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Oxovanadium Complex of Mebendazole: Synthesis, Spectroscopic and Physico-chemical Characterization

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ABSTRACT

The greener and cost-effective synthesis of an oxovanadium complex of mebendazole is described. The synthesis involves the use of distilled water as a solvent and refluxing, providing environmentally friendly advantages, simple work-up procedures, and a short reaction time with excellent yield. Characterization included UV-Vis and FTIR spectroscopy. The UV-Vis spectra showed intra-ligand transitions at 242 and 269 nm and charge transfer bands at 310 and 380 nm, indicating the formation of oxovanadium complex of mebendazole. The FTIR spectra confirmed coordination via the nitrogen and oxygen atoms of the ligand, evidenced by shifts in C-H, C=C, and C-O stretching bands, the appearance of a new V=O band at 977.94 cm^{-1}, and an OV-N bending band at 497.65 cm^{-1}. The metal complex with the formula $[VO(L)]SO_4$ was deduced, where L is mebendazole.

Keywords: Oxovanadium; Mebendazole; Synthesis; Characterization; Spectroscopy; UV-Vis; FTIR; Physico-chemical; Ligand; Antibiotic; Green synthesis; Coordination complex.

1. Introduction

The development of metal-based drugs has gained considerable attention in medicinal chemistry due to their superior therapeutic properties compared to organic compounds. Among transition metals, vanadium complexes have shown significant promise in pharmaceutical applications, thanks to their diverse biological activities and relatively low toxicity [1]. The coordination chemistry of vanadium, particularly in its +4 oxidation state as oxovanadium (VO^{2+}), has been extensively explored due to its stability and biological significance.

Mebendazole [methyl N-(6-benzoyl-1H-benzimidazol-2-yl)carbamate], a well-known anthelmintic drug, has demonstrated remarkable versatility beyond its primary antiparasitic role. Recent studies highlight its potential anticancer properties and its ability to function as a multidentate ligand in metal complex formation [2],[3]. Its multiple coordination sites, including the benzimidazole nitrogen, carbonyl oxygen, and carbamate groups, make it a compelling candidate for metal complexation.

The combination of oxovanadium with bioactive organic ligands has shown great potential in developing more effective therapeutic agents. Research indicates that metal complexation can enhance the biological activity of organic drugs through mechanisms such as increased lipophilicity, altered cell membrane permeability, and modified target interactions [4]. Notably, oxovanadium complexes have demonstrated superior anticancer, antidiabetic, and antimicrobial properties compared to their parent ligands.

Previous studies have explored the synthesis and characterization of metal complexes with benzimidazole-based ligands [5], reported significant improvements in biological activity when benzimidazole derivatives were complexed with metal ions Likewise, [6],[7] found that metal complexation enhanced the stability and biological activities of benzimidazole-based drugs. Despite extensive research on oxovanadium complexes and mebendazole separately, there remains a gap in understanding their combined properties as a metal-ligand system. The

interaction between oxovanadium and mebendazole could result in a complex with improved therapeutic potential while providing deeper insights into the coordination chemistry of benzimidazole-based drugs [8],[9]. Investigating this synergy may not only lead to novel therapeutic agents but also enhance our understanding of how metal ions influence drug efficacy and stability in biological systems.

Understanding the structural and physicochemical properties of these complexes is essential for assessing their therapeutic potential [10],[11]. Spectroscopic techniques such as UV-visible, infrared, and along with physico-chemical analysis such as solubility and stability measurements, offer valuable insights into metal-ligand bonding and overall complex biological activity [12],[13].

In this context, our research focuses on the synthesis, detailed spectroscopic characterization, and physicochemical analysis of a novel oxovanadium-mebendazole complex. This study aims to elucidate the coordination behavior of mebendazole with oxovanadium and define the structural characteristics of the resulting complex, laying the groundwork for future research into its potential therapeutic applications.

1.1. Study Objectives

The aims of this study are to achieve the following objectives:

(a) To synthesize an oxovanadium complex of mebendazole using a green and cost-effective approach, (b) To characterize the synthesized complex using spectroscopic techniques such as UV-Vis and FTIR, (c) To determine the physicochemical properties of the oxovanadium-mebendazole complex, including solubility and stability, (d) To elucidate the coordination behavior of mebendazole with oxovanadium and define the structural characteristics of the resulting complex, and (e) To provide insights into the application of metal-ligand interactions in medicinal and coordination chemistry.

2. Materials and Methods

The metal salt ($VOSO_4$) and mebendazole (Meb) were gotten from commercial sources and were used without any further purification. The complexes (materials) were further characterized using the JASCO V-730 Ultraviolet-Visible spectrophotometer. The FTIR spectra of the synthesized complex wer taken on Shimadzu 8400-S from the region of 4000-400cm^{-1}; the melting points of the complexes were determined using Stuart melting point (SMP 11) apparatus, and the solubility was determined in from these solvents: methanol, ethanol, distilled water and DMF.

2.1. Synthesis of [VOMeb]SO_4) Complex

0.590 g (2 mM) of mebendazole dissolved in 10 ml of sodium hydroxide (NaOH) solution of 0.2 M in a round bottom flask of 50 ml, swirled. It formed a milkfish colour and partially soluble. 0.163 g (1 mM) of $VOSO_4$ dissolved in 10 ml of distilled water was added into the solution forming a light blue colour, stirred for 1 hour. Then the solution was added 6 ml of ethanol and refluxed at 50 ^oC for 1 hour till the colour changed to green. The solution was washed with hot ethanol, filtered. The residue was kept for two weeks to dry at ambient conditions to obtain yellowish green solid used for analysis. The percentage yield was: 0.54 g (72%). UV-Vis (DMF): 310 nm, 380 nm.

3. Results and Discussion

3.1. Physico-Chemical Characterization

The newly synthesized complex is colored (yellowish green), stable at room temperature, partially soluble in common organic solvents such as ethanol, appreciably soluble in dimethylformamide (DMF) and insoluble in water. The physical properties of mebendazole and its metal complexes are given in table 1 below.

Table 1. Solubility of the ligands and metal complexes in different solvents

Compounds	Water	Ethanol	DMF
Mebendazole	S/S	S	S
[VO-Meb]SO_4 Complex	I	S/S	S/S

S/S= Slightly Soluble; S =Soluble; I =Insoluble.

The solubility result showed that mebendazole, is soluble in ethanol, and slightly soluble in water. It's oxovanadium complex is slightly soluble in ethanol and DMF but insoluble in water.

3.2. Electronic Spectra (UV-Visible spectra)

The electronic absorption spectral data of the ligand and its metal complexes in ethanol and DMF are presented in table 2. Please note that there is instrument error between 340 nm and 370 nm in the UV-Visible spectra.

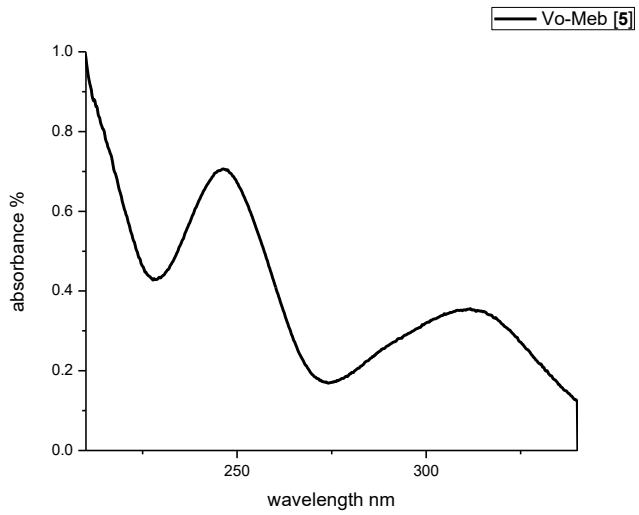

Figure 1. UV-Visible spectrum of [VO-Meb]SO_4 complex

Table 2. Spectroscopic data of the complex

Complexes	Product yield (%)	Colour	Appearance	Electronic transition in DMF/Ethanol	
				Ligand Transitions (nm)	Charge Transfer (nm)
[VO-Meb]SO_4 complex	72	Yellowish Green	Powdery	1	310, 380

The absorption spectra of the complex and respective ligand (mebendazole) were recorded in the range of 200-800 nm. The absorption spectra was recorded in DMF/Ethanol to solubilize the complex. The electronic spectra of this ligand and the complex was illustrated in table 2. Peaks ranging from 200-300 nm (242 and 269 nm) indicates intra-ligand transition (π-π*) while peaks at 301-399 nm (i.e. 310 and 380 nm) indicates charge transfer of ligands. Absence of d-d transition shows that the vanadium complex formed is probably V(V) as no peaks were observed in the visible region.

3.3. FTIR Spectrum of the Complex

The FTIR spectra of the synthesized complex was taken on Shimadzu 8400-S from the region of 4000-400cm^{-1}. The bonding sites of the complex through the heteroatoms (O and N) of the ligand were observed in the IR spectrum when the spectra of the original parent ligand and its metal complexes were compared. The assignment of the spectra of the parent mebendazole and the oxovandium complex are compiled in Table 3.

Table 3. FTIR spectra of mebendazole and its complexes (VO-Meb)

Mebendazole (cm^{-1})	**VO-Meb** (cm^{-1})	**Assignment**
3088.14	3059.20	C-H stretching of aromatics
2998	2949.26	C-H stretching of alkene
1593	1595.18	C=C stretching of alkene
1264.39	1261.49	C-O stretching
-	977.94	V=O stretching
-	497.65	OV-N bending of mebendazole

The FTIR spectra of the synthesized [VO-Meb]SO_4 complex provide key insights into the coordination of mebendazole with oxovanadium. The comparison of the FTIR data between free mebendazole and its oxovanadium complex reveals significant shifts in characteristic vibrational bands, confirming the formation of the metal-ligand bond.

A notable feature in the FTIR spectrum of the complex is the appearance of a new band at 977.94 cm^{-1}, which is attributed to the V=O stretching vibration. This band is a hallmark of oxovanadium(IV) complexes and confirms the presence of the vanadyl (VO^{2+}) moiety in the synthesized compound [8]. Additionally, the emergence of a band at 497.65 cm^{-1}, corresponding to OV-N bending, provides strong evidence of the coordination of vanadium through the nitrogen atom of the benzimidazole ring in mebendazole [8].

The characteristic C-H stretching vibrations of aromatic and aliphatic groups in mebendazole undergo slight shifts upon complexation. The aromatic C-H stretching, which appears at 3088.14 cm^{-1} in free mebendazole, shifts to 3059.20 cm^{-1} in the complex, while the aliphatic C-H stretching shifts from 2998 cm^{-1} to 2949.26 cm^{-1}. These shifts suggest changes in electronic distribution due to metal coordination. Similarly, the C=C stretching band of the benzimidazole ring, observed at 1593 cm^{-1} in free mebendazole, undergoes a slight shift to 1595.18 cm^{-1} in the complex, indicating possible changes in the aromatic system of the metal complex [8].

Furthermore, the C-O stretching band, present at 1264.39 cm^{-1} in mebendazole, is slightly shifted to 1261.49 cm^{-1} in the complex, suggesting metal coordination through the oxygen atom [8]. These spectral changes collectively confirm the successful coordination of mebendazole to oxovanadium through both nitrogen and oxygen donor atoms, supporting the proposed structural formula of the complex as $[VO(L)]SO_4$.

Overall, the FTIR results provide compelling evidence for the formation of the oxovanadium-mebendazole complex, reinforcing the role of metal-ligand interactions in altering the vibrational characteristics of the ligand. These findings lay the foundation for further studies on the structural, electronic, and biological properties of the synthesized complex.

4. Conclusion

This research study successfully synthesized and characterized an oxovanadium complex of mebendazole. The UV-Vis spectra revealed intra-ligand and charge transfer transitions, consistent with the formation of a V(IV) complex. FTIR analysis confirmed coordination through nitrogen and oxygen atoms of mebendazole, evidenced by characteristic V=O and OV-N bands.

The combined spectroscopic data provided strong evidence for the metal-ligand interaction and complex formation. Future work could involve further structural studies using X-ray crystallography to elucidate the detailed geometry of the complex. Also, biological activity assays should be performed to investigate the potential antimicrobial, anticancer, or antiparasitic properties of the oxovanadium-mebendazole complex while computational studies, including density functional theory (DFT) calculations, could provide deeper insights into the electronic structure and binding interactions of the complex.

In addition, investigation of the complex's pharmacokinetics and cytotoxicity in biological systems could facilitate its potential therapeutic applications while exploring the modification of mebendazole derivatives for improved metal complexation and bioactivity enhancement would be beneficial for future drug development.

Declarations

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Competing Interests Statement

The authors declare no competing financial, professional, or personal interests.

Consent for publication

The authors declare that they consented to the publication of this study.

Authors' contributions

Both the authors made an equal contribution in the Conception and design of the work, Data collection, Drafting the article, and Critical revision of the article. Both the authors have read and approved the final copy of the manuscript.

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