

Synthesis, Structures and Characterization of a Novel Schiff Base Ligand and their Three Homotrimeric Metal Complexes and study bioactivity them

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Authors' contributions

1- RAAM designed wrote the protocol, and wrote the first draft of the manuscript. 2- HQNA, YMSJ, AAA and AKA partly designed the study and managed the data analyses of the study. 3- RAAM and AAA managed the literature searches and performed the practical study. All authors read and approved the final draft

Abstract

A novel N-isopropylidene hydrazinedithiocarbamate Schiff base [(CH₃)₂C=Hy-dtc] was used as stabilizer ligand for three homotrimeric metal complexes prepared by condensation of ammonium hydrazinedithiocarbamate and acetone and to use them into in-situ reactions with metal chloride salts (M) in 3 : 2 molar ratio [M : L] in ethanol solution to yield Schiff base homotrimeric metal complexes of the general formula is {M₃[(CH₃)₂C=Hy-dtc]₂(Cl)₂(H₂O)₂} where M refers to Co(II) (1), Ni(II) (2) and Cu(II) (3). The structures of the metal complexes were characterized using elemental analysis, molar conductivity, FT-IR and UV-Vis spectroscopy and magnetic susceptibility measurements as well as MM2 theoretical calculations. The FT-IR spectra data suggest the Schiff base acts as a tetradentate attachment. Results confirmed that configuration around the central metal ion is the square planer and configuration around the two terminal metal ions distorted tetrahedral and their ammonium hydrazinedithiocarbamate ligand and Schiff base metal complexes showed different levels of in vitro inhibition activity against two bacterial species they Staphylococcus aureus (G+) and Escherichia coli (G-).

Keywords: Novel Schiff Base; Spectral, Magnetic, Antimicrobial Activities and 3D Molecular Modeling.

المخلص

استعملت قاعدة شيف الجديدة η-ايزوبروبيليدين هيدرازين ثنائي ثايوكارباميت [(CH₃)₂C=Hy-dtc] لاستقرار المعقدات الفلزية ثلاثية النوى المتجانسة التي حضرت بالتفاعل موضعيا وذلك بتكاثف الاسيتون والهيدرازين ثنائي ثايوكارباميت مع كلوريد الفلزات (M) ونسبة مولية 2:3 (فلز : ليجاند) في محلول الايثانول لإنتاج معقدات قواعد شيف الفلزية ثلاثية النوى والتي تحمل الصيغة العامة {M₃[(CH₃)₂C=Hy-dtc]₂(Cl)₂(H₂O)₂} حيث تمثل M ايونات الكوبلت (II) او النيكل (II) او النحاس (II). تراكيب المعقدات الفلزية لقاعدة شيف تم تشخيصها عن طرق التحليل الدقيق للعناصر والتوصيلية المولارية الكهربائية وأطياف الأشعة تحت الحمراء والأطياف الالكترونية والحساسية المغناطيسية بالإضافة الى استخدام برنامج MM2 لحساب اطوال الروابط والزوايا. تشير قياسات طيف الأشعة تحت الحمراء الى أن قاعدة شيف الجديدة تكون رباعية السن، كما تؤكد النتائج ان الترتيب حول ايون الفلز الوسطي مربع مستوى والترتيب حول ايوني الفلز في الاطراف رباعي سطوح مشوه، كذلك أظهر ليجاند امونيوم هيدرازين ثنائي ثايوكارباميت ومعقدات قواعد شيف الفلزية مستويات مختلفة من النشاط التثبيطي ضد نوعين من البكتيريا الموجبة (G+) للجرام (Escherichia coli) والسالبة (Staphylococcus aureus) للجرام (G-).

INTRODUCTION

Coordination chemistry of Schiff bases derived from dithiocarbamate with various metal ions leading to mono- or poly-nuclear complexes. Schiff bases and their metal complexes are becoming increasingly important in recent years due to their biological activity as antiviral [1], antibiotics [2] and anti-tumour agents [3] due to presence of their specific moiety and industrial applications as luminescence chemical probes sensors [4], catalysis [5] and antioxidants [6]. Also they are important due to their facile syntheses and multi-nuclear feature [7,8]. This successful strategy allows for the control of the nuclearity ingredients in the ingenious use of compartmental ligands [9,10] which are organic molecules able to hold together two or more metal ions. Moreover, discrete homo and heteropolynuclear complexes have contributed to understanding of the factors governing the sign and magnitude of exchange interaction between paramagnetic ions, either identical or different [11]. In the 70s, M. Iskander and L. El. Sayd. used hydrazinedithiocarboxylic acid, as a precursor for the synthesis of Schiff base which behaved as monobasic bidentate ligand and giving only mononuclear nickel (II) complex [12]. The aim of the present study is to synthesis and characterization of novel N-isopropylidene hydrazinedithiocarbamate Schiff base and their cobalt(II), nickel(II) and

copper(II) coordination complexes and study their bioactivity.

Experimental part

Materials and Solutions

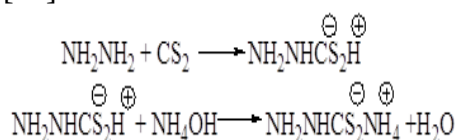
Hydrazine hydrate, carbon disulphide, ammonium hydroxide, $\text{CoCl}_2 \cdot 6\text{H}_2\text{O}$, $\text{NiCl}_2 \cdot 6\text{H}_2\text{O}$ and $\text{CuCl}_2 \cdot 2\text{H}_2\text{O}$, acetone and ethanol (96%) were of analytical reagent grade (BDH, Aldrich or Fluka).

Instrumentation

The ammonium hydrazinedithiocarbamate, ammonium and Schiff base metal complexes were analyzed for carbon, hydrogen and nitrogen using 1106 (Carlo Erba) microanalyser. Infrared absorption spectra were recorded on a Unicam SP-2000 spectrophotometer as CsI discs in the range $200\text{--}4000\text{ cm}^{-1}$. The magnetic susceptibility measurements were made by the Faraday method at room temperature using a Bruker B.M. 6 instrument. The electronic spectra were recorded on a Shimadzu UV/Vis spectrophotometer (range $200\text{--}1100\text{ nm}$), model 160 Koyoto (Japan) using acetonitrile as a solvent. Conductivity measurements were carried out on 10^{-3} M solutions of the metal complexes in acetonitrile at room temperature on a digital conductivity meter, model 4070 (Jenway). The 3D molecular modeling of a representative Schiff base complexes was carried out on a CSChem. 3D Ultra Molecular Modeling and analysis program [13]. Antibacterial screening was done at laboratories of Faculty of Education, University of Al-Baydha using agar diffusion technique

Synthesis of the Dithiocarbamate Ligand

Ammonium hydrazinedithiocarbamate (Hy-dtcNH₄) as shown in the Figure 1 was prepared by the reaction of hydrazine hydrate with carbon disulphide in presence of ammonium hydroxide is shown in the equation 1 [12].



Equation 1:

Preparation of the dithiocarbamate ligand

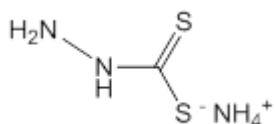
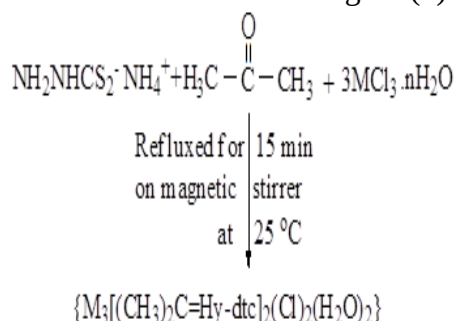


Figure 1: Chemical structure of the dithiocarbamate ligand

Synthesis of the Schiff base Metal Complexes

Aqueous solution of 0.033 mol of hydrated metal chloride (CoCl₂. 6H₂O, NiCl₂. 6H₂O and CuCl₂. 2H₂O) was added to an ethanolic solution of the 0.022 mol of ammonium hydrazinedithiocarbamate with 0.05 mol of dimethyl ketone. The mixture was refluxed for 15 min and then cooled to room temperature. The product was then washed with ethanol and dried over P₂O₅ in a desiccator vacuum for 24 h. The following equation general reaction 2 represent formation of the Schiff base metal complexes and the structure of the Schiff base is shown as in Figure (2).



Equation 2: General reaction for the synthesis of Schiff base metal complexes;

M= Co(II), Ni(II), n=6 and M=Cu(II), n=2

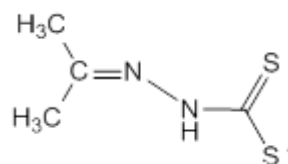


Figure 2: Chemical structure of the Schiff base

Antibacterial Assay

In vitro antibacterial activities of ammonium hydrazinedithiocarbamate ligand and Schiff base complexes of Co(II), Ni(II) and Cu(II) were tested against two bacterial species G(+) *Staphylococcus aureus* and G(-) *Escherichia coli* using disk diffusion technique [14]. An aliquot of the bacterial culture in the nutrient broth was similarly distributed on to the surface of the nutrient agar (NA) using a sterilized L-shaped glass rod. Sterilized filter paper disks (6 mm in diameter) were separately soaked in the different concentrations of tested compounds, Cephalexin, Ampicillin, and Amoxicillin solutions (w/v) [15].

The paper discs were then dried at room temperature under the laminar flow to avoid contamination. Antibiotics of Cephalexin, Ampicillin, and Amoxicillin were used as a positive control. Each of sterile disc was carefully placed on the surface of NA plates containing the bacterial inoculum. After 24 h of incubation at 37°C, the diameter of the inhibition zone surrounding the disks (disk diameter included) was measured.

Result and Discussion Syntheses and Physical Properties

The in-situ reaction of the ammonium hydrazinedithiocarbamate and acetone with metal chloride in (2:3) ligand to metal molar ratio afford the Schiff base metal complexes of the general formula $\{M_3[(CH_3)_2C=Hy-dtc]_2(Cl)_2(H_2O)_2\}$ as shown in Figure 3. They were characterized by using elemental analyses and magnetic susceptibility measurements as listed in the Table 1, the FT-IR data are listed in the Table 2 and the FT-IR spectra curves are shown in the Figures 4-7. The UV-Vis spectroscopy

and molar conductivities of the complexes as listed in the Table 3 and the electronic spectra curves are shown in the Figures 8-10. The antibacterial activity of the ammonium hydrazinedithiocarbamate ligand and Schiff base metal complexes are listed in the Table 4. The selected bond lengths and bond angles calculated are listed in the Tables 5-7 and the optimized 3D structures are shown in the Figures 11-13. They are quite stable in air and melt or decompose above 210 °C in the Table 1. They are insoluble in most organic solvent but soluble in DMSO and DMF.

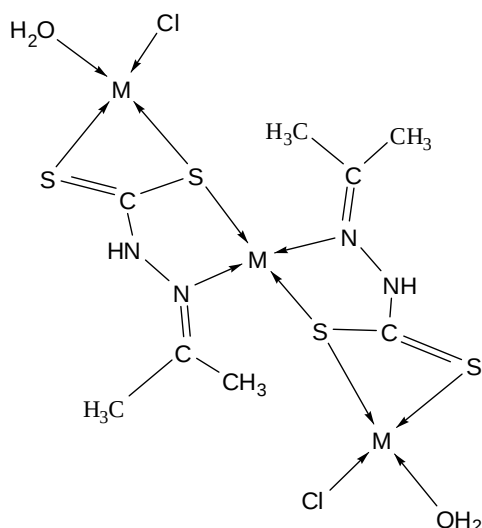


Figure 3: The structure of the synthesis complexes
M= Co(II), Ni(II) and M=Cu(II)

Table 1: Physical properties of the dithiocarbamate and Schiff base metal complexes

Compounds	Color	M.P (°C)	Yield %	% Analysis, found (calcd)			μ_{eff} (B.M)
				C %	H %	N %	
Hy-dtcNH ₄	White	110*	70	9.34 (9.60)	5.90 (5.60)	33.35 (33.60)	-
(CH ₃) ₂ C=Hy-dtc *	-	-	-	-	-	-	-
1	Dark green	270	52	15.44 (15.76)	9.26 (9.13)	2.16 (2.29)	2.90
2	White green	210	65	15.48 (15.70)	2.41 (2.29)	8.95 (9.15)	3.55
3	Bright green	240	74	15.08 (15.30)	3.37 (2.23)	8.77 (8.90)	1.37

*= Schiff base ligand has no results because it is formed during the synthesis of the metal complexes

Molar Conductivity Measurements

The Schiff base metal complexes were dissolved in DMSO solution and molar conductance 10^{-3} M of solution at 25°C was measured. The molar conductance values of the complexes fall in the range 8.80 to $13.50 \text{ ohm}^{-1}\text{cm}^2 \text{ mol}^{-1}$ indicating that these complexes are non-electrolytes [16].

Fourier Transform Infrared (FT-IR) Spectra

The FT-IR spectra of the Schiff base complexes were compared with those of the ammonium hydrazinedithiocarbamate ligand as shown in the Table 2 and the Figures 4-7. The FT-IR spectra of ligand is used in this study to compare it with Schiff base complexes due to the Schiff base free ligand can't be prepared it.

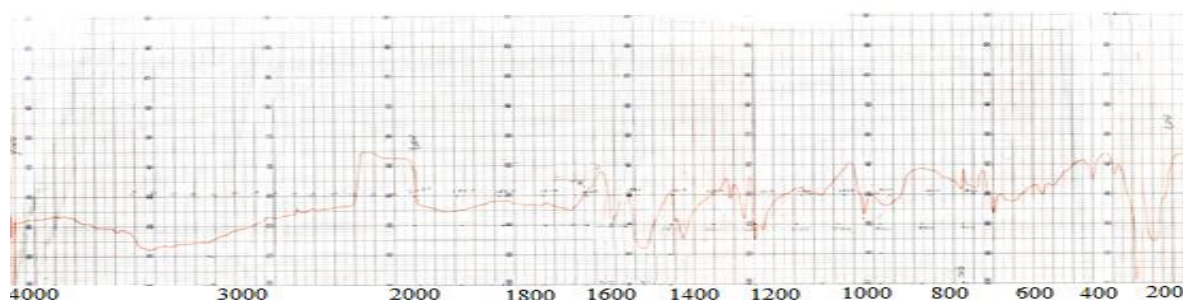


Figure 4: FT-IR spectra of Hy-dtcNH₄ ligand

In the FT-IR spectra of the Schiff base metal complexes, the $\nu(\text{NH}_2)$ band is absent in the three complexes [17] and new sharp bands observed in the range $1625\text{--}1643 \text{ cm}^{-1}$ were assigned to the $\nu(\text{C}=\text{N})$ band of the azomethine group, the shift to lower frequency in all the complexes, indicates the coordination of the azomethine nitrogen to the metal ion center [12,17]. The $\nu(\text{C}=\text{S})$ in the range $975\text{--}986 \text{ cm}^{-1}$ [12]. The spectra of $\nu(\text{C}-\text{S})$ bands appear in the range $1034\text{--}1053 \text{ cm}^{-1}$ in the complexes [12,18], the shift to higher frequency,

indicates that sulfur atom are coordinated with more than one metal ions and strongly supported that the complexes are homotrimeric [19]. The new bands $\nu(\text{M}-\text{N})$, $\nu(\text{M}-\text{S})$, $\nu(\text{M}-\text{O})$ and $\nu(\text{M}-\text{Cl})$ appear in the complexes in the range $458\text{--}475 \text{ cm}^{-1}$ [19,17], $358\text{--}390 \text{ cm}^{-1}$ [12,19-24], $480\text{--}542 \text{ cm}^{-1}$ [25-27] and $265\text{--}280 \text{ cm}^{-1}$ regions, respectively [28]. In the FT-IR spectra of the complexes, indicates coordination of the Schiff base through nitrogen and sulfur atoms and suggests tetradentate attachment.

Table 2: FT-IR spectra (cm^{-1}) of dithiocarbamate and Schiff basemetal complexes

Assignments	Compounds			
	Hy-dtcNH ₄	1	2	3
$\nu(\text{C}-\text{S})$	938 s	1048 m	1034 s	1053 m
$\nu(\text{C}=\text{S})$	890 s	981 (w)	986 (m)	975(w)
$\nu(\text{NH})$	3075 w	-	-	-
$\nu(\text{NH}_2)_{\text{as}}$	3200 m	-	-	-
$\nu(\text{NH}_2)_{\text{s}}$	3270 m	-	-	-
$\delta(\text{NH}_2)$	1580 s	-	-	-
$\nu(\text{C}=\text{N})$	-	1643 (m)	1625 (m)	1638 (m)
$\nu(\text{M}-\text{N})$	-	458 (m)	475 (w)	470 (m)
$\nu(\text{M}-\text{S})$	-	358(w)	390(m)	385(w)
$\nu(\text{M}-\text{O})$	-	480 (m)	542 (w)	535 (m)
$\nu(\text{M}-\text{Cl})$	-	265(s)	270(s)	280(s)

For IR spectra, s = strong; m = medium; w = weak

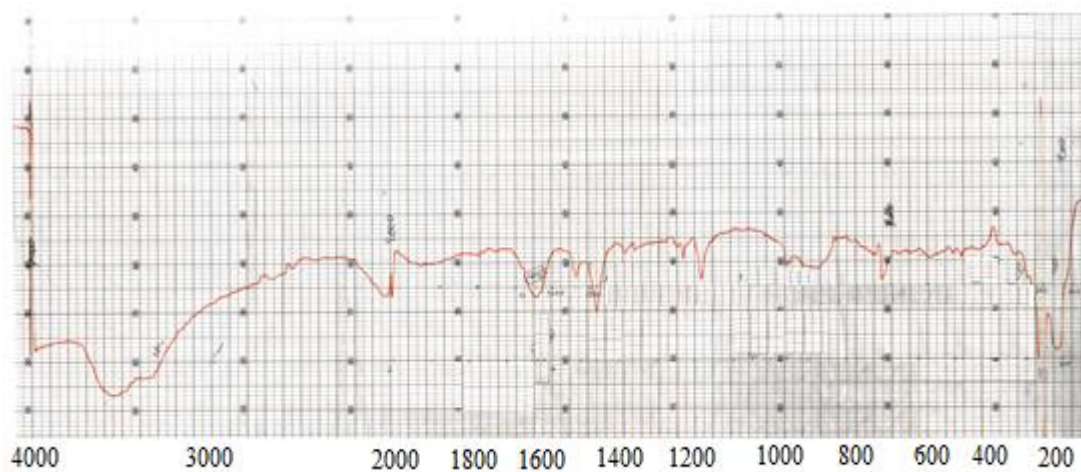


Figure 5: FT-IR spectra of cobalt complex 1

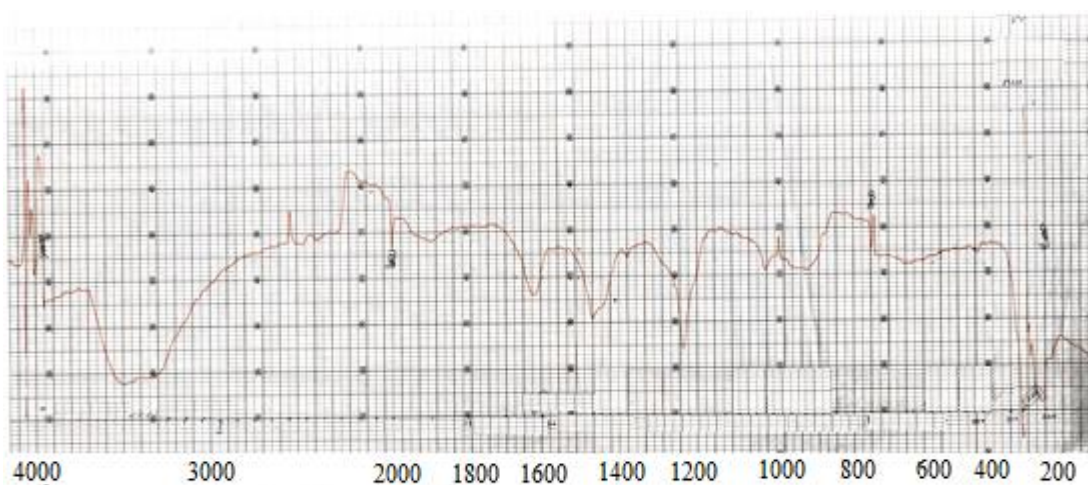


Figure 6: FT-IR spectra of nickel complex 2

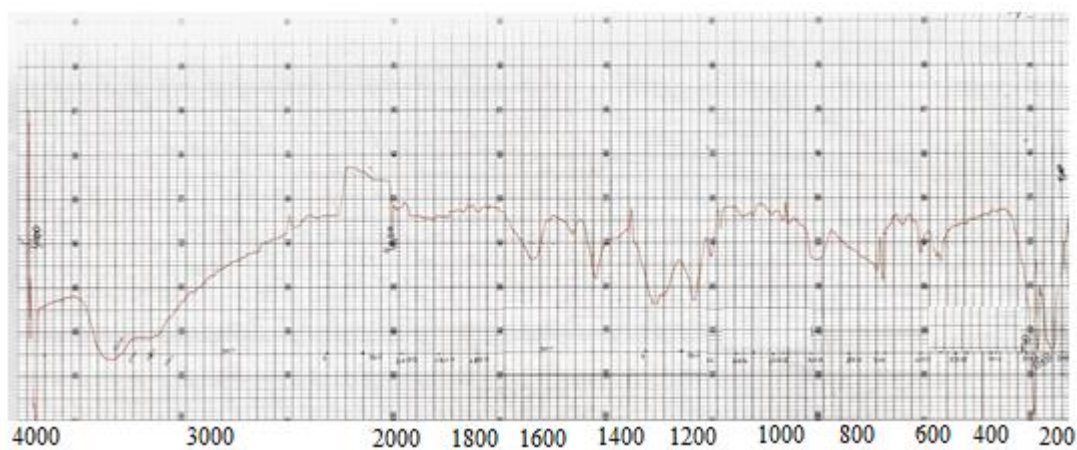


Figure 7: FT-IR spectra of copper complex 3

UV-Vis Spectra and Magnetic Moments

The electronic spectra of the Schiff base metal complexes were recorded in DMSO solution at 25°C as listed in Table 3. The magnetic properties of the cobalt (II) complex 1, exhibit μ_{eff} value of 2.90 B.M as shown in the Table 1, which is the lower value ascribed to antiferromagnetic interaction occurred between three cobalt ions, which strongly supported that the complex is homotrimeric [23, 29-33]. The electronic spectra of the cobalt (II)

complex is shown in Figure 8, the appearance of a band at 11,430 cm^{-1} , is attributed to the transition $^2A_{1g}(F) \rightarrow ^2E_{1g}$ in the square planer configuration around the central metal ion (Low spin) and could be also attributed the band in the transition $^4A_2(F) \rightarrow ^4T_1(P)$ (ν_2) in the distorted tetrahedral configuration around the two terminal metal ions (High spin) [34,35]. The bands at 14,331 cm^{-1} are due to the transition $^4A_2(F) \rightarrow ^4T_1(P)$ (ν_3) characteristic of strong distorted tetrahedral configuration [36,37].

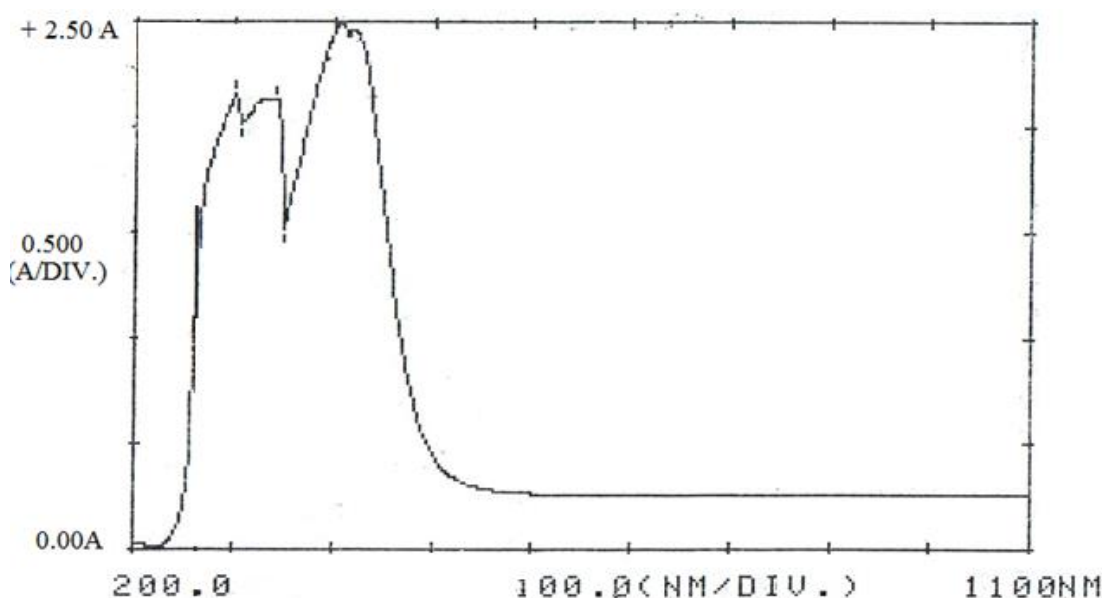


Figure 8: Electronic spectra of cobalt complex 1

The magnetic properties of the nickel (II) complex 2, display μ_{eff} value of 3.55 B.M as listed in the Table 1, the higher value may be attributed to orbital contribution occurring between the two terminal nickel while the central metal ion is diamagnetic, which strongly supported that complex is homotrimeric [23, 29, 31, 38-40]. The electronic spectra of the nickel (II) complex is shown in Figure 9. The appearance of a band at

16,500 cm^{-1} , is due to the transition $^3T_1(F) \rightarrow ^3T_1(P)$ (ν_3) in the distorted tetrahedral configuration around the two terminal nickel ions and could be also attributed to the transition $^1A_{1g} \rightarrow ^1A_{2g}$ in the square planer configuration around the central nickel ion [41]. The band at 22,462 cm^{-1} is ascribed to the transition $^1A_{1g} \rightarrow ^1B_{1g}$, which is again assigned to the square planer configuration [42,43].

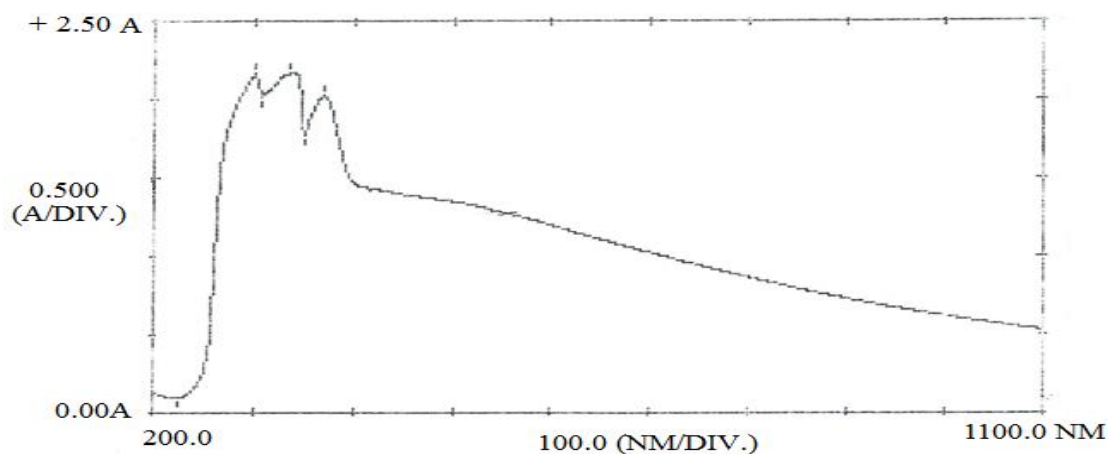


Figure 9: Electronic spectra of nickel complex 2

The copper (II) complex 3, showed magnetic properties with μ_{eff} value of 1.37 B.M is listed in the Table 1 [44], the lower value is clearly indicating that antiferromagnetic interaction occurred between three copper ions, which strongly supported that the complex is homotrimeric. The electronic spectra of the copper

(II) complex is shown in Figure 10. The band is observed at $11,835 \text{ cm}^{-1}$, which certainly indicates the distorted square planer configuration around the central copper ion, which the transition $^2B_{1g} \rightarrow ^2E_g'$. [44,45], since the distorted tetrahedral configuration does not, usually, give electronic band in the range $10000\text{-}20000 \text{ cm}^{-1}$.

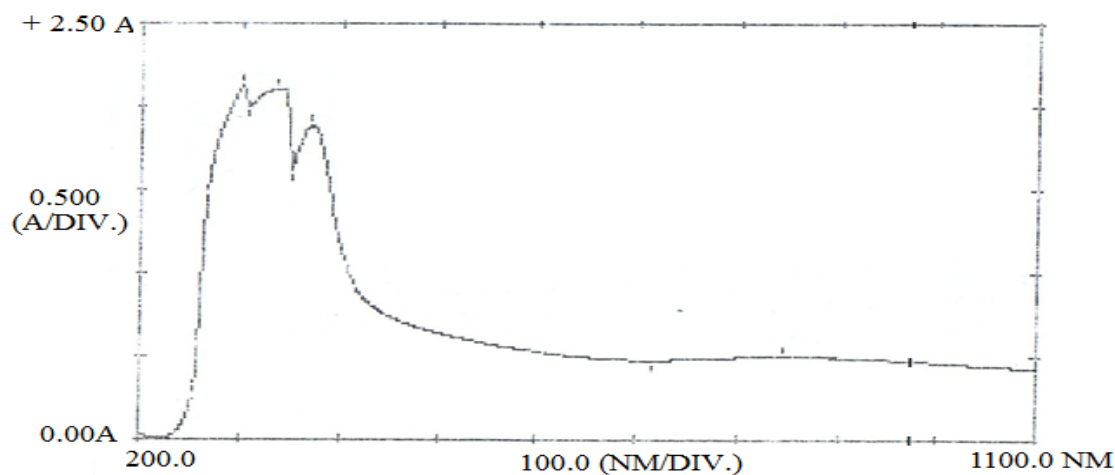


Figure 10: Electronic spectra of copper complex 3

Table 3: Electronic spectra and molar conductivity of the Schiff base metal complexes

Complexes	Spectra (cm^{-1})	Λ_M $\text{ohm}^{-1} \text{cm}^2 \text{mol}^{-1}$
1	11430, 14331, 29499, 33223	12.50
2	16500, 22462, 29851, 33223	8.80
3	11835, 16611, 26955, 299941, 33223	13.50

Antibacterial Activity

Obtained results (Table 4) from antibacterial assay revealed that tested compounds have different inhibition activities toward *Staphylococcus aureus* and *Escherichia coli*, however Schiff base complex 3 has the highest inhibition zone against two bacterial species compared with other compounds followed by Schiff base complex 1. Conversely, Schiff base complex 2 has the lowest inhibition efficacy against both bacterial species relative to the rest of the complexes studied.

Chemicals facing the biological system can have numerous effects such as antibacterial, antifungal, antiviral and antineoplastic effects. In addition, they may be inert [46]. The findings of the present work indicate that all the three complexes have different levels of inhibition activity against the target bacterial species compared to the activity of the antibiotics used as positive control. These differences can be due to the variance in their chemical structure and chemical/physical characteristics.

Table 4: Antibacterial activities of dithiocarbamate and Schiff base metal complexes

Compounds	Inhibition area <i>St. aureus</i> (+)	Inhibition area <i>E. coli</i> (-)
Hy-dtcNH ₄	++	++
1	++	+++
2	+	+
3	+++	+++
Ampicillin	+++	+
Amoxicillin	+++	+
Cephalexin	+++	+++

Not: (0-6)mm = - (Non active), (12) mm = + (Slightly active), (12-14) mm= ++ (Moderately active) and (14-20) mm= +++ (Highly active).

St. aureus =*Staphylococcus aureus* and *E. coli* =*Escherichia coli*.

3D Molecular Modeling and Analysis of Bonding Modes

We have optimized and MM2 calculated the molecular structure of the Schiff base and their metal complexes by using CsChem3D Ultra program package [13]. Therefore we could obtain the optimized geometry for each complex by competing the minimum steric energy and the theoretical physical parameters, such as bond lengths and bond angles. The optimized structures of the complexes are observed in the Figures 11-13, which were some selected calculated parameters in coordination sphere in the Tables 5-7. In complexes, coordination by chelation involving

the various modes of sulfur, nitrogen, oxygen and chloride are possible. These results reveal presence of mixed properties for both the square planar configuration around the central metal ion and the distorted tetrahedral configuration around the two terminal metal ions. All three studied of the Schiff base and three complexes reveals minimum steric energies values (3.032 kcal/mol⁻¹ for Schiff base, 210.12 kcal/mol⁻¹ for complex 1, 180.12 kcal/mol⁻¹ for complex 2 and 150.45 kcal/mol⁻¹ for complex 3). MM2 calculated is in good agreement with the experimental results and confirms the structures.

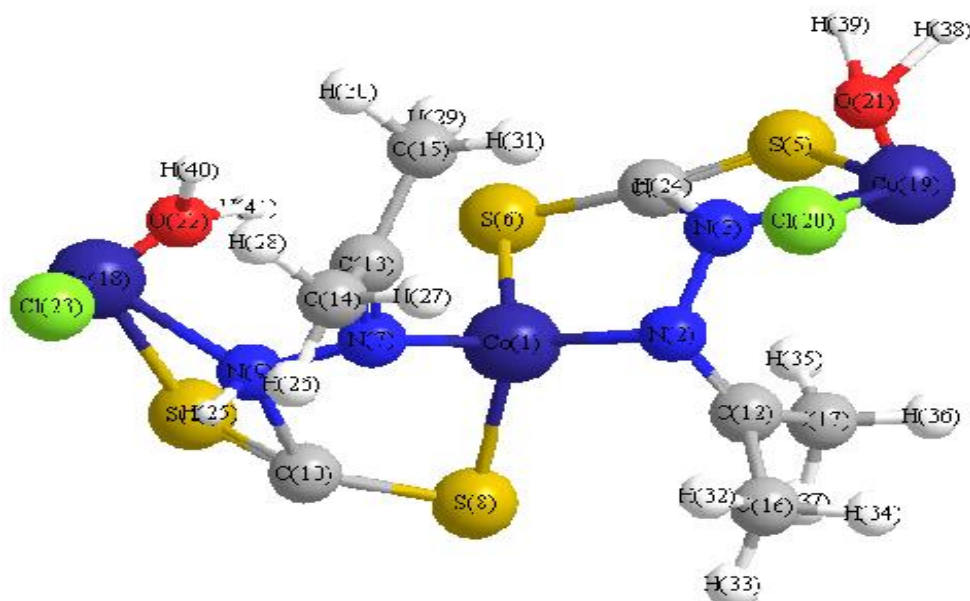


Figure 11: Optimized 3D structure of the cobalt complex 1

Table 5: Some selected calculated parameters of the cobalt complex 1

Bond lengths Å (Central ion)					
Co(19)-Cl(20)	2.1556	O(21)-Co(19)	1.1291	S(8)-Co(1)	2.1714
Cl(23)-Co(18)	2.1446	O(22)-Co(18)	1.1055	S(6)-Co(1)	2.1712
S(5)-Co(19)	2.1495	N(9)-Co(18)	2.0329	N(2)-Co(1)	1.8343
N(3)-Co(19)	2.0119	S(11)-Co(18)	2.1407	N(7)-Co(1)	1.8328
Bond angles° (Terminal ions)					
O(21)-Co(19)-Cl(20)	77.5508	Cl(23)-Co(18)-O(22)	99.9753	N(2)-Co(1)-S(6)	109.7618
O(21)-Co(19)-N(3)	87.5365	Cl(23)-Co(18)-N(9)	75.9975	N(2)-Co(1)-N(7)	111.384
O(21)-Co(19)-S(5)	79.514	Cl(23)-Co(18)-S(11)	114.1313	N(2)-Co(1)-S(8)	113.4677
Cl(20)-Co(19)-N(3)	72.5399	O(22)-Co(18)-N(9)	75.9225	S(6)-Co(1)-N(7)	114.1009
Cl(20)-Co(19)-S(5)	119.1671	O(22)-Co(18)-S(11)	101.3895	S(6)-Co(1)-S(8)	109.2683
N(3)-Co(19)-S(5)	50.8483	N(9)-Co(18)-S(11)	51.0362	N(7)-Co(1)-S(8)	98.5205

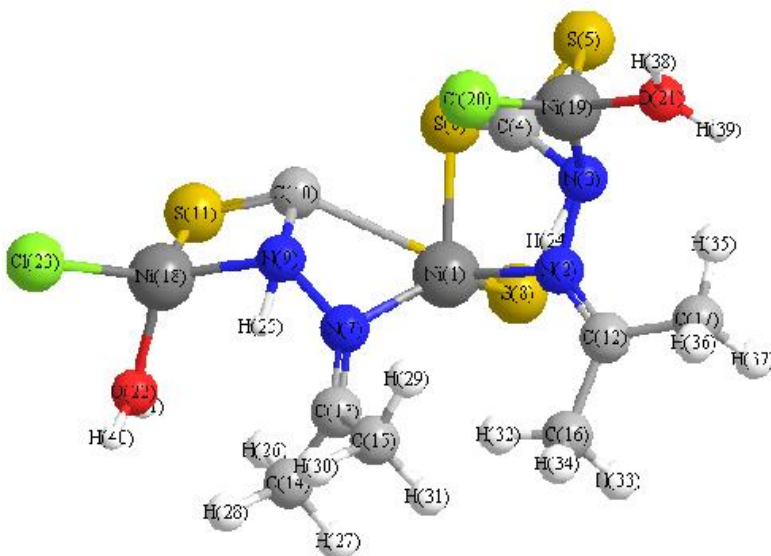


Figure 12: Optimized 3D structure of the nickel complex 2

Table 6: Some selected calculated parameters of the nickel complex 2

Bond lengths Å (Central ion)					
Ni(19)-Cl(20)	2.1323	O(21)-Ni(19)	1.8179	S(8)-Ni(1)	2.1639
Cl(23)-Ni(18)	2.1293	O(22)-Ni(18)	1.8133	S(6)-Ni(1)	2.1642
S(5)-Ni(19)	2.1269	N(9)-Ni(18)	2.0116	N(2)-Ni(1)	1.8222
N(3)-Ni(19)	2.011	S(11)-Ni(18)	2.1254	N(7)-Ni(1)	1.8227
Bond angles° (Terminal ions)					
O(21)-Ni(19)-Cl(20)	108.0591	Cl(23)-Ni(18)-S(11)	115.079	N(3)-N(2)-Ni(1)	116.5601
O(21)-Ni(19)-S(5)	113.6756	Cl(23)-Ni(18)-N(9)	87.449	S(8)-Ni(1)-N(7)	107.1336
O(21)-Ni(19)-N(3)	80.7472	O(22)-Ni(18)-S(11)	111.7745	S(8)-Ni(1)-S(6)	100.5803
Cl(20)-Ni(19)-S(5)	106.788	O(22)-Ni(18)-N(9)	78.6783	S(8)-Ni(1)-N(2)	108.3431
Cl(20)-Ni(19)-N(3)	81.0025	S(11)-Ni(18)-N(9)	51.9062	N(7)-Ni(1)-S(6)	107.668
S(5)-Ni(19)-N(3)	51.883	Cl(23)-Ni(18)-S(11)	115.079	N(7)-Ni(1)-N(2)	124.0319
Cl(23)-Ni(18)-O(22)	104.511	C(12)-N(2)-Ni(1)	107.2433	S(6)-Ni(1)-N(2)	106.6326

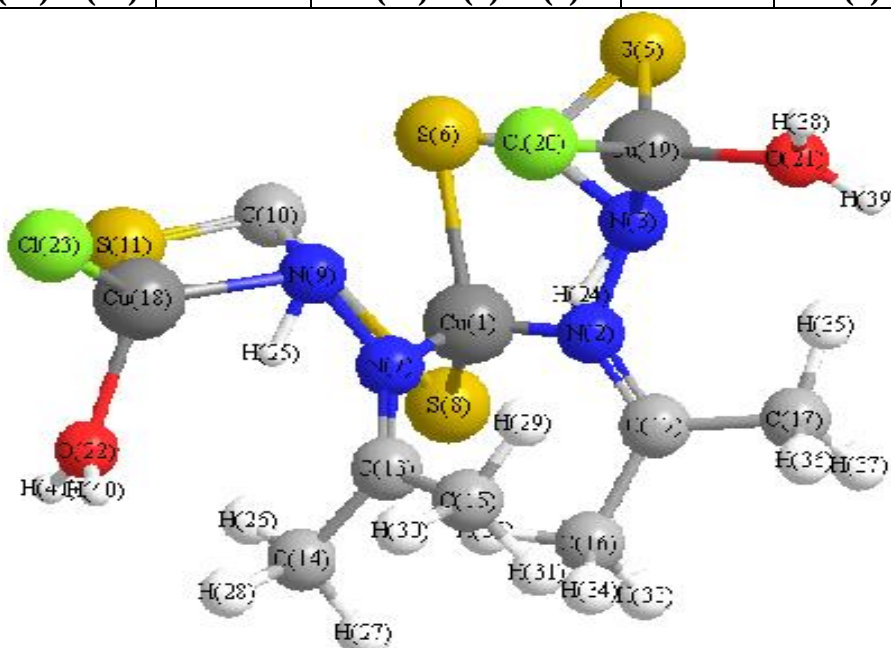


Figure 13: Optimized 3D structure of the copper complex 3

Table 7: Some selected calculated parameters of the copper complex 3

Bond lengths Å (Central ion)					
Cu(19)-Cl(20)	2.1553	O(21)-Cu(19)	1.832	S(8)-Cu(1)	2.2068
Cl(23)-Cu(18)	2.1556	O(22)-Cu(18)	1.8373	S(6)-Cu(1)	2.2159
S(5)-Cu(19)	2.1437	N(9)-Cu(18)	2.0007	N(2)-Cu(1)	1.3641
N(3)-Cu(19)	2.0021	S(11)-Cu(18)	2.1438	N(7)-Cu(1)	1.3611
Bond angles° (Terminal ions)					
O(21)-Cu(19)-Cl(20)	113.9631	Cl(23)-Cu(18)-O(22)	112.5239	C(12)-N(2)-Cu(1)	114.7648
O(21)-Cu(19)-S(5)	123.8416	Cl(23)-Cu(18)-S(11)	121.7194	N(3)-N(2)-Cu(1)	110.8249
O(21)-Cu(19)-N(3)	105.8112	Cl(23)-Cu(18)-N(9)	105.4861	S(8)-Cu(1)-N(7)	114.0136
Cl(20)-Cu(19)-S(5)	121.6008	O(22)-Cu(18)-S(11)	121.6111	S(8)-Cu(1)-S(6)	99.6038
Cl(20)-Cu(19)-N(3)	103.0617	O(22)-Cu(18)-N(9)	92.3949	S(8)-Cu(1)-N(2)	111.504
S(5)-Cu(19)-N(3)	55.505	S(11)-Cu(18)-N(9)	55.012	N(7)-Cu(1)-S(6)	102.0071
N(7)-Cu(1)-N(2)	114.4169	S(6)-Cu(1)-N(2)	114.0397		

Conclusion

New tetradentate N isopropylidene hydrazinedithiocarbamate Schiff base $[(CH_3)_2C=Hy-dtc]$ and their homotrinnuclear cobalt(II), nickel(II) and copper(II) complexes of the general formula $\{M_3[(CH_3)_2C=Hy-dtc]_2(Cl)_2(H_2O)_2\}$ were synthesized. The Schiff base was used as stabilizer ligand for homotrinnuclear metal complexes. The structures of Schiff base and their three complexes were determined by several methods such as elemental analysis, FT-IR, UV-Vis, magnetic susceptibility, molar conductivities and in addition to theoretical calculation using MM2 modeling program. The FT-IR spectra of data suggest the Schiff base acts as a tetradentate attachment. The Schiff base complexes of cobalt (II), nickel (II) and copper (II) have mixed properties for both the square planer configuration around the central metal ion and distorted tetrahedral configuration around the two terminal metal ions and according to the practical measurements and theoretical calculations. Accordingly, these experimental results correspond with the MM2 theoretical results and confirms the structures. The ammonium hydrazinedithiocarbamate ligand and their Schiff base metal complexes were found to be antibacterial activity against one strain of *Staphylococcus aureus* and one strain of *Escherichia coli*. The antibacterial activity is significantly increased on coordination.

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