

Synthesis, Spectroscopic Identification for Mixed-Ligand Complexes and Evaluating Their Biological Effectiveness

Marwah M. Al-Dulaimi *, Omar Hamad Shihab

Department of Chemistry, College of Science, University of Anbar, Ramadi, Iraq;



ARTICLE INFO

Received: 12 / 08 /2023

Accepted: 29 / 08 / 2023

Available online: 18 / 12 / 2023

DOI: 10.37652/juaps.2023.142224.1107

Keywords:

Dimidone, 1,2-dibenzothiophene, biological effectiveness, FT-IR, Mix ligand..

Copyright©Authors, 2022, College of Sciences, University of Anbar. This is an open-access article under the CC BY 4.0 license (<http://creativecommons.org/licenses/by/4.0/>).



ABSTRACT

Mix ligand composed of (HL1) Dimidone and (HL2) 1,2-dibenzothiophene were allowed to react with next metal ions: Co (III), Mn (II), Fe (III), Co (II), Ni (II), Cu (II), Zn (II) and Cd (II) individually forming stable metal complexes with different geometries as indicated using various techniques. The formation of the complexes as well as the geometries of the complexes were detected by Fourier-transform-infrared, mass_spectra, elemental analysis and electronic spectra. Moreover, the solubility of the compounds was tested in various solvents including: CHCl₃, THF, DMF, DMSO, C₂H₅OH and H₂O. Furthermore, the vital effectiveness was tested toward two types of bacteria gram negative bacteria (Spuedomonas & E.Coli) and positive bacteria (Staph. Aureas & Bacillus) and two types of fungi (Aspergillus niger & Fuzaium) giving different inhibition values (either effective or noneffective) as detailed in the manuscript.

1. INTRODUCTION

The mixed ligand complexes derived from the bioactive potent ligands containing N, O donor binding sites with M(II) ions are used in a number of fields like biological, analytical, agricultural industrial and therapeutic applications ^(1,2). Metal ions are fundamental elements for healthy life to human and higher animals ⁽³⁾ particularly the late first row transition metals such as, cobalt, nickel, copper and zinc are biologically relevant metals as they are associated with various biomolecules related to essential physiological activities. Metal complexes of biologically important ligands were sometimes more effective than free ligands ⁽⁴⁾. It was not surprising; therefore, that many authors have studied the coordination compounds of several central atoms. Mixed ligand complexes had a key role in biological chemistry ⁽⁵⁾ because the mixed chelation occurs commonly in biological fluids as millions of potential ligands were likely to compete for metal ions in-vivo ⁽⁶⁾.

These create specific structures ⁽⁷⁾ and have been implicated in the storage and transport of active substances through membranes. The transition metal complexes with oxygen donors are applied in various activities such as anticancer, antibiotic, antimicrobial and antifungal agents. Many of the metals such as Cu²⁺, Co²⁺ and Ni²⁺ have found widespread application in organic synthesis and biology ⁽⁸⁾. In this recent work, we describe the synthesis of mixed-ligand derived from dimedone and 1,2-dibenzothiophene with next transition metal salts: Co (III), Mn (II), Fe (III), Co (II), Ni (II), Cu (II), Zn (II) and Cd (II). The ligand and its mixed-ligand complexes are diagnosed using elemental_analysis, fourier transform-infrared, mass_spectra, magnetic susceptibility measurements, molar conductivity and electronic spectra to elucidate the molecular structure of the ligand transition metal.

2. MATERIALS AND METHODS

2.1 Instrumentation & Chemicals:

All the starting materials, chemicals and solvents for the prepared compounds were of analytical grade. Abs. EtOH, MeOH, dimethylsulfoxide and other solvents were of high purity and supplied by Merck Co.,

*Corresponding author at: Department of Chemistry, College of Science, University of Anbar, Ramadi, Iraq;
ORCID:<https://orcid.org/0000-0000-0000-0000>; Tel:+964000000000000
E-mail address: mhdymrwt65@gmail.com

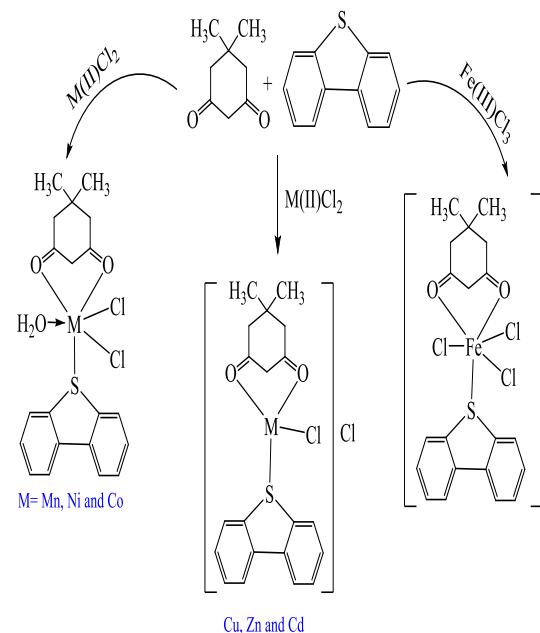
Fluka Co. and Sigma-Aldrich Co., Dimedon, 1,2-dibenzothiophene and metal salts [FeCl₃, ZnCl₂, CoCl₂.6H₂O, MnCl₂.4H₂O, NiCl₂.6H₂O, CuCl₂.2H₂O and CdCl₂.H₂O] were supplied by Sigma-Aldrich Co. and BDH Co., The melting point of the prepared ligands and complexes were measured by a Stuart electrothermal melting point apparatus. The elemental (H, N, O, S, C) micro-analysis, to search using the EA 3000 single V.3 model vector device. LC-MSQP50A(E170ev) Shimadzu device. Infrared spectra were measured with a device (Shimadzu-8000S) and the ultraviolet-visible spectra of the ligand and its complexes were recorded using a Shimadzu UV-Visible Spectrophotometer. Molar electrical conductivity measurements were carried out using BC3020 Professional Bench Top Conductivity device.

Complex preparation

2.2 Synthesis of Complexes:

(0.237 g, 1mmol.) from CoCl₂. 6H₂O dissolved in 10 mL of absolute EtOH placed in round bottomed flask (100 mL in size) with heating to perform the dissolving. Both ligands (HL1) Dimidone (0.140 g, 1mmol.) and (HL2) 1,2-dibenzothiophene (0.184 g, 1mmol.) were dissolved in 20 mL of EtOH and added immediately to cobalt salt solution. After reflux for one hour at 50 °C, the mixture was cooled until precipitates, then filtered, dried and recrystallized using absolute ethanol (1:1:1). Other metal complexes were synthesized in the same approach that followed with cobalt complex using their corresponding chloride metal salt for the next metal ions: Mn(II), Fe(III), Co(II), Ni(II), Cu(II), Zn(II), Cl(II) as detailed in table 1 and illustrated in scheme 1.

Scheme 1. Synthesis of complexes



Scheme 1. Synthesis of complexes

Table (1) Weights of metal salts and some physical properties of the resulting complexes

Metal Salt	Weight of salt (mmole 1g)	Complex	Yield%	Color	M.P.C	Decomposit ion
NiCl ₂ .6H ₂ O	0.237	[CoL ₁ L ₂ Cl ₂ .H ₂ O]	0.197	[MnL ₁ L ₂ Cl ₂ H ₂ O]	70	Yellow
[NiL ₁ L ₂ Cl ₂ .H ₂ O]	49	[FeL ₁ L ₂ Cl ₃]	65	[FeL ₁ L ₂ Cl ₃]	72	Dark brown
	410 – 412		280 – 283		298 – 301	212 – 214

CdCl ₂ .H ₂ O	ZnCl ₂	CuCl ₂ .2H ₂ O
0.201	0.136	0.170
[CdL ₁ L ₂ Cl]Cl	[ZnL ₁ L ₂ Cl]Cl	[CuL ₁ L ₂ Cl]Cl
60	47	63
Pale Yellow	Pale Yellow	Green
288 – 290	289 – 291	300 – 303

6, 7 and 8) can be applied for the rest of the complexes as detailed in table 2.

Table (2) FT-IR spectral incomes of ligands and their complexes

[FeL ₁ L ₂ Cl ₃]	[CoL ₁ L ₂ Cl ₂ .H ₂ O]	[NiL ₁ L ₂ Cl ₂ .H ₂ O]	[MnL ₁ L ₂ Cl ₂ H ₂ O]	1,2-dibenzothiophene (HL ₂)	Dimedone (HL ₁)	Comp. Symb.
-	3373 b 1597 msh	3365 b 1600 msh	3371 b 1587 msh	--	--	v(H ₂ O)
1616 wsh	1621 wsh	1624 wsh	1634 Msh	--	1695 m, sh	v(C=O)
3047 w	3050 w	3029 w	3071 w	3088 w	3029 w	v(C-H) Arom.
2922 Msh	2900 W	2930 W	2937 W	--	2929 w	v(C-H) Alipha.
516, 460 Ws	572, 420 w,w	592, 564 462 w, w, w	529, 472 w,w	--	--	M-O
		380,405 wsh	375,380 wsh	--	--	M-S
		345 msh	350 msh	--	--	M-Cl

3. RESULTS AND DISCUSSION

Spectroscopic studies

FT-IR Spectroscopy: According to FT-IR spectroscopy we can indicate about the formation of new complexes depending on the modifications that observed in the spectra of those complexes when compared with the spectra of each ligand individually. Those modifications may include change in the shape or intensities of the main bands or include shift in their wavelengths toward lower or higher wavelengths. In figure 1(a), (HL1) ligand gave the next stretching absorption bands: weak – strong band at 3029 cm⁻¹ for the vibration of C-H aromatic group, weak band at 2929 cm⁻¹ belongs to C-H aliphatic group and moderate, sharp band at 1695 cm⁻¹ for the vibrational mode of carbonyl group and bending absorption band for CH₃ group at 1421 cm⁻¹. Figure 1(b) for ligand (HL2) (1,2-dibenzothiophene) demonstrates the next absorption peaks: weak stretching absorption band of C-H aromatic group at 3088 cm⁻¹, stretching absorption band of C=C at 1688 cm⁻¹^(9,10). Figures 2 (a & b) for manganese complex demonstrates the same bands that found in both ligands in addition to the modifications in some bands because of the occurrences of coordination through these groups, those are C=O observed at 1634 cm⁻¹. Moreover, new absorption peaks are detected those are aqua water molecule, M-S, M-O and M-Cl as detailed in table 2⁽¹¹⁾. Same characterization⁽¹²⁾ in figures (3, 4, 5,

[CdL ₁ L ₂ Cl]Cl	[ZnL ₁ L ₂ Cl]Cl	[CuL ₁ L ₂ Cl]Cl
-	-	1626 msh
1625 ssh	1627 msh	3055 w

3088 b	3053 W	2920 Wsh
2926 W	2920 Wsh	2920 Wsh
495, 424 Wsh	582, 435 w, wsh	538, 435 wsh, w

380 wsh	380 B	
345 msh	345 W	

UV-Vis Spectroscopy: Ultra violet spectrum of (HL1) ligand dimedone in figure 9, demonstrates moderately broad absorption band at (271 nm, 36900 cm⁻¹) belongs to ($\pi\rightarrow\pi^*$) electronic transition, whereas the spectrum of ligand (HL2) (1,2-dibenzothiophene) in figure 10 demonstrates three absorption bands at (272 nm, 36764 cm⁻¹) corresponds to ($\pi\rightarrow\pi^*$) electronic transition, (301 nm, 33222 cm⁻¹) and (329 nm, 30395 cm⁻¹) both corresponding to (n \rightarrow π^*) electronic transition ⁽¹³⁾ as illustrated in table 3. Figure 11 demonstrates the spectrum of copper complex and the next transitions: ($\pi\rightarrow\pi^*$ and n \rightarrow π^*) +C. T M \rightarrow L at (255 nm, 39215 cm⁻¹) and (298 nm, 33557 cm⁻¹), the transitions of ligands with some shifting in their wavelengths because of coordination with metal. In addition to d-d transition at visible region (419 nm, 23866 cm⁻¹) ⁽¹⁴⁾. The UV-Vis spectra of the rest complexes illustrate the same absorption bands that found in ligands at ultra violet region with some modifications including shifting in their absorption bands because of the coordinative binding with metal ion. Moreover, those spectra illustrate new absorption peaks at visible region which in turn belonging to d-d transitions ⁽¹⁴⁾ as demonstrated in figures (12 \rightarrow 17) and table 3.

Magnetic Susceptibility

At a temperature of 25 °C, the Faraday method was used to determine the magnetic sensitivity of the

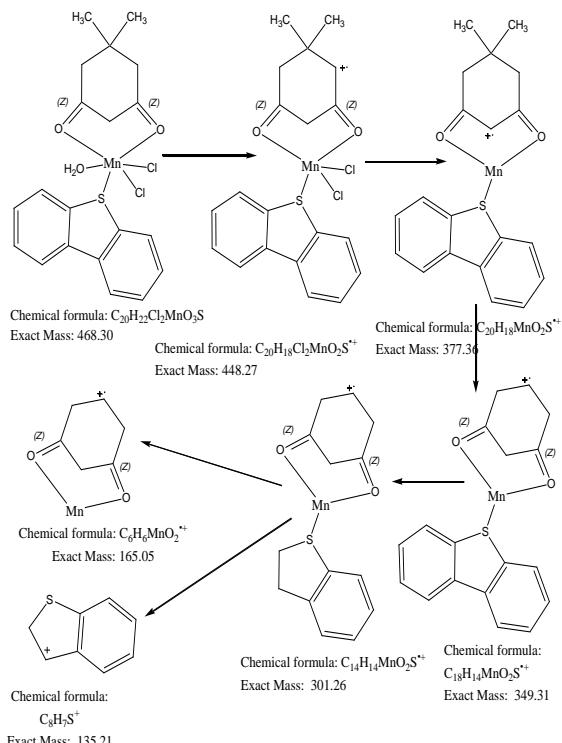
solid states. The oxidation state and electronic configuration of the transition metal atoms are inferred from measurements of the magnetic characteristics. Therefore, whether a compound has low-spin or high-spin is determined by the number of single electrons that make up a transition metal ion ^(22,23). The magnetic moment for the manganese (II) complex has been measured to be equal to (5.86B.M), whereas the magnetic moment for the iron complex was measured to be (5.80B.M). All complexes have highly twisted octahedral geometries, which are compatible with the magnetic moment of cobalt, which was measured to be (3.96B.M). The lists of magnetic sensitivity values of atoms in organic molecules (Pascal's constants) were used ⁽²⁴⁾, and the values of magnetic moments were fixed in Table (4).

Table (3) UV-Vis incomes of mix ligands and their complexes

Compounds	λ nm	ABS	$\tilde{\nu}$ (cm ⁻¹)	ϵ L.mol ⁻¹ cm ⁻¹	Assignment	Δm (S.cm ² .Mol ⁻¹)	Geometry
Dimedone (HL ₁)	271	3.311	36900	3311	$\pi\rightarrow\pi^*$
1,2-dibenzothiophene (HL ₂)	329	1.500	30395	1500	n \rightarrow π^*
	301	1.001	33222	1001	n \rightarrow π^*
	272	0.489	36764	489	$\pi\rightarrow\pi^*$
[CuL ₁ L ₂ Cl]Cl	419	0.557	23866	557	$^{2}T_2\rightarrow^{2}E$	44	Tetrahedral
	298	2.395	33557	2395	n \rightarrow π^* , M \rightarrow LCT
	255	2.663	39215	2663	$\pi\rightarrow\pi^*$

[FeL ₁ L ₂ Cl ₃]	[NiL ₁ L ₂ Cl ₂ H ₂ O]	[MnL ₁ L ₂ Cl ₂ H ₂ O]	[CoL ₁ L ₂ Cl ₂ H ₂ O]	[CdL ₁ L ₂ Cl]Cl	[ZnL ₁ L ₂ Cl]Cl
768 681 392 301	0.018 0.012 0.653 0.546	13020 14684 25510 33222	180 120 6530 5460	⁶ A _{1g} → ³ T _{1g} (G) ⁶ A _{1g} → ³ T _{1g} (G) M→LCT n→π*	382 307
596 582 501 461 301	0.273 0.293 0.286 0.288 0.601	16778 17182 19960 21691 33222	273 293 286 288 601	³ A _{2g} → ³ T _{1g} (F) ³ A _{2g} → ³ T _{1g} (P) M→LCT, n→π*	0.478 0.329
756 596 306	0.657 0.732 2.893	13227 16778 32679	657 732 2893	⁶ A _{1g} → ⁴ T _{1g} (O) ⁶ A _{1g} → ⁴ T _{1g} (G) ⁶ A _{1g} → ⁴ A _{1g} , ⁴ E _g M→LCT	0.789 1.426 0.675
				n→π*, M→LCT n→π*, π→π*	478 329
					789 1426 675
					41
					49
					41
					Tetrahedral

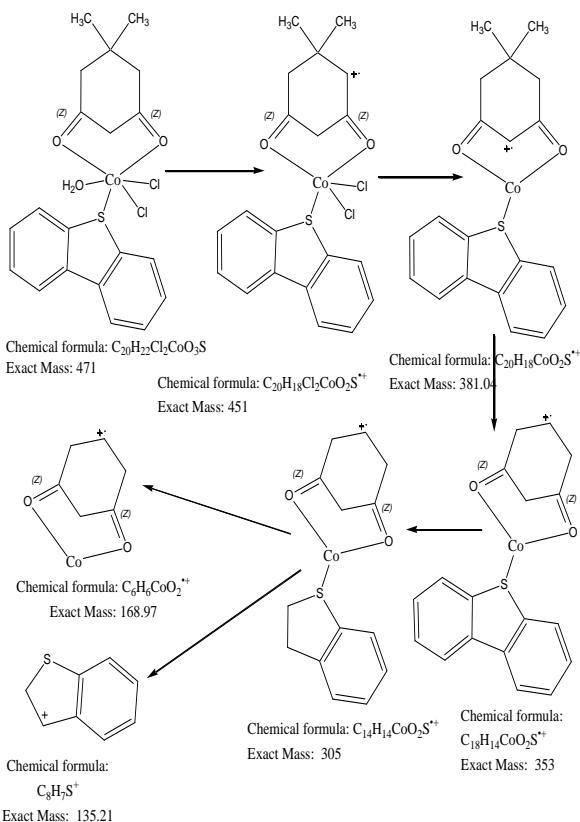
the complex. As for copper complex in Figure 20 and scheme 4 illustrates the molecular ion peak (M+) C₂₀H₂₀SCl₂CuO₂ at 422.44 m/z results from the partitioning of the complex. In addition, the spectrum of cadmium complex in Figure 21 and scheme 5 gave the main peak (M+) C₂₀H₂₀SCl₂CdO₂ at 472.99 m/z.



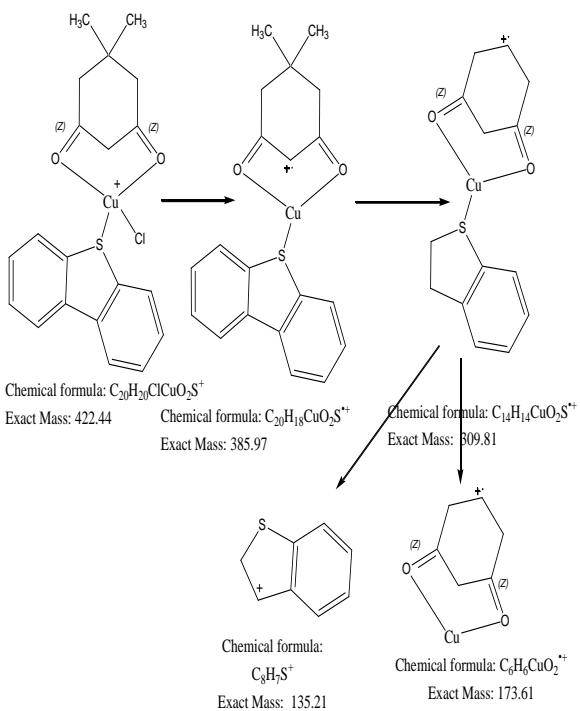
Scheme 2. Fragmentation analogues of manganese complex

LC-Mass spectroscopy:

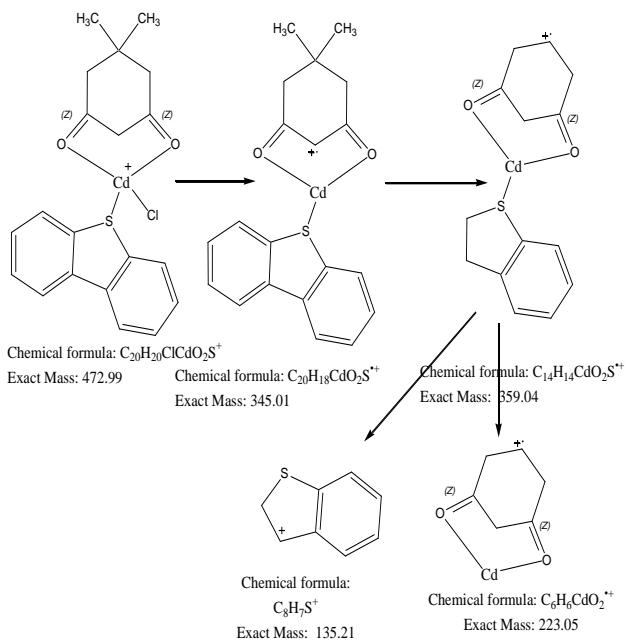
The LC-Mass spectra of the complexes gave compatible results with theoretical results when observe the obtained molecular formulas for each complex and comparing it with the calculated formula. Figure 18 and scheme 2 for manganese complex demonstrates the molecular ion peak (M+) for the formula C₂₀H₂₂SCl₂MnO₃ at 468.30 m/z which corresponds to the molecular weight of the complex. Figure 19 and scheme 3 for cobalt complex demonstrates the molecular ion peak (M+) for the formula C₂₀H₂₂SCl₂CoO₃ at 471 m/z which corresponds to the molecular weight of



Scheme 2. Fragmentation analogues of cobalt complex



Scheme 2. Fragmentation analogues of copper complex



Scheme 5. Fragmentation analogues of cadmium complex

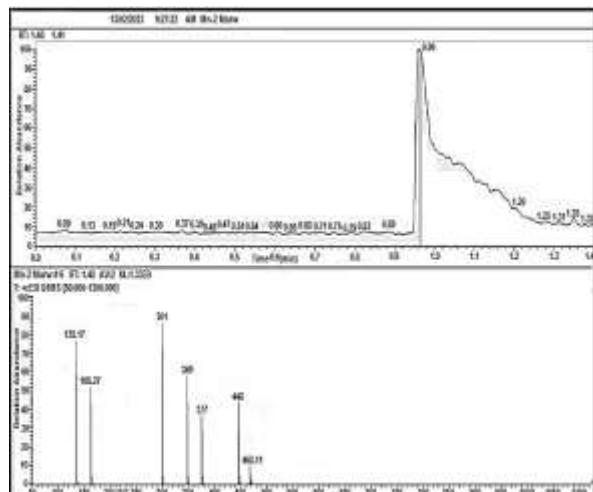


Figure 1. LC-Mas spectrum of manganese complex

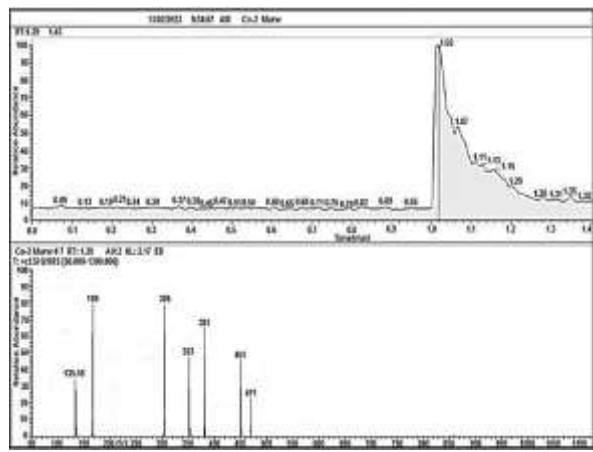


Figure 2. LC-Mas spectrum of cobalt complex

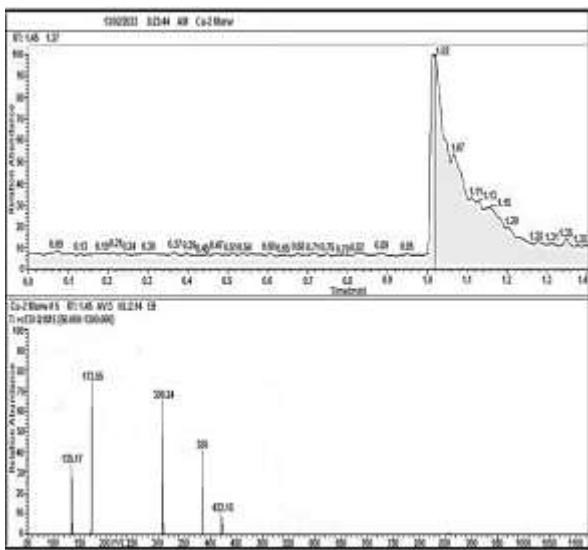


Figure 3. LC-Mas spectrum of copper complex

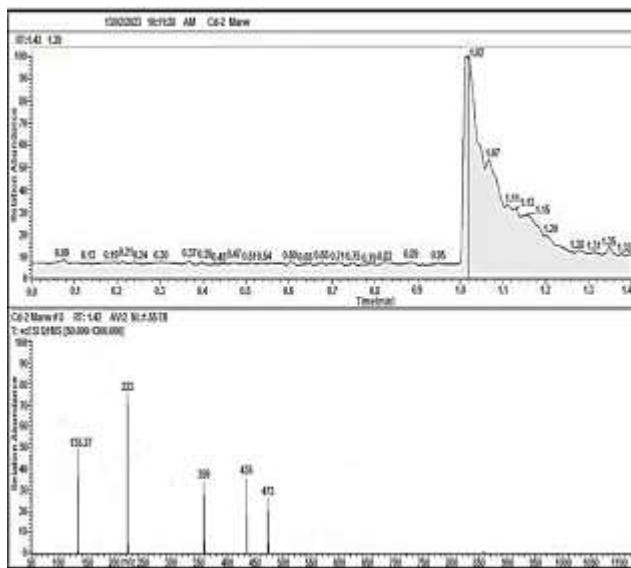


Figure 4. LC-Mas spectrum of cadmium complex

Elemental-micro-analysis (C. H. N. O. S) diagnosis:

The percentage for each element in synthesized complexes and also chloride involvement and metal ratio were estimated technically and calculated theoretically, then comparing the results. All estimated results were in good agreement with the theoretical results⁽¹⁵⁾ as illustrated in table 4.

antibacterial activity inhibition:

The inhibition effectiveness for the compounds in this work were tested against gram negative bacteria (Spuedomonas & E.Coli) and positive bacteria (Staph. Aureas & Bacillus) and two types of fungi (Aspergillus niger & Fuzaium). The samples of the cultivated

complexes showed varying results in terms of the zone of inhibition, and some of them showed ineffectiveness in inhibiting the growth of bacteria or fungi according to the concentrations prepared⁽¹⁶⁾ as shown in Tables 5 and 6, the inhibition values of the complexes according to the concentration prepared, as well as Figures 5 show the zones of inhibition for bacteria and fungi.

Table 4. Elemental analysis incomes of the complexes

Element micro analysis %, Estimated & (calculated)					
		Compounds (M. wt)			
C ₂₀ H ₂₀ SCl ₂ MnO ₃	C ₂₀ H ₂₀ SCl ₂ CuO ₂	C ₂₀ H ₂₀ SCl ₂ ZnO ₂ (460.73)	C ₂₀ H ₂₀ SCl ₂ NiO ₃ (472.05)	C	H
48.01 (47.31)	50.49 (51.30)	51.58 (52.35)	49.94 (50.86)	49.94 (50.89)	
4.09 (3.97)	3.77 (4.74)	4.11 (4.39)	3.52 (4.38)	3.88 (4.70)	
--	--	--	--	--	
6.89 (6.30)	11.04 (10.25)	7.08 (6.97)	5.99 (6.95)	11.12 (10.16)	
5.39 (6.32)	7.85 (6.85)	6.70 (6.99)	7.66 (6.96)	5.84 (6.79)	
14.38 (13.96)	14.84 (15.14)	16.11 (15.45)	16.60 (15.39)	16.00 (15.01)	
21.24 (22.14)	12.01 (11.73)	14.42 (13.85)	15.08 (14.19)	13.26 (12.48)	
				13.31 (12.43)	M

$C_{20}H_{20}SCl_3FeO_2$ (449.51)	50.11 (49.36)	4.72 (4.14)	:	5.73 (6.58)	6.89 (6.59)	20.91 (21.86)	11.64 (11.48)
--------------------------------------	------------------	----------------	---	----------------	----------------	------------------	------------------

Table 5. the bacterial inhibition values of the complexes

Sample	mg/ml	Gram positive		Gram negative	
		<i>Staph. aureas</i> Inh. zone cm	<i>Bacillus</i> Inh. zone cm	<i>Spudomonas</i> Inh. zone cm	<i>E.Coli</i> Inh. zone cm
[ZnL ₁ L ₂ Cl]Cl	0.033	-ve	-ve	0.8	-ve
[CuL ₁ L ₂ Cl] Cl	0.02	2	3	3.5	1.7
[MnL ₁ L ₂ Cl ₂ H ₂ O]	0.025	-ve	-ve	-ve	-ve
[CoL ₁ L ₂ Cl ₂ H ₂ O]	0.019	-ve	-ve	-ve	-ve
[CdL ₁ L ₂ Cl]Cl	0.0075	3.5	3.5	2.5	2
[FeL ₁ L ₂ Cl ₃]	0.0178	-ve	-ve	1	-ve
[NiL ₁ L ₂ Cl ₂ H ₂ O]	0.015	-ve	-ve	1.5	-ve

Inh. = inhibition

Table 6. the fungal inhibition values of the complexes

Sample	mg/ml	<i>Aspergillus niger</i>		<i>Fuzaium</i> growth cm	
		growth cm	cm	cm	cm
[CuL ₁ L ₂ Cl] Cl	0.02	-ve	-ve	-ve	-ve
[MnL ₁ L ₂ Cl ₂ H ₂ O]	0.025	-ve	-ve	-ve	-ve
[CoL ₁ L ₂ Cl ₂ H ₂ O]	0.019	-ve	-ve	-ve	-ve
[CdL ₁ L ₂ Cl]Cl	0.0048	-ve	-ve	-ve	-ve
[ZnL ₁ L ₂ Cl]Cl	0.008	-ve	-ve	-ve	-ve
[FeL ₁ L ₂ Cl ₃]	0.0178	-ve	-ve	-ve	-ve
[NiL ₁ L ₂ Cl ₂ H ₂ O]	0.015	-Ve	-Ve	-Ve	-Ve

Conclusion:

The synthesis of stable mixed-ligand complexes was carried out successfully using dimedone (HL1) and (HL2) 1,2-dibenzothiophene with next metal salts: Co (III), Mn (II), Fe (III), Co (II), Ni (II), Cu (II), Zn (II) and Cd (II) individually. The interaction of metal ions was carried out through oxygen atoms of (HL1) ligand and sulfur atom of (HL2) ligand. This binding was indicated by FT-IR spectra of the compounds by noticing M-O and M-S bands. Those spectra are also indicated the binding of aqua water molecule and chloride molecules. According to electronic spectra and molar conductivity measurements we could prove the obtained shapes of the complexes either octahedral or tetrahedral. LC-Mass spectra, the fragmentation

analogues of the complexes and also elemental analysis proved the gained molecular formulas. Finally, the inhibitory action of the compounds was tested toward bacteria and fungi giving variable effects as detailed in the manuscript.

References:

- Chen, M., Guo, Z., Lanier, M. C., Zhao, L., Betz, S. F., Huang, C.Q., Loweth, C.J., Ashweek, N.J., & Liu, X.J. (2007). Identification of 2-(4, 5, 6, 7-tetrahydro-1H-pyrrolo [3, 2-c] pyridin-3-yl)-ethylamine derivatives as novel GnRH receptor antagonists. Bioorganic & medicinal chemistry letters, 17(14), 3845-50. DOI: 10.1016/j.bmcl.2007.05.009.
- El-Sherif, A.A., & Eldebss, T.M. (2011). Synthesis, spectral characterization, solution equilibria, in vitro antibacterial and cytotoxic activities of Cu (II), Ni (II), Mn (II), Co (II) and Zn (II) complexes with Schiff base derived from 5-bromosalicylaldehyde and 2-aminomethylthiophene. Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy, 79(5), 1803-14. DOI: 10.1016/j.saa.2011.05.062.
- El-Dissouky, A., Shuaib, N.M., Al-Awadi, N.A., Abbas, A.B., El-Sherif, A. (2008) Synthesis, characterization, potentiometric and thermodynamic studies of transition metal complexes with 1-benzotriazol-1-yl-1-[(p-methoxyphenyl) hydrazone] propan-2-one. Journal of Coordination Chemistry, 61(4), 579-94. DOI:10.1080/00958970701365492.
- Buldurun, K. (2020). Synthesis, characterization, thermal study and optical property evaluation of Co (II), Pd (II) complexes containing Schiff bases of thiophene-3-carboxylate ligand. J. Electron. Mater, 4(3), 1935-43. <https://doi.org/10.1007/s11664-019-07876-2>.
- Mayans, J., Gómez, D., Font-Bardia, M., & Escuer, A. (2020) Chiral Oxazolidine Complexes Derived from Phenolic Schiff Bases. Crystal Growth & Design, 20(6), 4176-84. <https://doi.org/10.1021/acs.cgd.9b00381>.
- Mohamed, G.G., El-Sherif, A.A., Saad, M.A., El-Sawy, S.E., & Morgan, S.M. (2016) Mixed-ligand

complex formation of tenoxicam drug with some transition metal ions in presence of valine: Synthesis, characterization, molecular docking, potentiometric and evaluation of the humeral immune response of calves. *J. Mol. Liq.*, 22(3)1311-32. DOI:10.1016/j.molliq.2016.09.065.

7. Jiang, Y., Dey, S., Ke, H., Yang, Y., Sun, L., Xie, G., Chen, S., & Rajaraman, G. (2023). Steric hindrance effect of Schiff-base ligands on magnetic relaxation dynamics and emissive behavior of two dinuclear dysprosium complexes. *J. Rare Earths*, 41(7),1049-57. DOI:10.1016/j.jre.2022.04.019.
8. El-Sonbati, A. Z., Diab, M. A., Morgan. S. M., Abou-Dobara, M. I., & El-Ghettany, A. A. (2020). Synthesis, characterization, theoretical and molecular docking studies of mixed-ligand complexes of Cu (II), Ni (II), Co (II), Mn (II), Cr (III), UO₂ (II) and Cd (II). *J. Mol. Struct.*, 15(1200), 127065. DOI:10.1016/j.molstruc.2019.127065.
9. Reda SM, Al-Hamdani AA. Mn (II), Fe (III), Co (II) and Rh (III) complexes with azo ligand: Synthesis, characterization, thermal analysis and bioactivity. *Baghdad Science Journal*. 2022.
10. Al Zoubi, W., Jirjees, V., Suleiman, V., Al Hamdani, A. A., Ahmed, S. D., Kim, Y. G., & Ko, Y. G. (2019). Synthesis and bioactivity studies of novel Schiff bases and their complexes. *J. Phys. Org. Chem.*, 32(11), e4004. <https://doi.org/10.1021/acs.chemrev.7b00656>.
11. Al Zoubi, W., Kim, M. J., Salih, Al Hamdani A. A., Kim, Y. G., & Ko ,Y. G. (2019). Phosphorus-based Schiff bases and their complexes as nontoxic antioxidants: Structure–activity relationship and

mechanism of action. *Appl. Organomet. Chem.*, 33(11), e5210. DOI:10.1002/aoc.5210.

12. Kareem, M. J., Al-Hamdani, A. A., Ko, Y. G., Al Zoubi, W., & Mohammed, S.G. (2021). Synthesis, characterization, and determination antioxidant activities for new Schiff base complexes derived from 2-(1H-indol-3-yl)-ethylamine and metal ion complexes. *J. Mol. Struct.*, 5(1231), 129-669. DOI: <https://doi.org/10.21123/bsj.2022.7289>.
13. Obaid, S. M., Sultan, J. S., & Al-Hamdani, A. A. (2020). Synthesis, Characterization and Biological Efficacies from Some New Dinuclear Metal Complexes for Base 3-(3, 4-Dihydroxy-phenyl)-2-[(2-hydroxy-3-methylperoxy-benzylidene)-amino]-2-methyl Propionic Acid. *Indones. J. Chem.*, 20(6), 1311-22. <https://doi.org/10.22146/ijc.49842>.
14. Al-Qudsi, Z. N., & Abood, H. M. (2013) The Electronic Transition Behavior Cr (III), Fe (III), Fe (II) and Ni (II), Transition Metal Cations In Ammonium Alum-Urea Room Temperature Ionic Liquid. *ANJS.* 16(3),46-55. DOI: 10.22401/JNUS.16.3.06.
15. Patange, V. N., Pardeshi, R. K., & Arbad, B. R. (2008). Transition metal complexes with oxygen donor ligands: a synthesis, spectral, thermal and antimicrobial study. *J. Serb. Chem. Soc.*, 73(11),1073-82. DOI:10.2298/JSC0811073P.
16. Al Zoubi, W., Al Hamdani, A. A., Ahmed, S.D., & Ko, Y. G. (2018). A new azo-Schiff base: Synthesis, characterization, biological activity and theoretical studies of its complexes. *Appl. Organomet. Chem.*, 32(1), e3895. <https://doi.org/10.1002/aoc.3895>

تحضير وتشخيص معقدات والتحديد الطيفي لخلط معقدات الليكанд وتقدير فعاليتها البيولوجية

مروة الدليمي^{*} و عمر حمد شهاب^{**}

^{*} قسم الكيمياء ، كلية العلوم ، جامعة الانبار ، العراق

E-mail address: mhdymrwt65@gmail.com

الخلاصة:

اتجهت الدراسة المقدمة الى تحضير معقدات جديدة بالسماح لخلط الليكанд المكون من (HL1) ديميدون و 1,2 (HL2)-ثنائي بنزوثيوفين بالتفاعل مع أيونات المعادن التالية: (III) Mn، (II) Co، (III) Fe، (II) Co، (II) Ni و Zn (II) و Cu (II) و Cd (II) يشكلون بشكل فردي مجاميع معدنية مستقرة ذات أشكال هندسية مختلفة كما هو موضح باستخدام تقنيات مختلفة. تم الكشف عن تكوين المجاميع وكذلك الأشكال الهندسية للمعقدات بواسطة تحويل الأشعة تحت الحمراء، أطياف الكتلة، التحليل العنصري والأطياف الإلكترونية. علاوة على ذلك، تم اختبار ذوبان المركبات في مذيبات مختلفة منها: THF، CHCl₃، Spuedomonas & DMSO، DMF، C2H5OH و H₂O. علاوة على ذلك، تم اختبار الفعالية الحيوية تجاه نوعين من البكتيريا البكتيريا سالبة الجرام (E.Coli و Aspergillus niger & Fuzarium) و نوعين من الفطريات (Staph. Aureas & Bacillus). تطبيقيات مختلفة (سواء كانت فعالة أو غير فعالة) كما هو موضح في البحث.

الكلمات المفتاحية: (ديميدون، 1,2-ثنائي بنزوثيوفين)، (الفعالية البيولوجية)، الاشعة تحت الحمراء، ليكандات.