



**INVITRO ANTIBACTERIAL AND ANTIFUNGAL ACTIVITIES OF NITRITO-O
COMPLEX OF Hg(II) WITH BENZIMIDAZOLE**

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ABSTRACT

Transition metal complex of Benzimidazole (Bz) and nitrito-O (NO₂) ligands was synthesized and characterized based on elemental analysis, metal estimation, molar conductance, cyclic voltammetry, solid state reflectance (UV-Spectra), IR, Far-IR and NMR spectra. The data obtained from elemental analysis, metal estimation and molar conductance the proposed general formula of the complex is [M(L₁)₂(L₂)₂] where M = Hg(II), L₁ – Benzimidazole and L₂ – Nitrite ion (Nitrito-O). The complex is neutral in nature. Solid state reflectance depicts the tetrahedral geometry of the complex. Metal- chelate and complexation ability confirmed by their IR and Far-IR spectral data. Nuclear magnetic resonance spectra (¹H-NMR & ¹³C-NMR) conveniently predict the geometry of the complex. The mixed ligand complexes were evaluated for their biological activities against the bacterial strain *Klebsiella Pneumonia* and the fungal strain *C.albicans*. The complex was found to very good antibacterial and antifungal activities compared to the Benzimidazole ligand.

KEYWORDS: Hg(II) complex, Benzimidazole, Nitrito-O, *Klebsiella Pneumonia* and *C.albicans*.

INTRODUCTION

Nitrogen and oxygen based ligands are extensively used for the coordination complexes of transition metal ions. Benzimidazole is one the heterocycles which exhibit diverse biological activities.^[1] benzimidazole derivatives were used to antibacterial, antifungal, antiviral, antioxidant, anthelmintic, anti-inflammatory, anticancer, antihistaminic, anti-anxiety and anti hypertensive activities.^[2-4] microwave assisted organic synthesis is simple, clean, fast efficient and economic.^[5-6] microwave assisted synthesis have some advantages in the field of multistep total synthesis, medicinal chemistry, drug discovery, material science and nano technology.^[7-9] in this paper we have reported microwave assisted synthesis, spectral and biological activities of Hg(II) complex with Benzimidazole and nitrite ion ligands.

MATERIAL AND METHODS

All the chemicals used were of AR grade from Alfa Aesar and were used as such. Microwave irradiations were used for the synthesis of complexes from domestic microwave oven. The elemental analysis of the complex was carried out using (Thermo Finnegan make, Flash EA1112 series) CHNS(O) analyzer instrument. The metal ion estimated by gravimetrically using standard procedure. The molar conductance of 10⁻³ M complex in acetonitrile was conducted using Systronic Conductivity Bridge at 25⁰C. The cyclic voltammetry of the complex

were carried out using Princeton applied research cyclic voltammogram. The diffused reflectance spectra of the complex in the solid state were measured using Varian carry-5000 model UV-Visible spectrophotometer. IR spectra of the free Benzimidazole and its complex were carried out using Shimadzu FT-IR8400s spectroscopy at 4000-400 cm⁻¹ wave number with KBr pellet technique. The Far IR spectrum of the complex was recorded in a Bruker make, 3000 Hyperion Microscope with Vertex 80 FTIR system model instruments.

The antibacterial and antifungal activities of Benzimidazole and its complex were done by in-vitro Agar well diffusion method using Amikacin and ketoconazole as a standard for bacterial and fungal strain respectively.

Preparation of complexes

The Hg(II) complex was synthesized by mixing Benzimidazole 0.87 g (7.36 mmol) in 10ml methanol to the mercury chloride 1g (3.68 mmol) in 10ml methanol. The mixture was irradiated on a microwave oven for 10 sec, then sodium nitrite 0.50g (7.36 mmol), in 10 ml ethanol was added to the above mixture respectively. The whole mixture was irradiated on a microwave oven for another 10 sec. The precipitated colourless complex was filtered and washed with ethanol, dried in vacuum desiccators and kept in an airtight glass contained.

RESULTS AND DISCUSSION

i) Micro-analytical data

The elemental analysis and metal estimation of the prepared complex indicate their molecular formula. The metal and ligands are present in the complex by the ratio of (1:2:2) metal: Benzimidazole: nitrite is the

predominant evidence for the formula of the complex. The complex have the formula of $[\text{Hg}(\text{Bz})_2(\text{NO}_2)_2]$ which is monomeric in nature. The molar conductance value is $21.80 \text{ Ohm}^{-1}\text{cm}^2\text{mol}^{-1}$ in acetonitrile were measured, according to Geary *et al.*, the complex exhibit non-electrolyte (1:0 type) neutral^[10] complex.

Table 1: Micro analytical data.

S.No.	Complex	Colour	% Yield	Molecular weight (g/mol)	Elemental analysis				
					%C	%H	%N	%O	%M
1	$[\text{Hg}(\text{Bz})_2(\text{NO}_2)_2]$	colourless	65	574.85	29.22	2.08	14.61	11.13	34.89

ii) Solid state reflectance spectra

The solid state diffused reflectance spectra of the Hg(II) complex gives only charge transfer spectra at 36764 cm^{-1} (272 nm). 5d orbital of metal ion is completely filled; there are no unpaired electrons on taking electronic transitions and their fore C-T band only is observed.^[11]

iii) IR and Far-IR Spectra

Complexing ability and metal chelation of the complex predicted using IR and Far-IR spectral data. IR spectra of free Benzimidazole exhibits strong stretching frequencies at $1400\text{-}1650 \text{ cm}^{-1}$ indicating the $\nu(\text{C}=\text{N})$ of Benzimidazole ring which is shifted to 1672 cm^{-1} in the complex may exhibit the metal ion can coordinated through the nitrogen atom.^[12] The other frequencies $\nu(\text{N}-\text{H})$ at $3200\text{-}3100 \text{ cm}^{-1}$; $\nu(\text{C}-\text{N})$ at $1270\text{-}1290 \text{ cm}^{-1}$ and $\nu(\text{C}-\text{H})$ aromatic, at $3100\text{-}3300 \text{ cm}^{-1}$; are shifted to 3305 cm^{-1} , 1275 cm^{-1} and 3080 cm^{-1} respectively indicating

the Benzimidazole can enter into the coordination sphere. The mixed ligand nitrite ion shows $\nu_a(\text{NO}_2)$ at 1234 cm^{-1} and $\nu_s(\text{NO}_2)$ at 1362 cm^{-1} were also confirming the additional ligand also enter into the sphere.^[13] metal chelating ability of complex also predicted and confirming the $\nu(\text{M}-\text{N})$ and $\nu(\text{M}-\text{O})$ coordination.^[14] Hg-N (Imidazole nitrogen atom of C=N) at 435 cm^{-1} and Hg-O (Nitrito-O of NO_2 ion) at 346 cm^{-1} confirming metal chelation from Far-IR spectra.

iv) Cyclic voltammeter

Mercury metal ions have different oxidation state (+2, +1 0). The metal ion reduction and oxidation properties was perfectly depicted from cyclic voltammeter study.¹⁵ the cyclic voltammogram of Hg(II) complex show one electron quasi reversible reaction of Hg(II)/Hg(I) couple with Epc at -1.235V and Epa at -0.500V and $\Delta E_p = -0.735\text{V}$.^[15]

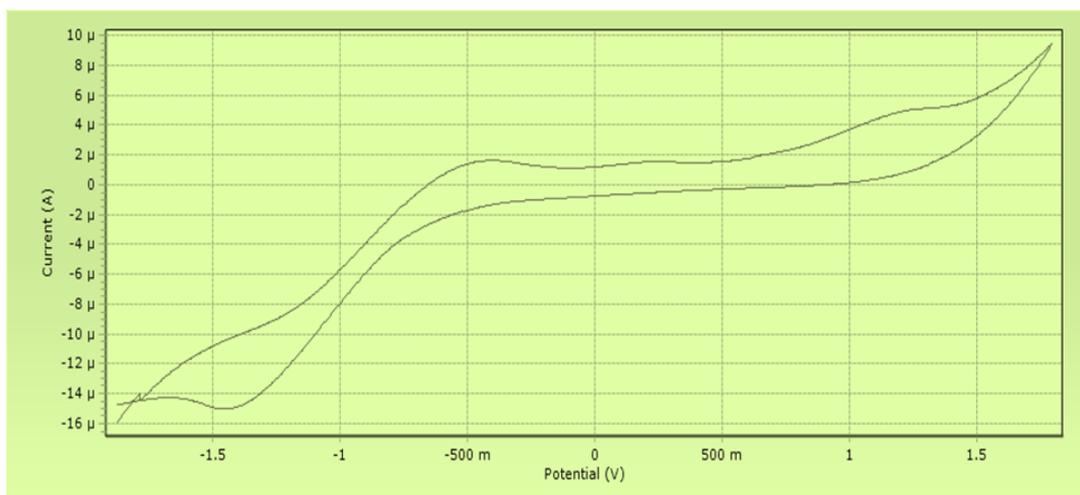


Figure-2: Cyclic voltammogram of Hg(II) complex.

v) ^1H and ^{13}C NMR spectra

Proton NMR and carbon NMR spectra of the diamagnetic Hg(II) complex were carried out in DMSO- d_6 using Tetramethylsilane as the internal standard. The ^1H -NMR spectra of free Benzimidazole shows chemical shift values at 12.53 ppm, 8.25 ppm and 7.17-7.20 ppm corresponding to N-H, H-C=N and aromatic C-H groups respectively these are shifted to downfield or up field at 12.58 ppm, 8.42 ppm and 7.19-7.20 ppm respectively in the complex confirming the complexation nature of

ligands to the metal ions.^[16] in ^{13}C -NMR of Benzimidazole gives the chemical shift values at 142.42 ppm, 122.20 ppm, 118.20 ppm and 113.07 ppm corresponding to four different carbon of ligand which are downfield/up field in the complex at 150.43 ppm, 140.10 ppm, 122.73 ppm and 116.88 ppm respectively.^[17]

vi) Bio-potential activities

Antibacterial and antifungal activities

The Invitro antibacterial and antifungal activities of Hg(II) complex were done by Agar well diffusion method using Amikacin and ketoconazole as the standards and DMSO as the solvent control. Metal-

chelates exhibit significant activities against *Klebsiella Pneumonia* and the fungal strain *C.albicans* than the ligand Benzimidazole. However chelate nature and neutral nature of complex shows its higher activity than the ligand.



Figure-3: Inhibition of Hg(II) and Benzimidazole of *Klebsiella Pneumonia* and *C.albicans*

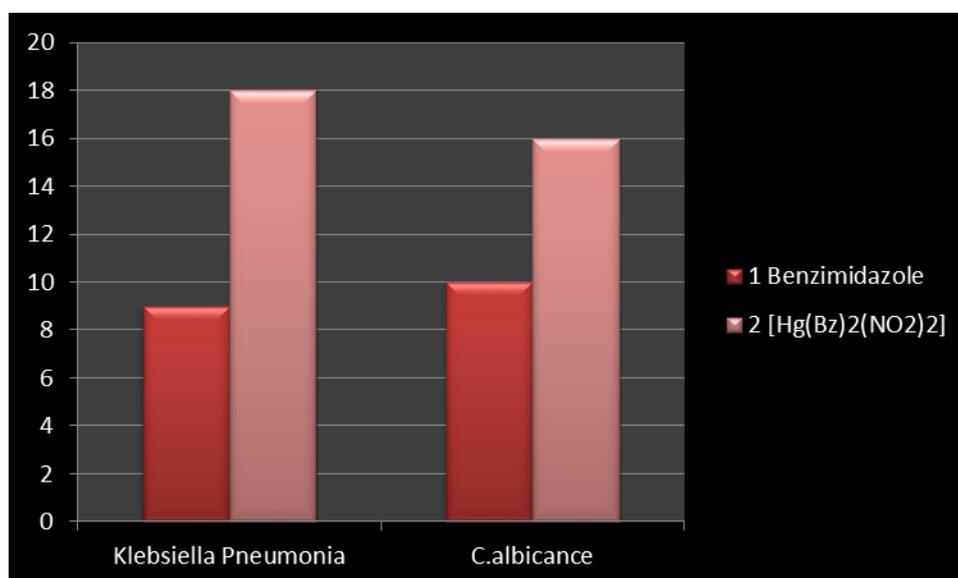


Figure 4: Comparative Bio-potential activities of Hg(II) and Benzimidazole of *Klebsiella Pneumonia* and *C.albicans*.

CONCLUSION

In this effort, the Hg(II) complex of Benzimidazole and nitrite ion was synthesized using microwave irradiated method and characterized on the basis of analytical, spectral, and Biological methods. The formulae of the Hg(II) complex $[\text{Cu}(\text{Bz})_2(\text{NO}_2)_2]$ and they are non-ionic, neutral and non-electrolyte. The solid state diffused reflectance spectra reveal that the complex has tetrahedral geometry. The bio-potential activities show the complex is biologically active against the tested microorganisms than the free ligand.

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