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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).

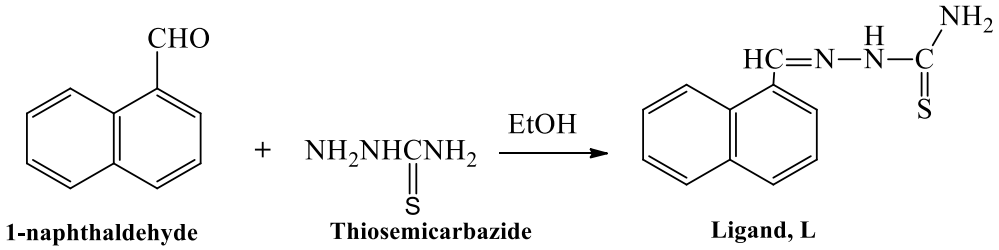
Transition metal complexes derived from NS-donor ligands appears as predominantly attractive because they can produce stable chelates with metal ions. Complexes of thiosemicarbazones and substituted thiosemicarbazones with appropriate metal ions through synergic effects, in addition to enhancing the 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 complexescan 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-napthaldehyde 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 complexwere 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-napthaldehyde (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 P_4O_{10}. 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 P_4O_{10}. 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 H_2SO_4 (500 µL) was added. It was fumed until dry and the process was repeated two times. Concentrated HNO_3 (500 µL) and $HClO_4$ (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).

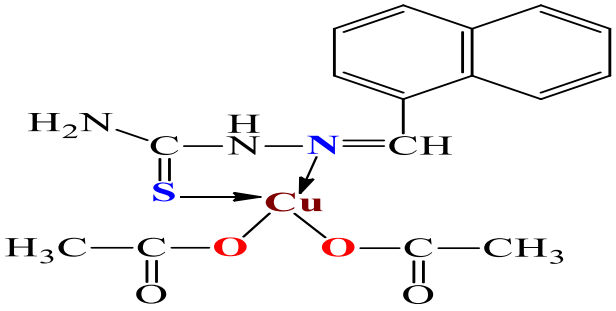


Fig 1: Proposed structure of the copper complex.

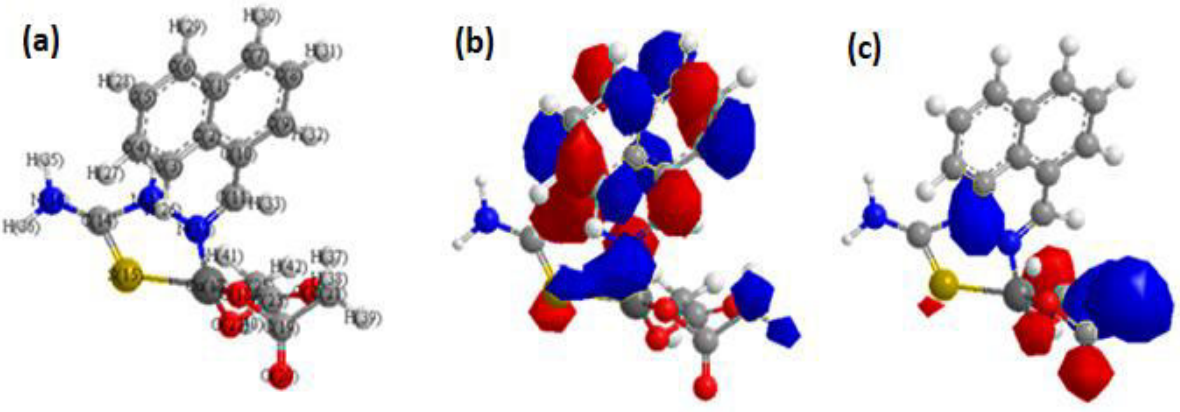


Fig 2: (a) 3D structure; (b) Highest Occupied Molecular Orbital (HOMO); (c) Lowest Unoccupied Molecular Orbital (LUMO) of the complex.

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 *Escherichiacoli*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 permitthe diffusion of chemicals, followed by incubation at 28 °C. Antibacterial activity was assessed by measuring theinhibition 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 complexwas 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 determinedat 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 $\mu_{eff} = 2.828(\chi_A T)^{1/2}$ where χ_A 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 discrete magnetically non-coupled copper(II) ion (Sallam *et al.*, 2002). The magnetic moment value of the copper complex was matched with the reported tetrahedral structure (Patel *et al*., 1989; Day, 1969, Reddy and Agarwala, 1987). The complex exhibited 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)

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**).

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

Compound	Empirical Formula	Formula Weight (g/mol)	M.P (ºC)	Color	Λm µs	Yield (%)	μ_{eff} (B.M.)
Ligand	$C_{12}H_{11}N_3S$	229.30	198	Brown	9	83	-
Complex	$C_{16}H_{17}CuN_3O_4S$	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 peakin 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.

Electrospray Ionization Mass Spectroscopy (ESI-MS) - ESI-MS spectrum of the ligand (L) shows molecular ion peakat 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 complexsupports the suggested molecular formula of the synthesized compounds.

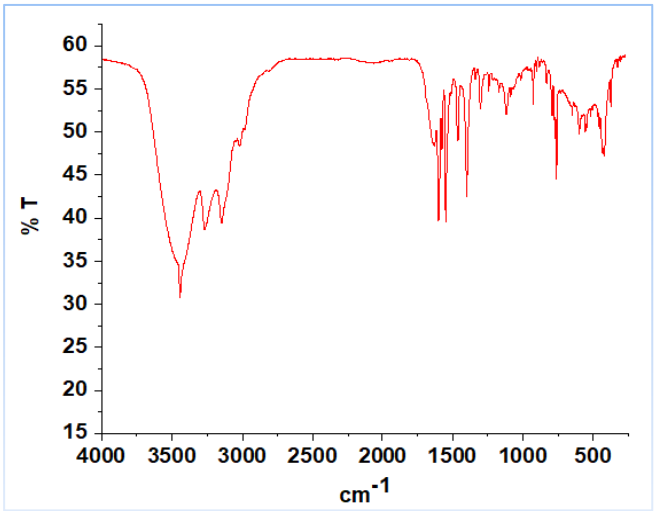


Fig 3: IR spectrum of the ligand, L.

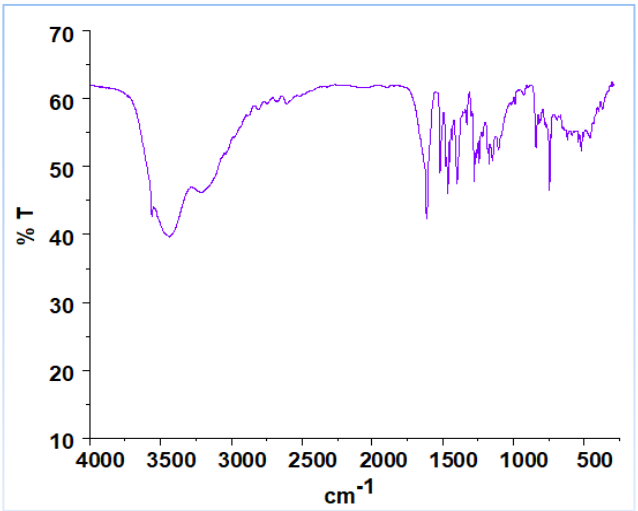


Fig 4: IR spectrum of the copper complex.

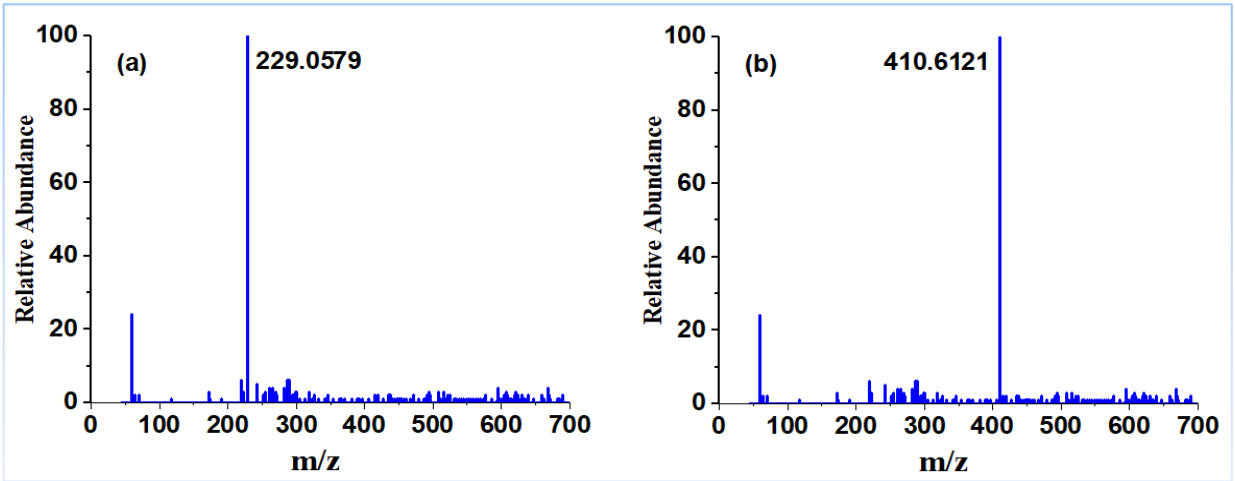


Fig 5: ESI-MS spectrum of (a) Ligand, and (b) Complex.

Table 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 $(COO^-)_{asym}$ & ν $(COO^-)_{sym}$	ESI-MS
Ligand	1600	757	-	-	-	-	229.0579
Complex	1597	737	516	450	362	1456 & 1390	410.6121

Antibacterial Activity Studies - The ligand, L and its Cu(II) complex were testedfor 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 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 º

Table 6: Computational data for the complex.

Formal Charge	0
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) isbidentate 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 rangeand 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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CONFLICTS OF INTEREST

The authors declared no potential conflicts of the interest with respect to the research, authorship of this article.

REFERENCES

1. Afrasiabi Z., Sinn, E., Padhye, S., & Powell, A. K. (2003). Transition metal complexes of phenanthrenequinone thiosemicarbazone as potential anticancer agents: synthesis, structure, spectroscopy, electrochemistry and in vitro anticancer activity against human breast cancer cell-line, T47D. *J. of Inorganic Biochemistry*, **95**, 306-314. https://doi.org/10.1016/S0162-0134(03)00131-4
2. Alam S. A. M. F., Ahmad T., Alam M. G., Maitra P., Mandol D., Uddin ME., Ahammed T. (2017). Synthesis of benzimidazole derivatives containing schiff base exhibiting antimicrobial activities. *International J. of Research Studies in Biosciences.* **5**(7), 18-24. https://doi.org/0.20431/2349-0365.0507003
3. Antonov L., Vladimirova, M., & Mitewa, M. (2001). Complexation properties of Schiff bases containing the N-phenylaza-15-crown-5 moiety. *J. of Inclusion Phenomena and Macrocyclic Chemistry*, **40**, 23-28. https://link.springer.com/article/10.1023/A:1011190403722
4. Basuli F., Peng, S.-M. & Bhattacharya, S. (1997). Steric control of the coordination mode of thesalicylaldehyde thiosemicarbazone ligand. Syntheses, structures, and redox properties of ruthenium and osmium complexes. *Inorganic Chemistry*, **36**, 5645-5647. https://pubs.acs.org/doi/abs/10.1021/ic9705094
5. Bisceglie F., Bacci, C., Vismarra, A., & Pelosi, G. (2020). Antibacterial activity of metal complexes based on cinnamaldehyde thiosemi-carbazone analogues. *Journal of Inorganic Biochemistry*, **203**, 110888. https://doi.org/10.1016/j.jinorgbio.2019.110888
6. Casas J., Garcıa-Tasende, M. & Sordo, J. (2000). Main group metal complexes of semi-carbazones and thiosemicarbazones. A structural review. *Coordination Chemistry Reviews*, **209**, 197-261. https://doi.org/10.1016/S0010-8545(00)00363-5
7. Day M. C. (1969). Theoretical inorganic chemistry. 2nd Edition, New York, NY: Van Nostrand Reinhold, p 608. https://cds.cern.ch/record/225164
8. Fostiak L. M., García, I., & West, D. X. (2003). Structural and spectral characterization of transition metal complexes of 2-pyridine-formamide N (4)-dimethylthiosemicarb-azone. *Polyhedron*, **22**, 83-92. https://doi.org/10.1016/S0277-5387(02)01330-X
9. Iakovidou Z., Papageorgiou, A., Demertzis, M., & Kovala-Demertzi, D. (2001). Platinum (II) and palladium (II) complexes with 2-acetyl-pyridine thiosemicarbazone: cytogenetic and antineoplastic effects. *Anti-Cancer Drugs*, **12**, 65-70.
10. John R. P., Sreekanth, A., Kurup, M. R. P. & Mobin, S. M. (2002). Synthesis and structural studies of novel Co (III) ternary complexes containing N (4)-substituted thiosemicarbazones of 2-hydroxyacetophenone and heterocyclic bases. *Polyhedron*, **21**, 2515-2521. https://doi.org/10.1016/S0277-5387(02)01227-5
11. Katwal R., Kaur, H. & Kapur, B. K. (2013). Applications of copper-Schiff's base complexes: a review. *Sci Rev Chem Commun*, **3**, 1-15.
12. Kovala-Demertzi D., Demertzis, M. A., & Filousis, G. (2001). Platinum (II) complexes with 2-acetyl pyridine thiosemicarbazone: synthesis, crystal structure, spectral properties, antimicrobial and antitumour activity. *J. of Inorganic Biochemistry*, **86**, 555-563. https://doi.org/10.1016/S0162-0134(01)00224-0
13. Liberta A. E. & West, D. X. (1992). Antifungal and antitumor activity of heterocyclic thiosemi-

carbazones and their metal complexes: current status. *Biometals*, **5**, 121-126. https://link.springer.com/article/10.1007/BF01062223

14. Matesanz A. I., Herrero, J. M., & Quiroga, A. G. (2020). New Platinum (II) Triazole Thiosemicarbazone Complexes: Analysis of Their Reactivity and Potential Antitumoral Action. *ChemBioChem*, **21**, 1226-1232. https://doi.org/10.1002/cbic.201900545
15. Melha K. S. A. (2008). In-vitro antibacterial, antifungal activity of some transition metal complexes of thiosemicarbazone Schiff base (HL) derived from N4-(7′-chloroquinolin-4′-ylamino) thiosemicarbazide. *Journal of Enzyme Inhibition and Medicinal Chemistry*, **23**, 493-503. https://www.tandfonline.com/doi/full/10.1080/14756360701631850
16. Mishra D., Naskar, S., Drew, M. G. & Chattopadhyay, S. K. (2006). Synthesis, spectroscopic and redox properties of some ruthenium (II) thiosemicarbazone complexes: Structural description of four of these complexes. *Inorganica Chimica Acta*, **359**, 585-592. https://doi.org/10.1016/j.ica.2005.11.001
17. Netalkar P. P., Netalkar, S. P. & Revankar, V. K. (2014). Nickel (II) complexes of thiosemicarbazones: synthesis, characterization, X-ray crystallographic studies and in vitroantitubercular and antimicrobial studies. *Transition Metal Chemistry*, **39**, 519-526. https://link.springer.com/article/10.1007/s11243-014-9827-8
18. Netalkar P. P., Netalkar, S. P. & Revankar, V. K. (2015). Transition metal complexes of thiosemicarbazone: Synthesis, structures and invitro antimicrobial studies. *Polyhedron*, **100**, 215-222. https://doi.org/10.1016/j.poly.2015.07.075
19. Patel B., Desai, K. & Thaker, B. (1989). Mixed azomethine mononuclear and binuclear copper (II) complexes with alkyl and aryl Schiff bases involving ONO and ONS donor atoms. *Synthesis and Reactivity in Inorganic and Metal-organic Chemistry*, **19**, 391-412. https://www.tandfonline.com/doi/abs/10.1080/00945718908048078
20. Prabhakaran R., Kalaivani, P., & Natarajan, K. (2012). Copper Ion Mediated Selective Cleavage of C–S Bond in Ferrocenyl-thiosemicarbazone Forming Mixed Geometrical [(PPh_3) Cu (μ-S) 2Cu $(PPh_3)_2$] Having Cu_2S_2 Core: Toward a New Avenue in Copper-Sulfur Chemistry. *Inorganic Chemistry*, **51**, 3525-3532. https://pubs.acs.org/doi/abs/10.1021/ic2022616
21. Prabhakaran R., Palaniappan, K., Huang, R., & Natarajan, K. (2011). Can geometry control the coordination behaviour of 2-hydroxy-1-naphthaldehyde-N (4)-phenylthiosemicarbazo-ne? A study towards its origin. *Inorganica Chimica Acta*, **376**, 317-324. https://doi.org/10.1016/j.ica.2011.06.045
22. Rahman MA, Ahmad T, Mahmud S, Barman NC, Haque MS, Uddin ME, and Ahmed R. (2019). Isolation, identification and antibiotic sensitivity pattern of *Salmonella* spp. from locally isolated egg samples, *Am. J. Pure Appl. Sci.*, **1**(1), 1-11. https://doi.org/10.34104/ajpab.019.019111
23. Ranford J. D., Sadler, P. J. & Tocher, D. A. (1993). Cytotoxicity and antiviral activity of transition-metal salicylato complexes and crystal structure of bis (diisopropylsalicylato)(1, 10-phenanthroline) copper (II). *Journal of the Chemical Society*, *Dalton Transactions*, 3393-3399. https://doi.org/10.1039/DT9930003393
24. Reddy P. & Agarwala, B. (1987). Synthesis and characterization of new Schiff Base complexes of 2-pyridinecarboxaldehyde and thiosemicarbazides. *Synthesis and Reactivity in Inorganic and Metal-Organic Chemistry*, **17**, 585-594. https://www.tandfonline.com/doi/abs/10.1080/00945718708059456
25. Sallam S. A., Orabi, A. S., & Lentz, A. (2002). Copper, nickel and cobalt complexes of Schiff-bases derived from β-diketones. *Transition Metal Chemistry*, **27**, 447-453. https://link.springer.com/article/10.1023/A:1015085023602
26. Sarker D., Karim, M. R., Haque, M. M., Zamir, R. & Asraf, M. A. (2019a). Copper (II) Complex of Salicylaldehyde Semicarbazone:

Synthesis, Characterization and Antibacterial Activity. *Asian J. of Chemical Sciences*, **6**, 1-8. https://doi.org/10.9734/ajocs/2019/v6i419001

27. Sarker D., Reza, M. Y., Haque, M. M., Zamir, R. & Asraf, M. A. (2019b). Synthesis, Characterization, Antibacterial and Thermal Studies of Cu (II) Complex of Thiophene-2-aldehyde Semicarbazone. *Asian Journal of Applied Chemistry Research*, **4**, 1-10. https://doi.org/10.9734/ajacr/2019/v4i430116
28. Schwarzenbach G. & Flaschka, H. A. (1969). Complexometric Titrations. 2nd Edition, United Kingdom. https://www.osti.gov/biblio/4764767
29. Shankar G., Premkumar, R. & Ramalingam, S. (1986). 4-Aminoantipyrine schiff base complexes of lanthanide and uranyl ions. *Polyhedron*, **5**, 991-994. https://doi.org/10.1016/S0277-5387(00)80140-0
30. Shawish H. B., Paydar, M., Looi, C. Y., & Maah, M. J. (2014). Nickel (II) complexes of polyhydroxybenz aldehyde N4-thiosemicarbazones: synthesis, structural characterization and antimicrobial activities. *Transition Metal Chemistry*, **39**, 81-94. https://link.springer.com/article/10.1007/s11243-013-9777-6
31. Shebaldina L., Kovalchukova, O., & Ivanova, T. (2004). Synthesis and Physicochemical Properties of d-and f-Metal Complexes with Alloxan. *Russian Journal of Coordination Chemistry*, **30**, 38-42. https://link.springer.com/article/10.1023/B:RUCO.0000011641.13455.ab
32. White R. E. & Coon, M. J. (1980). Oxygen activation by cytochrome P-4501. *Annual Review of Biochemistry*, **49**, 315-356. https://www.annualreviews.org/doi/pdf/10.1146/annurev.bi.49.070180.001531
33. Zoroddu M. A., Zanetti, S., Pogni, R. & Basosi, R. (1996). An electron spin resonance study and antimicrobial activity of copper (II)-phenanthroline complexes. *Journal of Inorganic Biochemistry*, **63**, 291-300.

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