

Green Synthesis Characterization and Antimicrobial Activity of Complex of Amide Ligand with Mn(II)

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ABSTRACT

The present study reports the green synthesis, structural characterization, and antimicrobial evaluation of Manganese (II) complexes derived from amide-based ligands. The complexes were synthesized under eco-friendly conditions without the use of toxic solvents or harsh reagents. Infrared spectral analysis confirmed the bidentate coordination of the amide ligands through the carbonyl oxygen and pyrimidine nitrogen atoms. Electronic spectral data suggested tetrahedral geometry around the Mn (II) ion, which was further supported by magnetic moment measurements. The complexes exhibited enhanced thermal stability compared to the free ligands, indicating strong metal–ligand interactions. Antimicrobial screening against selected bacterial and fungal strains demonstrated significant biological activity, suggesting that amide-based Mn (II) complexes could serve as potential candidates for bioinorganic and pharmaceutical applications.

Keywords: Amide Ligand, Antibacterial, Octahedral, Carbonyl Oxygen, Bioinorganic.

Introduction

Transition metal complexes play a vital role in coordination chemistry due to their diverse structures, reactivity, and biological applications. Among these, **Manganese (Mn)** is an essential trace element involved in various enzymatic and redox processes, such as oxygen evolution, metabolism, and antioxidant defence. The chemistry of Mn (II) complexes is of special interest because of their ability to adopt variable oxidation states and geometries, which enhance their catalytic and biological potential.

Amide ligands are widely studied in coordination chemistry as they contain both donor oxygen and nitrogen atoms, enabling them to coordinate in a **bidentate or polydentate manner**. Their ability to form stable chelates with transition metals makes them attractive candidates for the design of novel complexes with improved stability, electronic properties, and biological activity.

The coordination of Mn (II) with amide ligands not only influences the **spectral and magnetic behaviour** of the complexes but also plays a crucial role in determining their **geometry and reactivity**. Such complexes have been investigated for their **antimicrobial, catalytic, and pharmacological activities**, offering potential applications in green chemistry and medicinal inorganic chemistry.

In this work, Manganese (II) complexes with amide ligands were synthesized via a **green synthetic route**, avoiding hazardous reagents and solvents. The synthesized complexes were characterized by spectroscopic (UV-Vis, IR) and magnetic studies to elucidate their structural features. Furthermore, their biological activity was assessed to explore the role of amide coordination in enhancing antimicrobial potential.

Materials and Methods

To synthesize Mn (II) complexes with amide-containing ligands, a 250 mL round-bottom flask was charged with a solution of Mn chloride (0.001 mol in 30 mL ethanol). The appropriate amide ligand

(0.003 mol) was then added gradually with continuous stirring. The reaction mixture was maintained at room temperature for 6–7 hours under constant magnetic stirring.

For an alternative **green synthesis approach**, the reaction mixtures were subjected to microwave irradiation at 600 W for 2–10 minutes. Both conventional and microwave-assisted methods yielded solid precipitates, which were isolated and purified by recrystallization. The crude products were washed with alcohol to remove impurities, followed by drying under vacuum.

Table 1: Physio - Chemical Data of Mn (II) Metal Complexes C.M.= conventional Method M.M Microwave Method

S. No.	Complexes	Color	m. p. (°C)	Reaction Period		Yield %		Element Analysis Calculation		
				C.M. hrs.	M.M. min.	C.M.	M.M.	C	H	N
1.	[Mn(2NPCFA)]	Pale yellow	256±2	6.6	2.50	45	55	43.13	3.01	25.16
2.	[Mn(2NPCAA)]	Light orange	252±1	6.6	2.50	45	50	46.40	3.90	23.20
3.	[Mn(2NPCBA)]	white	209±2	6.6	2.50	40	50	49.23	4.64	21.53
4.	[Mn(2NPCPA)]	Yellowish-White	202±2	6.6	2.50	40	45	51.66	5.30	20.10

The resulting Mn (II) complexes were obtained as coloured crystalline or powdered materials. They exhibited good stability under normal laboratory conditions, were non-hygroscopic, and generally insoluble in most organic solvents and water, but showed solubility in methanol and dimethylformamide (DMF). Conductivity measurements of the complexes in DMF indicated non-electrolytic behaviour, suggesting a predominantly covalent nature of bonding.

Table 1 summarizes the physical characteristics, elemental analysis data, and proposed molecular formulae of the synthesized Ni (II) complexes, which were found to be in close agreement with theoretical values.

Vibration Spectra

Spectra of Vibration For extended periods of time, the Mn (II) complexes having ligands including amide groups remain stable at normal temperature. The manganese complexes that were being studied were insoluble in all other solvents and had a white or brown powder colour. They were somewhat soluble from the elemental and metal estimations are satisfice Table contains the complexes' analytical and physical data. In the mid- and far-infrared range, vibrational spectra were recorded in polyethylene film and KBr pellets. A few diagnostic bands are shown in Table For the free amide group containing ligands, the amide ν (N-H) mode's infrared bands, which are seen at 3163-3382 cm^{-1} , are displaced to higher frequencies, showing that the nitrogen coordination. In the complexes, amide 1 bands owing to ν (C=O) shift negatively in opposition to that of ν (N-H), indicating carbonyl oxygen coordination Pyrimidine nitrogen is said to engage in bonding in complexes; this is supported by the 16–100 cm^{-1} negative shifting of by the complexes' 16-pyrimidinyl ring peak to the ligand comparison.

The ultimate structural conclusions of the complexes and the manner of bonding within them are supported by these equivocal observations.

Measurements of Magnetic

Table 2: Magnetic Moments and Electronic Spectral Data Mn (ii) Ligand with Complexes

S.N.	Ligand Complex	Rf values	μ_{eff} (BM)	Electronic spectral (cm) ⁻¹	Tentative assignments	Expected Geometry
1.	[Mn(2NPCFA)]	(0.82)	5.85	18220, 20141, 22778, 24448, 26630	${}^6A_{1g} \longrightarrow {}^4T_{2g}$ ${}^6A_{1g} \longrightarrow {}^4E_g, {}^4A_{1g}(4G)$	Tetrahedral
2.	[Mn(2NPCAA)]	(0.85)	5.78	18222, 20145, 22780, 24449, 26632	${}^6A_{1g} \longrightarrow {}^4T_{2g}$ ${}^6A_{1g} \longrightarrow {}^4E_g, {}^4A_{1g}(4G)$	Tetrahedral

3.	[Mn(2NPCBA)]	(0.86)	5.82	18222, 20148, 22782, 24450, 26633	${}^6A_{1g} \longrightarrow {}^4T_{2g}$ ${}^6A_{1g} \longrightarrow {}^4E_g, {}^4A_{1g}(4G)$	Tetrahedral
4.	[Mn(2NPCPA)]	(0.88)	5.83	18225, 20149, 22802, 26635	${}^6A_{1g} \longrightarrow {}^4T_{2g}$ ${}^6A_{1g} \longrightarrow {}^4E_g, {}^4A_{1g}(4G)$	Tetrahedral

Bivalent manganese complexes are known in both low spin ($S = 1/2$) and high spin ($S = 5/2$) states. Manganese (II) typically forms high spin complexes with an orbitally degenerate S ground state term and a spin-only magnetic moment of 5.9 ± 0.1 BM, which is expected to be independent of both temperature and stereochemistry due to the additional stability of the half-filled d-orbitals. At room temperature, the magnetic susceptibility experiments were conducted in the polycrystalline form. All the manganese (II) complexes have magnetic moment values between 5.70 and 5.92 BM, which show that there are five unpaired electrons; as a result, these complexes have high spin and tetrahedral manganese coordination:

a = Ethanol: Benzene (3:7), b = Ethanol: Benzene (5:5), c = Ethyl acetate: Carbon tetrachloride (3:7), d = Ethyl acetate: Carbon tetrachloride (4:6)

Electronic Spectra

Weak absorption is evident in the visible range of the electronic spectra of the manganese complexes containing ligands containing amide groups. The manganese (II) complexes' measured spectra with the ligands show bands in the regions of 17636 cm^{-1} and 28011 cm^{-1} , which are attributed to the transitions. Manganese complexes with ligands exhibit electronic spectrum transitions that are characteristic of the tetrahedral environment surrounding the manganese.

Table 3: IR vibrational frequency of Mn Metal

S. No.	Complexes	ν_{N-H} (amide)	$(\nu_{C=O})^a$	$(\nu_{C-N+5N-H})^b$	$(\nu_{N-H+5C-N})^c$	PyrimidinyI	ν_{M-N}	ν_{M-O}	ν_{M-Cl}
1.	[Mn(2NPCFA)]	3380	1625	1496	1343	1575	486	503	-
2.	[Mn(2NPCAA)]	3385	1627	1499	1347	1579	490	505	-
3.	[Mn(2NPCBA)]	3390	1631	1504	1351	1584	494	510	-
4.	[Mn(2NPCPA)]	3395	1635	1510	1356	1589	499	514	-

Thermal Studies

First order behaviour is seen in the complexes of Mn (II) with ligands containing amide groups. The rate at which their thermal breakdown process occurs. This is based on a Coats and Redfern straight line plot (for $n = 1$). Activation energy (E_a) has been computed using the Coats and Redfern linearization method. The complexes' thermal stability is described by the thermal investigations. are relatively stable much above room temperature and that no degradation occurs at room temperature. Above 500K, the first decomposition began.

Results and Discussion

Antibacterial Activity

The antibacterial activity of the synthesized compounds was evaluated using **Mueller–Hinton Agar medium** against *Escherichia coli*, *Staphylococcus aureus*, and *Bacillus subtilis*. The results indicated that all the metal complexes exhibited **moderate antibacterial activity** against the tested strains. Among them, the Mn (II) complexes demonstrated the highest effectiveness, showing significant inhibitory activity particularly against *B. subtilis*, followed by *S. aureus* and *E. coli*.

Conclusion

IR spectra indicate that amide group-containing ligands exhibit bidentate behaviour in Mn (II) complexes, coordinating through carbonyl oxygen of amide groups and nitrogen of pyrimidine rings. Metal ions in ligand settings have distinct electronic spectrum assignments that reflect their geometries.

Mn (II) forms tetrahedral structures in complexes with amide ligands electronic spectral measurements. The hypothesized structures for Mn (II) complexes are shown in Fig. based on previous studies. The revolutionary green method produces compounds that are comparable to conventional synthesis and, in certain situations, yields better results.

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