Nat. Volatiles & Essent. Oils, 2021; 8(5): 12341-12347

NVEO
Natural Volatiles & Essential Oils

Synthesis, Characterization and Antibacterial Activity of Cobalt chloride complex with 2-(*p*-thiomethyl phenyl)benzimdazole

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Abstract

The reaction of 2-(p-thiomethyl phenyl) benzimdazole (tmpbi) with the appropriate metal halide yielded the coordination product $Co(tmpbi)_2Cl_2$. Elemental analyses, conductance measurements, FT-IR, UV-visible, and magnetic susceptibility measurements were used to describe the complex. For this complex, a tetrahedral geometry has been proposed. The N-benzimidazole coordination is visible in the ligand tmpbi. The ligand and its complex of Co were evaluated in vitro for antimicrobial (antibacterial) activity using the paper disc diffusion method, with the selected strains being Streptococcus aureus and Escherichia coli, which represent the gramme positive and gramme negative bacterial groups, respectively. These bacteria were chosen because they are potential human pathogens that can cause dysentery and food poisoning, respectively. Against E. coli and Streptococcus aureus, the cobalt chloride complex is more effective than the ligand. When compared to the activity of the free ligand, the complex has a higher activity.

Keywords: Cobalt chloride complex; 2-(*p*-thiomethyl phenyl) benzimdazole (tmpbi); Antibacterial activity.

Introduction:

In the course of the last decade, benzimidazole subordinates containing thiazolyl, ester, carboxyl, alkyl, and amine bunches have shown to be productive antibacterial and antifungicidal drugs [1-14]. Change metal coordination mixtures of benzimidazole subsidiaries have remedial potential also. Cytotoxic, antiviral, and antiamoebic activities have been seen in complexes containing 2-substituted benzimidazole [15-17]. 5,6-dimethylbenzimidazole provides one of the five nitrogen atoms coupled to cobalt(II) in vitamin B12, which has generated interest in benzimidazole and its derivatives research [19]. The synthesis, structure, and antibacterial investigations of the Cobalt chloride complex of tmpbi are presented here.

2. Experimental

2.1. Materials and physical measurements

Since each of the synthetics were reagent grade, they didn't should be refined any further. Standard methods were utilized to sanitize methanol, ethanol, N, N-dimethylformamide, acetonitrile, and other compound solvents. An advanced conductivity meter (Elico model-180) was utilized to quantify the conductivity of the complex in nitrobenzene at room temperature (10-3M). The examinations were done utilizing the elementar Vario EI III and Carlo Erba-1108 gear. The FTIR spectra of tmpbi and its complex in KBr pellet were gained utilizing a Nicolet sway 400D spectrometer in the 4000-400 cm^{-1} territory. An electrothermal melting point equipment was used to obtain melting points. The mull approach was used to record solid state electronic spectra in the 200-2000 nm range using a UV-Vis-NIR spectrophotometer [20]. Magnetic susceptibility measurements of powdered sample ware at room temperature were recorded using the Faraday method on a Johnson-Mathey DG8 5HJ balance.

2.2. Antibacterial activity measurements

The paper circle dissemination strategy [21] was utilized to assess the antimicrobial (antibacterial) conduct of the ligand and its mix with cobalt chloride in vitro, utilizing G (+) Staphylococcus and G (-) Escherichia coli as the strains of decision. The liquid medium containing the bacterial subcultures was autoclaved for 20 minutes at 121°C and 15 lb strain going before immunization. The microorganisms were then produced for 24 hours at 36 degrees Celsius in an incubation facility. A nutritious agar plate was put inside and permitted to set. A 10 mm measurement channel paper circle was plated in the focal point of every agar plate with the test synthetic substances (DMF arrangements). From that point onward, the plates were hatched for 1 hour at 50°C prior to being moved to a 360°C hatchery. The width of the development hindrance zone encompassing the plate was estimated following 24 hours of brooding. Now, four reproductions have been finished.

2.3. Syntheses of compounds

2.3.1. Synthesis of the ligand 2-(*p*-thiomethylphenyl) benzimidazole (tmpbi)

For 2 hours, a combination of o-phenylenediamine (10 mmol) and p-thiomethylbenzaldehyde (10 mmol) in benzene (100 mL) was refluxed in a steam shower. Subsequent to being left for the time being, it separated into a yellow translucent strong. The item was isolated through filtration and afterward washed with an answer of water and n-hexane. It was recrystallized from ethanol to create light yellow gems that were vacuum dried over P_2O_5 (Yield 90%).

2.3.2. Synthesis of Cobalt chloride complex

Independently, an answer of divalent cobalt (1 mmol) in ethanol (25 mL) was ready, and an answer of tmpbi (2 mmol) in hot ethanol was added to each of these (15 mL). It was refluxed for around 6 hours for metal halides. The subsequent strong was sifted, washed with cold ethanol broadly, and dried in vacuo more than P_2O_5 (yield 85–90%).

3. Results and discussion

3.1. Syntheses

The insightful information for tmpbi and its metal complex are recorded in Table 1. As per the information, the complex has the overall recipe $[M(tmpbi)_2X_2]$ (where M=Co and X=Cl-). They are genuinely steady at room temperature. The compound is insoluble in most natural solvents aside from N,N-dimethylformamide, nitrobenzene, and dimethyl sulfoxide. In the mass spectra of tmpbi, the atomic particle top at m/z 240, which relates to the M+1 species, was apparent. The molar conductance esteems for nitrobenzene (10^{-3}M) show that the edifices are non-electrolytes, demonstrating that the halogen particles are facilitated to the metal [20]. The substances were portrayed utilizing the techniques recorded beneath.

Table 1

Data on the substances' physical and analytical properties

Compound	Empirical formula (mol.wt)	Colour	Anal.found (Cald) (%)			
			C	H	N	S

tmpbi	$C_{14}H_{12}N_2S$ (240)	Yellow	69.71 (76.74)	4.32 (5.04)	12.41 (11.66)	12.95 (13.32)
$Co(tmpbi)_2Cl_2$	$C_{28}H_{24}N_4S_2Cl_2Co$ (609.8)	Blue	55.51 (55.09)	4.09 (3.93)	9.43 (9.18)	9.17 (9.15)

3.2. Spectral studies

3.2.1. Infrared spectra

Table 2 shows the IR spectrum data for tmpbi and its complex. The bending modes of vibration of different groups present in the organic molecule have been assigned to the numerous bands found in the IR spectrum of ligand tmpbi. Table 2 contains a summary of the assignments completed. The peak detected at 1471 cm^{-1} in the IR spectra of tmpbi is attributable to the NH of the benzimidazole ring. The stretching vibrations (C=N) and (C-N) are attributed to the bands at 1604 and 1331 cm^{-1}, respectively. The symmetrical C-H stretching mode of the S-CH_3 group is responsible for the peak at 2800 cm^{-1}. The in-plane C-H deformation mode of the p-substituted benzene ring of the ligand is allocated to a band at 1130 cm^{-1}. The C=N stretching band appears in the spectra of the metal complex containing tmpbi in the region 1593-1615 cm^{-1}. In the spectra of mind boggling, a solid band around 1604 cm^{-1} in the free ligand credited to the C=N extending mode is moved to lower or higher frequencies, inferring that the benzimidazole ring's tertiary nitrogen directions to the metal ion. The benzimidazole ring vibrations are allocated to the bands at 1284, 1016, 602, and 457 cm^{-1}, which are not depicted in Table 2. Between 1322 and 1370 cm^{-1}, the C-N stretching band can be found. The lower frequency region, which is typical of metal halide vibrations, is of special interest. The development of metal halide bonds is supported by the presence of a band in the complex about 455 cm^{-1}. It's worth noting that the chemical isn't an electrolyte. The conductivity measurements corroborated this.

Table 2

tmpbi's infrared spectral data (cm^{-1}) and its complicated

Compound	ν(C=N)	ν(C-N)	δNH	ν(S-CH_3)
tmpbi	1604	1331	1471	2800
$Co(tmpbi)_2Cl_2$	1593	1322	1436	2814

3.2.2. Electronic spectra

Table 3 shows the electronic absorption spectra of the cobalt chloride complex in the visible range. Tetrahedral structure is supported by the spectra of the Co(II) complex [23, 24]. Around 15,000-17,000 cm^{-1}, the cobalt complex exhibits an absorption band with fine structure (Table 3). The $^4A_2 \rightarrow {}^4T_1$

(P) transition is responsible for this pretty strong absorption band. The fine structure observed in this region is typical of the tetrahedral complex, and it is caused by spin-orbit coupling in the T state [24]. The $^4A_2 \rightarrow {}^4T_1$ (F) transition is responsible for the broad absorption band in the 6000-9000 cm^{-1} range. The $^4A_2 \rightarrow {}^4T_1$ transition produces a low energy band about 5000 cm^{-1} in the present complexes, which is expected for tetrahedral complexes. When Cl was substituted by Br, the band for the $^4T_2 \rightarrow {}^4T_1$ (P) transition redshifted in accordance with the spectrochemical series, and the absorbance increased in the order of the hyperchromic effect [27, 25, 26]. The halogen ions are shown to coordinate with the centre cobalt ion.

Table 3

Cobalt chloride complex magnetic moment and electronic spectral data using tmpbi.

Substance	Magnetic moment (B.M.)	Absorption maxima (cm^{-1})
$Co(tmpbi)_2Cl_2$	4.50	16,760 14,650

3.3. Magnetic measurement studies

The complexes are paramagnetic at room temperature, according to magnetic moment measurements in the solid state. To a certain extent, the magnetic moment values can be used to distinguish octahedral and tetrahedral complexes of Co(II). Co(II) octahedral high spin complexes have moments in the range of 5.0 B.M., while tetrahedral complexes have moments in the range of 4.4 - 4.8 B.M. [28]. Table 3 shows that the magnetic moment values of the cobalt complex are in the range of 4.50 B.M., indicating that the complex has a tetrahedral structure. Because of spin – orbit interaction, the value is higher than that expected by the spin solely value, i.e. 3.87 B.M.

3.4. Antibacterial activity

The following five major aspects have been considered while developing metal compounds with antibacterial activity: The chelate effect I bipyridine, phenanthroline, and o-phenyldiamine are ligands that are attached to metal ions in a bidentate way and have stronger antibacterial efficacy than complexes with unidentified N-donor ligands, such as pyridine [29]. For two reasons, benzimidazole ligands with a phenyl group at position 2 were chosen as the complex's 'carrier ligands' in this investigation. Sterically hindering ligands may lower the rate of thiol-containing compounds detoxification.

The antibacterial activity of the ligand and its metal complex was tested against two bacteria, S. aureus and E. coli, which represent the gramme positive and gramme negative bacterial groups, respectively. Table 4 shows the findings of an antimicrobial investigation of the complex as a function of the concentration of the complexes. DMF was used as a control and had no effect on bacteria. The complex was tested at four different concentrations: 5, 10, 15, and 20 mM. Discs of paper were created and dipped into the various solutions. The size of the inhibitory diameter was used to measure the susceptibility of various bacteria strains to the metal complex. E. coli and Streptococcus aureus, two bacterial pathogens, were found to have growth inhibitory effects. Against E. coli and Streptococcus aureus, the complex is more effective than the ligand. Escherichia coli is a type of bacteria that lives in

the human colon and is usually harmless. Water or undercooked food contaminated with the 0157:H7 strain, on the other hand, can cause serious, sometimes fatal infections. In almost 90% of cases, an increased quantity of Streptococcus aureus bacteria is identified on the skin of people with atopic eczema. In tests against S. aureus and E. coli, the complex was found to have more activity than the free ligand. As a result, complexes could be effective antibacterial agents against microorganisms.

Table 4

The ligand tmpbi and its metal complexes have antibacterial action.

Compound	Zone of inhibition (in mm)							
	Streptococcus aureus (conc. in mM)				*E. coli* (conc. in mM)			
	5	10	15	20	5	10	15	20
DMF (control)*	-	-	-	-	-	-	-	-
tmpbi	2	4	6	8	3	5	6	8
$Co(tmpbi)_2Cl_2$	3	5	14	18	3	6	14	18

*No effect upto 24 hours

4. Conclusion

The synthetic and physicochemical features of the mononuclear $M(tmpbi)_2X_2$ complex (M=Co; X=Cl) have been addressed. According to biological testing of the ligand and its metal complex, the complex has more antibacterial action against microorganisms than the ligand.

Acknowledgement

"One of the authors (MNM) is thankful to the Vision Group on Science and Technology, Department of Information Technology, Biotechnology and Science & Technology, Government of Karnataka, for providing funds under the K-FIST (L1), GRD No.770 to carry out the present work by means of a sponsored project in our esteemed Institute. Our sincere thanks are due to the Raman Research Institute, Bangalore, for the elemental analysis. Our thanks are also because of Prof. D.N. Sathyanarayana, IISc, Bangalore for their valuable suggestions. MNM also thanks Prof. K.R. Nagasundara, Central College, Bangalore University, Bangalore for his constant support and encouragement".

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