



# **Novel benzothiazolinone ligand and its transition metal complexes chemical preparation, structure and antimicrobial activity**

Research Project

Submitted to the department of (Chemistry) in partial fulfillment of the requirements for the degree of **B.A** or **BSc.** in (science)

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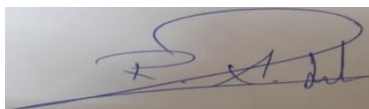
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## Supervisor recommendation

I am the student's supervisor, **rahel hamadamin mustafa**. I support that the student has completed all the requirements for submitting the research drawn entitled ‘Novel Benzothiazolinone ligand and its transition metal complexes chemical preparation, structure and antimicrobial activity’ according to the numbered administrative order **// on oct.** in accordance with the instructions of Salahaddin university quality assurance and it is ready for discussion.



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## **Dedication**

This research project is dedicated to our almighty God, who gave me strength and knowledge for completing this research project, also to my mam and family that helps and supports me. Finally, to teachers, mentors, and many friends and classmates how never left our side in supporting me throughout the process.

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Muhammad, may Allah bless you.

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**Rahel hamadamin mustafa**

## **Abstract**

My research about synthesis and characterization of transition metal complexes with benisothiozolate (bit) ligand. Benisothiozolate is a 7-membered ring compound containing one nitrogen, one oxygen and one sulfur atom with chemical formula  $C_7H_5NOS$ . belongs to heterocyclic class containing Nitrogen-Sulfur with extensive antimicrobial utilization. Benisothiazolinone (Hbit) has potent antimicrobial and anti-fungicidal properties and it is potentially a versatile poly-functional ligand that could coordinate with metal centers in various coordination modes. Based on the reported literature the bit ligand form complexes with metals such as Mn(II), Co(II), Ni(II), Pd(II), Pt(II), Cu(II) and Hg(I), in which the bit ligand bound to the metal ions through either monodentate N-atom or bidentate N,O-atoms in a tetrahedral, square planar, square pyramidal or octahedral geometry.

**Keywords:** *Transition Metal complexes, Benzothiazolinone ligand, review.*

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## **Part One: Introduction**

### **1.Introduction**

#### **1.1Coordination compound**

Coordination compounds also known as coordination complexes, complex compounds, or simply complexes. The essential feature of coordination compounds is that coordinate bonds form between electron pair donors, known as the ligands, and electron pair acceptors, the metal atoms or ions (House, 2008).

Coordination chemistry is, quite simply, the chemistry of coordination compounds. The coordinated groups, called ligands, may be neutral molecules or ions. (McCLEVERTY, 1987). Ligand is a molecule or ion carrying suitable donor groups capable of binding (or coordinating covalently) to a central atom. The central atom that is the focus of ligand coordination is most commonly a metal, although a central metalloid atom can take on the same role. In order for a pair of electrons to be donated from a ligand to a metal ion, there must be an empty orbital on the metal ion to accept the pair of electrons. This situation is quite different from that where covalent bonds are being formed because in that case, one electron in a bonding pair comes from each of the atoms held by the bond (House, 2008). The coordinate bonds are the result of Lewis acid-base interactions, the number of species that can form complexes with metal ions is large. Lewis bases such as H<sub>2</sub>O, NH<sub>3</sub>, F, Cl, Br, I, CN, SCN, NO<sub>2</sub>, all form a wide range of coordination compounds/ Ligands may be molecules with heteroatom (e.g. H<sub>2</sub>O, NH<sub>3</sub>, PPh<sub>3</sub>) having lone pair (Astruc, 1992). anions (e.g. CN<sup>-</sup>, F<sup>-</sup>, Cl<sup>-</sup>, SCN<sup>-</sup>), unsaturated hydrocarbons (H<sub>2</sub>C=CH<sub>2</sub>, C<sub>4</sub>H<sub>4</sub>) or aromatics (C<sub>6</sub>H<sub>6</sub>). Ligands can be group into different classes based on the number of donor atoms (sites) they possess. A ligand with one donor site is called monodentate (e.g. H<sub>2</sub>O, NH<sub>3</sub>, CN<sup>-</sup>, Cl<sup>-</sup>

). Bidentate ligands are those with two binding sites e.g. ethylenediamine ( $\text{H}_2\text{NCH}_2\text{CH}_2\text{NH}_2$ ), oxalate ( $\text{C}_2\text{O}_4^{2-}$ ) etc. These ligands are capable of forming ring structure (Chelate) with central metal. A ring of this type is known as a chelate (pronounced “key-late”) ring (from the Greek word *chelos*, meaning “claw”). Tridentate ligands possess three donor atoms e.g. diethylenetriamine ( $\text{H}_2\text{NCH}_2\text{CH}_2\text{NHCH}_2\text{CH}_2\text{NH}_2$ ). They have capacity to form two ring structure around the central metal. Ligands with four donor sites are said to be quadridentate e.g. triethylenetetraamine ( $\text{H}_2\text{NCH}_2\text{CH}_2\text{NHCH}_2\text{CH}_2\text{NHCH}_2\text{CH}_2\text{NH}_2$ ), they are capable of forming complexes with four ring structures. Polydentate ligands have many donor sites e.g. EDTA (ethylenediaminetetraacetate). Another category of ligands are called ambidentate ligands because they have two heteroatoms and any can be used to coordinate to metal depending on the reaction conditions e.g.  $\text{SCN}^-$  (it can either coordinate through S or N),  $\text{NO}_2^-$  (it can coordinate through O or N (LAWAL)). The geometric shape of the fixed positions occupied by ligating atoms is the coordination polyhedron. The common coordination polyhedra are the tetrahedron, square plane, trigonal bipyramid, square pyramid, octahedron and trigonal prism, for coordination numbers four, five and six (McCLEVERTY, 1987).

## 1.2 Transition Metals

Transition metals include the three series of elements that are positioned between the first two groups and the last six groups in the periodic table (**Fig. 1.1**). These series have as their general characteristic that a set of d-orbitals is being filled in progressing from one involves filling the 3d orbitals. The second- and third-row transition metals correspond to those in which the 4d and 5d orbitals are being filled. Because a set of d-orbitals can hold a maximum of 10 electrons, here are 10 elements in each series. The groups containing the transition metals are sometimes designated as the “B” groups or as



groups 3 through 10. Most of the first-row transition metals and several in the second and third groups have important uses. For example, iron is the basis of the enormous range of ferrous alloys in which other first-row metals are often combined (House, 2008).

H																	Ho
Li	Be											B	C	N	O	F	Ne
Na	Mg											Al	Si	P	S	Cl	Ar
K	Ca	Sc	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn	Ga	Ge	As	Se	Br	Kr
Rb	Sr	Y	Zr	Nb	Mo	Tc	Ru	Rh	Pd	Ag	Cd	In	Sn	Sb	Te	I	Xe
Cs	Ba	La	Hf	Ta	W	Re	Os	Ir	Pt	Au	Hg	Tl	Pb	Bi	Po	At	Rn
Fr	Ra	Ac	Rf	Db	Sg	Bh	Hs	Mt	Ds	Rg	Uub						

Ce	Pr	Nd	Pm	Sm	Eu	Gd	Tb	Dy	Ho	Er	Tm	Yb	Lu
Th	Pa	U	Np	Pu	Am	Cm	Bk	Cf	Es	Fm	Md	No	Lr

**Figure 1.1 Periodic table of elements; d-block elements are highlighted**

**Table 1.1 Examples of ground-state electronic configurations**

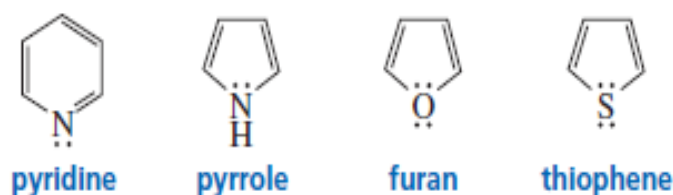
Sc	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn
$d^1s^2$	$d^2s^2$	$d^3s^2$	$d^5s^1$	$d^5s^2$	$d^6s^2$	$d^7s^2$	$d^8s^2$	$d^{10}s^1$	$d^{10}s^2$

The transition metals have always held a special interest for inorganic chemists. Whereas the compounds of the main group metals are almost always white, the transition metal compounds come in every color of the rainbow. Chemists were fascinated by the fact that it was sometimes possible to make compounds of the same formula but in different colors. For example, chromium (III) chloride hexahydrate,  $\text{CrCl}_3 \cdot 6\text{H}_2\text{O}$ , can be synthesized in purple, pale green, and dark green forms. Inorganic chemists generally restrict the term transition metal to an element that has at least one simple ion with an incomplete outer set of d electrons (Geoff Rayner-Canham, 2010, 2006, 2003, 2000).

### 1.3 Heterocyclic compound

A heterocyclic compound is a cyclic compound in which one or more of the ring atoms is an atom other than carbon. A ring atom that is not carbon is called a heteroatom. The name comes from the Greek word heteros, which means “different”. The most common hetero atoms found in heterocyclic compounds are N, O and S (bruice, 2003).

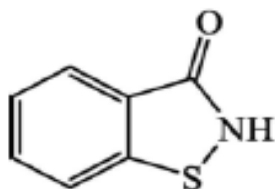
Heterocyclic chemistry is the branch of chemistry dealing with synthesis, properties, and applications of heterocycles. A heterocyclic compound is a cyclic compound that has atoms of at least two different elements as members of its ring (Astruc, 1992). The counterparts of heterocyclic compounds are homocyclic compounds, the rings of which are made of a single element. Although heterocyclic compounds may be inorganic, most contain at least one carbon. Since in organic chemistry non-carbons usually are considered to replace carbon atoms, they are called heteroatom, meaning different from carbon and hydrogen. The simplest of the five-membered heterocyclic compounds are pyridine, pyrrole, furan, and thiophene (**Fig. 1.2**) (Morrison and Boyd, 2002).



**Figure 1.2 Structure of Pyrrole, furan and thiophene**

### 1.4 Benzisothiazolinone (bit) ligand

The coordination chemistry of the related benzisothiozolate (bit) anion (**Fig. 1.3**), resulting from deprotonation of the acidic imine hydrogen in benzisothiazolinone (Al-Jibori et al., 2021, Al-Jibori et al., 2017)



**Figure 1.3 Structure of Benzisothiazolinone ligand**

Benzisothiazolinone (Hbit) has potent antimicrobial and anti-fungicidal properties and it is potentially a versatile poly-functional ligand (Al-Jibori et al., 2017). Benzisothiazolinone which is structurally similar to saccharin has potent antimicrobial and anti-fungicidal properties (Al-Jibori et al., 2018, Al-Jibori et al., 2015). Benzisothiazolinone coordination chemistry and have recently shown that it can bind to Pd(II) in a monodentate fashion through the amide nitrogen (Al-Jibori et al., 2019a, Al-Jibori et al., 2018). The benzisothiazolinone (bit) anion results upon deprotonation of the acidic imine hydrogen and like saccharinate is potentially a versatile poly-functional ligand. However, while saccharinate complexes of the transition and heavy non transition metals are common. Benzisothiazolinone also named 1,2-benzisothiazol-3(2H)-one which is a poly functional heterocyclic ligand, containing sulfur, nitrogen in addition to oxygen atoms that could coordinate with metal centers in various coordination modes (Alheety et al., 2019). The coordination chemistry of the related benzisothiazolinone anion, resulting from deprotonation of the acidic imine hydrogen in benzisothiazolinone, remains virtually unexplored (Al-Jibori et al., 2017)

## 2. Part two: Literature Review

### 2.1 Complexes of benzisothiazolinone (bit) ligand

In 2010, Griffith and coworkers, synthesized and characterized *cis*-[Pd(en)(bit.1H)<sub>2</sub>] (Fig. 2.1) and *cis*-[Pt(NH<sub>3</sub>)<sub>2</sub>(bit.1H)<sub>2</sub>] (Fig. 2.2) complexes as a result of reaction of benzisothiazolinone (bit) with *cis*-[Pd(en)(H<sub>2</sub>O)<sub>2</sub>](NO<sub>3</sub>)<sub>2</sub> and *cis*-[Pt(NH<sub>3</sub>)<sub>2</sub>(H<sub>2</sub>O)<sub>2</sub>](NO<sub>3</sub>)<sub>2</sub>, respectively. In both complexes, the bit ligand is bound to the metal centers through the deprotonated isothiazolinone N-atom in a square planar geometry (Griffith et al., 2010)

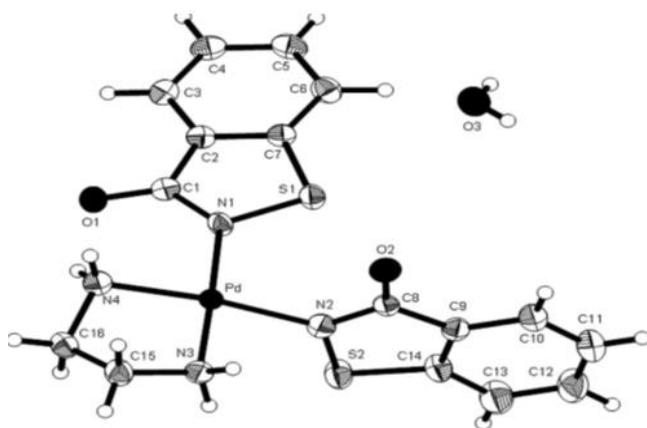


Figure 2.1 Molecular structure of *cis*-[Pd(en)(bit.1H)<sub>2</sub>]

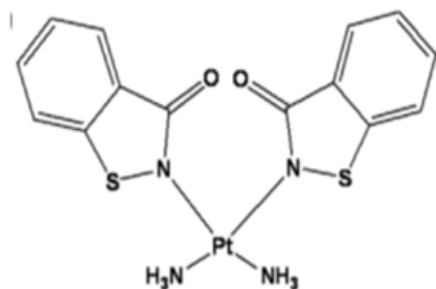
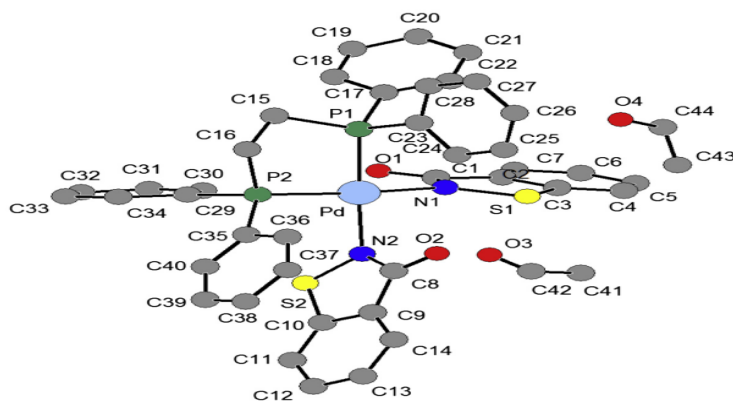


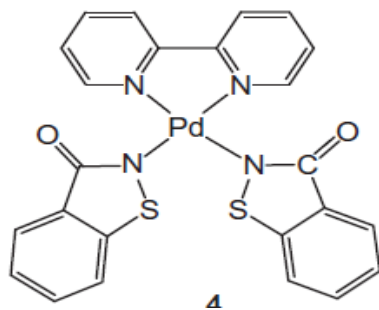
Figure 2.2 Molecular structure of *cis*-[Pt(NH<sub>3</sub>)<sub>2</sub>(bit.1H)<sub>2</sub>]

In 2015, Al-Jibori and coworkers, synthesized and characterized a series of Pd(II) and Pt(II) complexes containing bit ligand of the type; [Pd(bit)<sub>2</sub>(dppe)] (Fig. 2.3), *cis*-[Pd(bit)<sub>2</sub>(bipy)] (Fig. 2.4) (where **bipy** = 2,2'-bipyridin), *cis*-[PdCl(bit)(dppb)] (Fig. 2.5)

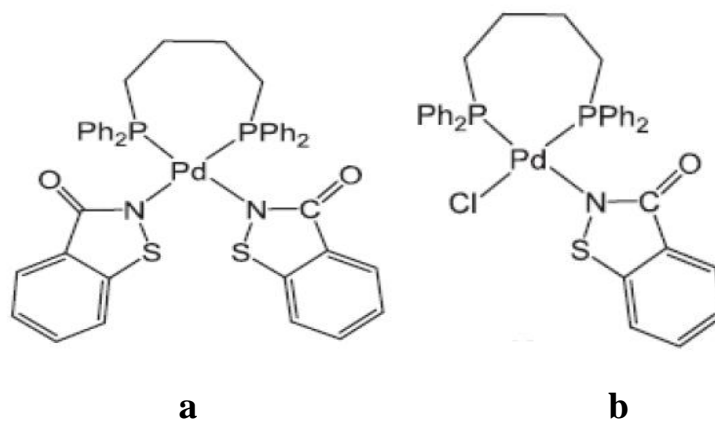
and *cis*-[Pd(bit)<sub>2</sub>(dppb)] (**Fig. 2.5**). A crystal structure of *cis*-[Pd(bit)<sub>2</sub>(dppe)] reveals that the bit ligands are bonded in a monodentate fashion through N-atom and this binding mode is proposed for all of the synthesised complexes. (Al-Jibori et al., 2015)



**Figure 2.3** Molecular structure of *trans*-[Pd(bit)<sub>2</sub>(dppe)]



**Figure 2.4** Structure of *cis*-[Pd(bit)<sub>2</sub>(bipy)]



**Figure 2.5** Structure of **a**: *cis*-[Pd(bit)<sub>2</sub>(dppb)] and **b**: [PdCl(bit)(dppb)]

In 2016, Al-Jibori and coworkers, synthesized and characterized a square planar *cis*-[Pd(bit)<sub>2</sub>(H<sub>2</sub>NBz)<sub>2</sub>] (Fig 2.6) complex. A complex was obtained by reaction of *trans*-[PdCl<sub>2</sub>(H<sub>2</sub>NBz)<sub>2</sub>] (where H<sub>2</sub>NBz = benzylamin) with Nabit ligand. The crystal structure of the synthesized complex reveals that the bit ligand coordinated to the palladium metal through N-atom in a square planar arrangement (Al-Jibori et al., 2017)

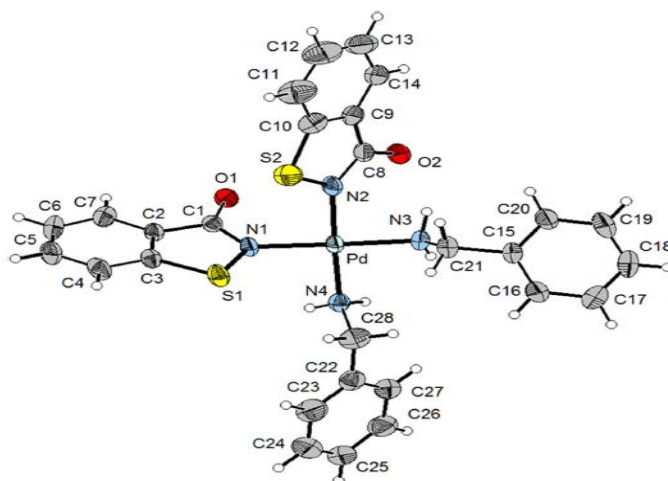
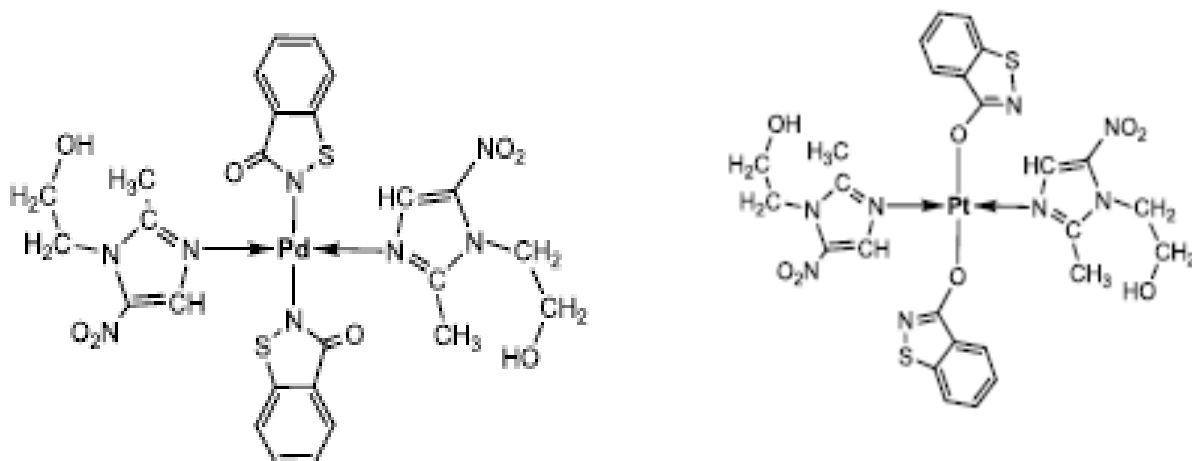


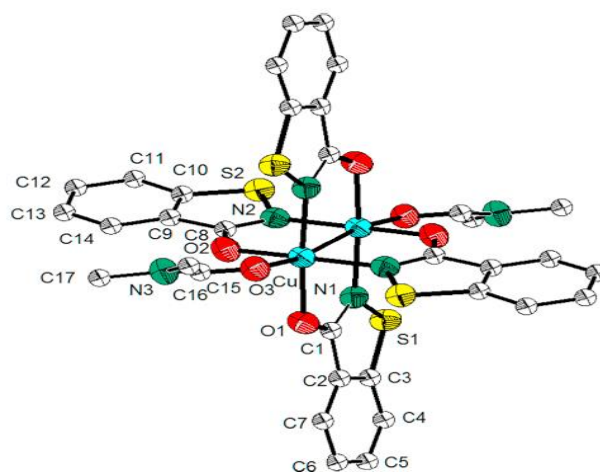
Figure 2.6 Molecular structure of *cis*-[Pd(bit)<sub>2</sub>(H<sub>2</sub>NBz)<sub>2</sub>]

In 2019, Al-Jibori and coworkers, synthesized and characterized complexes of the type *trans*-[M(bit)<sub>2</sub>(mnz)<sub>2</sub>] (Fig. 2.7), where M = Pd or Pt, **mnz** = metronidazole. The prepared complexes have been characterized by elemental analysis, conductivity measurements, infrared and <sup>1</sup>H-NMR spectra. Characterization data showed that the **mnz** ligand in both complexes is coordinated to metal centers through the imidazole N-atom, while the (bit) anion ligand is coordinated to metal centers through the N-atom in the palladium complex and through the O-atom of the carbonyl group in the platinum complex. The geometry of the Pd(II) and Pt(II) complexes is a square planar geometry (Al-Jibori et al., 2019a).

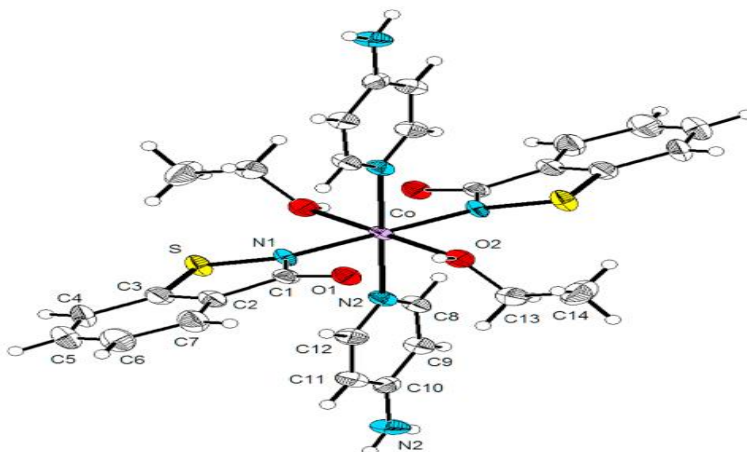


**Figure 2.7** Structure of *trans*-[M(bit)<sub>2</sub>(mnz)<sub>2</sub>], M = Pd or Pt

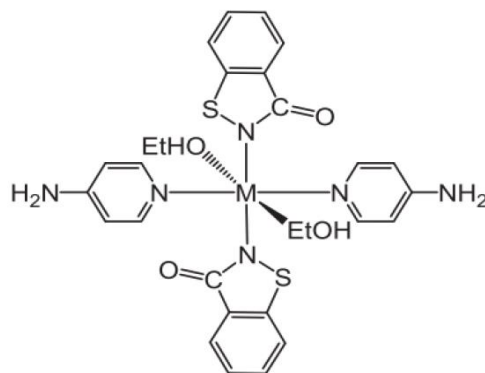
In 2019, Al-Jibori and coworkers, reported the synthesis of a series of mixed ligand complexes containing bit ligand. The benzisothiazolinate-bridged paddlewheel dimer complexes of the type [M<sub>2</sub>(μ-bit)<sub>4</sub>.2H<sub>2</sub>O], where M = Mn, Co, Ni, Cu, were synthesized up on addition of sodium benzisothiazolinate Nabit to metal salts MX<sub>2</sub>·nH<sub>2</sub>O. Addition of 4-aminopyridine (4-ampy) in ethanol leads to cleavage of dimers and formation of all *trans*-[M(4-ampy)<sub>2</sub>(bit)<sub>2</sub>(EtOH)<sub>2</sub>] (M = Co (**Fig. 2.9**), Ni (**Fig. 2.10**), the bit ligand binding in a monodentate fashion through the amide-nitrogen. With a slight excess of ethylenediamine (en) a similar cleavage occurs to afford *trans*-[M(bit)<sub>2</sub>(en)<sub>2</sub>] (M = Co (**Fig. 2.11**), Ni (**Fig. 2.11**), Cu (**Fig. 2.12**). For nickel and copper, the intermediate five-coordinate mono-diamine derivatives *cis*-[M(bit)<sub>2</sub>(en)(H<sub>2</sub>O)] (M = Ni, Cu) have also been isolated. Direct reactions of MX<sub>2</sub>·nH<sub>2</sub>O with either 1,4-bipyridine (bipy) or 1,10-phenanthroline (phen) and Nabit lead to *cis*-[M(bit)<sub>2</sub>(bipy)(H<sub>2</sub>O)<sub>2</sub>] (M = Co, Cu) and *cis*-[M(bit)<sub>2</sub>(phen)(H<sub>2</sub>O)L] (M = Mn (**Fig. 2.13**), Co, L = H<sub>2</sub>O (**Fig. 2.13**) M = Cu, L = EtOH (**Fig. 2.14**) respectively. Molecular structures of [Cu<sub>2</sub>(μ-bit)<sub>4</sub>.2dmf].2dmf, *trans*-[Co(4-ampy)<sub>2</sub>(bit)<sub>2</sub>(EtOH)<sub>2</sub>] and [Cu(bit)<sub>2</sub>(en)(H<sub>2</sub>O)].H<sub>2</sub>O have been determined (Al-Jibori et al., 2019b).



**Figure 2.8** Molecular structure of  $[\text{Cu}_2(\mu\text{-bit})_4(\text{dmf})_2]\cdot\text{dmf}$



**Figure 2.9** Molecular structure of  $[\text{Co}(\text{bit})_2(4\text{-ampy})_2(\text{EtOH})_2]$



**Figure 2.10** Structure of  $[\text{Ni}(\text{bit})_2(4\text{-ampy})_2(\text{EtOH})_2]$



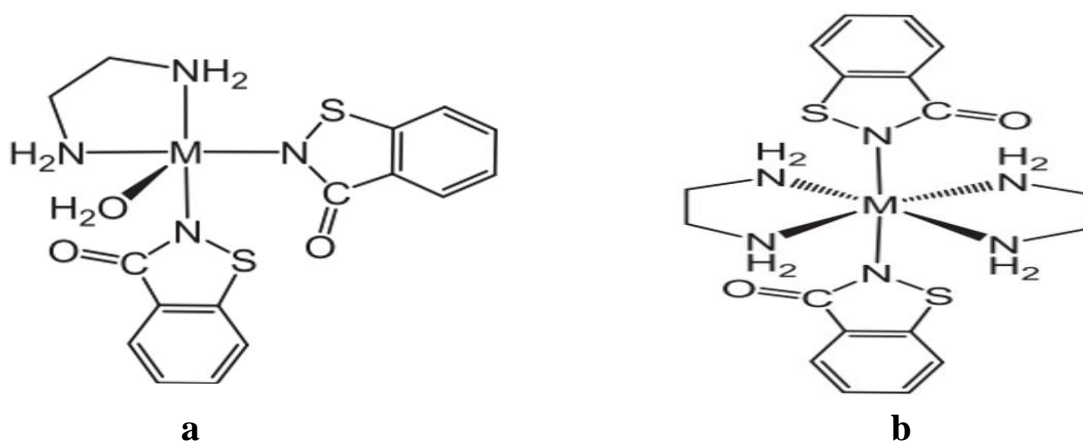


Figure 2.11 Structure of a:  $[M(\text{bit})_2(\text{en})(\text{H}_2\text{O})]$  (where  $M = \text{Ni}, \text{Cu}$ ) and b:  $[M(\text{bit})_2(\text{en})_2]$  (where  $M = \text{Ni}, \text{Co}, \text{Cu}$ ).

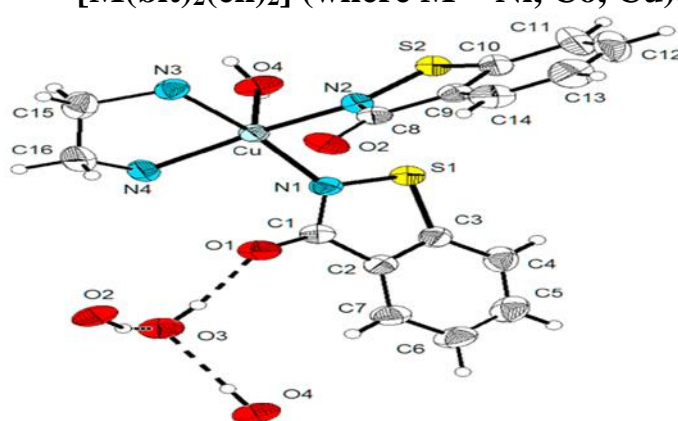


Figure 2.12 Molecular structure of  $[\text{Cu}(\text{bit})_2(\text{en})(\text{H}_2\text{O})_2] \cdot \text{H}_2\text{O}$

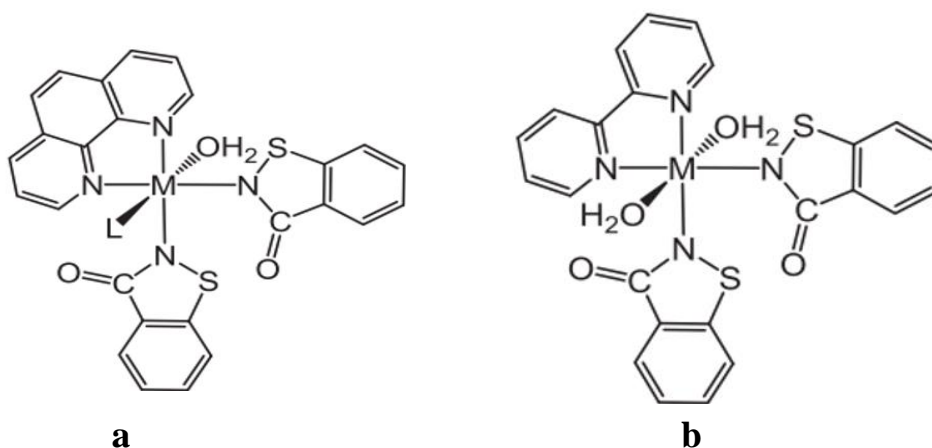
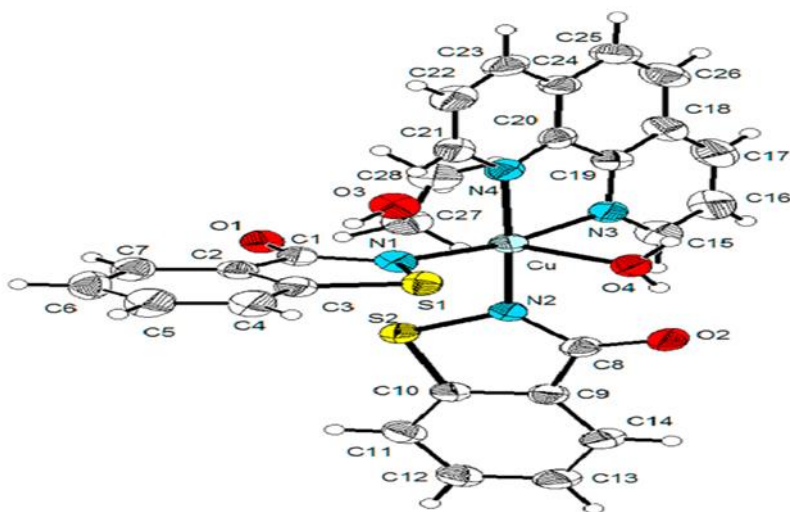
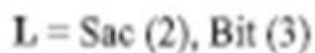
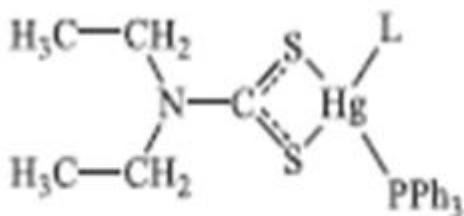


Figure 2.13 Structure of a:  $[M(\text{bit})_2(\text{phen})_2\text{L}]$  where  $M = \text{Mn}$  ( $\text{L} = \text{H}_2\text{O}$ ),  $\text{Co}$  ( $\text{L} = \text{H}_2\text{O}$ ),  $\text{Cu}$  ( $\text{L} = \text{EtOH}$ ). b:  $[M(\text{bit})_2(\text{phen})_2(\text{H}_2\text{O})_2]$  where  $M = \text{Co}, \text{Cu}$



**Figure 2.14** Molecular structure of  $[\text{Cu}(\text{bit})_2(\text{phen})(\text{EtOH})(\text{H}_2\text{O})]$

In 2019, Al-Nassiry and coworkers, synthesized mixed ligand Hg(II) complex containing bit ligand of the type  $[\text{Hg}(\text{Et}_2\text{Dt})\text{L}(\text{PPh}_3)]$  (Fig 2.15), where  $\text{Et}_2\text{Dt}$  = diethyl dithiocarbamate and  $\text{L}$  = benzisothiazolate. The synthesized complex was characterized by elemental analysis, molar conductivity, FT-IR, and NMR ( $^1\text{H}$  and  $^{31}\text{P}$ ) spectroscopic techniques. The characterization data reveals that the bit ligand bonded as monodentate N-donor atom to afford a tetrahedral geometry around the Hg(II) ion (Al-Nassiry et al., 2020).



**Figur 2.15** Structure of  $[\text{Hg}(\text{Et}_2\text{Dt})\text{L}(\text{PPh}_3)]$

In 2021, Al-Jibori and coworkers synthesized  $[\text{Hg}(\text{bit})_2(\text{bipy})]$  (Fig. 2.16) and  $[\text{Hg}(\text{bit})_2(\text{phen})]$  (Fig. 2.17) complexes by reaction of  $[\text{Hg}(\text{bit})_2]$  with bidentate ligands; 2,2-bipyridine (**bipy**) or 1, 10-phenanthroline (**phen**) in an absolute ethanol. The crystal structure of  $[\text{Hg}(\text{bit})_2(\text{bipy})]$  and  $[\text{Hg}(\text{bit})_2(\text{phen})]$  showing a distorted tetrahedral geometry around mercury with the two bit ligands being coordinated via N-atom and lying almost perpendicular to each other. (Al-Jibori et al., 2021)

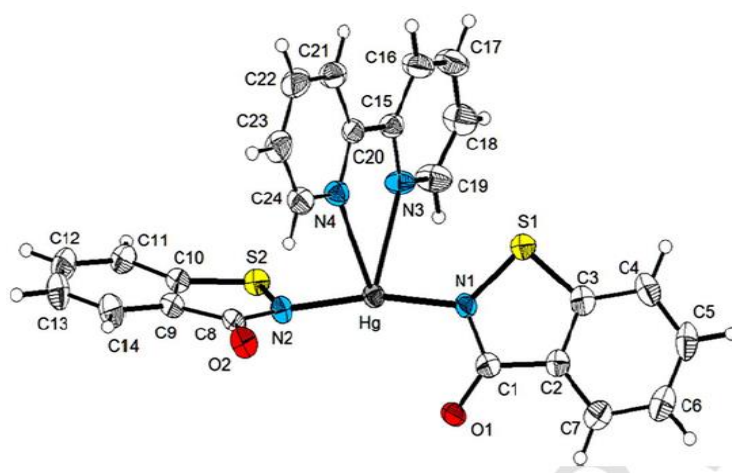


Figure 2.16 Molecular structure of  $[\text{Hg}(\text{bit})_2(\text{bipy})]$

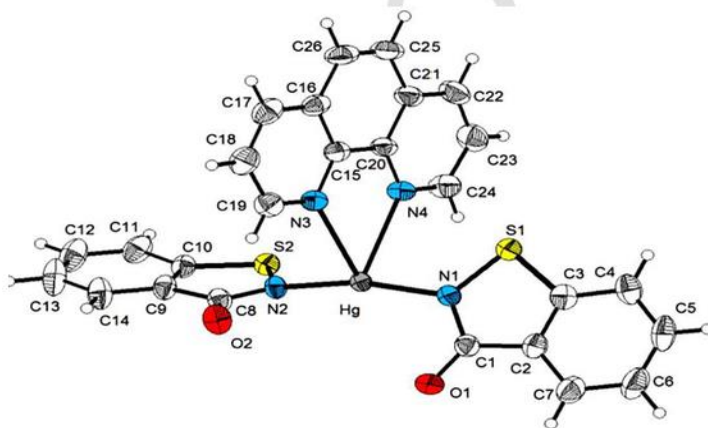


Figure 2.17 Molecular structure of  $[\text{Hg}(\text{bit})_2(\text{phen})]$

## **Discussion**

This study is a review project, aims to collect transition metal complexes of benzenethiozolate (bit) ligand. According to the reported literature, bit ligand form complexes with metals such as Mn(II), Co(II), Ni(II), Pd(II), Pt(II), Cu(II) and Hg(I), in a tetrahedral, square planar, square pyramidal or an octahedral coordination geometry. Characterization data as well as X-ray structure of the reported complexes reveal that the bit ligand functions as a monodentate ligand coordinating to the metal ions through either N-atom or as bidentate bridging ligand coordinating to the metal ion through N,O-atoms to form binuclear complexes.

## **Conclusion**

Benzenethiozolate (bit) ligand is aromatic heterocyclic ligand that functions as a monodentate ligand coordinating to the metal ions through nitrogen atom or it can form binuclear complex in which the bit ligand acts as a bidentate bridging ligand that bind to the metal ions through both nitrogen and oxygen atoms.

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