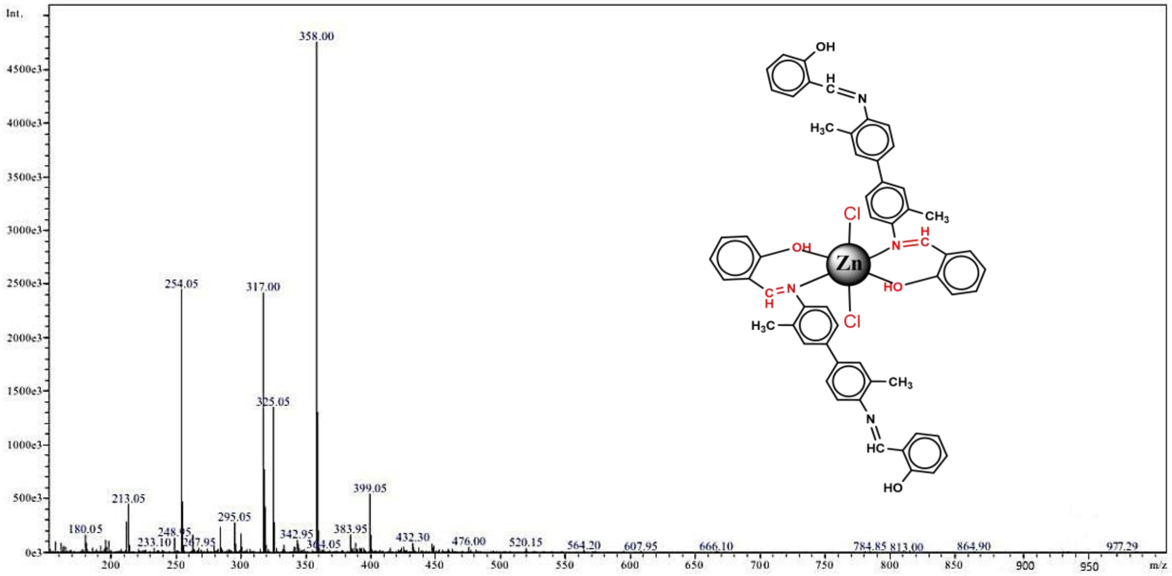


Figure 8. Mass spectrum of the complex (5)

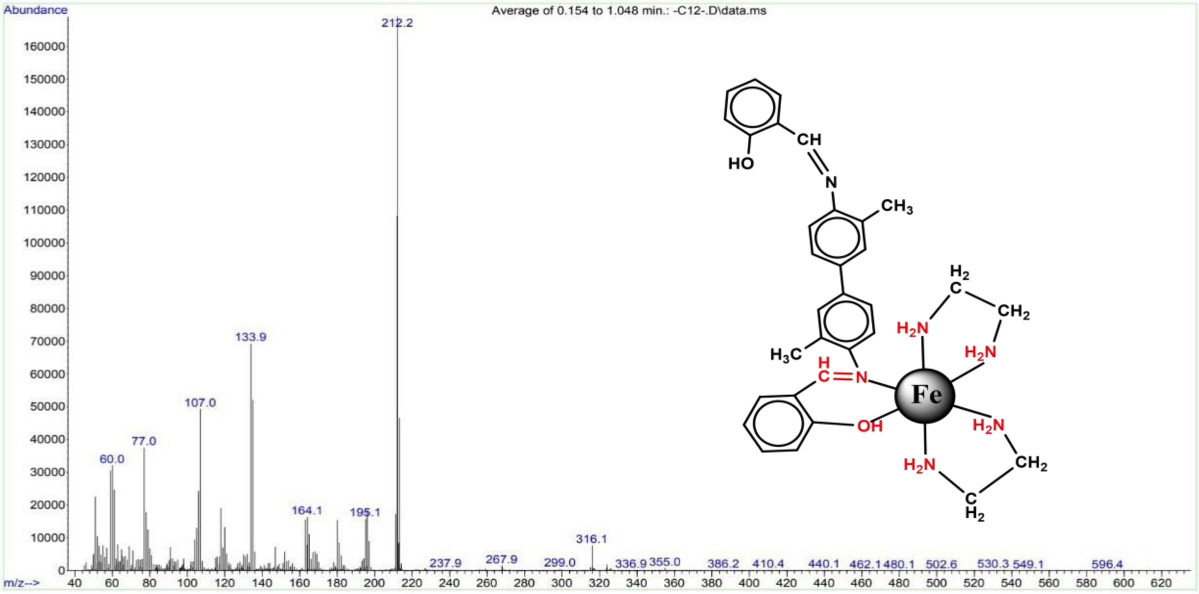


Figure 9. Mass spectrum of the complex (12)**.**

3.8- ^{1}H-NMR, ^{13}C-NMR Spectroscopy

The nuclear magnetic resonance (1H-NMR) spectrum of the prepared Schiff base proton was measured where it was dissolved in (DMSO-d^{6}) solvent and at a frequency of (400 MHz) using a tetramethylsilane reference, and the spectrum showed signals that were highly consistent with the proposed structural formula of the prepared Schiff base. The spectrum showed a single sharp signal at (13.30 ppm), attributed to the protons of the phenolic hydroxyl groups (–OH). These appeared in this weak region due to the formation of a strong internal hydrogen bond with the nitrogen atom in the isomethen group (–CH=N–). Signals also appeared at (2.3–2.5 ppm), attributed to the protons of the methyl groups (–CH_3) attached to the aromatic rings. A signal appeared at (8.7–9.2 ppm), attributed to the isomethen proton (HC=N), which confirms the formation of the isomethen bond and the completion of the reaction. Furthermore, multiple signals appeared in the range (6.8–7.7 ppm), attributed to the protons of the aromatic rings (Ar–H). The overlap of these signals is attributed to the large number of aromatic rings and the different chemical environments resulting from various substitutions. The absence of any signal in the (9.7–10 ppm) field confirms the completion of the reaction and the lack of unreacted starting materials, indicating the disappearance of the aldehyde proton and the completion of the reaction).Alemu, 2017(

The 13C-NMR spectrum of the prepared Schiff base compound also showed multiple signals belonging to the aromatic carbonates and the two isomethen bonds. Peaks were observed at 162–165 ppm, belonging to the aromatic ring carbonates attached to the hydroxyl group (C-OH). Similarly, the two carbon atoms in the isomethenine groups (C=N) exhibited a series of signals in the range of 115-155 ppm, attributed to the various benzene-ring carbonates in the extended aromatic system of the compound. The methyl groups (CH) showed weak signals in the range of 20-30 ppm, and their low number compared to the aromatic carbonates explains their weak signal. The solvent (DMSO-D6) registered a signal at 38 ppm. The 1H-NMR and 13C-NMR results confirm the successful formation of the Schiff double base and are consistent with the proposed structure of the compound. The 13C-NMR spectroscopy of the prepared Schiff base compound also showed multiple signals attributed to the aromatic carbonates and the two isomethenine bonds. Peaks were observed at 162-165 ppm, belonging to the aromatic-ring carbonates attached to the hydroxyl group (C-OH). Likewise, to the two carbon atoms in the two isomethen groups (C=N), a group of signals appeared in the range (115-155 PPM) that are attributed to the different benzene ring carbonates in the extended aromatic system of the compound. As for the methyl group carbonates (CH), they appeared with weak signals in the range (20-30 PPM), and due to their small number compared to the aromatic carbonates, they appeared weakly. The solvent (DMSO-D6) recorded a signal at (38 ppm). The results of (1H-NMR) and (13C-NMR) confirm the formation of the Schiff double base successfully and are consistent with the proposed structure of the compound.(Gavali et al., 2024)

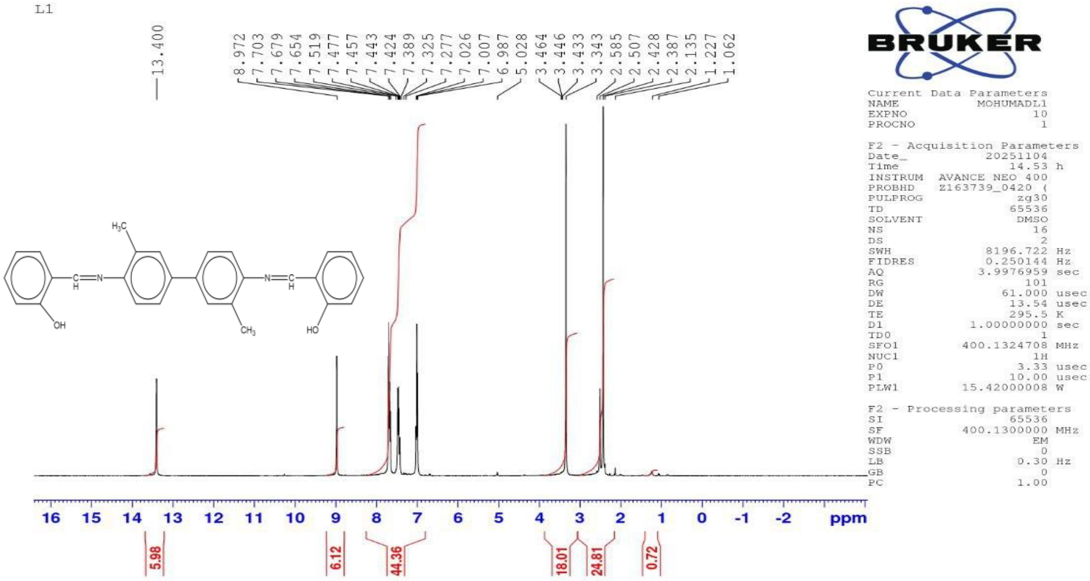


Figure 10: 1H-NMR spectrum of the ligand (ScB)

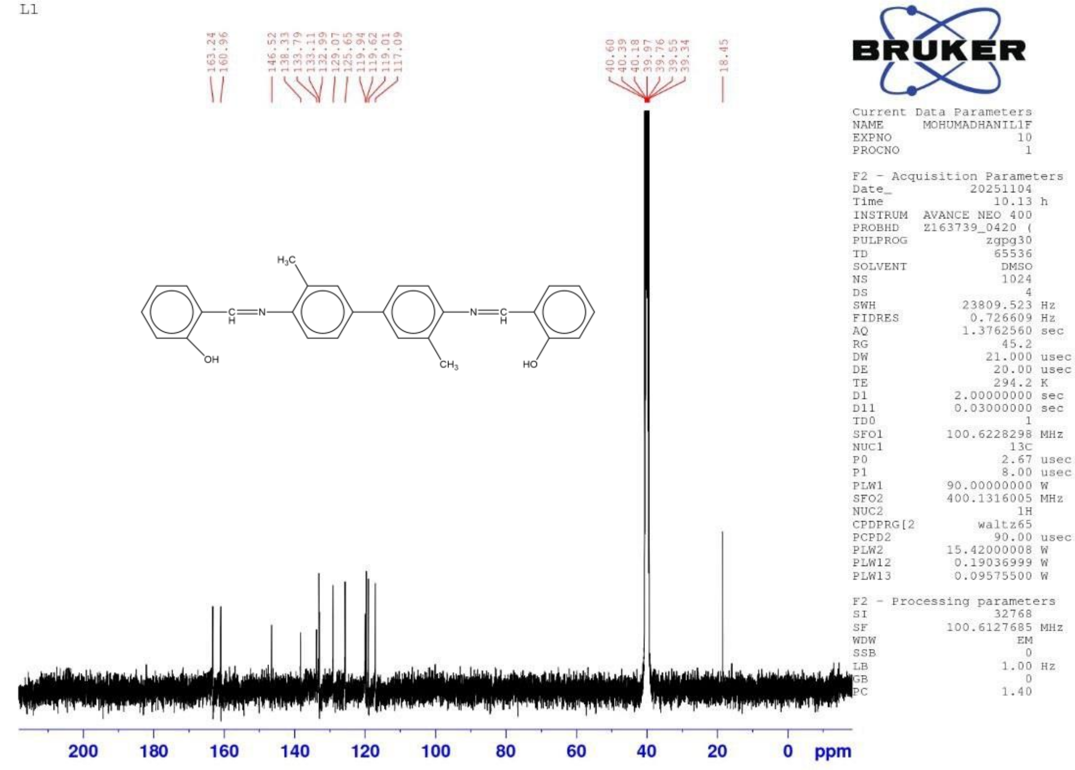


Figure 11: ^{13}C-NMR spectrum of the ligand (ScB)

3.9-Thermogravimetric analysis

The thermal behavior of the as-selectively prepared complex was studied at a heating rate of 5 °C per minute in a temperature range of (25–1000°C).). The complex decomposed in four distinct stages. The first stage involved a very slight weight loss at (25-150) , attributed to the evaporation of surface-absorbed moisture or residual solvents. The second stage involved a gradual weight loss began, attributed to the decomposition of organic groups such as CH_3, OH, NH. The third stage involved the greatest weight loss in the sample, resulting from the decomposition of Schiff bases and Nitrogenous bases. In the final stage,. it indicates the presence of inorganic residues such as metal oxides,.

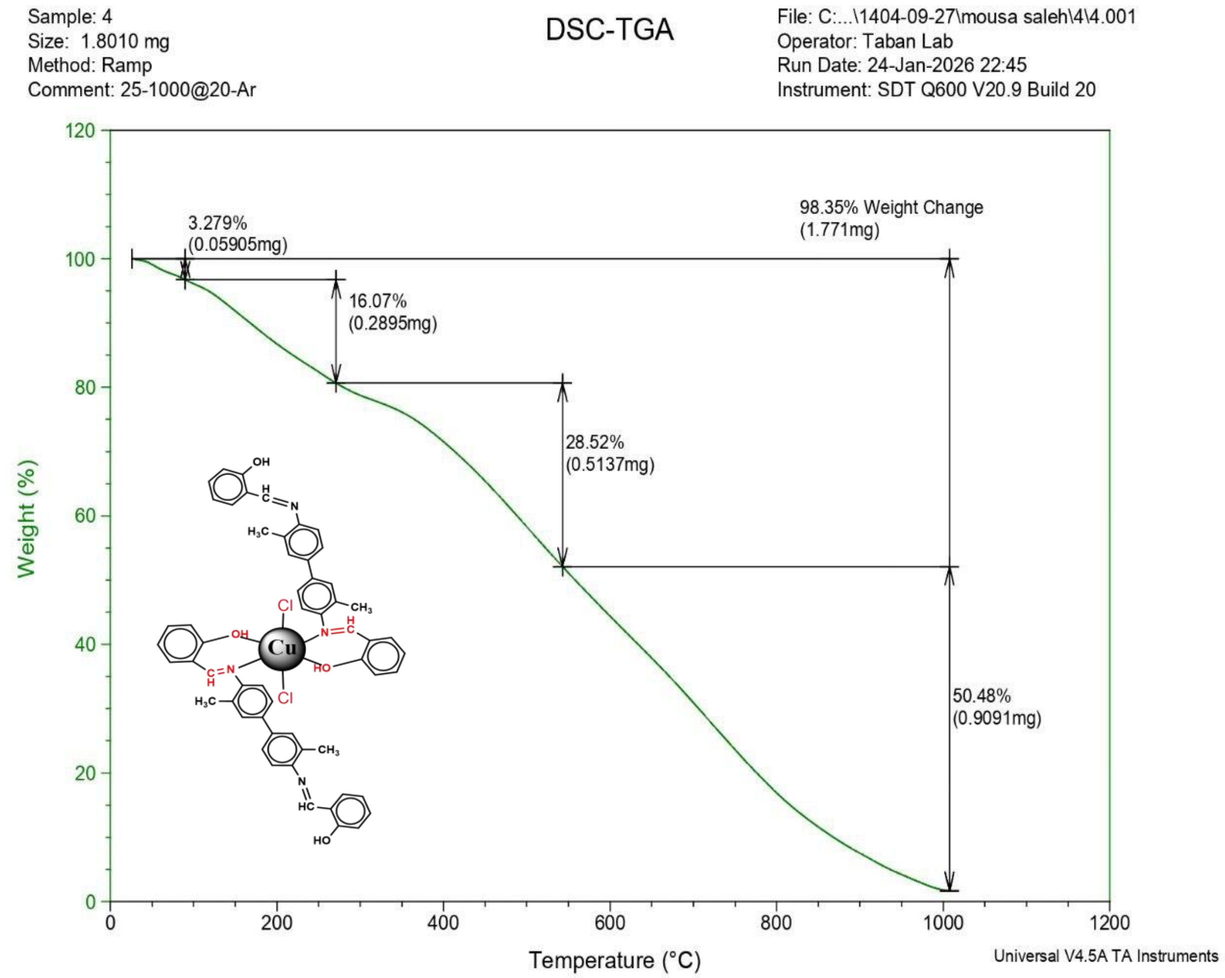


Figure 12: Thermogravimetric analysis (TGA) of complex (4)

3.10-Bioactivity Evaluation

The biological activity of the prepared ligands and compounds was measured against bacteria. E.coli and Staphylococcus aureus. The results showed that the free ligand exhibited no biological activity against the studied bacterial species. This is attributed to its lack of the necessary physical and chemical properties for interaction with these bacteria, despite containing active sites on the nitrogen atom and a hydroxide group as a substitute. The study also showed that most of the prepared ligand compounds possessed biological activity, while others lacked any activity. This confirms previous studies indicating that Schiff base compounds have better biological activity than their free-ligand counterparts. The results obtained were converging with the inhibitory activity of the antibiotics used, as shown in the tables below..(Thakur et al., 2024)

Table 4: Biological activity of ligands and complexes against types of bacteria**.**

No.	E.coli	Staphylococcus aureus
ScB	Zero	Zero
DMSO	Zero	Zero
Gentanycin	19 mm	14 mm
Ciprofloxacin	21mm	23mm
1	Zero	Zero
2	14 mm	11 mm
3	18 mm	17 mm
4	Zero	Zero
5	Zero	Zero
6	Zero	Zero
7	19 mm	18 mm
8	16 mm	16 mm
9	12 mm	Zero
10	Zero	Zero
12	12 mm	13 mm
13	16 mm	13 mm
14	16 mm	11 mm
15	12 mm	9 mm

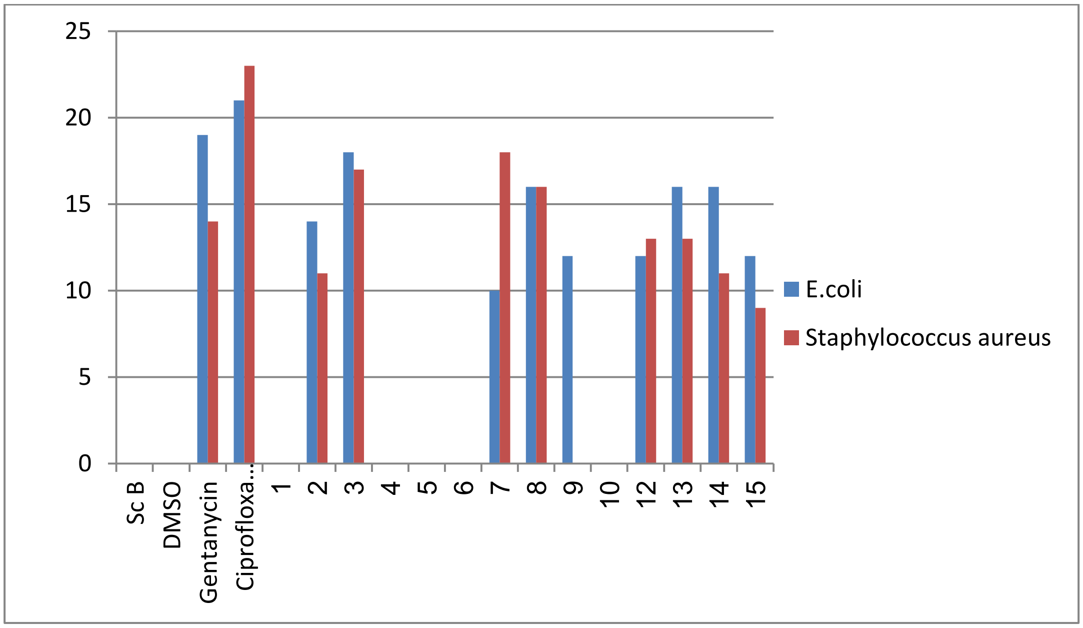


Figure 13 : The biological efficacy of the compounds prepared against bacteria E.coli and Staphylococcus aureus**.**

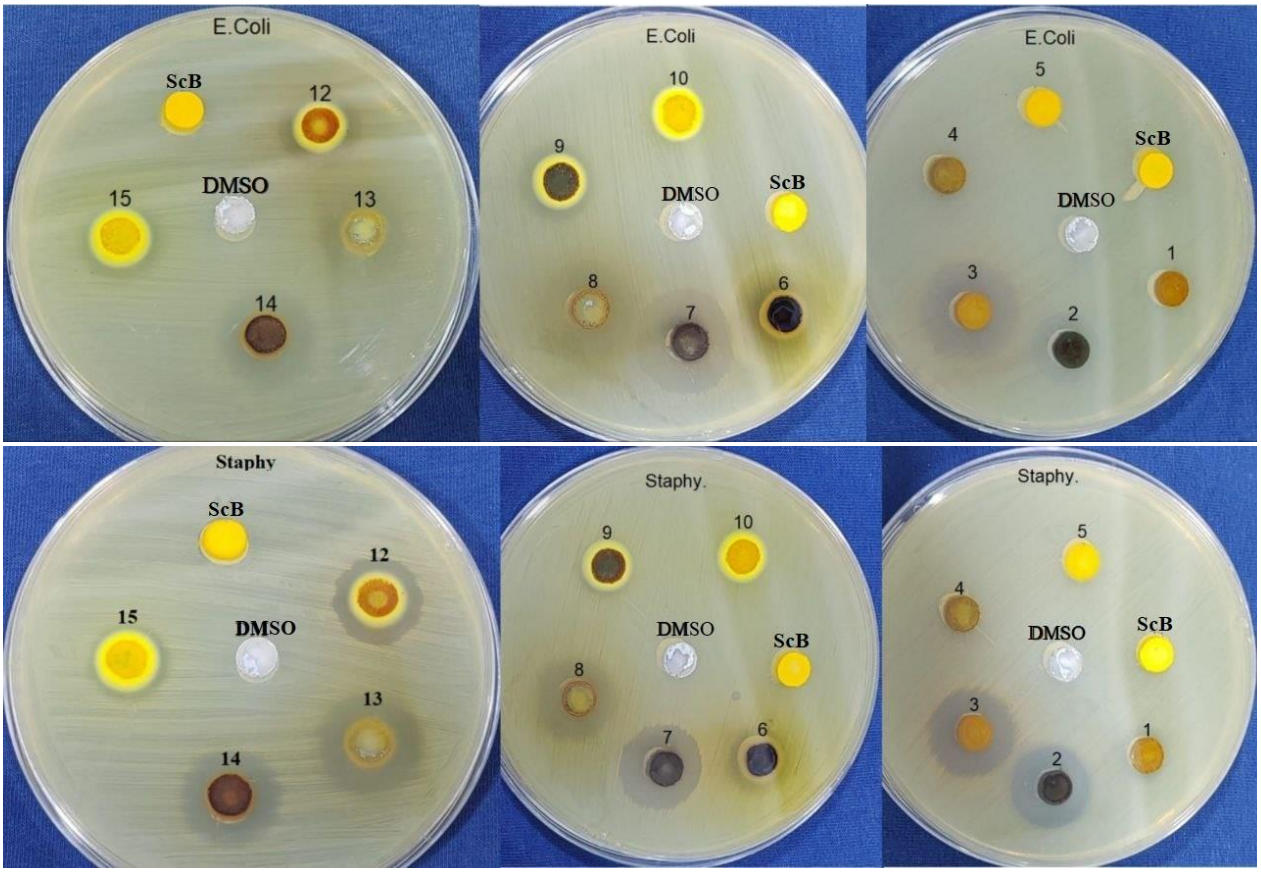


Figure 14 : Biological activity against E.coli and Staphylococcus aureus.

4-Conclusions

1- In this research, we prepared new compounds that possess distinctive physical and chemical properties. Based on the results of the chemical, physical and, and spectral measurements, it was confirmed that the prepared Schiff base ligand acts as a bidentate (kelite) ligand when in coordination with the metal ion

2- The result of the complexes (1-5) roved are not conductive, while the rest of the complexes were connected by a ratio of (1:2).

3- The coordination takes place through the azomethine nitrogen and the hydroxyl oxygen atoms which confirms the octahedral geometry of the prepared complexes . $[M(ScB)_2Cl_2]$, $[M(ScB)_2(en)]Cl_2$, $[M(ScB)(en)_2]Cl_2$

4- Biological measurements showed that the prepared Schiff base ligand had no biological activity, while the prepared complexes had good biological activity, supporting their potential future use in the pharmaceutical industry.

5-Reference

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