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COBALT(II) COMPLEX OF PYRAZOLONE: SYNTHESIS, SPECTROSCOPIC AND *IN-VITRO* BIOLOGICAL STUDIES

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ABSTRACT

The research work investigates the synthesis, spectroscopic characterization, and *in vitro* antibacterial activity of a Co(II) transition metal complex. The metal complex was synthesized by reacting the respective pyrazolone-based ligand. The synthesized ligand was characterized by ^{1}H NMR, mass, IR, UV, and elemental analysis, while the respective complex was characterized by IR, UV, and elemental analysis. The results confirmed that the synthesized Co(II) metal complex has promising antibacterial activity against Gram-positive (Bacillus megaterium) and Gram-negative (E. coli) microorganisms, which makes it a potential candidate for the development of a new antibacterial agent.

Keywords: Cobalt complex, Schiff base, Phenyl hydrazine, Pyrazolone and antibacterial activity

INTRODUCTION:

Among pyrazolone derivatives, 4-acyl pyrazolone is notable for its dual characteristics as a significant class of β-diketones, exhibiting diverse coordination modes similar to traditional β-diketones. Coordination chemistry, a rapidly advancing field, often involves 4-acyl pyrazolone due to its multiple electron-rich donor sites **[1]** and its wide range of applications **[2-13]**. Pyrazolone scaffolds are present in a variety of medicines and naturally occurring bioactive alkaloids **[14, 15]**. Additionally, acyl pyrazolone is known for its tautomeric behavior, existing in both keto and enol forms in solid or solution states.

Only a few cobalt complexes are known to play biochemical roles. One prominent example is vitamin B12, which is a type of cobaloxime—a cobalt complex with a glyoxime ligand. Vitamin B12 stands out as one of the few naturally occurring organometallic complexes, characterized by a metal-carbon bond **[16]**. In the present work, building on our previous research on pyrazolone-based complexes, we have synthesized Co(II) complex and carried out an evaluation of their biological activity.

Experimental

Materials and Methods

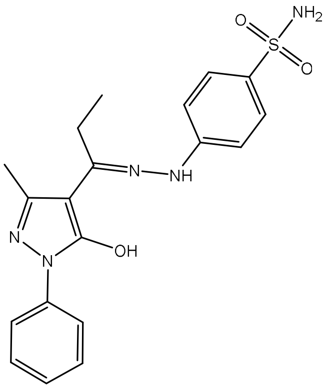
The compounds l-phenyl-3-methyl-5-pyrazolone, 4-sulphonamide phenyl hydrazine and $CoCl_2.6H_2O$were purchased from TCI (Japan). Acylchloride was purchased from spectrochem, Mumbai (India).

Method

Fourier Transform Infrared (FT-IR) Spectroscopy: The FT-IR spectra were recorded using potassium bromide (KBr) pellets on a Shimadzu 8201 PC spectrometer. Proton Nuclear Magnetic Resonance (^{1}H NMR) Spectroscopy: The ^{1}H NMR spectra was obtained using a Bruker Advance 400 FT-NMR instrument, with DMSO-d6 as the solvent.

General Procedure for pyrazolone-based phenylhydrazone ligand (A1)

Accordingly, as a continuation of our earlier work, we have synthesized a pyrazolone-based ligand. A 1:1 molar ratio of 4-acyl-3-methyl-1-phenyl-2-pyrazolin-5-one (amphp) and 4-sulfonamide phenyl hydrazine was combined in 50 ml of methanol. The mixture was heated for 3-4 hours with the addition of a catalytic amount of acetic acid. The progress of the reaction was monitored using thin-layer chromatography (TLC). After the reaction was complete, the resulting product was crystallized from 50 ml of methanol and washed with diethyl ether. The synthesized ligand was characterized by ^{1}H NMR, mass, IR, and UV spectroscopy **(Figures 2-4) [17]**. The final structure of ligand **A1** is shown in **Figure 1**.



A1

Figure 1: Structures of ligand A1

Ligand A1: M.F- $C_{19}H_{21}N_5O_3S$ Yield 76%; M.P. 215°C Cream powder; FT-IR (KBr,cm^{-1}): 3348 ν(O–H), 3251 ν(N–H), 1600 ν(C=O), 1539 ν(C=N); ^{1}H NMR (400 MHz,DMSO-d_6): δ (ppm) = 2.5 (3H,s,-CH_3); 1.20-1.24 (3H,t,-CH_3);2.76-2.78(2H,q,-CH_2) 6.89-7.99 (Ar-H). Elemental analysis found (%) C, 57.15; H, 5.32; N, 17.55 calculated for $C_{19}H_{21}N_5O_3S$: C, 57.13; H, 5.30; N, 17.53. M/Z=400.

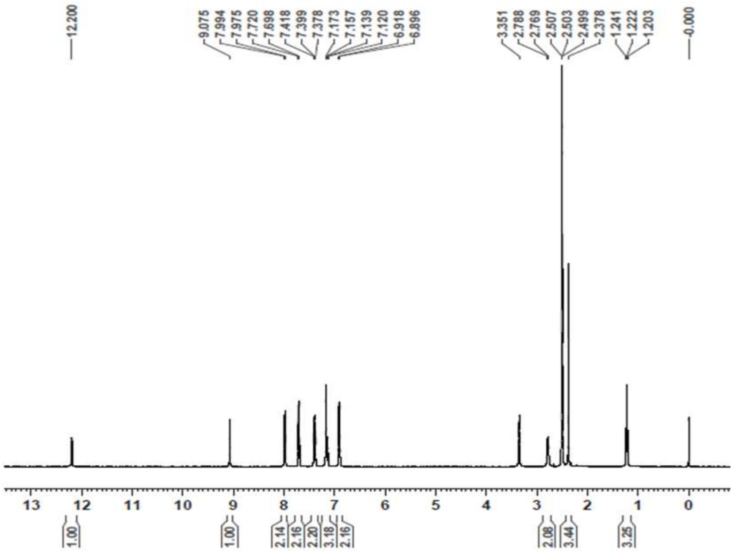


Figure 2: 1H NMR spectra of ligand A1

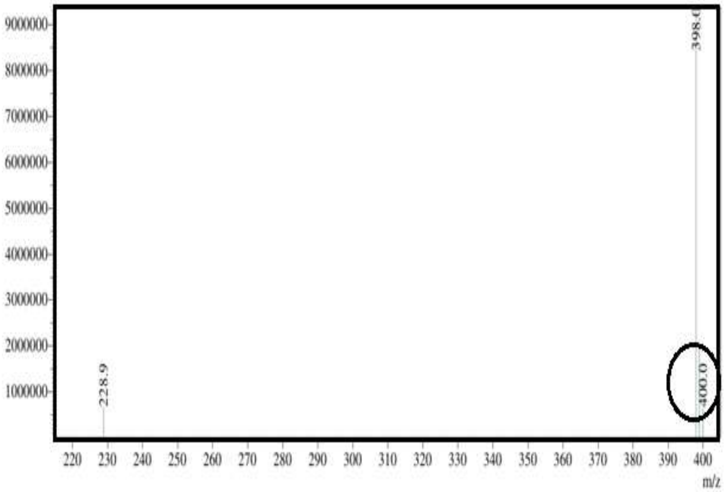


Figure 3: Mass spectra of ligand A1

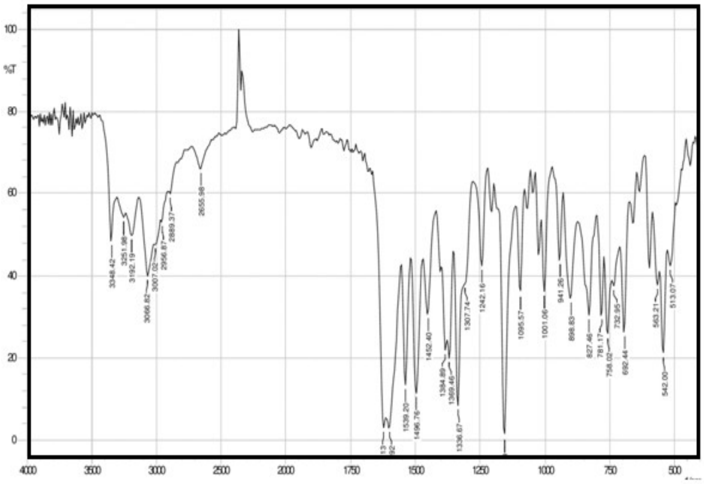


Figure 4: IR spectra of ligand A1

General Procedure for Co(II) complexes

A general method was adopted for the preparation and isolation of the complex. A hot methanolic solution of $CoCl_2 \cdot 6H_2O$ (10 mmol) and a solution of the respective Schiff base (10 mmol) were mixed in a 1:1 molar ratio. The pH was maintained between 8-9 by adding an aqueous solution of NaOH. The mixture was heated for 4 hours at 70°C and then left overnight at room temperature. The obtained colored crystals were washed with water, methanol, and finally with diethyl ether, and dried in air. The synthesized complex was characterized by IR, UV, and elemental analysis **(Figure 5 and Figure 6)**. The proposed structure of complex **CoA1** is represented in **Figure 2**.

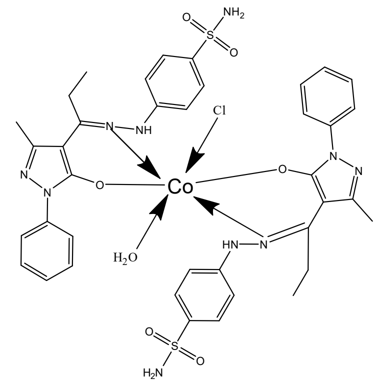


Figure 2: Proposed structure of CoA1 complex

Physical and Spectral Data of complexe (CoA1)

CoA1: Yield:79%; Orange; Elemental analysis (Cal.) C, 50.19%; H, 4.66%; N, 15.40%; Co, 6.48%; Found C, 50.22%; H, 4.69%; N, 15.88%; Co, 6.77%.

Table 1: FT-IR data of ligands And Metal Complexes (KBr, cm-1)							
Sr. No.	**Ligand/complex**	**v(O-H)**	**v(N-H)**	**v(C=O)**	**v(C=N)**	**v (M-O)**	**v (M-N)**
1	**A1**	**3348**	**3251**	**1600**	**1539**	**-**	
3	**CoA1**	**3253**	**3199**	**1566**	**1498**	**547**	**513**

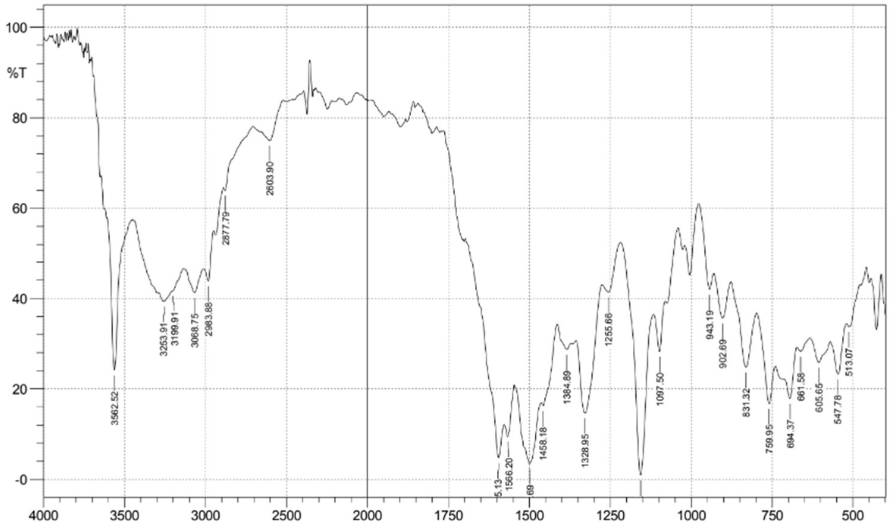


Figure 5: IR spectra of Complex CoA1

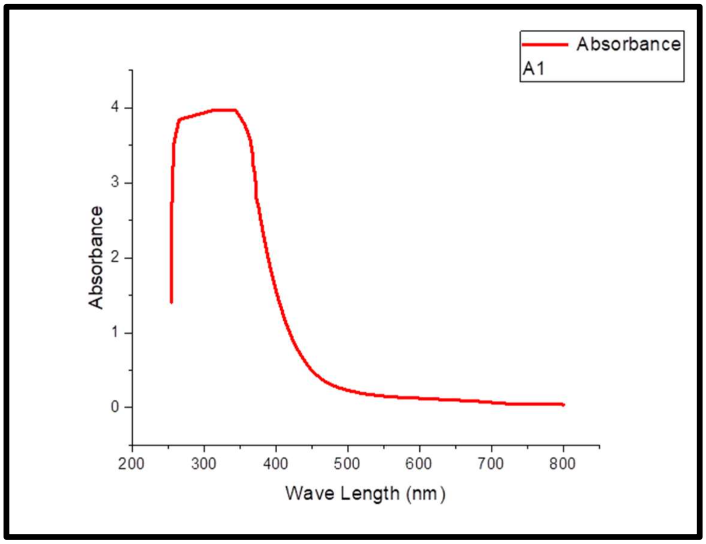


Figure 6: UV spectra of Complex CoA1

RESULTS AND DISCUSSION

The structural investigation of the prepared pyrazolone based ligand was carried out using elemental analysis, IR spectroscopy and ^{1}H NMR and its complex was investigated through IR, UV and elemental analysis as described in the experimental section.

Infrared Spectra

By carefully comparing the IR spectra of the ligand and its corresponding complex, a broad peak at 3348 cm^{-1} is observed, corresponding to the υ(O-H) stretching of the pyrazolone moiety. This peak exhibits a low-energy shift in the Co metal complex, indicating the involvement of oxygen in the metal complex formation through deprotonation. Additionally, the Schiff base ligand **(A1)** shows a sharp and intense band at 1539 cm^{-1}, corresponding to the υ(C=N) stretch of the acyclic azomethine group. In the metal complex, this band shifts to a lower frequency, suggesting that the azomethine nitrogen atom participates in complex formation.

Furthermore, when comparing the υ(C=O) stretching frequencies in the ligand and its metal complex, a significant negative shift is observed in the complex, which indicates coordination through the oxygen atom of the ligand. New bands appearing at 547 cm^{-1} and 513 cm^{-1} in the complexes are attributed to the ν(M–O) and ν(M–N) vibrations, respectively. These observations confirm that the formation of the complex occurs through the interaction between the ligands and the metal ion.

Electronic spectra

The geometry of the **Co(II) complex** can be inferred from its electronic spectral data. The electronic spectrum of the free ligand **(A1)** exhibits an intense band at 38,167cm^{-1}, which is likely due to intra-ligand charge transfer (ILCT). In contrast, the **Co(II)**

complex displays a band at 25,839 cm⁻¹, which can be attributed to a d-d transition. Given that the complex is six-coordinated, it is likely to adopt either an octahedral or distorted octahedral geometry.

Anti-bacterial Activity

The antibacterial activity of the ligand **(A1)** and its corresponding complex **(CoA1)** was thoroughly evaluated, revealing that both compounds exhibit significant bactericidal effects against Gram-positive and Gram-negative microorganisms. Notably, the **CoA1** complex demonstrated superior antibacterial activity compared to its parent ligand, **A1**. This enhanced efficacy is attributed to the overtone concept and chelation theory, which explain the increased ability of the complex to interact with and disrupt bacterial cell structures.

According to the overtone concept, the complex's ability to penetrate bacterial cell walls is improved due to reduced polarity and increased lipophilicity, allowing it to more effectively traverse lipid membranes. Chelation theory further supports this by suggesting that the complex's rigid structure enhances its binding affinity to bacterial enzymes or proteins, leading to more effective inhibition of bacterial growth. Together, these factors account for the superior antibacterial properties of the **CoA1** complex, making it a promising candidate for developing new antibacterial agents **[18]**.

Table 2: Antibacterial activity of ligand and Co(II) complex, Zone of inhibition(mm)

Sr. No.	Compound	Gram-Positive	Gram-Negative
		Bacillus Megaterium	*E. Coli*
Ref. Drug	Penicillin	35	28
1	A1	06	07
2	CoA1	21	13

CONCLUSION

The research successfully synthesized and characterized a Co(II) transition metal complex using a pyrazolone-based ligand. Comprehensive spectroscopic techniques, including ^{1}H NMR, Mass, IR, UV, and elemental analysis, were employed to characterize the ligand, while the Co(II) complex was analyzed using IR, UV, and elemental analysis. The findings confirm that the synthesized Co(II) complex exhibits significant antibacterial activity against both Gram-positive (Bacillus megaterium) and Gram-negative (E. coli) bacteria. These results highlight the potential of the Co(II) complex as a promising candidate for the development of new antibacterial agents.

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