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SYNTHESIS AND CHARACTERIZATION OF SOME BIVALENTMETAL COMPLEXES OF BIOACTIVE LIGANDS HAVINGBENZIMIDAZOLEMOIETY

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ABSTRACT

Cadmium, Mercury, and lead are three of the most harmful metal contaminants to human health and well-being. Cd (II), Hg (II), and Pb II complexes of the type [M(L1-3)X2] have been produced with three of the ligands, namely 2,5-bis (2-thiomethylenyl- benzimidolozolyl) 1,3,4-thiadiazole and 2-(picolinyl)-2-(benzimidozolyl) ether. It is clear from the 2917 cm-1 medium band in the free ligands due to (NH) vibration that these ligands remain in Keto form when solidified. There is no enolisation or deprotonation of ligands in complexes and they remain neutrally attached to the bivalent metal ions. It appears that picolinic N, etherial O/S, and azomethenic nitrogen in complexes can be coordinated by newly discovered bands in the far infrared range. At 1535-1540 and 1365-1370 cm-1, two lines in the Pb (II) spectra support the coordination of the acetate group to the Pb (II) ion through one octahedral oxygen, which indicates the monodentate acetate group's coordination to Pb

.**Keywords:**Complexes of metals, bioactive ligands, and benzimidazole are all examples of these.

INTRODUCTION

Ninety of the 118 elements that have been discovered so far are found in nature. Of these, nine of them are radioactive, while most of the rest of them are essential for life. Metals of varying types make up sixty-one of the items. Metals make up 3% of our body weight. Our bodies need a variety of metals in differing amounts, and they also play a critical role in medicine for a variety of ailments. However, if consumed in excess of the recommended dosage, they can be harmful to our health. cadmium, mercury, and lead are among the metals that pose the greatest threat to human life. 3,4

In both humans and animals, lead is a very lethal cumulative poison. Lead pollution in the environment is a prevalent problem. Gasoline with lead is the most common human source of this element. In addition to causing venous damage, cadmium may also interfere with the kidneys' ability to regulate the calcium and phosphate balance. Organisms are susceptible to its carcinogenic action. As an industrial waste or bi-product, the environmental impact of 4,7 Cadmium is significant. Dyslexia, ADHD, intellectual impairment, and autism are just a few of the neurological disorders linked to mercury exposure. As with Pink disease, it's possible that Mercury vapour causes Kawasaki disease. 6

Toxic metal ions such as cadmium, mercury, and lead, as well as the mechanisms by which they cause harm to living organisms, were therefore deemed critical in the current context and warranted in-depth investigation. sequence of compounds containing the cadmium ions

The ligands used to make [MLX2] were selected from the Ether, Thioether, and Thiadiazole groups. The molar conductance of these complexes ranges from 6 to 14 ohm-1 cm2 mol-1, indicating that they are non-electrolytic in nature.

The medium band at 3357 cm-1 in the ligand's spectra is attributed to the (NH) vibration. Medium band at 2917 cm-1 in the unattached ligand suggests that the ligand is still in Keto form in solid state because of (NH) vibration. There is no enolization or deprotonation of the ligand in the complexes, and the ligands are coordinated in their neutral state. When C=O (ethereal) Oxygen and C=S (thioethereal) sulphur are involved in coordination, a band at 1700 cm-1 in the ligand shifts to a lower frequency. For all complexes, bands in the 1681-1686 cm-1 range indicate the ligand is in the Keto form. At 1600 cm-1 in L, the distinctive C=N group can be found. Complexes with azomethine nitrogen coordinating to metal show this band shifting somewhat lower in frequency. 9,10 It is bolstered by the appearance of a new band, which measures between 460 and 487 centimeters.

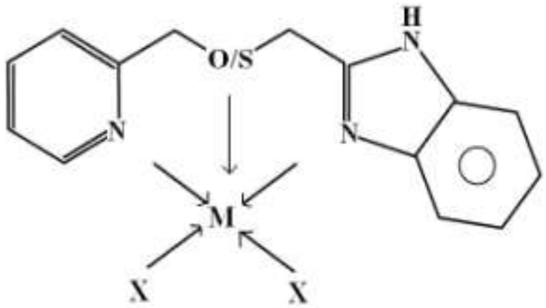
Support for the coordination of picolinic N, etherial O/S and azomethinic N in complex is provided by the appearance of additional bands in the far-infrared region. In the 385-370 cm-1 range, the M-S band appears, as does the M-N band (470-460 cm-1).

In this case, M-Cl (410-400 cm-1).

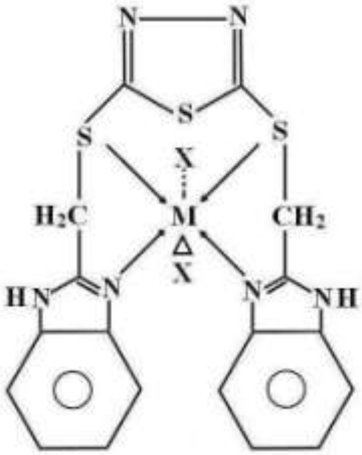
These complexes [PbL1–3(ac)2] contain bands that correspond to unidentified types of unidentified acetate groups. There were two distinct bands in the spectra of Pb(II) complexes, one at 1535-1540 cm–1 and the other at 1365-1370 cm–1. Pb(II) coordination was facilitated by these two prohibitions' existence.

The acetate group, which contains only one oxygen atom, serves as a monodentate ligand.9,10,11

Cadmium (II) anologous complexes with ligands L1 and L2 are discovered to be distorted tetrahedral



Structure of $[\mathrm{M\,L}^{1\text{-}2}\,\mathrm{X}_2]$
M=Cd(II), Hg(II); X=Cl^-
M=Pb(II), X=ac^-



Structure of $[\mathrm{M\,L}^{3}\,\mathrm{X}_2]$
M=Cd(II), Hg(II); X=Cl^-
M=Pb(II), X=ac^-

and those with L3 to be octahedral by X-ray single crystal structure. Thus, the metal complexes are represented in the diagram below.

2- (picolinyl)-2- (benzimidozolyl) ether and 2-(picolinyl)-2- (benzimidozolyl) ether were synthesized and characterized in this study (benzimidozolyl)

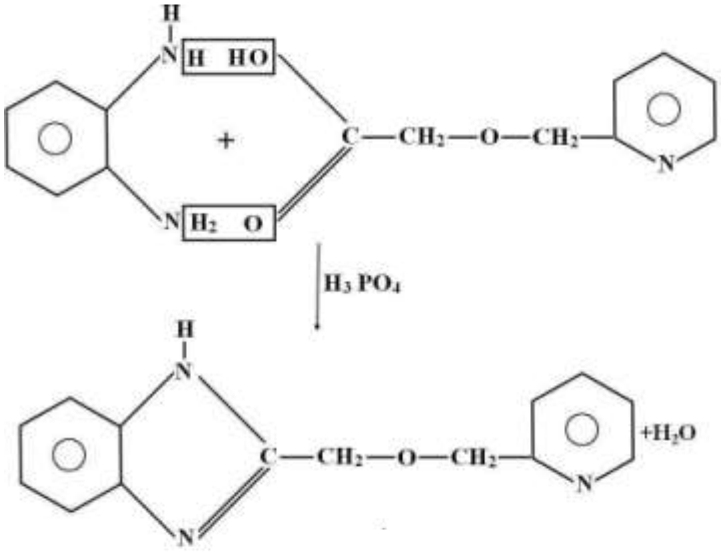
thethioethers, 2,5-bis (2-thiomethylenyl) benzimidazolyl) 1,3,4-thiadiazoles, and their complexes with Hg (II), Cd (II) and Pb (ii) (II).

EXPERIMENTAL

Ligands were synthesized using the method described. The following procedure was used to make 2-(picolinyl)-2-(benzimidozolyl) ether, also known as L1.

Benzimidazole derivatives are formed when picolinyloxoacetic acid is condensed with orthophenylenediamine in the presence of phosphoric acid.

5.6

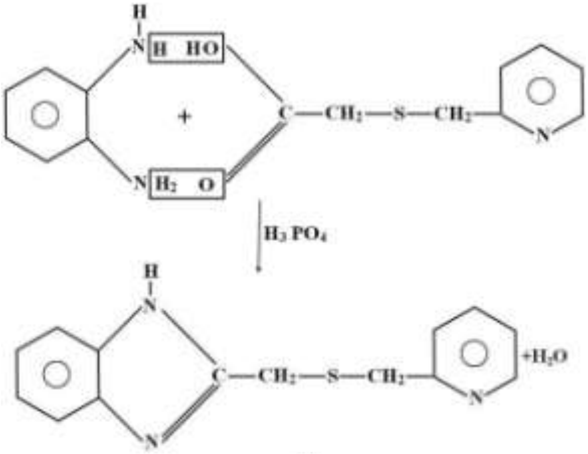


L

(M.FC14H13N3O)

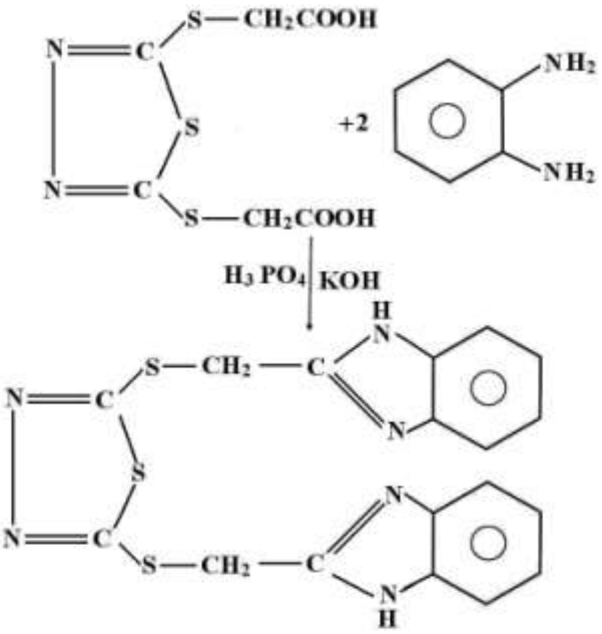
Similarly,L2 andL3weresynthesiseasshown below

Synthesis ofL2 :



L2

(M.F.C14H13N3S)



Synthesis ofL3 :

L3

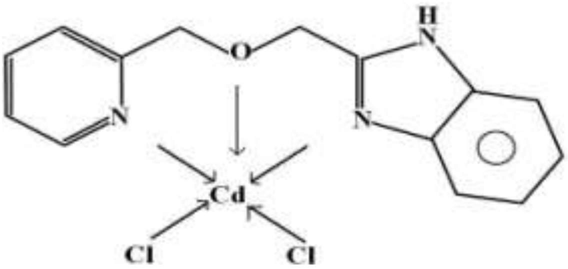
(M.F.C18H14N6S3)

The following procedure was used to prepare complexes. Reactions with all three ligands, L1, L2 and L3, were performed on each bivalent metal ion. The following steps show how to make cadmium complex with ligand L1.

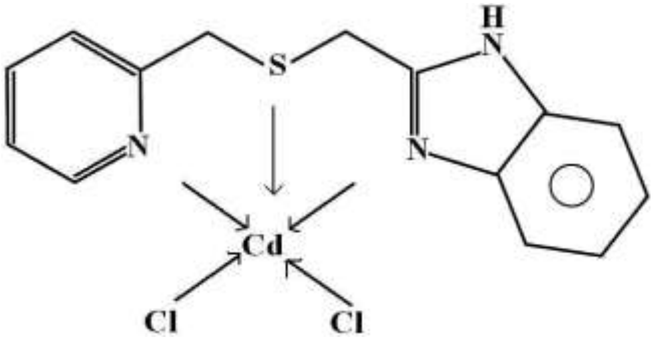
[Cd (L1) Cl2] is the product of a chemical reaction involving Cd (II) and L1.

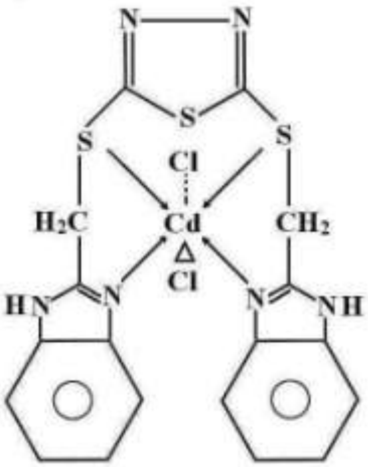
$$\mathrm{Cd\ Cl_2 \cdot 2H_2O} + \mathrm{L^1} \xrightarrow[\mathrm{Et\ OH}]{\Delta} [\mathrm{Cd\ L^1 Cl_2}] + \mathrm{2H_2O}$$

Thestructureofthesynthesisedcomplexshowingmodeofcoordinationofthe ligandwithmetal ionis shown



below.
[CdL1Cl2]Likewise,thestructuresofCd-complexesofL2 andL3areshownasunder.





[Cd L2Cl2]

[CdL3Cl2]

xAs with cadmium, mercury and lead have bivalent ion structures that are identical to those of cadmium complexes with ligands L1, L2, and L3.

In contrast to mercury, cadmium and lead were estimated spectrophotometrically. The following tables provide the results of elemental analysis and Infrared spectrum data based on the experiments that were carried out.

Table-1AnalyticalDataofLigands& complexes

Ligand/complexes	**Observed%(Calculated%)**						**$\wedge_M$ (Ohm^{-1}cm^{2}mol^{-1}**
	C	**H**	**N**	**S**	**Cl**	**M**	
L_1	70.02 (70.29)	5.41 (5.43)	12.46 (12.57)	–	–		–
L_2	65.88 (65.62)	5.01 (5.09)	16.47 (16.32)	12.55 (12.46)	–		–
L_3	54.32 (54.50)	3.49 (3.51)	20.88 (21.00)	23.96 (24.00)	–		–
[Cd L^1Cl_2]	39.58 (39.77)	3.00 (3.07)	9.68 (9.94)	–	16.76 (16.80)	26.32 (26.61)	10
[CdL^2Cl_2]	38.02 (38.32)	2.95 (2.96)	9.48 (9.58)	7.26 (7.29)	16.02 (16.19.)	25.42 (25.64)	08
[CdL^2Cl_2]	36.96 (37.02)	02.38 (02.40)	9.12 (9.25)	16.38 (16.45)	12.02 12.17	19.13 (19.26)	06
[HgL^1Cl_2]	32.76 (32.86)	2.53 (2.54)	8.20 (8.22)	–	13.74 (13.89)	39.01 (39.25)	12
[HgL^2Cl_2]	31.76 (31.90)	2.40 (2.46)	7.85 (7.97)	6.02 (6.07)	13.32 (13.48)	37.96 (38.10)	10

$[HgL^3Cl_2]$	31.12 (32.16)	2.03 (2.08)	12.38 (12.50)	14.22 (14.25)	10.48 (10.57)	29.76 (29.86)	13
$[PbL^1Cl_2]$	38.02 (38.23)	3.34 (3.36)	7.28 (7.44)	–	–	36.38 (36.72)	07
$[PbL^2Cl_2]$	36.98 (37.22)	3.25 (3.27)	7.23 (7.24)	5.43 (5.51)	–	35.62 (65.71)	09
$[PbL^3Cl_2]$	36.12 (36.40)	2.73 (2.75)	11.41 (11.58)	13.02 (13.23)	–	28.36 (28.57)	14

xAlso, the IR spectra of the free ligands and the related complexeswere determined,7,9,12 and the concerned data obtained are being presented inthefollowingtable.

Table-2IRSpectraldata

Ligands/Complexes	υ_{N-H}	$\upsilon_{C=N}$	υ_{M-Cl}	υ_{M-S}	υ_{M-N}	υ_{M-O}
L_1	3185	1610	–	–	–	–
L_2	3180	1615	–	–	–	–
L_3	3190	1612	–	–	–	–
$[Cd\ L^1Cl_2]$	3180	1600	410	–	460	585
$[Cd\ L^2Cl_2]$	3185	1595	415	380	468	–
$[Cd\ L^3Cl_2]$	3178	1597	412	372	472	–
$[HgL^1Cl_2]$	3188	1598	406	382	–	578
$[HgL^2Cl_2]$	3196	1596	408	385	463	–
$[HgL^3Cl_2]$	3175	1599	412	376	465	–
$[PbL^1Cl_2]$	3194	1601	414	374	–	581
$[PbL^2Cl_2]$	3174	1590	407	381	470	–
$[PbL^3Cl_2]$	3191	1585	409	382	475	–

RESULTS&DISCUSSION

For the Cd, Hg, and Pb complexes, a series of ligands have been chosen to interact with them, including 2-(picolinyl)-2- (benzimidozolyl)ether, 2-(picolinyl)-2- (benzimidozolyl)thioether, and 2,5-bis (2-thiomethylenlybenzimidazolyl) 1,3,4-thiodiazole [ML1–3X2] where X=Cl for Cd- and Hg-complexes, X=ac for Pb-complexes. Based on the results of the elemental analysis, the resulting molecular formulae are shown in Table 1. They are non-electrolytic because the molar conductivity is in the range of 6-14 ohm-per-cm2 cm2 mol-1 that is listed in the table.

There is a lot to learn from infrared spectral data. Without an advanced technology like X-ray crystallography, IR spectra have proven to be the most reliable method for determining the mode of

ligand-metal ion bonding. 11-13. The IR spectra of free ligands were compared to the spectra of corresponding complexes in order to analyze the binding manner of the metal ions to the ligands. 14–17

Using the 4000-400 cm-1 range as a guide, the ligands L1-3 are tentatively assigned their primary IR bands in Table 2. A medium band at 3357 cm-1 in the ligand's spectra is attributed to the (NH) vibration. This middle band at 2917 cm-1 suggests that the free ligand is still in the Keto form in the solid state because of the (NH) vibration. 10-

Because the ligand has not been enolized or deprotonated, this band is present in the complexes and L1 is coordinated in its neutral state. C=O (etheral) Oxygen/C=S (thioethereal) Sulphur are shown to be involved in coordination by shifting a band at 1700 cm-1 in the ligand to a lower frequency in the complexes. In all the complexes, there is a band in the 1681-1686 cm-1 range that supports the Keto form of ligand. The characteristic C=N group is responsible for a sharp band at 1600 cm-1 in L1. There are a few complexes8-15,16 where the azomethine nitrogen is covalently bound to the metal. The development of additional bands at 460-487 cm–1 adds credence to this argument. In the complexes [PbL1–3(ac)2], stretching bands of unidentate type of acetate group11–13 are present in asymmetric and symmetric forms.

A novel band in the far infrared supports the coordination of picolonic N, ethereal O/S, and azomethinic N in complexes produced. M–S(385-370) cm-1, M–N(470-460) cm-1, and M–Cl(410-400) cm-1 are the locations of the bands. These two bands, at 1535-1540 cm–1 and 1365-1370 cm–1, are attributed to COO(s) and COO(s), respectively.

COO(as)+ in this case. For the acetate group to be monodentate, these two bands must be present in order for it to coordinate to Pb(II) through one oxygen atom, which is clearly the case. 14,15,19

Review articles13,18 on the stereochemistry of lead (II) complexes with high coordination numbers (CN) have recently emerged in peer-reviewed journals.

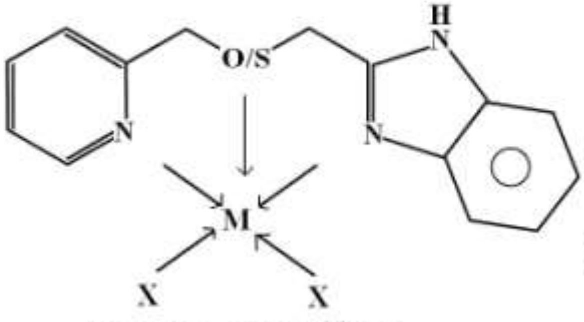
VSEPR theory has been used to discuss the initial coordination sphere of Pb(II) ions in the crystal structure of lead(II) complexes. There are four types of coordination: Tetrahedral, Trigonalbipyramidal, Octahedral, pentagonal bipyramidal with an axial or equitorial unoccupied spot in the first coordination sphere. 21–23 For Pb(II) with a d10 structure, electronic spectroscopy does not reveal any information about stereochemistry. X-ray crystallographic studies are the only ones that can provide a solid picture

of structure. Unfortunately, we have no access to any facilities in this part of the world. Based on X-ray research, we've come up with our own structure. Proposed structures for two tridentate ligands L1 and

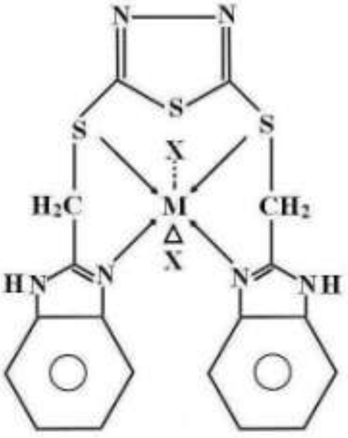
L2 with (3 + E) and (6 + E) cases are octahedral and tridentate, respectively, for complexes with L3. The diamagnetic properties of all complexes are the same. 24,25

According to the results of biological screening, complexes are more effective than ligands but less effective than the standard medicine. This is important to note.17,18,20

In light of the foregoing, it is postulated that the bivalent Cd, Hg, and Pb complexes with the aforementioned ligands have the following structures:



Structure of [M L^{1-2} X_2]
M=Cd(II), Hg(II); X=Cl^-
M=Pb(II), X=ac^-



Structure of [M L^3 X_2]
M=Cd(II), Hg(II); X=Cl^-
M=Pb(II), X=ac^-

Complexes of thebivalentmetalions Complexes of the bivalent metalusedwithfirsttwo ligands
ions used with third ligands

CONCLUSIONS

With the comparison of data obtained from the experimental investigation of Infra red spectrum with the data reported so far in the literature, the cadmium complexes with ligands L1 and L2 have distorted tetrahedral structures, while those with L3 have octahedral structures. X-ray single crystal structures of Cadmium (II) similar complexes support this. The comparison of current research findings with those previously reported in context of Hg complexes shows that the distorted tetrahedral structures of Hg(II) complexes with the first two ligands, namely L1 and L2, and those with L3 are the same. The isomorphous compounds were studied using X-ray crystallography, and this supports it. 21-25

With these ligands, the structures of bivalent plumbum complexes with these ligands are tetrahedral with L1 and L2 and octahedral with L3.

As evidenced by X-ray crystallographic research and earlier reports, as well as other evidence.17,19,23

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