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Synthesis, Characterization, and Biological Evaluation of Mixed-Ligand Cadmium Cd (II) Complexes Containing 5-Benzylthio-1*H*-Tetrazole and Phosphine Ligands

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Keywords: *(*5-Benzylthio-1*H*-tetrazole), Cd (II) complexes, phosphines, and bioactivity.

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Abstract:

This study reports the synthesis and characterization of a series of novel mixed-ligand cadmium(II) complexes derived from 5-(benzylthio)-1*H*-tetrazole (L) in combination with mono- and bidentate phosphine ligands . Three complexes, namely $[CdL_2(PPh_3)_2]Cl_2$, $[Cd_2L_4(\mu\text{-dppm})_2]Cl_2$, and $[CdL_2(dppp)]Cl_2$ were succefully synthesized and fully characterized . The structural characterization was performed using Fourier-transform infrared spectroscopy (FT-IR), proton nuclear magnetic resonance (^{1}H-NMR), phosphorus nuclear magnetic resonance (^{31}P-NMR) , elemental (CHN) analysis, and scanning electron microscopy (SEM). Spectroscopic investigations confirmed that the tetrazole ligand acts as a bidentate ligand through coordination via nitrogen donor atoms, whereas the phosphine ligands coordinate through phosphorus atoms. SEM images revealed that the synthesized complexes possess well –defined and homogeneous nanostructured morphologies .Furthermore, the biological activities of the prepared complexes were evaluated against selected bacterial and fungal strains as well as cancer cell lines . The obtained results

demonstrated promising biological properties, highlighting the potential of these cadmium (II) complexes as candidates for further pharmaceutical investigation . Overall , this work provides valuable insights into the design of biologically active metal complexes and broadens their potential application in medicinal and environmental chemistry .

Keywords: *(*5-Benzylthio-1*H*-tetrazole) , Cd (II) complexes, phosphines, and bioactivity

تحضير , تشخيص , و تقييم الفعالية الحيوية لمعقدات الكادميوم ثنائي التكافؤ [Cd(II)] المتحدة مع الليكاندات المحتوية على (٥-بنزيل ثيو -1*H*- تيترازول) و الفوسفينات .

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الخلاصة :

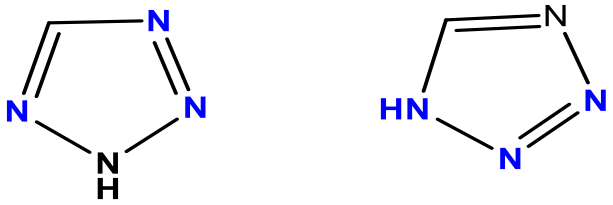
تتناول هذه الدراسة تحضير وتوصيف سلسلة من معقدات الكادميوم (II) الجديدة ذات الليكاند المختلط المشتقة من مركب ٥-(بنزيل ثايو)-١-*H*- تيترازول (L) بالاتحاد مع ليكاندات الفوسفين أحادية وثنائية السن. حيث تم بنجاح تحضير و توصيف ثلاثة معقدات بشكل كامل, وهي: $[CdL_2(PPh_3)_2]Cl_2$ ، $[Cd_2L_4(\mu\text{-dppm})_2]Cl_2$ و $[CdL_2(dppp)]Cl_2$ وقد اجري توصيف الهيكلي (البنيوي) باستخدام مطيافية الأشعة تحت الحمراء (FT-IR) ، الرنين المغناطيسي النووي للبروتون (^{1}H-NMR) ، الرنين المغناطيسي النووي للفوسفور (^{31}P-NMR)، التحليل الدقيق للعنصري(CHN) ، بالإضافة الى المجهر الإلكتروني الماسح (SEM) . وأكدت الدراسات الطيفية أن ليكاند التيترازول يسلك سلوك ليكاند ثنائي السن من خلال التناسق عبر ذرات النيتروجين المانحة ، في حين تتناسق ليكاندات الفوسفين عبر ذرات الفوسفور .كما كشفت صور المجهر الإلكتروني الماسح (SEM) أن المعقدات المحضرة تمتلك هياكل نانوية متجانسة و محددة بدقة . علاوة على ذلك، تم تقييم الأنشطة البيولوجية للمعقدات المحضرة ضد سلالات مختارة من البكتيريا والفطريات بالإضافة إلى خطوط خلايا السرطان. أظهرت النتائج المحصل عليها خصائص بيولوجية واعدة، مما يسلط الضوء على امكانية هذه المعقدات من الكادميوم (II) كمرشحات لاجراء المزيد من الدراسات الصيدلانية. وبشكل عام، يقدم هذا العمل رؤى قيّمة حول تصميم المعقدات الفلزية النشطة بيولوجياً ويوسع نطاق تطبيقاتها المحتملة في الكيمياء الطبية والبيئية.

كلمة المفتاحية: (٥- بنزيل ثيو--١*H*- تيترازول)، مركبات(II) Cd ، الفوسفينات، و الفعالية الحيوية .

Introduction:

Tetrazoles are unsaturated heterocyclic organic compounds (aromatic) comprising one carbon atom and four nitrogen atoms arranged in a five-membered ring, and the general molecular formula for the basic ring is CH_2N_4. These compounds mostly exist in the form of yellow crystalline solids with a distinctive odor, and they have the ability to dissolve in water and polar organic solvents such as alcohol and water [1]. Tetrazoles receive extensive attention and have a several uses in medical and pharmaceutical chemistry as a result of their multiple

biological and pharmacological activities [2]. Structurally, the unsubstituted tetrazole exists in a dynamic equilibrium between two tautomeric forms:



The most common method for preparing a tetrazole ring is by adding hydrazoic acid or an azide to compounds containing an unsaturated nitrogen bond, such as carbodiimines, cyanates, thiocyanates, and cyanides. During this reaction, the intermediate compound, imideazides, is formed, which undergoes cyclization to form the tetrazole ring [3], The synthesis of the tetrazole ring involves the reaction of compounds containing an unsaturated nitrogen bond with hydrazoic acid or azides, followed by the formation of an intermediate that undergoes cyclization to produce the tetrazole ring, as illustrated in Figure 1.

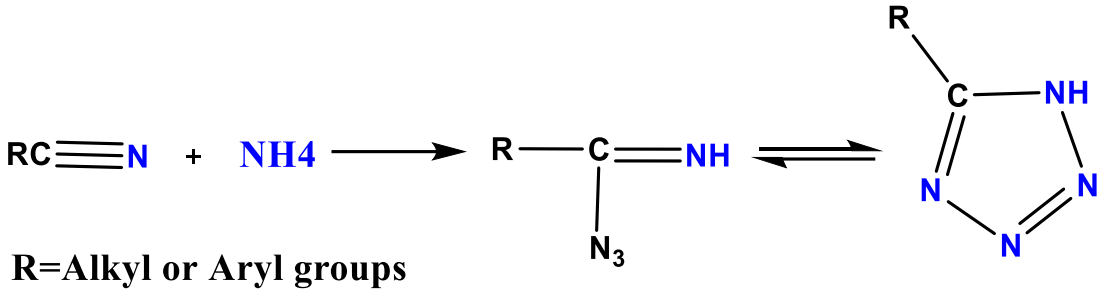


Figure (1) : This figure show how to prepare tetrazole ring

Material and methods :

The substances were synthesized using unpurified ingredients and solvents. The phosphines used in the research were: triphenylphosphine (PPh_3) and 1,2-bis(diphenylphosphino)ethane (dppe).

The melting points of the prepared complexes were measured using an automatic melting point apparatus (SAM30). The infrared spectra (FT-IR) of the complexes were recorded as KBr pellets using a SHIMADZU 8400S spectrometer between (400 and 4000) cm^{-1}. The magnetic nuclear resonance (NMR) spectra were captured with a 400 MHz Varian Unity Spectrometer. in DMSO-d^6. To determine the properties of thick or thin samples of the material, observe their shape, and identify the nanoscale or crystalline dimensions of the particles, a TESCAN MIRA3 device was used.

Practical steps:

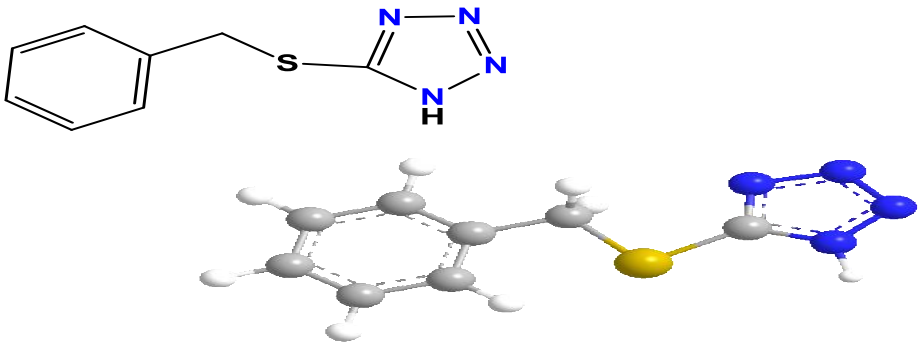


Figure (2): 5-(Benzylthio-)1*H*-Tetrazole

Step one:

Preparation of the complex $[CdL_2(PPh_3)_2]Cl_2$:

A solution of the ligand LH ,Cadmium chloride (0.16 g, 0.86 mmol) in 5 ml of ethanol was mixed with (0.1 g, 0.5 mmol) in 5 ml of ethanol. forming a milky-colored mixture. The solution was heated at 70 °C for two hours, then PPh3 The mixture was supplemented with (0.13 g, 0.5 mmol) in 5 ml of ethanol. After two more hours of heating, the precipitate was filtered while still hot, cleaned with cold ethanol, and left to dry at room temperature. (wt = 0.08 g, %=50%, m.p = 160-163 °C).

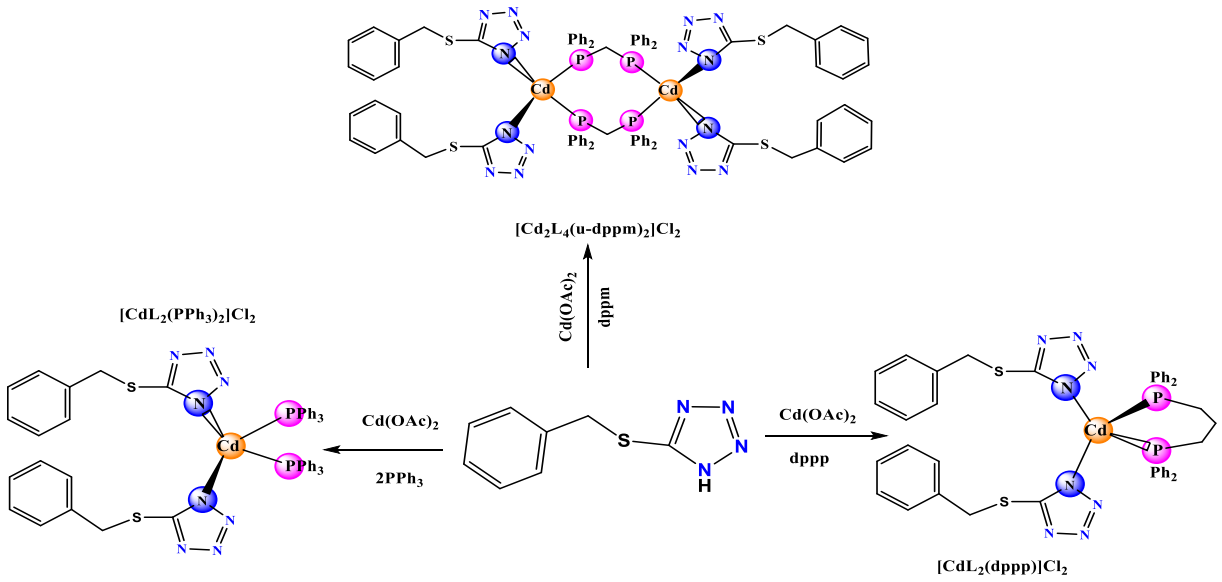
Preparation of the complex: $[CdL_2(dppm)]Cl_2$:

Add the ligand (0.129 g, 0.62 mmol) to cadmium chloride (0.1 g, 0.31 mmol) in a round-bottom flask, then add to the mixture 25 ml of chloroform. A colorless.

solution forms, stirring for two hours at 50 °C, resulting in a milky suspension. Then add to it a solution of (0.119 g, 0.31 mmol) dppm in 5 ml of chloroform. Stir the mixture at 70 °C for two hours until a colorless solution forms. Place it in a beaker and leave to dry at room temperature. (wt = 0.18 g, %=60%, m.p. = 194-196 °C).

Preparation of the complex $[CdL_2(dppp)]$:

Prepared as described in the method mentioned in paragraph (A). (wt = 0.2 g, %=66%, m.p = 163-165 °C).



[CdL2(dppp)]Cl2 , [Cd2L4(μ-dppm)2] Cl2 , [CdL2 (PPh3)2] Cl2

Figure(3) : Schematic diagram of the prepared complexes

[CdL2]Cl2: White Powder, (0,14 g), rendementde 77%, pointde fusion :(182-184)ºC. FTIR (KBr).**:** 3058m ν(C-H)Arom, 2991m ν(C-H)aliph, 1620s ν(C=N), 1346m ν(N=N), 1242s ν(N-N), 769m ν(C-S), 422w ν(M-P) .

ʾH NMR: (DMSO-d6) δ(PPm): 7,62 (d, 3J = 7.88 Hz, 4H, Ha), 7.39 (t, ($^4J_{H-H}$= 7.70 Hz,$^3J_{H-H}$= 1.20 Hz) 4H, H_b), 7.26 (t, $^4J_{H-H}$= 7.66 Hz,$^3J_{H-H}$= 1.16 Hz, H_c), 4.25(s, 4H,CH2).**^{13}C-{^{1}H}-NMR:** 157.69 (C1), 137.99 (C2), 129.33 (s,C3), 128.81 (s,C4), 127.66 (m,C5), 36.91 (m,C6).

]CdL2 (PPh3)2]Cl2: White powder (0.4 g), yields 86%, m.p.(175-178) ºC. FTIR (KBr): 3031m (C-H)Arom, 2921m (C-H)aliph, 1618s (C=N), 1552s (C=C), 1433s (P-Ph), 1249s (N-N), 750s (C-S), 696m (P-C), and 424s ν (M-P).1H NMR (DMSO-d6) δ(PPm): 7.45 (d, 3J = 8.11 Hz, 4H, Ha), 7. 26.30 (b, 30H, HPh), 7.18 (t, 3J = 7.56 Hz, 3J = 1.24 Hz, 4H, Hb), 7.14 (t, 4JH-H = 1.16 Hz, 3JH-H = 7.48 Hz, 2H,Hc), 7.32 (s, 3*J* = 4.06 Hz, 4H, CH2.^{31}P{^{1}H}NMR=25.63(s).

[CdL2(dppm)]Cl2: 60% of the white powder (0.18 g) has a m.p. of (194–196) ºC. FTIR (KBr): 3076m (C-H)Arom, 2983m (C-H)aliph, 1625s (C=N), 1560s (C=C), 1433s (P-Ph), 1244s (N-N), 748s (C-S), 696m (P-C), and 426s ν (M-P).7.44 (d, 3J = 7.48 Hz, 4H, Ha), 7.40 (m, 2H, HPh), 7.25 (b, 18H, HPh), 7.34 (t, 3J = 7.50 Hz, 3J = 1.22 Hz, 4H, Hb), 7.29 (t, 4JH-H = 1.14 Hz, 3JH-H = 7.45 Hz, 2H, Hc), and 7.32 (s, 3J = 4.19 Hz, 1H, CH2).**^{31}P{^{1}H}NMR**=23.59(s).

[CdL$_2$(dppp)]Cl$_2$: 0.2 g of white powder gives 66%, m.p. (163-165) ^{o}C. FTIR (KBr): 3049m (C-H)Arom, 2923m (C-H)aliph, 1629s (C=N), 1431s (P-Ph), 1240s (N-N), 769s (C-S), 692m (P-C), and 432s v (M-P).1H NMR (DMSO-d6) δ(PPm): 7,64 (d, 3J = 8.10 Hz, 4H, Ha), 7.58 (m, 20H, HPh), 7.47 (t, 4JH-H = 1.20 Hz, 3JH-H = 7.48 Hz, 4H, Hb), 7.38 (b, 4JH-H = 1.26 Hz, 7.58 Hz, 8H, Hb), and 4.34 (s, 4H,CH2), 3.62 (t, 4H, CH).**^{31}P{^{1}H}NMR**=28.13(s).

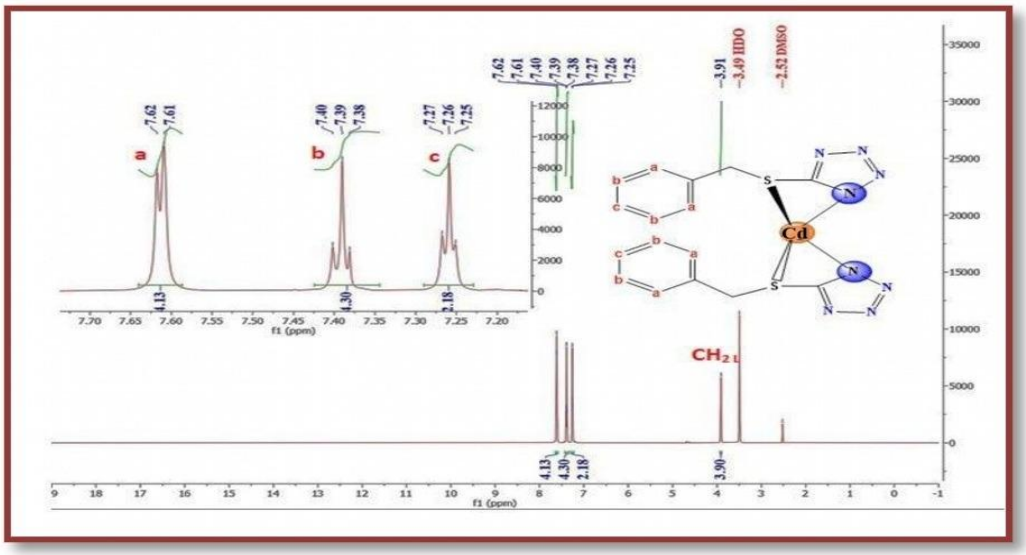


Figure (4): Proton Nuclear Magnetic Resonance Spectrum of the Complex [CdL$_2$]Cl$_2$

Results and Discussion:

Infrared Spectrum of the Complex [CdL$_2$]Cl$_2$:

The infrared spectrum of the complex [CdL$_2$]Cl$_2$ showed the disappearance of the N-H band that was present in the ligand at the frequency (3199 cm^{-1}) and the complex's band's emergence at the frequency (1620 cm^{-1}) attributed to ν(C=N) [4]. There was a band at (1589 cm^{-1}) assigned to ν(C=C) of the aromatic ring [5], and a band at the frequency (1346 cm^{-1}) attributed to ν(N=N) [6]. Another band appeared at (1242 cm^{-1}) ascribed to ν(N-N) [7], and a band at the frequency (769 cm^{-1}) assigned to ν(C-S) [8]. In addition, a medium band at the frequency (3058 cm^{-1}) was attributed to ν(C-H) of the aromatic group [9], and a band at the frequency (2991 cm^{-1}) assigned to ν(C-H) of the aliphatic group [10]. A band appeared at the frequency (422 cm^{-1}) attributed to ν(Cd-N) [11]. Meanwhile, The produced complexes' infrared spectra revealed a novel signal between 1433 s and 1429 s and 1097 m and 1095 m, which was ascribed to υ(P-Ph) and υ(P-C), respectively, and a signal in the range (1629 s - 1618 s) assigned to the ν(C=N) group, as well as a signal within the ranges (2983 m - 2912 w) and (3076 s - 3031 m) attributed to Alph. ν(C-H) and Ar

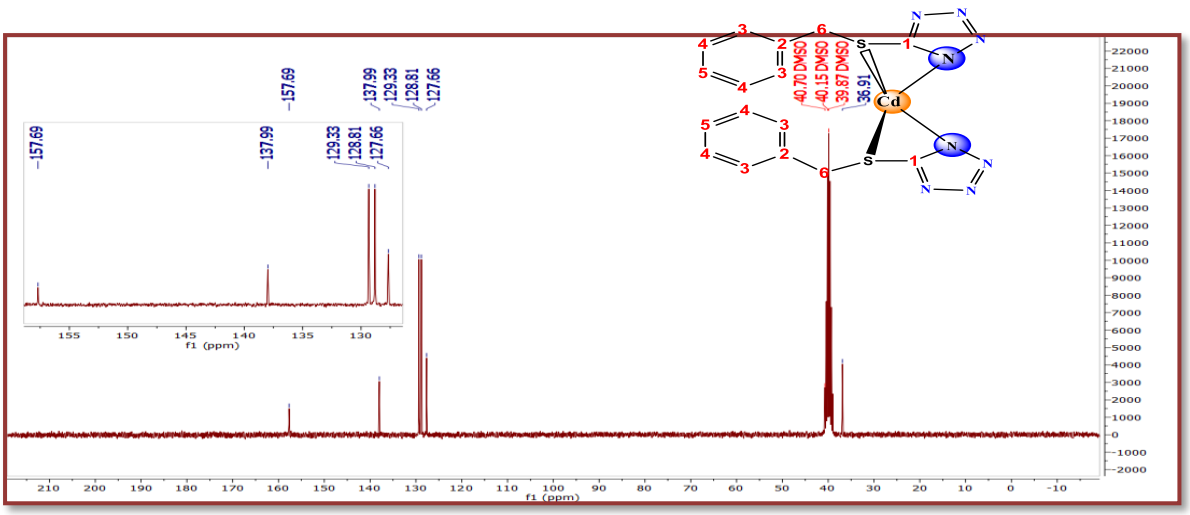


Figure (5): Proton Nuclear Magnetic Resonance Spectrum of the Complex $[CdL_2]Cl_2$

The proton nuclear magnetic resonance (^1H NMR) spectrum of the produced compounds (1-2) displayed many indications.: six signals at the chemical shifts (7.45, 7.84, 7.26, 7.27, 7.56, 7.58) due to protons Ha, HPh, Hb, respectively. In addition, a singlet was observed at the chemical shifts (4.30, 4.25) due to (CH_2) protons, and a singlet at δH = 2.08 ppm integrating for four protons corresponding to (CH) in the (dppe) complex. The $^{31}P\{^1H\}$ NMR spectrum showed signals at the chemical shifts 30.06, 25.63, 23.59, respectively [12].

Detailed analysis of the elements :

The proportions of carbon, hydrogen, cadmium, nitrogen, phosphorus, and sulfur in the prepared compounds were estimated. These experimentally obtained proportions showed agreement with the theoretically calculated values for the proposed formulas of the ligands and complexes. The closeness of the results supports the accuracy of the proportions used in the preparations, as shown in the table below :

Table (1): detailed analysis results for elements

Seq	compounds	C	H	Cd	N	P	S
١	L	49.95 (49.98)	4.16 (4.19)		29.09 (29.14)		16.66 (16.68)
٢	$[CdL_2(pph_3)_2]Cl_2$	61.24 (61.27)	4.33 (4.35)	11.01 (11.03)	10.96 (10.99)	6.06 (6.08)	6.25 (6.29)
٣	$[CdL_4(\mu\text{-dppm})_2]Cl_2$	35.75 (35.72)	2.82 (2.83)	19.66 (19.69)	19.61 (19.63)	10.83 (10.85)	11.22 (11.23)
٤	$[CdL_2(dppp)_2]Cl_2$	38.07 (38.10)	3.35 (3.37)	18.73 (18.77)	18.67 (18.71)	10.32 (10.34)	10.68 (10.71)

SEM Outcomes :

The majority of coordination compounds with regular geometric structures can be produced at the nanoscale, according to recent investigations on their geometric structure. A few complexes made with the SEM method had their microstructure's morphological appearance examined**.**

Through scanning electron microscope analysis of the complex $[Cd(L)_2(dppp)]$ Cl_2, the average peak of the complex body radii was 70 nm, which falls within the range of nanoparticles.

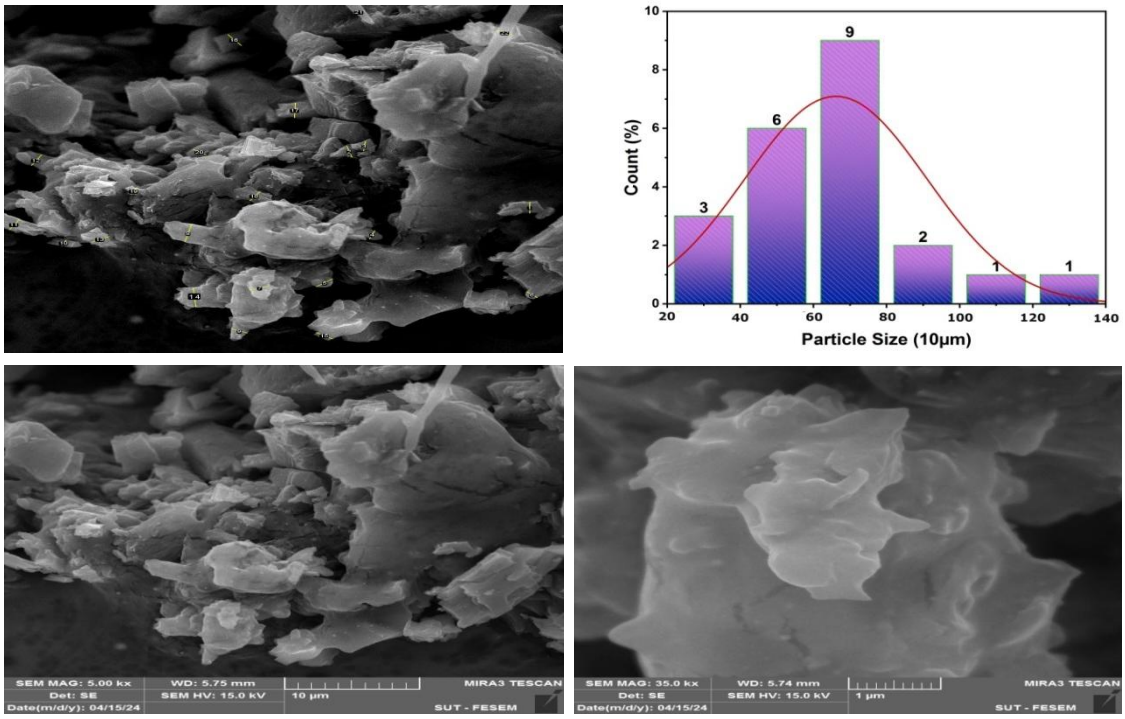


Figure (6): (a) SEM image of the complex $[Cd(L)_2(dppp)]Cl_2$ at 1 µm and 10 µm Graph (1): (b) Particle sizes and Gaussian curve for the complex $[Cd(L)_2(dppp)]Cl_2$ at 10 µm

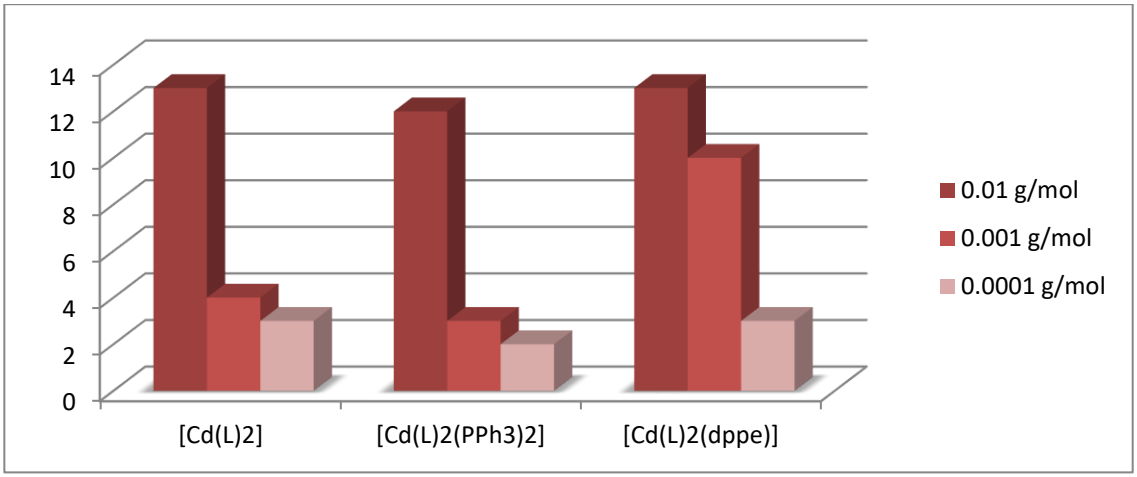
Biological Activity :

The Using the antibiotic Amikacin as a reference, the biological activity of the complexes was evaluated against four bacterial species: Escherichia coli (-), Acinetobacter baumannii (-), Staphylococcus aureus (+), and Enterococcus faecalis (+) at doses of 0.01, 0.001, and 0.0001 mg/mL. As seen in Figure 3, every complex exhibited action against the bacterial species. The concentration of ten showed weak activity against the bacterial species, while complex (1) showed the highest inhibition percentage at concentration 103 against (-)

Acinetobacter baumannii and (-) Escherichia coli. Complex (2) showed the highest inhibition percentage at concentration 180 against (+) Staphylococcus aureus and Enterococcus faecalis.

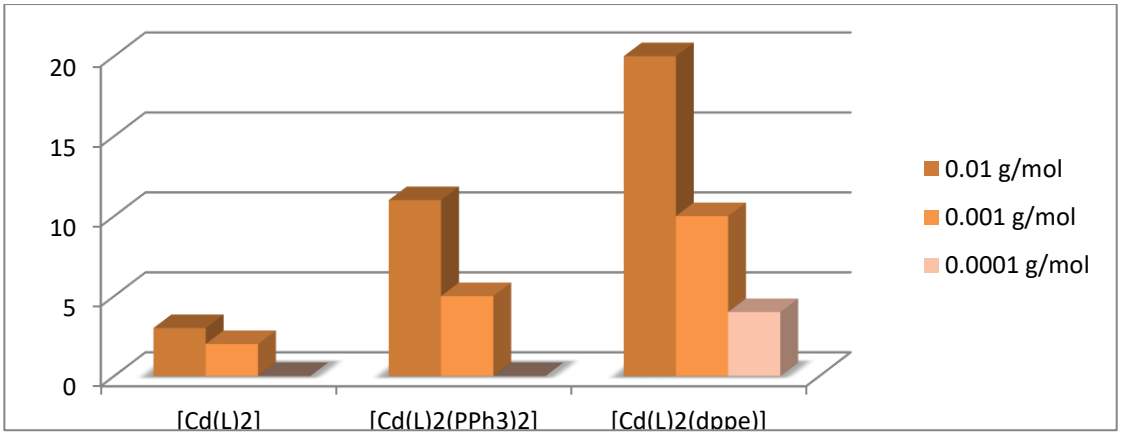
Complex (1) showed the highest activity at concentration 10 against ((Escherichia coli), while complex (2) showed the highest activity at the same concentration for the other species.

Acinetobacter baumannii (-)



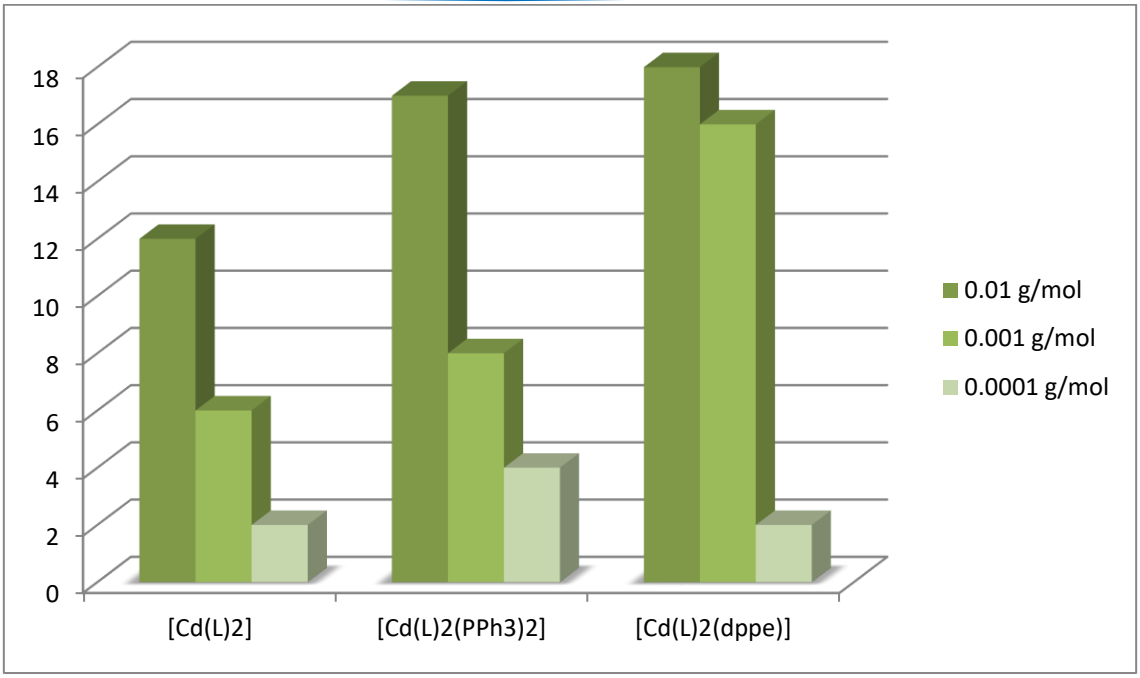
(a)

Escherichia coli(-)



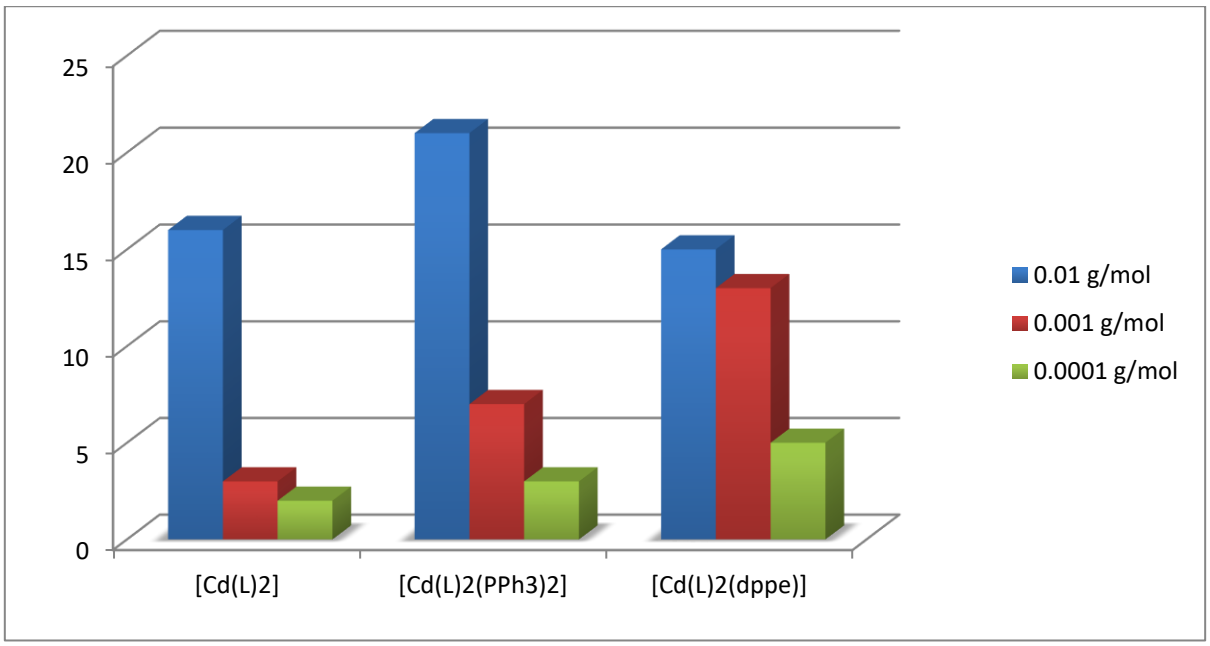
(b)

Staphylococcus aurous(+)



(c)

Enterococcus faecalis(+)



(d)

Figures (7) : The the prepared compounds' ability to suppress the development of a number of Gram-positive and Gram-negative bacteria (a, b, c, and d)

Conclusions:

1- A new series of novel mixed-ligand cadmium(II) complexes was successfully synthesized using 5-(benzylthio)-1}H tetrazole (L) in combination with mono- and bidentate phosphine ligands, yielding three specific complexes:$[CdL_2(PPh3)_2]Cl_2$, $[Cd_2L_4(\mu\text{-dppm})_2]Cl$, and $[CdL_2(dppp)]Cl_2$.

2- Spectroscopic and elemental analyses (FT-IR, ^{1}H-NMR, ^{31}P-NMR, and CHN) confirmed that the tetrazole ligand acts as a bidentate donor coordinating via nitrogen atoms, while the phosphine ligands coordinate through phosphorus donor atoms.

3- Scanning Electron Microscopy (SEM) analysis revealed that the synthesized complexes exhibit well-defined, homogeneous nanostructured surface morphologies .

4- valuated complexes demonstrate promising biological properties, showing activity against selected bacterial and fungal strains as well as cancer cell lines.

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