

## Synthesis, Characterization, Theoretical Crystal Structure and Antibacterial Activities of Some Transition Metal Complexes of The Thiosemicarbazone (Z)-2-(Pyrrolidin-2-Ylidene)Hydrazinecarbothioamide

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### Abstract

**Problem statement:** In Iraq like most third world countries, attempts to discovered a new antibiotic drugs derived from thiosemicarbazied and its metal complexes moreover develop the branch of applied in organic chemistry.

**Approach:** New (Z)-2-(pyrrolidin-2-ylidene) hydrazinecarbo thioamide (L) was synthesized in a good yield by the reaction of pyrrolidone with thiosemicarbazide. Co(II), Ni(II), and Cu(II) complexes of (L) were prepared, and characterized by FT-IR, UV/visible spectra, <sup>1</sup>HNR, and CHN analysis moreover charge, bond length, bond angle, twist angle, heat of formation and steric energy were calculate by using of ChemOffice program. The free ligand and its metal complexes were tested *in vitro* against a number of microorganisms (*Staphylococcus aurous*, *E.coli*, *Proteus vulgaris*, *Pseudomonas*, and *Klebsiella*) in order to assess their antimicrobial properties.

**Results:** The study indicates that these complexes have octahedral geometry, in addition it have high activity against tested bacteria.

**Conclusion/Recommendations:** Based on the reported results, it may be concluded that ligand act as bidentate uninegative ligand, coordinating through one of the nitrogen atom and the sulfur atoms.

Keywords: Thiosemicarbazone, hydrazinecarbothioamide, antibacterial activity.

### Introduction

The chemistry of thiosemicarbazones has received considerable attention in view of their variable bonding modes, promising biological implications, structural diversity, and ion-sensing ability [1–3]. They have been used as drugs and are reported to possess a wide variety of biological activities against bacteria, fungi, and certain type of tumors and they are also a useful model for bioinorganic processes [4–6]. The activity of these compounds is strongly dependent upon the nature of the heteroatomic ring and the position of attachment to the ring as well as the form of thiosemicarbazone moiety [7]. These are studied extensively due to their flexibility, their selectivity and sensitivity towards the central metal atom, structural and similarities with natural biological substances, due to the presence of imine group (–N=CH–) which imparts the biological activity [8-12]. There is

no report on the complexes of (Z)-2-(pyrrolidin-2-ylidene) hydrazinecarbothioamide (L). We now present details of the complexes of (L) with cobalt (II), nickel (II), and copper (II) ion.

### Materials and Methods

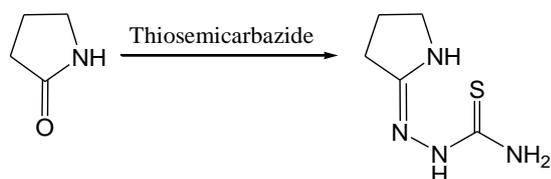
#### General:

All chemical used were of reagent grade (supplied by either Merck or Fluka) and used as supplied. The FTIR spectra in the range (4000–200) cm<sup>-1</sup> were recorded as cesium iodide disc on FTIR 8300 Shimadzu Spectrophotometer. Proton NMR spectra were recorded on Bruker -DPX 300 MHz spectrometer with TMS as internal standard in Jordan University. The UV-Visible spectra were measured in ethanol using Shimadzu UV-Vis. 160 A spectrophotometer in the range (200-1000) nm. Magnetic susceptibility measurement for complexes were obtained at

room temperature using (Magnetic susceptibility Balance Model MSB-MKI). Flame atomic absorption of elemental analyzer, shimadzu AA-670 was used for metal determination. Elemental micro analysis, was carried out using C.H.N elemental analyzer model 5500-Carlo Erba instrument. Gallen Kamp M.F.B.600.010 F melting point apparatus was used to measure the melting point of all the prepared compounds.

**Synthesis of (Z)-2-(pyrrolidin-2-ylidene)hydrazinecarbothioamide (L):**

Pyrrolidone (0.01 mole) in hot ethanol (20 mL) was mixed with hot ethanolic solution of thiosemicarbazide (0.01 mole). The mixture was refluxed for 6 hours on a water bath, on cooling the contents the precipitate was separated out, filtered, washed with 50% cold ethanol and dried in vacuum over  $P_4O_{10}$ , melting point  $176\text{ }^\circ\text{C}$ , yield 73% of yellow crystal (Z)-2-(pyrrolidin-2-ylidene)hydrazinecarbothioamide. The proposed structure can be shown according to the following reaction:



Proton NMR (1.4 t(2H) for  $\text{CH}_2$ , m. 2.0(2H) for  $\text{CH}_3$ , t. 2.9(2H) for  $\text{CH}_2$ , 2.4 for NH, 8.7 for  $\text{NH}_2$ , 10.8 for NH). Elemental analysis found % C 37.10(37.95), H 6.12(6.37), N 34.85(35.41) calculated for  $\text{C}_5\text{H}_{10}\text{N}_4\text{S}$ , Molecular weight: 158.

**Synthesis of the complexes:**

Metal salt (0.005 mole) in hot ethanol (20 mL) was mixed with hot ethanolic solution of the ligand (0.01 mole) and refluxed for 4 h

on a water bath, on cooling the contents, the colored complexes separated out in each case. The product was filtered, washed with cold 50% ethanol and dried in vacuum over  $P_4O_{10}$ . Purity of the complexes was checked by Thin Layer Chromatography (TLC).

**Study of complex formation in solution:**

The complexes of the ligand with metal ions were studied in DMF, in order to determine M:L ratio in the complex following the molar ratio method. A series of solutions were prepared having a constant concentration ( $10^{-3}$  M) of the metal ion and (L). The M:L ratio was determined from the relationship between the absorption of light and the mole ratio of M:L. The results of complexes formation in solution were listed in Table (1).

**The biological activity for the ligand and its complexes:**

All tests with the microorganisms were obtained from the *biotechnology division, department of applied science, University of Technology* which were follows: *Escherichia coli*, *Klebsiella pneumoniae*, *Proteus vulgaris*, *Pseudomonas aeruginosa*, and *Staphylococcus aureus*. Antibacterial activities of the ligand and the soluble complexes were evaluated by the disc diffusion technique [13]. Filter paper (Whatman No. 4) discs (6 mm diameter) were soaked in a solution of the test compounds of  $0 \times 5 \text{ mg cm}^{-3}$  concentration in DMF and placed on nutrient agar-plates after drying to remove the solvent. The inhibition zones were measured after 24 h. DMF was used as control. The results are shown in Fig.(2).

**Results**

**General:**

The complexes were synthesized by reacting ligand with the metal ions in 1:2 molar ratio in ethanolic medium.

Table (1)

Analytical conductivity, colors, elemental analysis and magnetic moment data of the complexes.

Complex	Yield %	M.P. °C	Analysis: Found (cal.) %				M:L	Color	$\Omega m\ ohm^{-1}\ cm^2\ mol^{-1}$
			Metal	C	H	N			
Co(C <sub>5</sub> H <sub>10</sub> N <sub>4</sub> S) <sub>2</sub> Cl <sub>2</sub>	75	Over 300	13.21 (12.7)	26.91 (26.4)	4.52 (4.22)	25.11 (24.87)	1:2	Dark brown	70
Ni(C <sub>5</sub> H <sub>10</sub> N <sub>4</sub> S) <sub>2</sub> Cl <sub>2</sub>	60	Over 300	13.16 (12.65)	26.93 (25.12)	4.52 (4.12)	25.12 (24.16)	1:2	light green	65
Cu(C <sub>5</sub> H <sub>10</sub> N <sub>4</sub> S) <sub>2</sub> Cl <sub>2</sub>	77	260	14.09 (13.39)	26.64 (25.94)	4.47 (4.30)	24.85 (24.43)	1:2	green	30

**Infrared spectroscopy:**

A study and comparison of infrared spectra of free ligand and its metal complexes (Table (2)) imply that the ligand behaves as

neutral bidentate and its metals are coordinated through N and S of the thio-keto group (See Fig.(1)).

Table (2)

Infrared absorption frequencies (cm<sup>-1</sup>) of Co (II), Ni (II) and Cu (II) complexes.

Compounds	$\nu(N-H)$	$\nu(C=N)$	$\nu(C-N)$	$\nu(N-N)$	$\nu(C=S)$	$\frac{\nu(M-N)}{\nu(M-S) / \nu(M-Cl)}$
Ligand	3395 s 3275 s	1600 s	1330 s 1200 m	1035 m	855 s 770 s	–
Co(C <sub>5</sub> H <sub>10</sub> N <sub>4</sub> S) <sub>2</sub> Cl <sub>2</sub>	3330 m 3265 m	1570 s	1380 s 1240 m	1075 m	850 s 780 m	525 m 440 m 350 <sub>w</sub>
Ni(C <sub>5</sub> H <sub>10</sub> N <sub>4</sub> S) <sub>2</sub> Cl <sub>2</sub>	3320 m 3260 m	1565 s	1380 s 1235 m	1070 m	835 s 780 m	535 m 420 m 355 <sub>w</sub>
Cu(C <sub>5</sub> H <sub>10</sub> N <sub>4</sub> S) <sub>2</sub> Cl <sub>2</sub>	3385 m 3275 m	1575 s	1365 s 1240 m	1060 m	840 s 795 m	520 m 430 m 360 <sub>m</sub>

Strong bands in the 3394, and 3275 cm<sup>-1</sup> region in the ligand was observed due to (N–H) vibrations. The negligible effect on these frequencies after complexation precludes the possibility of complexation at this group. The absorption at 1600 cm<sup>-1</sup> in free ligand can be attributed to (C=N) stretching vibration of imine nitrogen, which is in a good agreement with previous observations. On complexation this frequency was observed to be shifted to a lower wave number (Table (2)). These observations suggest the involvement of unsaturated nitrogen atoms of the azomethine groups in bonding with the metal ions. Coordination of sulfur with the metal ion would result in the displacement of electrons towards the latter, thus resulting in the weakening of the (C=S) bond. Hence, on complexation (C=S) stretching vibrations should decrease and those of (C–N) should

increase. The IR spectral bands in the ligand is practically unchanged in the complexes, but show some new bands with medium to weak intensity in the 520-440 cm<sup>-1</sup> region tentatively assigned to (M–N) and (M–S). (M–Cl) is tentatively assigned in the 360-350 cm<sup>-1</sup> region [14-15].

**Magnetic susceptibility:**

At room temperature all the complexes under study show the magnetic moment in the range 2.1-4.7 B.M. corresponding to the unpaired electrons. The magnetic moment of Co(II) complex is 4.1 BM indicating that the Co(II) complex is typically high spin complex and having octahedral structure [16]. For Ni(II) complex the observed magnetic moment value is 3.0 BM which is well within the expected range for Ni (II) complex with octahedral stereochemistry (2.83-4.0BM). The

magnetic moment for Cu (II) complex is 2.0 BM. The reported values for the Cu (II) complex having no major spin orbital interactions (1.75-2.20 BM) [16-17]. Thus the present Cu (II) complex is devoid of any spin orbital interaction with octahedral geometry. In octahedral Cu (II) complex the ground state is  $^4T_{1g}$  and large spin orbital contribution to the magnetic moment is expected.

### Uv-visible spectroscopy

#### Cobalt (II) complexes:

The electronic spectra of Co(II) complex recorded in DMF solution display three absorption bands at 8100, 16500 and 22000  $\text{cm}^{-1}$  corresponding to the following transitions respectively.  $^4T_{1g}(F) \rightarrow ^4T_{2g}(F)$ ,  $^4T_{1g}(F) \rightarrow ^4A_{2g}(F)$ ,  $^4T_{1g}(F) \rightarrow ^4T_{1g}(P)$  This indicates that these complexes have octahedral geometry.

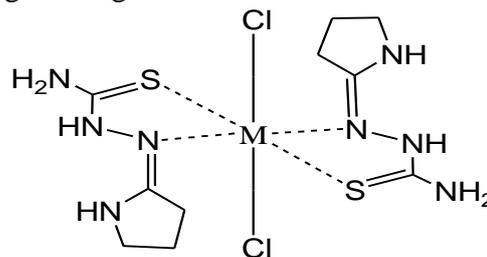
#### Nickel (II) complexes:

The electronic spectra of the Ni (II) complex show absorptions bands at 9000, 13000 and 24000  $\text{cm}^{-1}$  and may be assigned to the transitions  $^3A_{2g} \rightarrow ^3T_{2g}$ ,  $^3A_{2g} \rightarrow ^3T_{1g}(F)$ ,  $^3A_{2g}(F) \rightarrow ^3T_{1g}(P)$  corresponding to an octahedral geometry.

#### Copper (II) complex:

The Cu (II) complex under study display absorption band 13400 and 16000  $\text{cm}^{-1}$ . These bands were assigned to the following transitions form a distorted

octahedral geometry [18].  $^2B_{1g} \rightarrow ^2A_{1g}$ ,  $^2B_{1g} \rightarrow ^2B_{2g}$

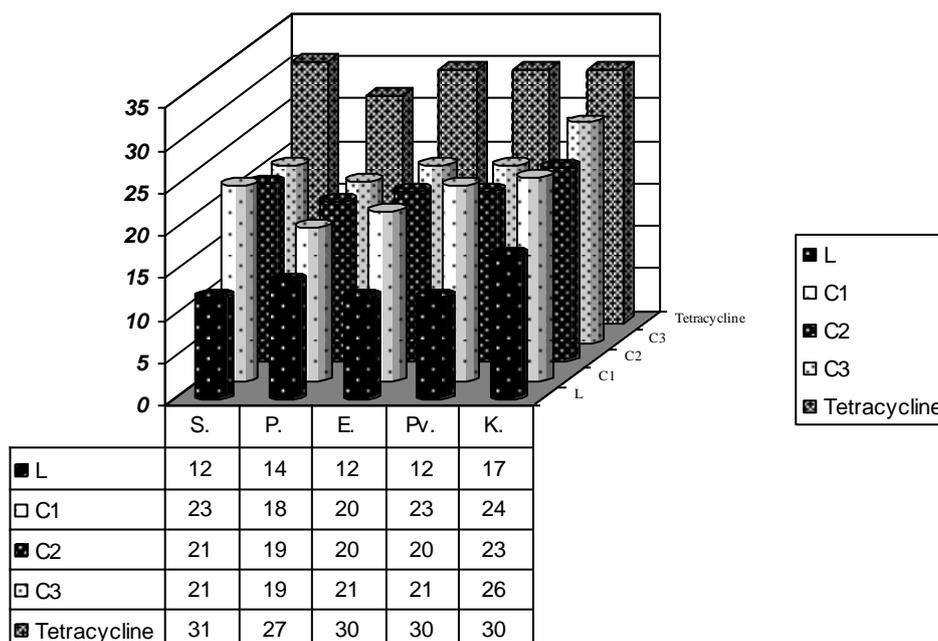


M = Co, Ni , Cu

Fig. (1) Structures of the complexes.

### Biological activity:

It is known that chelation tends to make the ligand act as more powerful and potent bactericidal agents, thus killing more of the bacteria than the ligand. It is observed that, in a complex, the positive charge of the metal is partially shared with the donor atoms present in the ligands, and there may be  $\pi$ -electron delocalization over the whole chelate [19]. This increases the lipophilic character of the metal chelate and favours its permeation through the lipid layer of the bacterial membranes. The increased lipophilic character of these complexes seems to be the reason of their enhanced potent antibacterial activity. There are other factors which also increase the activity, which are solubility, conductivity, and bond length between the metal and the ligand.

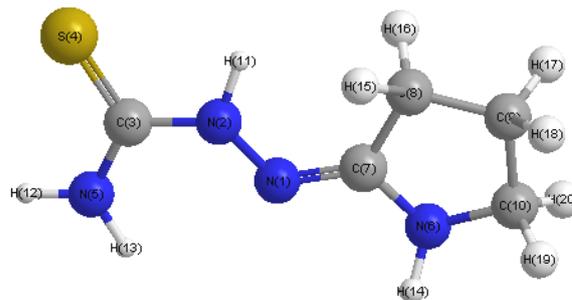


S.= *Staphylococcus aureus*, E.= *E.coli*, Pv.= *Proteus vulgaris*, P.= *Pseudomonas*, and K.= *Klebsiella*.

Fig.(2) : Antibacterial activity of the ligand and it metal complexes.

**Stability study:**

These data show that the atomic charge was affected by the presence of substituent of rings as shown in Tables (3-5). As a reference compound the unsubstituted Ligand (Fig.(3)) the data for minimized geometry (Tables (3-5)) and the 3d-geometrical structure (Fig.(3)) is shown in.



**Fig.(3) The 3d-geometrical structure for the ligand.**

**Table (3)  
Bond lengths of the ligand.**

Bond	Actual	Optimal	Bond	Actual	Optimal	Bond	Actual	Optimal
N(2)-H(11)	1.0117	1.0120	C(8)-H(15)	1.1188	1.1130	N(5)-H(13)	0.9906	1.0120
H(20)-C(10)	1.1242	1.1130	C(9)-C(8)	1.5256	1.5230	H(12)-N(5)	0.9929	1.0120
C(10)-H(19)	1.1246	1.1130	C(7)-N(1)	1.3204	1.2600	C(3)-N(5)	1.3652	1.3690
H(18)-C(9)	1.1167	1.1130	C(7)-C(8)	1.5251	1.4970	C(3)-S(4)	1.6285	1.5760
C(9)-H(17)	1.1169	1.1130	H(14)-N(6)	0.9976	1.0500	N(2)-C(3)	1.4145	1.3690
C(10)-C(9)	1.5399	1.5230	C(10)-N(6)	1.4571	1.4700	N(1)-N(2)	1.3414	
C(8)-H(16)	1.1188	1.1130	C(7)-N(6)	1.4224	1.4620			

**Table (4)  
Bond Angles of the ligand.**

Angle	Actual	Optimal	Angle	Actual	Optimal
H(20)-C(10)-H(19)	108.0742	109.4000	C(7)-C(8)-H(15)	110.1767	109.4100
H(20)-C(10)-C(9)	110.8390	109.4100	C(7)-C(8)-C(9)	105.3224	109.5000
H(20)-C(10)-N(6)	107.3801		N(1)-C(7)-C(8)	128.1179	115.1000
H(19)-C(10)-C(9)	110.4255	109.4100	N(1)-C(7)-N(6)	121.7403	126.0000
H(19)-C(10)-N(6)	111.8302		C(8)-C(7)-N(6)	110.0955	125.3000
C(9)-C(10)-N(6)	108.2648		C(10)-N(6)-H(14)	115.3567	
H(18)-C(9)-H(17)	108.0210	109.4000	C(7)-N(6)-H(14)	116.0931	118.0000
H(18)-C(9)-C(10)	110.5216	109.4100	C(7)-N(6)-C(10)	109.1525	
H(18)-C(9)-C(8)	111.1762	109.4100	H(12)-N(5)-H(13)	119.3842	118.8000
C(10)-C(9)-H(17)	110.4261	109.4100	C(3)-N(5)-H(13)	123.4115	
H(17)-C(9)-C(8)	110.9742	109.4100	H(12)-N(5)-C(3)	117.1111	
C(10)-C(9)-C(8)	105.7415	109.5000	N(5)-C(3)-S(4)	122.0027	124.3000
H(15)-C(8)-H(16)	108.4617	109.4000	N(2)-C(3)-N(5)	120.9560	120.0000
C(9)-C(8)-H(16)	111.3872	109.4100	N(2)-C(3)-S(4)	116.9829	124.3000
C(7)-C(8)-H(16)	110.1951	109.4100	C(3)-N(2)-H(11)	112.0942	117.4000
C(9)-C(8)-H(15)	111.2857	109.4100	N(1)-N(2)-H(11)	120.3309	
C(10)-C(9)-H(17)	110.4261	109.4100	N(1)-N(2)-C(3)	122.2156	

**Table (5)**  
**Atomic Charge of the ligand.**

Atoms	Charges	Atoms	Charges	Atoms	Charges	Atoms	Charges
N -0.431	[N(1)]	N 0.081	[N(6)]	H 0.068	[H(11)]	H 0.040	[H(16)]
N 0.263	[N(2)]	C 0.222	[C(7)]	H 0.101	[H(12)]	H 0.031	[H(17)]
C 0.233	[C(3)]	C -0.122	[C(8)]	H 0.104	[H(13)]	H 0.028	[H(18)]
S -0.696	[S(4)]	C -0.066	[C(9)]	H 0.091	[H(14)]	H 0.011	[H(19)]
N -0.049	[N(5)]	C 0.036	[C(10)]	H 0.038	[H(15)]	H 0.018	[H(20)]

### Discussion

All the solid complexes are stable in air. The metal complexes are soluble in DMF and DMSO. Table (1) shows the colors, elemental analyses and molar conductivities of the cobalt (II), nickel (II), and copper (II) complexes. Thiosemicarbazones can coordinate with metal ions as neutral ligand. The C, H, N data indicate that the complexes of neutral ligand is coordinated to the metal ion and the other coordination positions were occupied by chlorine, as confirmed by the IR spectra of the complexes.

The antibacterial screening (Fig.(2)), indicate that the the complexes, inhibit the growth of *Staphylococcus aurous*, and *Klebsiella*, whereas other complexes have less activity against other tested bacteria.

The theoretical data obtained show that the heat of formation is 52.61737 kcal/mole, and the highest atomic charge in ligand molecule is at [S<sub>4</sub> -0.696] the next charge value is at [N<sub>1</sub>-0.431]. These data show clearly that these atoms are the most reactive toward the bonding with the metal. The determined bond angle and 3D-geometrical (Fig.(3)) structure, indicate that this molecule is planar.

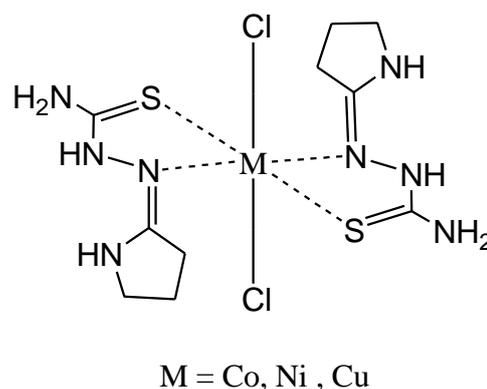
The stability for the prepared complexes were studied theoretically by the Density Function Theory (DFT). The total energy for the complexes was calculated and it was shown that the copper complex is the most stable and the cobalt complex is the least stable as follows:



### Conclsions

Based on the reported results, it may be concluded that ligand act as bidentate uninegative ligand, coordinating through one of the nitrogen atom and the sulfure. In the present work, which facilitates formation of five member rings, shifts the nitrogen atom of

the other ring away from the coordination site. In the present investigations, all the complexes are found to be mononuclear, based on the FT-IR spectral data. The coordination number five is attained by coordination with the two bidentate ligand molecules and to two chloride atoms. Based on the physicochemical and the spectral studies the tentative structures proposed for the complexes are shown in Fig.(4).



**Fig.(4) Structure of the complexes.**

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### الخلاصة

تم تحضير المشتق الجديد 3-امينو-2-مثيل كوينازولين-4 (3هيدرو)-ون من تفاعل استرة البايروليدينون بالايثانول مع الثايبوسيميكاريزايد. تم اختبار كلوريدات لبعض العناصر الانتقالية [ الكوبالت، النيكل، و النحاس الثنائية] كأملاح نقية لتفاعلها وتعقيدها مع المخلب الجديد 3-امينو-2-مثيل كوينازولين-4(3هيدرو)-ون. تم تشخيص المعقدات الجديدة بعد عزلها بطيف الأشعة تحت الحمراء المعززة بتحويلات فورير F.T.I.R، الرنين النووي المغناطيسي (للمخلب الجديد) والأطياف الإلكترونية بالإضافة الى تحديد النسبة المولية ليكاند : فلز، فضلا عن قياس الموصلية المولارية لمحاليل المعقدات في مذيب N,N-ثنائي مثيل فورم اميد وقياس العزم المغناطيسي المؤثر للمعقدات الصلبة، كما تم حساب اطوال الاواصر وزوايا التاصرووشحنة الذرة باستخدام برنامج الكم اوفيس. تم دراسة الفعالية المضادة للجراثيم لكل من المخلب ومعقداته على خمسة أنواع من البكتريا هي (*Staphylococcus aureus*, *E. coli*, *Proteus Vulgaris*, *Pseudomonas*, and *Klebsiella*).