Molecular Computation and Antibacterial Activity of Cu (II) Complex of Naphthaldehyde Thiosemicarbazone

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ABSTRACT
Copper (II) complex of naphthaldehyde thiosemicarbazone (L) have been synthesized and characterized by melting points, conductance, magnetic, infrared and ESI-MS spectral measurements in addition to elemental analysis. Tetrahedral structure is suggested for the complex. The antibacterial activities of the complex and ligand were evaluated by the disc diffusion technique. Pure bacteria cultures of Bacillus subtilis (Gram positive) and Escherichia coli (Gram negative) were used to check the antibacterial activities of the synthesized compounds. Antibacterial activities were compared by measuring the inhibition zone diameter and chloramphenicol was used as reference. Both the compounds showed significant antibacterial activity in different range against gram positive & gram negative bacteria. The antibacterial activity data also show that the Cu(II) complex to be more effective than the parent ligand. Molecular geometry of the complex has been optimized by ChemDraw Ultra 12.0 and then MM2 calculation has been done.

Keywords: Ligand, Metal complex, Antibacterial activity, Thiosemicarbazone, and Molecular computation.

INTRODUCTION
Nitrogen and sulfur donor ligands for the synthesis of metal complexes have expanded during the last few years as one of the core research areas in transition metal chemistry. Thiosemicarbazones and their metal complexes have gainedextensive attention among the nitrogen/sulfur compounds in view of their flexible binding modes, structural diversity and encouraging biological implications (Casas et al., 2000; Netalkar et al., 2014; Mishra et al., 2006; Sarker et al., 2019a; Sarker et al., 2019b; Matesanz et al., 2020; and Bisceglie et al., 2020). A good number of reasons can be mentioned to be responsible for their flexibility in coordination, such as intramolecular H-bonding, steric crowding on the azomethine carbon atom, bulkier coligandand stacking interactions (Prabhakaran et al., 2012; Basuli et al., 1997; and Netalkar et al., 2015). NS-donor ligands can coordinate to the metal ion in a neutral or deprotonated form, producing poly or mononuclear complexes with transition metals (Shebaldina et al., 2004; Prabhakaran et al., 2011; and Shawish et al., 2014).

Transition metal complexes derived from NS-donor ligands appears as predominantly attractive because they can produce stable chelates with metal ions. Complexes of thiosemicarbazones and substituted thiosemicarbazones with appropriate metal ions through synergic effects, in addition to enhancing the biological activity, also lead to reduced toxicities and have become a dependable source for discovering novel biologically active compounds (Iakovidou et al., 2001; and Kovala-Demertzi et al., 2001).
Thiosemicarbazones and their metal complexes can act as antibacterial, anti-fungal, anti-tumor, anticancer and anti-inflammatory agents (Melha, 2008; Liberta and West, 1992; Afrasiabi et al., 2003; and Katwal et al., 2013). It is also reported that Cu(II) complexes of various ligands possess remarkable antimicrobial activity and have been employed as antimicrobial agents (Ranford et al., 1993; and Zoroddu et al., 1996). Furthermore, thiosemicarbazone derivatives seem to be a probable pharmacophore in several pharmacologically active agents. Hence, we decided to prepare copper complex with thiosemicarbazone as possible antimicrobial agents which could provide better therapeutic results. In continuation of our current research on the synthesis and biological evaluation of Schiff base metal complexes, we have prepared Cu(II) complex of thiosemicarbazone and evaluated its potency against antimicrobial agents. We also report here molecular computation of the complex.

MATERIALS AND METHODS

Materials and Physical Measurements - Starting materials for synthesis have been purchased commercially and used as received. 1-naphthaldehyde and thiosemicarbazide were purchased from Aldrich and was used as such. To identify the melting points of synthesized compounds, a digital melting point apparatus (METTLER TOLEDO) was used. IR spectra of the ligand and its copper complex were recorded using KBr disc technique on a Nicolet 170 SX FT-IR spectrometer. ESI-MS spectra were recorded with an Agilent Technologies MSD SL Trap mass spectrometer with ESI source coupled with an 1100 Series HPLC system for the confirmation of molecular formulas of compounds. The magnetic susceptibility was measured on Faraday balance at room temperature using Hg[Co(SCN)4] as a calibrant. The ligand and complex were analyzed for carbon, hydrogen and nitrogen using a Thermo quest elemental analyzer. Molar conductivities of freshly prepared 1.0×10⁻³ mol/dm⁻³ DMSO solutions of the synthesized compounds were measured using Jenway 4010 conductivity meter. Molecular graphics were generated using ChemDraw Ultra (ChemBio3D HotLink).

**Synthesis of the Ligand, L** - 1-naphthaldehyde (10 mmol) in hot ethanol (30 mL) was mixed with hot ethanolic solution of thiosemicarbazide (10 mmol). The mixture was refluxed for 6 hours on a water bath. On cooling, the precipitate was separated out, filtered and washed with ethanol and dried in vacuum over P₂O₅. The proposed structure of the ligand can be shown according to **Scheme 1**.

**Scheme 1**: Preparation of the ligand, L.

**Synthesis of the Cu(II) Complex** - Copper acetate salt (5 mmol) in hot ethanol (30 mL) were mixed with hot ethanolic solution of the ligand (5 mmol) and refluxed for 4 hours on a water bath. On cooling, the colored complex separated out. The product was filtered, washed with ethanol and dried in vacuum over P₂O₅. Purity of the complex was checked by thin layer chromatography (TLC).

**Metal Content Estimation** - A known quantity of metal complex was put into a conical flask whose weight was known. Then, concentrated H₂SO₄ (500 µL) was added. It was fumed until dry and the process was repeated two times. Concentrated HNO₃ (500 µL) and HClO₄ (500 µL) were then added and the mixture was further fumed until dry. The process of adding acids and fuming was continued until there was no black material. 100 mL distilled water was added to dissolve the residue. Finally, the weight of the metal was estimated complexometrically using EDTA (Ethylenediamine tetraacetic acid) (Schwarzenbach and Flaschka, 1969).
**Fig 1:** Proposed structure of the copper complex.

**Fig 2:** (a) 3D structure; (b) Highest Occupied Molecular Orbital (HOMO); (c) Lowest Unoccupied Molecular Orbital (LUMO) of the complex.

**Antibacterial Activity** - Sterilized antibiotic discs (8 mm) was used for antibacterial screening of the compounds. A McFarland standard method was utilized to standardize the density of the bacterial suspension. All the tests were carried out at 28 ± 3°C. Bioassay of the ligand and its copper complex were assessed using the bacterial cultures of the gram negative bacteria *Escherichia coli* and the gram positive bacteria *Bacillus subtilis* by the disc diffusion technique (White and Coon, 1980). Chloramphenicol was used as a standard reference antibiotic and positive control for the tested bacteria whereas DMSO was used as a negative control. In this technique, liquefied agar medium with uniform thickness were poured in Petri-dishes (Rahman et al., 2019).

After solidification dishes were inoculated with test micro-organisms, after which filter paper discs dipped into the solution of the compounds dissolved in DMSO and standard drug solution dissolve in DMSO (each 10 μg/mL) were placed in each quadrant of the dishes.

The tested compounds diffused into the agar medium preventing the growth of bacteria and produced a clear zone of inhibition. Dishes were first kept at 4 °C for 2 h to permit the diffusion of chemicals, followed by incubation at 28 °C. Antibacterial activity was assessed by measuring the inhibition zone diameters (mm) as depicted in Table 4 against the test bacteria after 24 h of incubation.

**RESULTS AND DISCUSSION**

The complex was soluble in organic solvents like DMSO, DMF, hot alcohol and acetonitrile. Spectroscopic and analytical data for the complex indicates a 1:1 (M: L) stoichiometry.

**Elemental Analysis** - The microanalysis data (Table 1) indicated that the complex is mononuclear. These data also revealed that the metal-to-ligand ratio for the synthesized complex was 1:1. The proposed structure of the ligand and complex were consistent with elemental analysis data.
Molar Conductivity and Magnetic Measurements - The molar conductivity of the synthesized compounds were determined at room temperature at a concentration of 10^{-3} M in DMSO. The conductance value exposed that the complex is non-electrolyte in nature (Table 2) (Antonov et al., 2001). Magnetic moment was calculated by the equation $\mu_{\text{eff}} = 2.828 (\chi_\lambda T)^{1/2}$ where $\chi_\lambda$ is the magnetic susceptibility per copper. Room temperature magnetic susceptibility measurements (Gouy method, powdered sample) show that the Cu(II) complex has a magnetic moment close to 1.73 BM as projected for powdered sample) show that the Cu(II) complex has a magnetic moment 1.57 BM, which is less than the spin only value (1.73 BM). Low magnetic value can be expected for complexes having antiferromagnetic effect, with spin-orbital coupling in the ground state for spin doublet species (Day, 1969).

Table 1: Microanalysis data of the ligand and its copper complex.

| Compound | Found (Calculated) (%) | Cu | C | H | N |
|----------|------------------------|----|---|---|---|
| Ligand   |                        | 62.86 (62.69) | 4.84 (4.76) | 18.33 (18.12) |
| Complex  | 15.46 (15.32)          | 46.76 (46.52) | 4.17 (4.04) | 10.23 (10.11) |

Table 2: Physical data of the Ligand, L, and its Cu(II) complex.

| Compound | Empirical Formula | Formula Weight (g/mol) | M.P (ºC) | Color | $\Lambda_m$ | Yield (%) | $\mu_{\text{eff}}$ (B.M.) |
|----------|-------------------|-------------------------|----------|-------|------------|-----------|----------------------|
| Ligand   | C_{12}H_{11}N_{3}S | 229.30                  | 198      | Brown | 9          | 83        | -        |
| Complex  | C_{16}H_{17}CuN_{3}O_{4}S | 410.93 | 255 | Yellow | 13 | 78 | 1.57 |

This finding undoubtedly indicates the non-involvement of -NH_{2} group in coordination to the metal center. The band due to $v$(C=N) at 1600 cm^{-1} in the free ligand is shifted in the complex, suggesting the coordination via azomethine nitrogen atom to Cu(II) ion. Coordination of the azomethine N is also consistent with the presence of a new peak at 450 cm^{-1} in the infrared spectrum of the complex which is assignable to $v$ (Cu–N) for the complex. The absorption band observed in the infrared spectrum of the ligand due to $v$(C=S) is shifted in the complex indicating the participation of the S atom in complex formation (John et al., 2002).

Coordination of C=S group through S atom to copper ion is confirmed by the existence of a new peak in the complex due to $v$(Cu–S) at362 cm^{-1} (Fostiak et al., 2003). In the copper (II) complex, derived from copper acetate, presence of acetate group is noticed. For the coordinated unidentate acetate ion, the asymmetric stretching for COO^- occurs at 1456 cm^{-1} and the symmetric stretching for COO^- is observed 1390 cm^{-1} (Shankar et al., 1986). The band at 516 cm^{-1} in the complex due to $v$(Cu-O) also supports the coordination of acetate ion to the Cu(II) ion.

IR Spectral Studies - The band at 3448 cm^{-1} in the IR spectrum (Fig 3) of the ligand (L) can be assigned to the asymmetric $v$(N-H) vibration of the terminal NH_{2} group. Another two bands at 3268 and 3145 cm^{-1} may be due to the symmetric $v$(N-H) vibrations of the imino and amino groups respectively. The symmetric and asymmetric bands due to the terminal primary amine are present in the complex (Fig 4).

Electrospray Ionization Mass Spectroscopy (ESI-MS) - ESI-MS spectrum of the ligand (L) shows molecular ion peak at 229.0579. The ESI-MS spectrum of the complex shows molecular ion peak at 410.6121 (Fig 5). Electrospray ionization mass spectroscopy studies of the ligand and complex supports the suggested molecular formula of the synthesized compounds.
**Antibacterial Activity Studies** - The ligand, L and its Cu(II) complex were tested for their antibacterial activities against a gram positive and gram negative bacteria particularly *B. subtilis* and *E. coli* by disc diffusion technique at a concentration of 10 μg/mL. The growth inhibitory ability of the tested compounds were compared with that of standard drug, Chloramphenicol (CP). The metal complex was found to inhibit growth of *B. subtilis* and *E. coli* (Table 4). The antibacterial activity of the copper complex was found to be comparable with CP.

### Table 3: Key Infrared bands (cm⁻¹) and molecular ion peaks (m/z) of the ligand, L and its Cu(II) complex.

| Compound | ν (C=N) | ν (C=S) | ν (Cu-O) | ν (Cu-N) | ν (Cu-S) | ν (COO⁻)ₘₙₘ & ν (COO⁻)ₘₘₘ | ESI-MS |
|----------|---------|---------|----------|----------|----------|----------------------------|--------|
| Ligand   | 1600    | 757     | -        | -        | -        | -                          | 229.0579|
| Complex  | 1597    | 737     | 516      | 450      | 362      | 1456 & 1390                | 410.6121|

**Fig 3:** IR spectrum of the ligand, L.

**Fig 4:** IR spectrum of the copper complex.

**Fig 5:** ESI-MS spectrum of (a) Ligand, and (b) Complex.
**Table 4:** Antibacterial activities of the ligand, L and its copper complex.

| Compounds          | *Bacillus subtilis* | *Escherichia coli* |
|--------------------|--------------------|-------------------|
| Ligand             | 15                 | 17                |
| Copper Complex     | 24                 | 26                |
| Chloramphenicol    | 25                 | 27                |

Each value represents the inhibition zone diameter in mm.

**Table 5:** Selected bond lengths and bond angles for the Cu(II) complex obtained from MM2 calculation.

| Bond lengths and bond angles \(^a\) | Actual        | Optimal         |
|-------------------------------------|---------------|-----------------|
| Cu(17)-O(22)                        | 1.8067        | 1.8067          |
| Cu(17)-O(18)                        | 1.8066        | 1.8066          |
| S(15)-Cu(17)                       | 2.1692        | 2.1692          |
| Cu(17)-N(12)                       | 1.4391        | 1.3030          |
| Cu(17)-S(15)-C(14)                 | 124.5133      | 124.5133        |
| O(22)-Cu(17)-O(18)                 | 119.1825      | 119.1825        |
| O(22)-Cu(17)-S(15)                 | 114.1466      | 114.1466        |
| O(22)-Cu(17)-N(12)                 | 113.5681      | 113.5681        |
| O(18)-Cu(17)-S(15)                 | 115.4039      | 115.4039        |
| O(18)-Cu(17)-N(12)                 | 113.1432      | 113.1432        |
| S(15)-Cu(17)-N(12)                 | 72.5625       | 72.5625         |
| Cu(17)-N(12)-N(13)                 | 129.3109      | 129.3109        |
| Cu(17)-N(12)-C(11)                 | 112.2595      | 112.2595        |

\(^a\) Bond lengths are in Å and bond angles are in °

**Table 6:** Computational data for the complex.

| Formal Charge                  |                   |
|-------------------------------|-------------------|
| Connolly Accessible Area      | 569.238 Angstroms Squared |
| Connolly Molecular Area       | 302.885 Angstroms Squared |
| Connolly Solvent Excluded Volume | 293.393 Angstroms Cubed |
| Principal Moment              | 749.186, 3054.018, 3661.819 |
| Ovality                       | 1.41849282335958  |

**CONCLUSION**

In this work, we have successfully prepared copper (II) complex of naphthaldehydethiosemicarbazone. The synthesized ligand and complex were characterized by using FTIR, ESI-MS, melting point, magnetic and conductivity measurements. Based on stoichiometry and analytical data of the ligand, naphthaldehyde thiosemicarbazone (L) is bidentate and coordinated to Cu(II) ion through the “N” and “S” atoms, respectively. Another two coordination sites of the metal have been occupied by two acetate groups. Antibacterial activity of the metal complex and ligand were evaluated. The complex and ligand exhibited significant antibacterial activity in different range and have a potential to be used as drugs. Moreover, we have calculated different bond lengths and angles and different parameters of the complex through MM2 calculation using ChemDraw Ultra 12.0.
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