

Journal of Applicable Chemistry

2015, 4 (5): 1477-1485 (International Peer Reviewed Journal)



Synthesis of some transitional metal ion complexes derived from $2-{(E)-[(6-amino-2-phenylpyrimidin-4-yl) imino] methyl}-5-chlorophenol$

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Accepted on 7th August 2015

ABSTRACT

Novel complexes of 2-{(E)-[(6-amino-2-phenylpyrimidin-4-yl) imino]methyl}-5-chlorophenol with Mn(II), Co(II), Ni(II), Cu(II), Zn(II) and Pd(II) were prepared. On the basis of some analytical and physicochemical techniques they are characterized by elemental analysis, molar conductivity, UV-Vis, IR, magnetic susceptibility, TGA, Mass and X-Ray Powder diffraction spectra. Electronic and magnetic susceptibility measurements of the complexes were octahedral geometry for Pd (II) and Ni (II) and square planar geometry for all the other complexes. The ESR spectral data provide information about their structures on the basis of Hamiltonian parameters and the degree of covalence parameters. These metal complexes were also screened for its anti-bacterial activities for its inhibiting potential.

Keywords: Schiff base, Spectral studies, Magnetic moments, Microbial studies.

INTRODUCTION

Schiff base compounds were prepared from the condensation of aldehyde with amines and their complexes [1, 2] played a significant role in the improvement of co-ordination / inorganic chemistry. As broadly studied co-ordination compounds are increasingly vital as biochemical, analytical and Anti-microbial reagents [3, 4]. Such type of Schiff base compounds were used for anti-bacterial, anti-fungal, anti-cancer, anti-tubercular and hypothermic reagents [5, 6]. Such compounds are great potential and have recently been demonstrated in the synthesis of conjugated linear polymers [7], in the thermo-stable optical material industry [8]. Azomethine is one example of a Schiff based compound. According to the previous research [9-10], azomethine has shown some applications in therapeutic applications to exert anti-tumor activity. A novel Schiff base formed by the condensation of 4- chloro-2-hydroxy benzaldehyde and 2-phenyl pyrimidine-4, 6 - diamine has been carried out. These studies shown that, the compound exists in two major forms and the Schiff base exhibits positive absorption have investigated Ni(II) and Cu(II) metal complexes. Their work antibacterial activity was investigated and square planar geometry was proposed for Mn (II) and Cu(II) complexes. Azo- compounds are very important molecules and have attracted much attention in both academic and applied research [11-13]. Our interest in this molecule stems from its ability to act as a diamine and also from the fact that the electron-withdrawing CN groups affect the coordinating capacity itself and have the potential to modulate the electronic properties of resulting coordination complexes and also their chemical reactivity. Hence the present work deals with the synthesis and characterization of the Schiff base ligand and its Mn(II), Co(II), Ni(II), Cu(II), Zn(II), Pd(II) complexes and biological activity, electrochemical behavior of complexes are also examined.

MATERIALS AND METHODS

All reagents used were of AR grade and all the solutions were prepared in doubly distilled water. Mass spectra recorded at IPCA Laboratory, infrared spectra recorded Perkin -Elmer paragon-500 Spectrophotometer using KBr Pallets. Electronic spectra recorded on Cintra-5 GBC UV-Visible Spectrophotometer. Magnetic Susceptibility measurement were carried out using [HgCO (CNS)₄] as a calibrate, X-ray powder diffraction was recorded on Joel-8030 double Goniometer X-ray powder Diffractometer . The densities of the complexes were calculated using specific density bottle in toluene solvent. TGA, DTA were recorded on Mettler Toledo star^e system, in the range 25⁰ to 1000 °C in atmospheric Nitrogen. The conductivity measurements were made on an Elico conductivity bridge. Elemental analysis, electron spin resonances were carried out at IIT Mumbai.

Synthesis of Schiff base: In a round bottom flask 1.50 g of 4- chloro-2-hydroxy benzaldehyde was taken and 1.87 g of 2-phenylpyrimidine-4, 6-diamine was dissolved in 100 cm³ of alcohol. Then this resulting mixture was refluxed for about ≈ 4 h at 70-80° C using few drops of acetic acid. The reaction mixture was cooled to room temperature and it was then poured in to cold water, then precipitate separates out. The precipitate was filtered through Whatman's paper 41 and washed with distilled water. The residue is dried at 60 °C for 12 h in hot air oven. The percentage yield of the product obtained is 85%.



Physical Properties of Schiff base:

Appearance: brown colour powder Molecular weight: 325.76 Molecular Formula: $C_{17}H_{14}ClN_4O$ Melting point: 165-167 °C

Elemental Analysis:

| | C% | H% | N% |
|----------------------|---------------|------------|-------------|
| $C_{17}H_{14}ClN_4O$ | 62.68(62.32)* | 4.33(3.08) | 17.2(16.87) |

Synthesis of metal ion complexes: All the Metal Chlorides/ Nitrates (MnCl₂/NO₃, CoCl₂, NiCl₂/NO₃, CuCl₂/NO₃ and ZnCl₂/NO₃) solutions were prepared in double distilled water. The 0.1M concentration of stock solutions is prepared for synthesis of schiff base complexes. The solution of Schiff base (0.1M) was

prepared in alcohol and metal chloride (M= Mn (II), Co(II),Ni(II),Cu(II) and Zn(II) solution was prepared in double distilled water. The equimolar solutions of Schiff base (L-1) 0.1M and of metal chloride solution (0.1M) were refluxed for 3-4 h with constant magnetic stirring on hot plate. After complete refluxing, 2-3 drops of alcoholic ammonia were added drop wise till precipitate was obtained. This precipitate was cooled, filtered and washed with distilled water followed by alcohol. The residue is dried at 70 °C in dry oven for 12 h. The yield of the resulting complex was 54-65 %.

RESULTS AND DISCUSSION

The physical and analytical data of Schiff base and its newly prepared metal ions complexes are given in table 1. All these complexes are colored except Zn (II) complex and stable at room temperature. The complexes are mostly insoluble in organic solvents , but they are soluble in dimethyl sulfoxide and dimethyl formamide. They are decomposed in the range 205-242 °C. The melting point and decomposition point reported in open capillary and which is uncorrected. The molar conductivity values are in agreement with electrolytic nature of the complexes. The conductivity values of the complexes are observed in dimethyl sulfoxide in 10^{-3} molar solution [14]. It is non -electrolytic in nature.

| Schiff base / complexes | % yield | MP/DP ⁰ C | C% | N% | M% | Ω^{-1} ol ⁻¹ cm ² | BM.µeff |
|---|---------|----------------------|--------|--------|--------|--|---------|
| $(C_{17}H_{14}ClN_4O)$ | 85 | 165-167 | 62.68 | 17.20 | - | 19.0 | - |
| | | | 62.32* | 16.87* | - | | |
| [Mn(C ₁₇ H ₁₃ ClN ₄ O) ₂ .2H ₂ O] | 64.7 | 205-207 | 57.15 | 15.63 | 07.69 | 22.0 | 5.29 |
| | | | 56.84 | 15.37 | 07.17* | | |
| [Co(C ₁₇ H ₁₃ ClN ₄ O) ₂ .2H ₂ O] | 62.5 | 211-213 | 56.83 | 15.59 | 08.02 | 17.8 | 4.32 |
| | | | 56.44 | 15.11 | 07.76 | | |
| [Ni(C ₁₇ H ₁₃ ClN ₄ O) ₂ .2H ₂ O] | 58.9 | 217-219 | 54.85 | 15.61 | 08.17 | 15.8 | 3.19 |
| | | | 56.48 | 15.32 | 07.84 | | |
| [Cu(C ₁₇ H ₁₃ ClN ₄ O) ₂ .2H ₂ O] | 57.3 | 225-227 | 56.74 | 15.50 | 08.79 | 19.1 | 1.77 |
| | | | 56.26 | 14.96 | 08.44 | | |
| [Zn(C ₁₇ H ₁₃ ClN ₄ O) ₂ .2H ₂ O] | 55.2 | 237-239 | 56.32 | 15.46 | 09.02 | 14.2 | Dimag |
| | | | 55.94 | 14.08 | 08.81 | | |
| [Pd (C ₁₇ H ₁₃ ClN ₄ O) ₂ .2H ₂ O] | 54.1 | 238-241 | 53.31 | 14.63 | 13.89 | 18.4 | - |
| | | | 52.98 | 14.30 | 13.66 | | |

 Table 1: Analytical and Physical data (* Experimental Values)

Infrared spectra of Schiff base and complexes: This is an invaluable technique in organic molecule structure determination and verification involves the class of electromagnetic radiation with band frequencies in between 4000 and 350 cm⁻¹ (wave length). The categories of electromagnetic radiation are termed infrared radiation and their application to organic chemistry is called as Infrared spectroscopy. The important IR frequencies of the ligands and Complexes, along with their assignments are reported in table 2 and figures 1 and 2. The following observations were made from the comparison of the IR spectra of the ligands and their metal chelates. (a) The IR spectra of the ligands are almost identical to those of the metal chelates in the region 390-580 cm⁻¹.(b) The ligand shows the absence of bands at about 1635 cm⁻¹, 3250 cm⁻¹ and 3420 cm⁻¹ due to the characteristic azomethine v(>C=N-), amino $v(NH_2)$ and hydroxyl group(-OH) stretching vibrations of the respective starting materials [19-20 35-36]. Instead, the appearance of new bands in the spectra of the chelates at 1635 cm⁻¹ due to the azomethine linkage v(>C=N) clearly suggested (Yong-xiang et al., 1989; Nakamoto, 1970) the formation of the proposed Schiff-base ligands [15-16] The shifting of this azomethine band to the higher frequency side (10-25 cm⁻¹) furthermore provided evidence in support of the involvement of azomethine nitrogen in coordination to the metal atom. (c) Some characteristic bands due to amino group at lower frequency side (35-55 cm⁻¹) in the spectra of their metal chelates, which suggested that coordination of the ligands, took place through the nitrogen of the amino group of nitrogen atoms to the metal atom at 3185-3210 cm⁻¹. (d) A broad band at 3420 cm⁻¹ was observed in the spectra of all the ligands due to v(OH) stretching vibrations. This band disappeared in the spectra of all the chelates; instead a new band appeared at 1270 -1290 cm⁻¹ due to the v(C-O) frequency, which strongly supports the observation that during chelation, deprotonation of the hydroxyl group occurred.(e) Moreover, in the far infrared region the bands at 370-415 cm⁻¹ and 545-580 cm⁻¹ attributed to v(M-O) and v(M-N) were observed for all the complexes[17-18]. However, that the amino group of nitrogen, (Agarwal, 1988) azomethine nitrogen and deprotonated oxygen of the phenol moiety are all involved in the chelation process. The two new bands occur at higher region 3450-3470 and 3510-3530 for two coordinate water molecule in co-ordination sphere.

| | | 1 | 1 | | | | |
|-----------|-------|------------|------|-----------|------|--------|-----------|
| Complexes | vOH | νNH_2 | vC-O | $\nu C=N$ | vM-N | vM-O | $2H_2O$ |
| comprenes | , 011 | | | | | 1111 0 | 21120 |
| | | | | | | | |
| Ligand | 3420 | 3250 | - | 1635 | | | 3452,3518 |
| 8 | | | | | _ | _ | ,, |
| Mn(II) | - | 3192 | 1278 | 1612 | 570 | 425 | 3450,3527 |
| | | | | | | | |
| Co(II) | - | 3185 | 1270 | 1620 | 575 | 414 | 3455,3530 |
| Ni(II) | - | 3204 | 1290 | 1617 | 562 | 422 | 3470 3522 |
| i u(ii) | | 5201 | 1220 | 1017 | 502 | 122 | 3110,3322 |
| Cu(II) | - | 3210 | 1282 | 1615 | 580 | 427 | 3462,3510 |
| Zn(II) | _ | 3198 | 1274 | 1618 | 545 | 438 | 3454 3525 |

Table 2: Infrared spectra of Schiff base L-1 and complexes (cm⁻¹)





Figure 1: Infrared spectra of (C₁₇H₁₄ClN₄O) Schiff base Figure 2: IR spectra of [Mn (L)₂.2H₂O] complex

Electronic Spectra of Complexes: The electronic spectra were very useful for the calculations, spectral parameters and other methods of structural investigation. The electronic spectral measurements were used for assigning various parameters like bonding, covalency, many more of metal complexes based on its positions and number of d-d transition peaks. The electronic absorption spectra of metal ion complexes were recorded in 10⁻⁴ molar concentration of each complex in DMF in the range 300–900 nm at room temperature (Table 3). The electronic absorption spectra of manganese (II), cobalt (II) in 10⁻⁴ M solutions, the spectra were noisy in both the visible and the UV regions. The spectrum of [Mn (C₁₇H₁₃ClN₄O)₂.2H₂O] complex exhibits three bands at 24,390 cm⁻¹ (410 nm), 19305 cm⁻¹ (518 nm) and 12092 cm⁻¹ (832 nm) cm⁻¹ which may be assigned to ${}^{4}T_{1g} \rightarrow {}^{6}A_{1g}$, ${}^{4}T_{2g}(G) \rightarrow {}^{6}A_{1g}$ and ${}^{4}T_{1g}(D) \rightarrow {}^{6}A_{1g}$ transitions respectively, which suggests an octahedral geometry[19-20]. The electronic spectrum of [Co (C₁₇H₁₃ClN₄O)₂.2H₂O] complex generally showed three absorption bands in the region at 22,124 cm⁻¹ (452nm), 13348 cm⁻¹ (748nm) and 11862 cm⁻¹ (842nm), which assigned to ${}^{4}T_{1g} \rightarrow {}^{4}T_{2g}(F)$, ${}^{4}T^{1g} \rightarrow {}^{4}A_{2g}(F)$ and ${}^{4}T_{1g} \rightarrow {}^{4}T_{g}(P)$ transitions, showing an octahedral geometry[21] around the Co(II) ion.

| Complexes Bands maximum cm ⁻¹ | | β | 1-β | η | b ^{1/2} | δ% |
|---|---------------------------|--------|--------|--------|------------------|------|
| [Mn (C ₁₇ H ₁₃ ClN ₄ O) ₂ .2H ₂ O] | 12092, 19305, 24390 | 0.9648 | 0.0352 | 0.0181 | 0.0938 | 1.84 |
| [Co (C ₁₇ H ₁₃ ClN ₄ O) ₂ .2H ₂ O] | 11862, 13348, 22124 | 0.9702 | 0.0298 | 0.0151 | 0.0863 | 1.58 |

Table 3: Electronic Spectral Parameters complexes

Electron spin resonance spectra of complex: The ESR spectra of the complexes are recorded at room temperature. The parameters are listed in table 4. At room temperature, the spectra of Cu^{2+} complex exhibit a 4 line hyperfine splitting signals which rare due to the interaction between the single d-electron of the copper and the copper-63 nuclear spin. At liquid nitrogen temperature, the ESR spectrum of Cu^{2+} complex shows the hyperfine splitting lines for the copper nucleus with the g values are given in table. The presence of the two separate resonances for Cu^{2+} nuclei suggests that the interaction between the terminal metal atoms with ligand is weak. If there is a strong interaction between the metal ions, a septet of sextets is expected for the presently studied complexes, but the spectra of the complexes show two separate resonances for the individual ions. Hence interaction between the metal ions is weak.

Electron spin resonance spectra of the [Cu (C₁₇H₁₃ClN₄O)₂.2H₂O] complex were recorded at room temperature and liquid nitrogen temperature . There are four well resolved peaks in the low field region corresponding to $g \parallel (2.254)$ and $g^{\perp} (2.0417)$. The trend $g \parallel (2.254) > g (2.0417) > ge (2.0023)$ observed for the copper complex suggests that the unpaired electron is localized in the dx^2-y^2 orbital of the copper ion[22-23]. The fact that the unpaired electron lies predominately in the dx^2-y^2 orbital is also supported by the value of the exchange interaction term *G* estimated from expression: $G = (g \parallel -2.0023) / (g^{\perp} -2.0023)$ If G > 4.0, the local axis are aligned parallel or only slightly misaligned. If G < 4.0, significant exchange coupling is present and the misalignment is appreciable. The observed value for the exchange interaction parameter for the Cu(II) complex (G = 6.50) suggests that the local tetragonal axes are aligned parallel or slightly misaligned and that the unpaired electron is present in the dx^2-y^2 orbital. The spin orbit coupling constant, λ (value: -15745 cm^{-1}), calculated using the relation, $g_{av} = 1/3(g \parallel + 2 g^{\perp})$ and $g_{av} = 2(1 - 2\lambda/10Dq)$, is less than that for the free Cu(II) ion, -11989 cm^{-1} , which also supports the covalent character of M–L band in the complex had some covalent character in the ligand environment [24-26]. The observed $g \parallel$ value for the copper complex was less than 2.3, suggesting a covalent character of the M–L bond, which is in agreement with the observation of Kivelson and Neiman.

Table 4: Electron spin Resonance spectral parameters

| Complexes | ge | g | g | g _{av} | g ^H | g _{iso} | | | |
|---|--------|-------|--------|-----------------|----------------|------------------|--|--|--|
| [Cu (C ₁₇ H ₁₃ ClN ₄ O) ₂ .2H ₂ O] | 2.0023 | 2.254 | 2.0417 | 2.112 | 6.50 | 2.105 | | | |

Mass Spectra of Schiff base and complexes: The mass spectra recommended that, all the complexes were in a monomeric environment. These complexes show molecular ion peaks in excellent contact with the empirical formula suggested by elemental analysis. The mass spectra of prepared Schiff base (C₁₇H₁₄ClN₄O) and their complexes such as [Ni (C₁₇H₁₃ClN₄ O) $_2.2H_2O$] were recorded at room temperature, and they were used to compare their stoichiometric composition. The ESI mass spectra of the metal complexes recorded at room temperature are used to compare their composition and are listed in figures 3 and 4. The Schiff base (C₁₇H₁₄ClN₄ O) shows a molecular ion peak at m/z 325.8, which corresponds to peak as the calculated m/z being 325.76. The mass spectra of [Ni (C₁₇H₁₃ClN₄ O) $_2$] complex shows a molecular ion peak at m/z = 719.1. The spectra of the Schiff base and complexes shows characteristic molecular ion peaks at their m/z values confirming their monomeric forms. Here the molecular weight of metal complex is shown without water molecule, which is corrected [27].



Figure 4: Mass spectra of (C₁₇H₁₄ClN₄O) Schiff base



Thermal analysis of Schiff base Complex: The complexes were losses its molecular weight due to exothermic and endothermic reactions. This complex is thermally stable at Room temperature and decomposes in three stages. The decomposition occurred in three stages; represented generally as follows. The thermo gravimetrical analysis curves indicate that the loss of weight starts from 50-290 °C for the zinc complexes and at much higher temperature for the zinc complex. The decomposition continues to about 300-360 °C at which point most of the organic part of the complex has been lost. The zinc complex shows three decomposition peaks in the thermo gram. The first decomposition peak, which has the highest weight loss, corresponds to the loss of co-ordinated water molecule and some organic part of the complex. In accordance with stoichiometric calculation, the product of the second decomposition step for the most organic part of the complex which lost in the temperature range 300-360 °C. The differential thermal analysis peak is due to the endothermic loss percentage. In the final stage entire organic part of the complex were lost and formation of stable metal oxide in the range 370-1000°C. The detailed scheme-I of the complex decomposition is given as below:

Scheme-I. For
$$[Zn (C_{17}H_{13}ClN_4O)_2.2H_2O]$$
 Complex

$$\begin{bmatrix} Zn(C_{34}H_{26}Cl_2N_4O_2)_2.2H_2O] & \xrightarrow{50-290 \circ C} & [Zn(C_{30}H_{20}Cl_2N_4O_2)] & \xrightarrow{300-370 \circ C} \\ & -2H_2O, C_4H_6 & [Zn(C_{30}H_{20}Cl_2N_4O_2)] & \xrightarrow{-C_{10}H_{12}N_2Cl} \\ & [Zn(C_{20}H_8ClN_2O_2)] & \xrightarrow{380-1000 \circ C} & ZnO & \\ \end{bmatrix}$$

X-ray Powder diffraction complex: The X-ray diffractogram of the [Pd ($C_{17}H_{13}ClN_4O$)₂.2H₂O] complex were recorded and scanned in the range 5–40° at a wavelength of 1.543 A°. The diffractogram associated data depict the 2θ value for each peak, the relative intensity and interplanar spacing (*d*-values). The X-ray diffraction patterns of these complexes with respect to major peaks of relative intensity greater than 10 % were indexed using a powdin and powdout computer programme [28]. This indexing method also yields the Miller indices (*hkl*), the unit cell parameters and the unit cell volume and density of complexes were calculated and listed in figure 6 and table 5.

Calculated parameters of [Pd (C₁₇H₁₃ClN₄O)₂.2H₂O] complex:

| System: Monoclinic-P | Lambda= 1.5418 Ű | | |
|----------------------|------------------|-------------------|----------------------------|
| A= 21.71 A° | B= 21.19 A° | C= 99.46 A° | |
| a=16.8195 A° | b= 16.7325 A° | c=07.8585 A° | |
| E= 17.15 | beta=100.63D | $V = 2131.61 A^3$ | D=1.212 g cm ⁻³ |
| | | | |

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Figure 6: X-ray Powder diffraction of [Mn(C₁₇H₁₃ClN₄O)₂.2H₂O] complex

| | d spa | ace A ^o |] | Indice | s | Sir | nθ | 2θ Deg | | I/Io | |
|----|--------|--------------------|---|--------|---|-------|-------|--------|-------|-------|-----|
| No | Obs. | Cal. | h | k | 1 | Obs. | Cal. | Obs. | Cal. | Diff. | |
| 1 | 8.3861 | 8.3663 | 0 | 2 | 0 | 84.4 | 84.8 | 10.54 | 10.57 | -0.03 | 40 |
| 2 | 8.3075 | 8.2653 | 2 | 0 | 0 | 86 | 86.8 | 10.64 | 10.69 | -0.05 | 55 |
| 3 | 7.7148 | 7.7234 | 0 | 0 | 1 | 99.7 | 99.5 | 11.46 | 11.45 | 0.013 | 52 |
| 4 | 7.5443 | 7.5522 | 1 | 0 | 1 | 104.2 | 104 | 11.72 | 11.71 | 0.012 | 32 |
| 5 | 7.3689 | 7.4105 | 2 | 1 | 0 | 109.3 | 108 | 12 | 11.93 | 0.068 | 45 |
| 6 | 7.0527 | 7.0124 | 0 | 1 | 1 | 119.3 | 120.7 | 12.54 | 12.61 | -0.07 | 100 |
| 7 | 6.7051 | 6.5491 | 1 | 0 | 1 | 132 | 138.3 | 13.19 | 13.51 | -0.32 | 47 |
| 8 | 6.3656 | 6.2476 | 2 | 0 | 1 | 146.4 | 152 | 13.9 | 14.16 | -0.26 | 51 |
| 9 | 6.1287 | 6.0986 | 1 | 1 | 1 | 158 | 159.5 | 14.44 | 14.51 | -0.07 | 45 |
| 10 | 5.87 | 5.8798 | 2 | 2 | 0 | 172.2 | 171.6 | 15.08 | 15.05 | 0.025 | 76 |
| 11 | 5.4801 | 5.5102 | 3 | 0 | 0 | 197.6 | 195.4 | 16.16 | 16.07 | 0.089 | 65 |
| 12 | 5.1451 | 5.157 | 1 | 2 | 1 | 224.1 | 223.1 | 17.22 | 17.18 | 0.04 | 59 |
| 13 | 5.0462 | 5.0058 | 2 | 2 | 1 | 233 | 236.8 | 17.56 | 17.7 | -0.14 | 54 |
| 14 | 4.5276 | 4.5217 | 0 | 3 | 1 | 289.4 | 290.2 | 19.59 | 19.62 | -0.03 | 35 |
| 15 | 4.3858 | 4.4077 | 2 | 2 | 1 | 308.4 | 305.4 | 20.23 | 20.13 | 0.102 | 75 |
| 16 | 4.2427 | 4.2463 | 1 | 3 | 1 | 329.6 | 329 | 20.92 | 20.9 | 0.018 | 55 |
| 17 | 4.055 | 4.0553 | 1 | 4 | 0 | 360.8 | 360.8 | 21.9 | 21.9 | 0.002 | 59 |
| 18 | 3.9638 | 3.9605 | 4 | 0 | 1 | 377.6 | 378.2 | 22.41 | 22.43 | -0.02 | 23 |
| 19 | 3.6971 | 3.6968 | 3 | 3 | 1 | 434 | 434.1 | 24.05 | 24.05 | 0 | 34 |
| 20 | 3.5588 | 3.5529 | 1 | 2 | 2 | 468.5 | 470 | 25 | 25.04 | -0.04 | 35 |
| 21 | 3.4035 | 3.4057 | 3 | 1 | 2 | 568.6 | 511.5 | 26.16 | 26.14 | 0.017 | 54 |
| 22 | 3.3556 | 3.3465 | 0 | 5 | 0 | 588.5 | 529.8 | 26.54 | 26.61 | -0.07 | 59 |
| 23 | 3.2852 | 3.28 | 1 | 5 | 0 | 549.7 | 551.5 | 27.12 | 27.16 | -0.04 | 69 |
| 24 | 3.2303 | 3.2292 | 4 | 3 | 1 | 568.6 | 569 | 27.59 | 27.6 | -0.01 | 46 |
| 25 | 3.175 | 3.175 | 0 | 3 | 2 | 588.5 | 588.6 | 28.08 | 28.08 | 0 | 25 |
| 26 | 3.0681 | 3.0706 | 0 | 5 | 1 | 630.3 | 629.2 | 29.08 | 29.05 | 0.025 | 67 |
| 27 | 2.9597 | 2.9515 | 3 | 3 | 2 | 677.3 | 681 | 30.17 | 30.26 | -0.09 | 43 |
| 28 | 2.8932 | 2.8985 | 4 | 3 | 1 | 708.8 | 706.2 | 30.88 | 30.82 | 0.058 | 40 |
| 29 | 2.8589 | 2.8603 | 3 | 5 | 0 | 725.9 | 725.2 | 31.26 | 31.24 | 0.016 | 62 |
| 30 | 2.7979 | 2.803 | 2 | 4 | 2 | 757.9 | 755.1 | 31.96 | 31.9 | 0.06 | 51 |
| 31 | 2.7249 | 2.724 | 6 | 1 | 1 | 799.1 | 799.4 | 32.84 | 32.85 | -0.01 | 39 |
| 32 | 2.5866 | 2.5864 | 3 | 3 | 2 | 886.8 | 886.9 | 34.65 | 34.65 | 0 | 25 |
| 33 | 2.5293 | 2.529 | 0 | 5 | 2 | 927.4 | 927.6 | 35.46 | 35.46 | 0 | 24 |
| 34 | 2.3534 | 2.3519 | 5 | 5 | 0 | 1071 | 1073 | 38.21 | 38.23 | -0.02 | 34 |

Table 5: X-ray Powder diffraction of $[Mn(C_{17}H_{13}ClN_4O)_2.2H_2O]$ complex

APPLICATIONS

Anti-bacterial activity of Schiff base and complexes: Schiff base and their complexes have been screened in -vitro against the following bacterial species by well diffusion method using agar as nutrient medium. Here streptomycin has been used as a standard [29-30]. The microbial activity of the Schiff base compound and its complexes are listed in table 6. The Schiff base compound of $2-\{(E)-[(6-amino-2-phenylpyrimidin-4-yl)imino]methyl\}$ -5-chlorophenol (C₁₇H₁₄ClN₄O), have shown activity against all both micro-organisms while its [Co(C₁₇H₁₃ClN₄O)₂.2H₂O] and [Ni(C₁₇H₁₃ClN₄O)₂.2H₂O] complexes show more moderate but enhanced activity. However, the [Cu (C₁₇H₁₃ClN₄O)₂.2H₂O] complex is more active against both the bacterial strains.

| No | Complexes/compound | Gram nega | tive Bacteria | Gram Posit | ive bacteria |
|----|------------------------------------|------------------|---------------|------------|--------------|
| | | E. Coli S. typhi | | S. aureus | B. subtilis |
| 1 | $(C_{17}H_{14}ClN_4O)$ | 12 | 13 | 11 | 10 |
| 2 | $[Co(C_{17}H_{13}ClN_4O)_2.2H_2O]$ | 16 | 22 | 15 | 14 |
| 3 | $[Ni(C_{17}H_{13}ClN_4O)_2.2H_2O]$ | 19 | 17 | 15 | 21 |
| 4 | $[Cu(C_{17}H_{13}ClN_4O)_2.2H_2O]$ | 20 | 25 | 17 | 27 |

Table 6: Anti-bacterial activity of Schiff base and complexes

CONCLUSIONS

Schiff base of $2-\{(E)-[(6-amino-2-phenylpyrimidin-4-yl) imino]methyl\}-5-chlorophenol was synthesized and characterized by some analytical techniques mentioned above. Novel transition metal complexes with Mn(II), Co(II), Ni(II), Cu(II), Zn(II) and Pd(II) was prepared. Characterized and their microbial activities was screened. It can be concluded that Metal complexes of transition metals of the ligand have better activity against above bacteria. The results of the screening of the Schiff base and transition metal complexes for antimicrobial activity indicate that the antimicrobial activity of the Schiff base was enhanced on complex formation with metal in all cases studied. From the Electronic spectra concluded that complexes have covalent in nature and x-ray diffraction studies indicates that complex are Monoclinic with Density of =1.212 g cm⁻³.$

ACKNOWLEDGMENTS

Authors thanks to the Director, Regional Sophisticated Instrumentation Centre, IIT-Mumbai, C-MET Pune, Principal and Head of Department Sathaye College and finally Lalita, Mayuri and Vishant encourage me for research activities.



Structure of Schiff base Complex [M=Mn(II), Co(II), Ni(II), Cu(II)₂, Zn(II), Pd(II)]

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