مجلة الدراسات التربوية والعلمية - كلية التربية - الجامعة العراقية
العدد السابع والعشرون - المجلد العاشر - علوم الكيمياء - نيسان 2026 م
doi.org/10.52866/esj.2026.10.27.19

# Preparation, characterization and evaluation of the biological activity of Cd and phosphine complexes derived from 2-thiouracil

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**Abstract:**

This study included the synthesis of a number of cadmium complexes by reacting cadmium chloride with one mole of thiauracil and two moles of sodium hydroxide to produce the complex $[Cd(L)_2]$ to be the nucleus in the formation of the rest of the complexes, and then reacting this complex L2 to produce the complex $[Cd(L)_2(dppm)]$ and reacting with (dppe) to produce $[Cd(L)_2(dppe)]$, respectively. Spectroscopic investigations, including infrared spectra and nuclear magnetic spectra of protons and phosphorus, validated the validity and precision of these complexes. Furthermore, two types of negative bacteria - Escherichia coli and positive Staphylococcus aureus - were used to test the complexes' efficacy, and the results indicated that the complexes were effective against both of these bacteria. Even if the complexes are more effective against Staphylococcus aureus, they may still be useful medicinal substances.

**Keywords:** coordination chemistry, 2-thioracil, Biological activity**.**

# تحضير وتشخيص وتقييم الفعالية البايولوجية لمعقدات Cd والفوسفين المشتقة من -2ثاييوراسيل

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**مستخلص:**

تضمنت هذه الدراسة تحضير عدد من معقدات الكادميوم من خلال تفاعل كلوريد الكادميوم مع مول واحد من الثايويوراسيل واثنين مول من هيدروكسيد الصوديوم لتكوين المعقد $[Cd(L)_2]$، والذي اعتُمد كنواة لتحضير بقية المعقدات. بعد ذلك، تم تفاعل هذا المعقد مع (dppm) لتكوين المعقد $[Cd(L)_2(dppm)]$، ومع (dppe) لتكوين المعقد $[Cd(L)_2(dppe)]$ على التوالي. جرى توصيف المعقدات المحضرة باستخدام تقنيات طيفية شملت طيف الأشعة تحت الحمراء وطيف الرنين المغناطيسي النووي للبروتون والفوسفور، مما أكد صحة ودقة البنية المقترحة لهذه المعقدات. علاوة على ذلك، تم تقييم الفعالية الحيوية لهذه المعقدات ضد نوعين من البكتيريا، إحداهما سالبة الغرام (Escherichia coli) والأخرى موجبة الغرام (*Staphylococcus aureus*)، وأظهرت النتائج أن المعقدات فعّالة ضد كلا النوعين، مع فعالية أعلى تجاه بكتيريا *Staphylococcus aureus*، مما يشير إلى إمكانية توظيفها كمركبات دوائية واعدة.

الكلمات المفتاحية: الكيمياء التناسقية ، 2-ثايويوراسيل ، الفعالية البايولوجية .

## 1. Introduction

Coordination chemistry has been the most popular form of inorganic chemistry for less than 10 years, having studied and developed numerous complexes. It is important in biochemistry, where it studies metal-containing molecules and how they bind within biological systems. It is involved in the formation of metal-containing drugs [1]. Because the antimicrobial activity of metal chelates is generally higher than that of the chelating molecules themselves, inorganic biochemistry is becoming increasingly important in the field of inorganic chemistry. Because of their uses in biology, medicine, and agriculture, pyrimidine derivatives are very interesting [2]. Numerous research have recently focused on pyrimidine-metal complexes because of their diverse biological activities, which include antimalarial, antibacterial, anticancer, and antiviral properties[3,4]. Many studies have explored the role of uracil thioesters, thiouracils, and pyrimidines in biological processes by providing metal ion binding sites [5]. In 1817 AD, the Germans Heymann and Friedrich Stromeyer first discovered cadmium. Cadmium metal is characterized by its delicate white color and pungent odor. It emits toxic fumes when burned. According to the World Health Organization, cadmium is one of the most dangerous compounds in the world due to its severe pollution [6] Cadmium has the electrical composition $4s^2 4d^{10}$ and two oxidation states, II and III. [7] Its atomic number is (48).

## 2. Materials and Methods:

### 2.1. Chemicals and Instruments

All research materials were collected from well-known companies such as Al-Aldrich , Falaka and Merck.

### 2.2. Preparation of Complex (L1) [8,9]:

Equal moles (1 mol) of each of the materials sodium hydroxide (1 g) and (0.312 g) of 2-thiouracil were mixed with cadmium chloride (1.12 g) in absolute ethanol for 3 hours at 25 °C until a Portuguese precipitate was given. The precipitate was recrystallized by DMF, the product was filtered, and the material was collected.

[Cd(L)2]

*Orange yield: 71%; mp = 195–197*

*°C; I.R ν(cm⁻¹)= 3245(N-H), 3141(=C-H), 3066(Ar-CH),1654 (C=O), 1596 (-C=C-), 1103 (-C=S-), 520 (-Cd-O), 466(Cd-N) cm⁻¹; ¹H-N.M.R: δ(ppm) = 7.44-7.43 (2H, d, =C-H), 7.40 (2H, s, N-H), 6.79,6.78 (2H, d, H-C=).*

**2.3. Preparation of Complex (L2) [10]:**

Equal quantities of (1 mol) of L1 (0.15 g) were mixed with dppm solution (0.1 g) in absolute ethanol until a brown precipitate was given. The material was then filtered and dried in an oven. [$Cd(L)_2$(dppm)]

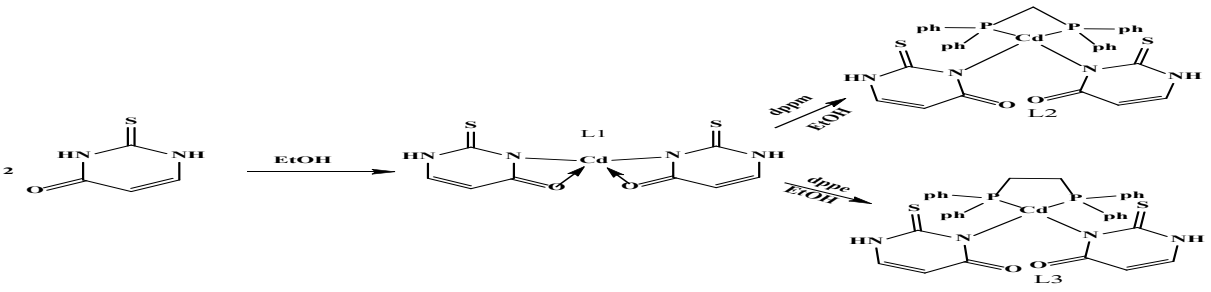
*Brown yield: 78%; mp = 278–280 °C; I.R ν(cm⁻¹)= 3211(N-H), 3171(=C-H), 3036(Ar-C-H), 2941, 2858 ($CH_{Aliphatic}$), 1653 (C=O), 1600 (-C=C-), 1541, 1491 (Ar-C=C-), 1437 (P-Ph),1103 (-C=S-), 1014 (-C-P), 495 (-Cd-O), 434(-Cd-N) cm⁻¹; ¹H-N.M.R: δ(ppm) = 7.492) H, s, NH), 7.42,7.40 2)H, d, =CH), 7.32-7.2320) H, m, ph), 5.65, 5.632) H, d, HC= ), 2.012) H, s, $CH_2$); ³¹P-NMR: δ(ppm) = 27.84 (P)*

**2.4. Preparation of Complex (L3) [11]:**

Equal quantities of (1 mol) of L1 (0.15 g) were mixed with dppesolution (0.1 g) in absolute ethanol until a *Green* precipitate was given. The material was then filtered and dried in an oven. In accordance with all laboratory safety regulations, solutions of cadmium (Cd) and its complexes were disposed of by chemical precipitation ($Na_2S$ or NaOH) to produce insoluble deposits. These were then gathered and dried in designated containers with hazardous waste and sent to the unit for the safe disposal of heavy metals.

[$Cd(L)_2$(dppe)]

*Green yield: 73%; mp = 263–265 °C; I.R ν(cm⁻¹)= 3254(N-H), 3130(=C-H), 3036 (Ar-C-H), 2958, 2848 ($CH_{Aliphatic}$), 1656 (-C=O), 1610(-C=C-), 1535, 1489 (Ar-C=C-), 1438 (P-Ph),1111 (-C=S), 1057 (-C-P),497 (-Cd-O), 462 (Cd-N) cm⁻¹; ¹H-N.M.R: δ(ppm) = 7.772) H, s, NH), 7.53,7.52 2)H, d, =CH), 7.51-7.34 (20H, m, ph), 5.68, 5.662) H, d, H-C= ), 1.12-1.08 4)H, t, -$CH_2$-$CH_2$); ³¹P-N.M.R: δ(ppm) = 27.95 (P)*




**Scheme 1: Preparation of complexes (L1-L3)**

### 2.5. Biological activity evaluation

*Staphylococcus aureus* and *Escherichia coli*, two bacteria found in the central laboratories of Tikrit University, were used to create a Mueller-Hunton agar culture medium. 39 grams of bacteria were dissolved in a liter of water, stirred, and then heated in a sterile pressure vessel at 1.5 bar for 14 minutes at 120°C. They were cooled, transferred to Petri dishes, and dried at 25°C [12,13]. Three doses of each complex (0.01, 0.001, and 0.0001) mg/ml were then prepared in dimethyl sulfoxide solvent. After that, the dried bacteria in their designated plates were used to wipe the dishes in which the medium was poured in three different directions in order to thoroughly spread the bacteria. The solutions were then poured into the three holes made in the dishes by piercing them with a 6 mm cork piercer. *Amoxicillin* was used as a control sample, and the plates were then stored in a dedicated container at 37°C for a whole day. The findings were then measured with a ruler in millimeters [14,15].

## 3. Results and discussions

### 3.1. Characterization of complexes (L1-L3)

Spectral measurements, including FT-IR, confirmed the validity of the prepared complexes as they showed the presence of new bands in the [Cd(L)2] complex, including a band at (466) cm-1, which was attributed to the (Cd-N) stretching, and another band at (520) $cm^{-1}$, which was attributed to the (Cd-O) bond stretching, while the reduction of the (C=O) bond stretching appeared at (1654) $cm^{-1}$. The remaining bonds also retained their positions as the

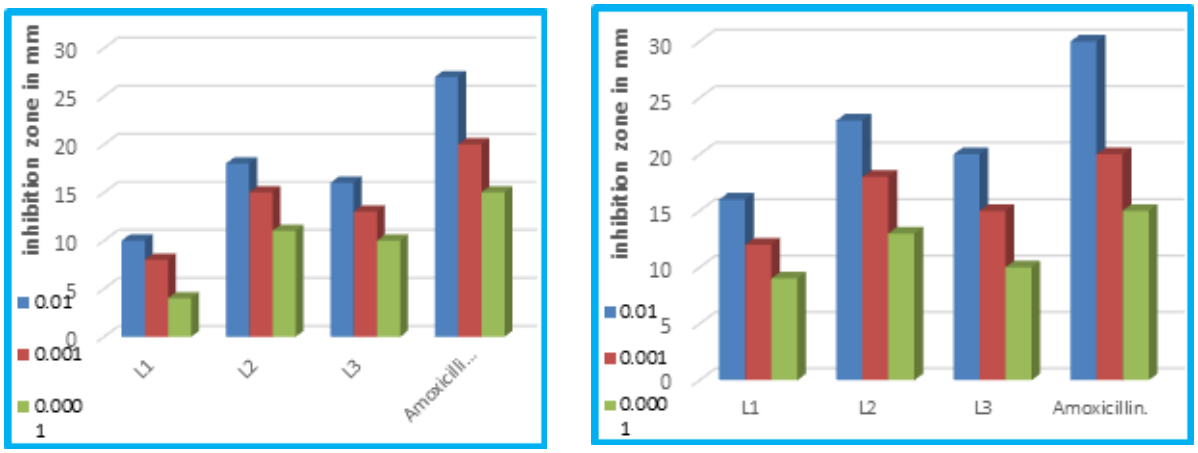
(NH) band appeared at (3245) $cm^{-1}$ and the band at (1103) $cm^{-1}$, which was attributed to the (C=S) stretching[16].As for the complexes $[Cd(L)_2(dppm)]$ and $[Cd(L)_2(dppe)]$, the presence of new bands was shown. A band appeared in the range (1489-1541) $cm^{-1}$ attributed to the benzene rings linked to the phosphines, and another band at (1438, 1437) $cm^{-1}$ was for (P-Ph) stretching. It also showed a band at (1014, 1057) $cm^{-1}$ for stretching (C-P) bonds, in addition to the presence of (Cd-N) and (Cd-O) bands in the same ranges at (434, 462 & 495, 497) $cm^{-1}$, respectively [17]. Through the $^{1}H$-NMR study, the formation of the complex $[Cd(L)_2]$ was confirmed by the appearance of a double signal at (7.44, 7.43) ppm attributed to (=CH), a single signal at (7.40) ppm, usually (NH), as well as a double signal at (6.79, 6.78) ppm attributed to (=CH). For the $[Cd(L)_2(dppm)]$ and $[Cd(L)_2(dppe)]$ complexes, a multiple signal was observed at 7.23 and 7.51 ppm, attributed to the benzene rings attached to the phosphine [18]. The $[Cd(L)_2(dppm)]$ complex showed a single signal at (2.01) ppm, typically for ($CH_2$), while the $[Cd(L)_2(dppe)]$ complex showed a triple signal at (1.12–1.08) ppm, which was for ($CH_2$–$CH_2$) [19]. A $^{31}P$-NMR study of the $[Cd(L)_2(dppm)]$ and $[Cd(L)_2(dppe)]$ complexes revealed that the presence of a single signal indicates a single isomer at positions (27.84–27.95) ppm [20].

**3.2. Biological activity test results**

The results we obtained through the biological activity of the complexes against the two types of bacteria used under study show that they have promising antibacterial activity, especially at high concentrations. Naturally, the formed complexes had a greater effect against Staphylococcus aureus bacteria compared to Escherichia coli bacteria, which was less effective [21]. This is consistent with previous studies indicating that pathogenic bacteria have an outer membrane containing lipopolysaccharides, which reduces the waste of compounds inside these bacteria, while positive bacteria have a less complex wall than is the case in negative bacteria. Despite the success of the antibiotic amoxicillin, these complexes can be promising pharmaceutical compounds [22,23].

**Table (1): Antibacterial activity of compounds (mm).**

| Comp. No. | *E.coli*.mg/ml | | | *Staph. aureus* mg/ml | | |
|---|---|---|---|---|---|---|
| | **0.01** | **0.001** | **0.0001** | **0.01** | **0.001** | **0.0001** |
| $L_1$ | 10 | 8 | 4 | 16 | 12 | 9 |
| $L_2$ | 18 | 15 | 11 | 23 | 18 | 13 |
| $L_3$ | 16 | 13 | 10 | 20 | 15 | 10 |
| *.Amoxicillin* | 27 | 20 | 15 | 30 | 20 | 15 |




**Scheme (2): L1-L3 inhibitory action against Staph. aureus and E. coli**

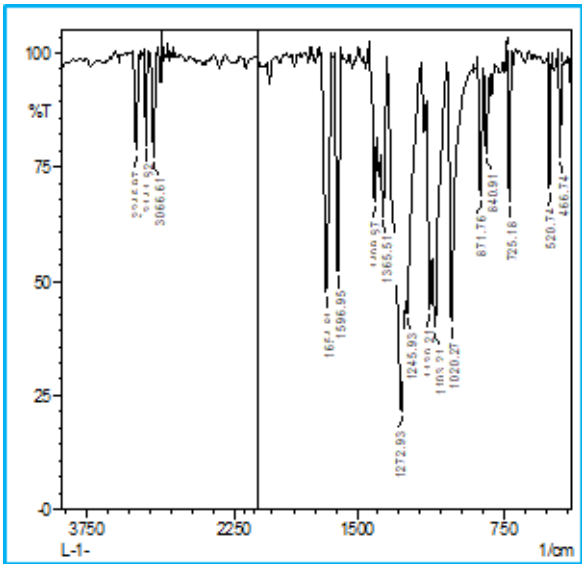



**Fig (1): FT-IR of (L1)**

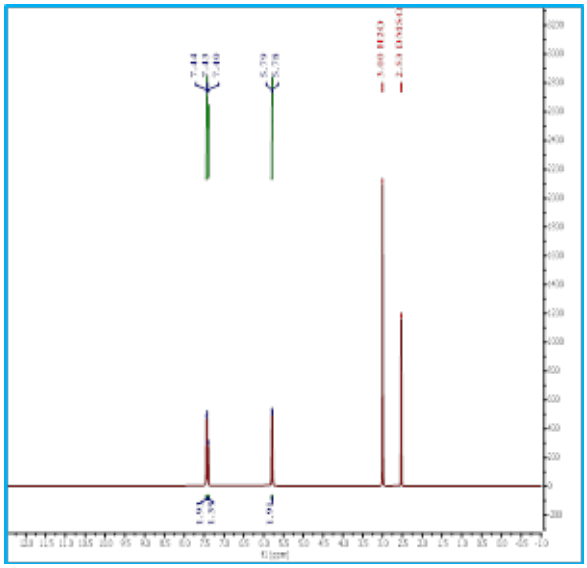


**Fig (2): $^1$H-NMR of (L1).**

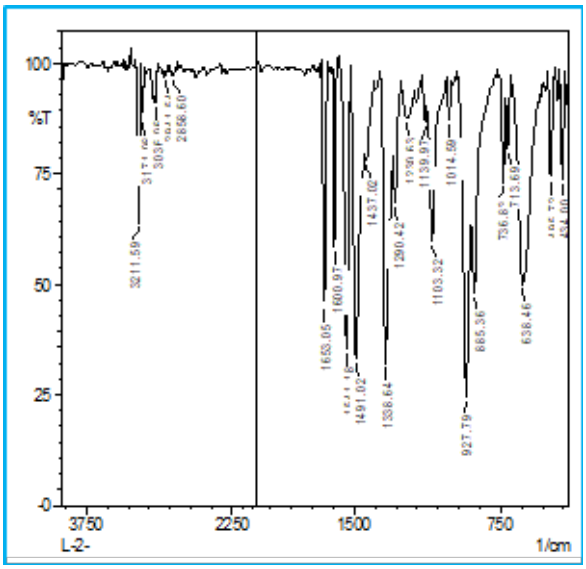



Fig (3): FT-IR of (L2)

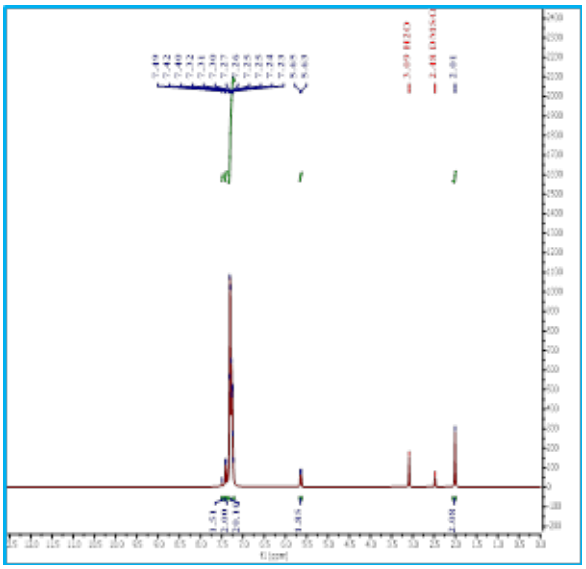


Fig (4): $^{1}$H-NMR of (L2).

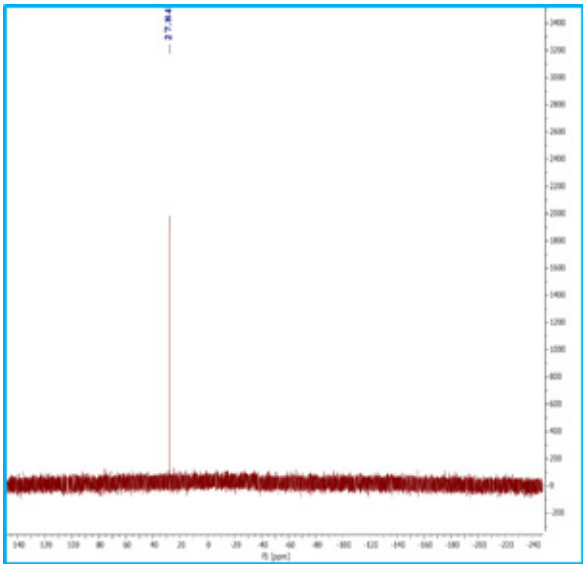


Fig (5): $^{31}$P-NMR of (L2).

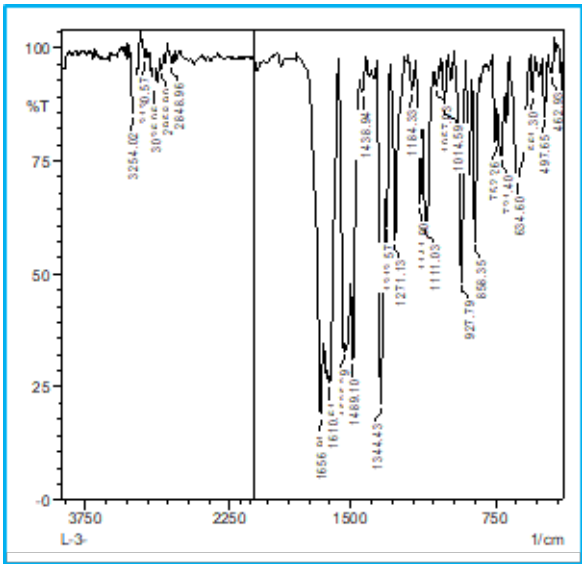



Fig (6): FT-IR of (L3).

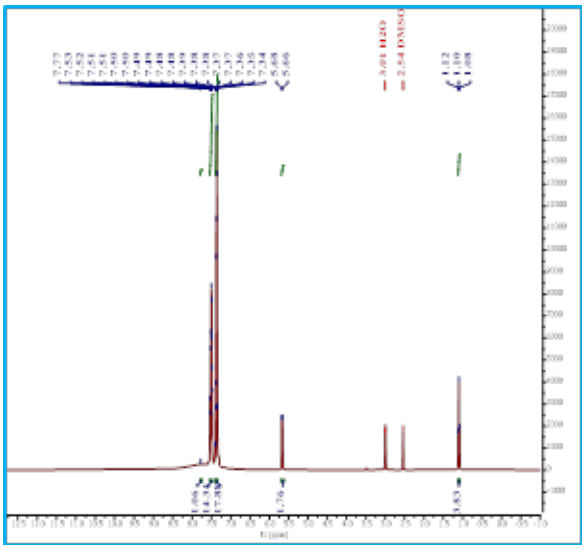


Fig (7): $^{1}$H-NMR of (L3).

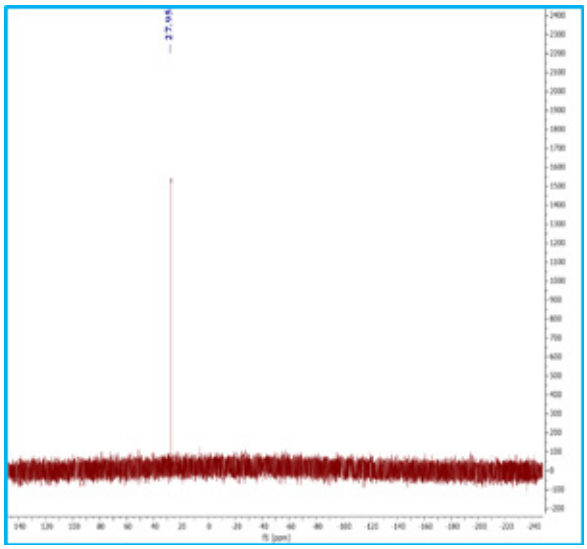


Fig (8): $^{31}$P-NMR of (L3).

## 4. Conclusions:

Phosphine compounds were made with thiouracil. By using spectroscopic measurements, which showed the appearance of bands like (P-Ph) and (C-P), which indicated the binding of phosphine to cadmium, as well as bands belonging to (Cd-N) and (Cd-O), which indicated the metal binding to the ligand, the accuracy and validity of the results were verified. The compounds containing phosphine have just one isomer, as shown by the single signal in the $^{31}$P-NMR spectrum. The complexes successfully fought off the negative and positive bacteria that were being studied. The chemical that proved more effective against the two kinds of bacteria under investigation was L2.

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