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Synthesis, Characterization and Antimicrobial Studies on Cu(II), Co(II), Ni(II), Zn(II), Cd(II) and Hg(II) Complexes with Biologically Active Benzothiazole Schiff Bases

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Abstract

Novel Schiff bases derived from 7-chloro-6-fluoro-2-aminobenzothiazole with substituted salicylaldehydes and its transition metal complexes of Cu(II), Co(II), Ni(II), Zn(II), Cd(II) and Hg(II) have been synthesized and characterized by elemental analysis, conductivity measurements, magnetic susceptibility, X-ray, electronic, IR, ¹HNMR, ESR spectra, Elemental analysis, TGA and DTA studies. These studies indicates the formation of 1:2 complexes of the type $ML_2(H_2O)_2$. The spectral results indicate that, the ligands coordinate through azo-methine nitrogen and phenolic oxygen to the metal ions. The study projects octahedral geometry for these complexes. X-ray powder diffraction studies of copper complexes reveal that, these form hexagonal or tetragonal structures. The antimicrobial activities of the ligands and their metal complexes have also been studied.

Key-Words: Schiff bases, Antimicrobial activity, Benzothiazoles

Introduction

Benzothiazoles and their derivatives are well known biologically active compounds. They possess CNS antiviral², depressant¹, anti-inflammatory³, antimicrobial⁴. antitubercular⁵. antiallergic⁶, anticonvulsant⁷, diuretic⁸, sedative⁹ and anticancer¹⁰ activities etc. In addition, benzothiazole forms an important pharmacophore in herbicidal 11 and insecticidal 12 agents. The azomethine of benzothiazole considerable Schiff bases exhibits biological importance¹³. The biological activity of these compounds may be connected to their ability to form complexes with certain metal ions which may lead to "locked geometry" via coordination mechanism so that, only certain substances are able to become attached to the frame work of this interaction¹⁴. Schiff base can be considered as a useful chelating agent when a suitable functional groups like -OH, -SH, -COOH etc., are present sufficiently close to azo-methine group so as to form five or six member chelate ring upon reaction with metal ion^{15,16}.

* Corresponding Author E.mail: proftsuresh@gmail.com By changing nature and position of the donor atoms and groups, it is possible to control the size of the chelate ring formed and exploit the effect of substitution. All these factors make Schiff bases good chelating agents and potential analytical reagents. As the biological activity is often augmented when the ligand forms the complexes, the resulting complex may be of potential biological importance¹⁷.



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Therefore, in this paper, we report the synthesis of highly stable six member chelate ring metal complexes of Cu(II), Co(II), Ni(II), Zn(II), Cd(II) and Hg(II) with benzothiazole Schiff bases derived from 2-amino-7chloro-6-fluorobenzothiazole (Fig.1). These complexes were characterized by elemental, spectral, thermal and magneto-chemical studies. Preliminary antibacterial and antifungal activities of the ligands and their complexes have also been screened.

Material and Methods

IR spectra of the ligands and complexes were recorded in KBr matrix using Parkin Elmar 1000 FTIR spectrometer in the range of 4000 - 250 cm⁻¹. Electronic spectra of the complex in DMSO solution were recorded using Hitachi 150-20 model spectrophotometer in the range of 200-1100 nm. Magnetic susceptibility of the metal complexes were measured at a temperature of 25°C, using Guoy method. The ESR spectra of copper (II) complexes in polycrystalline state were recorded on Varian Хband ESR spectrometer. The proton magnetic resonance spectra of the few ligands and their complexes in CDCl₃ were recorded on a Brucker NMR spectrometer using TMS as internal standard. The X – ray data were recorded on Philips Pw 1050/70 X - ray machine attached with diffractogram using Cu Ka radiation ($\lambda = 1.54178$ A°), Nickel filter at voltage of 30 KV and current strength of 15 mA.

Experimental

Substituted salicylaldehydes and 2-amino-7-chloro-6-fluorobenzothiazole were prepared as reported earlier^{18,19}.

Preparation of 2-Amino-7-Chloro-6-Fluoro benzothiazole Schiff Bases

2-Amino-7-chloro-6-fluorobenzothiazole and 5substituted salicylaldehyde in 1:1 molar ratio in ethanolic medium were refluxed for about 5-6 hours in presence of catalytic amount of sulphuric acid. The reaction mixture was concentrated and cooled. The product separated is filtered and recrystallized from ethanol.

Synthesis of Metal Complexes

An ethanolic solution of the ligand (0.02 mol) and metal (II) chloride (0.01 mol) was refluxed on water bath for about three hours. About 1.0g of sodium acetate was added and the refluxation was continued for another hour. The reaction mixture was cooled and added to crushed ice. The complex was filtered, dried and purified by Soxhelet extraction with alcohol.

Results and Discussion

The analytical data and the conductance values are presented in Table-1. Elemental analysis confirms

formation of complexes of 1:2 stoichiometry with the empirical formula $ML_2(H_2O)_2$.

The molar conductance values of all the complexes were measured in DMF at 10^{-3} M concentration. The values are too low to account for their electrolytic behavior. Hence, these complexes were regarded as non-electrolytes.

IR spectra Important IR frequencies of ligands, complexes and their assignments are given in Table-2. In the ligands, a high intensity band was observed in the region 1594-1572 cm⁻¹ has been assigned to v(C=N) azo-methine vibrations in view of previous reports ^{20, 21}. A medium intensity band in the region 1580-1528 cm⁻¹ was observed in the complexes, this has been assigned to v(C=N) of azo-methine. The shifting of v(C=N) of azo-methine band to the lower frequency as compared to the ligands indicates the involvement of C=N in coordination with metal atom^{20, 21}.

The band appearing in the region $2800-2731 \text{ cm}^{-1}$ of the ligands disappears in the complexes indicating the deprotonation of phenolic –OH group with the formation of coordinated bond with the metal during complexation²². A band appears in the region $3527-3442 \text{ cm}^{-1}$ indicates the presence of coordinated water in these complexes²². In addition to these, the new bands observed in the region $596-534 \text{ cm}^{-1}$ and $470-440 \text{ cm}^{-1}$ have been assigned to v(M-N) and v(M-O) vibrations respectively²⁰⁻²².

¹HNMR spectra

The NMR spectrum of the ligand CFBIMP exhibit a peak at δ 12.10 due to the phenolic OH integrating for one proton and multiplet in the region of δ 7.00 to 8.00 due to six aromatic protons and one N=CH-R proton appeared at δ 9.25.

The disappearance of a singlet at δ 12.10 in the Zn(II) and Hg(II) complexes of CFBIMP can be attributed to the deprotonation of the phenoloic OH upon complex formation ²³.

Other characteristic peak due to azo-methine proton at δ 9.25 shows considerable downfield shift of δ 0.2 to 0.3 in the Zn(II) and Hg(II) complexes of CFBIMP, suggesting that coordination of azo-methine group with metal ions²³.

Magnetic measurements

The magnetic susceptibility measurements were used in combination with electronic spectral data to establish the structure of complexes. The effective magnetic moment (μ_{eff}) values observed at room temperature (300 K) for the complexes have been listed in Table-3. The observed magnetic moment values for Co(II) complexes of CFBIMP, CFBIMMP and CCFBIMP fall in the range 4.58-4.65 BM which indicates



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octahedral geometry for Co(II) complexes²⁴. These values lie in the range expected for μ_s and μ_{s+1} . This is due to the partial quenching of orbital contribution to the magnetic moment.

The magnetic moment values for Ni(II) complexes of ligands CFBIMP, CFBIMMP and CCFBIMP fall in the range 3.33-4.42 BM which are well within the range expected for octahedral geometry around the central metal ion²⁵⁻²⁶.

The observed magnetic moment values for Cu(II) complexes of ligands CFBIMP, CFBIMMP and CCFBIMP are 1.90,1.75 and 1.86 B.M respectively. These magnetic moment data are agreeable to the spin only value for Cu(II) systems and the values suggest that there is no major coupling interaction in these complexes. Hence, observed magnetic moment for the Cu(II) complexes indicates distorted octahedral²⁷ configurations.

Electronic spectra

The electronic spectra of Co(II), Ni(II) and Cu(II) complexes were recorded in DMSO solution at 10^{-3} M concentration and are given in the Table-3.

In the present investigation, the electronic spectra of Co(II) complexes of ligands exhibited bands in the region 10416.66-10438.41 cm⁻¹, 17857.14-18115.94 cm⁻¹ and 22988.50- 23640.66 cm⁻¹ due to the ${}^{4}T_{1g}(F) \rightarrow {}^{4}T_{2g}(F)(v_1), {}^{4}T_{1g}(F) \rightarrow {}^{4}A_{2g}(F)(v_2)$ and ${}^{4}T_{1g}(F) \rightarrow {}^{4}T_{1g}(P)(v_3)$ transitions respectively. These transitions suggest octahedral geometry for the Co(II) complexes. These assignments are in good agreement with the reported values ${}^{28-29}$.

The electronic spectra of Ni(II) complexes of all the ligands exhibited three bands in the region 10869.56 – 11111.11 cm⁻¹, 15151.51 – 15408.32 cm⁻¹ and 23809.52 – 24390.24 cm⁻¹ respectively. These bands are assigned ${}^{3}A_{2g}(F) \rightarrow {}^{3}T_{2g}(F)(v_1)$, ${}^{3}A_{2g}(F) \rightarrow {}^{3}T_{1g}$ (F) (v_2) and ${}^{3}A_{2g}(F) \rightarrow {}^{3}T_{1g}$ (P) (v_3) transitions respectively. All these observations favour octahedral geometry for Ni(II) complexes³⁰.

Cu(II) complexes of ligands showed broad band at 15873.01, 15974.44 and 16155.08 cm⁻¹ respectively. The observed broad band in the case of present Cu(II) complex of ligands can be assigned to envelope of ${}^{2}B_{1g} \rightarrow {}^{2}E_{g}$, and ${}^{2}B_{1g} \rightarrow {}^{2}E_{2g}$ transitions in distorted octahedral geometry³⁰.

ESR spectra

In order to obtain more information about the magnetic environment of the Cu(II) complexes, powder samples were used to record X-band ESR spectra of the complexes at room temperature using DPPH as a reference standard. Copper(II) complexes measured in polycrystalline sample at room temperature, gave values: $g_{\parallel} = 2.06$, $g_{\perp} = 2.13$ for the [Cu(CFBIMMP)₂2H₂O] and g_{||}=2.03, g \perp =2.10 for the [Cu(CFBIMP)₂2H₂O]. The trend, g_{||} < g \perp showed that the electron is delocalized in d_z² orbital of the ground state of Cu(II) and the spectra are characteristic of axial (compressed octahedral) symmetry. The parameter G, determined as G = (g_{||} -2) / (g \perp -2), is found to be much less than 4 suggesting considerable interaction in the solid state³¹.

X-ray studies

Powder XRD pattern for Cu(II) complexes of the ligands CFBIMMP and CFBIMP have been studied. The diffraction pattern for the Cu(II)CFBIMMP and Cu(II)CFBIMP complex showed 17 and 9 reflections in the range 0-40° (2 θ) arising from the diffraction of X-rays by planes of Cu(II) complexes. The interplanar spacing 'd' has been calculated from the positions of intense peaks using the Bragg's relation $n\lambda = 2d$ Sin θ . The calculated inter planar spacing together with relative intensities with respect to most intense peaks are recorded in Table-4. The 20 values with maximum intensities of the peak for the complexes were found to be 6.360, 15.620 and 27.380 (2 θ), that correspond to d = 13.8864, 5.6686 and 3.2570 A° for Cu(II) complexes respectively. All the important peaks have been indexed and the observed values of inter planar distances have been compared with the calculated ones. It was observed that there is good agreement between the calculated and observed values.

The experimental values of $\text{Sin}^2\theta$ is common factor are recorded for each peak in the Table-4. The $((h^2+k^2+l^2))$ values obtained were 1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14, 15, 16, 17, 18, 19, 20, 21, 22, etc., in all the complexes. The presence of forbidden numbers 7, 15 indicated that compounds may belong to hexagonal or tetragonal system³²

Thermal analysis

TGA and DTA studies of few selected Cu(II) complexes have been studied and the results are summarized as follows:

TGA analysis of Cu(CFBIMP)₂H₂O indicates first stage decomposition is observed in the range 141-184 °C and the weight loss corresponds to 4.9% (calculated 5.1%) which attributes decomposition of two molecules of water from the complex. The second stage decomposition occurs in the temperature range 500-600°C and the weight loss observed is 51.7% against 52.2% (calculated) due to the decomposition of L(H₂O)₂. At temperature higher than 1000 °C, the weight loss corresponds to 88.8% (calculated 88.9%) due to decomposition of ligand moiety with the formation of copper oxide.



On the basis of elemental analysis, infrared, electronic, ESR, XRD and thermal studies reveals the following structure for these complexes.



Fig (2): Metal complexes of Substituted 2-amino-7chloro-6-fluorobenzothiazole Schiff base. Where M= Cu(II), Co(II), Ni(II), Zn(II), Cd(II) and Hg(II) and R= H, CH₃, Cl

Antimicrobial activity

Antimicrobial activity was carried out by the Cup-plate method²². The ligands and their Cu(II), Co(II), Ni(II), Zn(II), Cd(II) and Hg(II) complexes have tested for their antibacterial and antifungal activities. The antibacterial and antifungal results of the ligands and its complexes were tabulated in Table-5.

All the ligands have shown moderate to good activity against the bacteria, *E. coli & S. aureus* and fungi *A.niger* and *F.oxysporum* respectively.

The Cu(II), Co(II), Zn(II) and Mn(II) complexes of all the ligands synthesized have shown moderate to good activity against the pathogenic bacteria, whereas, the Cu(II) and Ni(II) complexes have displayed moderate to good activity against the tested fungi *A.niger* and *F. oxysporum*. Especially, Zn(II), Cd(II) and Hg(II) complexes of the ligands have shown very good activity against the fungi *A.niger* and *F. oxysporum*. The Co(II), Zn(II), Cd(II) and Hg(II) complexes of the ligands showed good activity against *E. coli & S. aureus*. This enhanced activity of the complexes compared to that of ligands can be attributed to the presence of metal ions and stereo chemical configurations in the molecule.

Conclusion

Condensation of 2-amino-7-chloro-6-fluoro benzothiazole and 5-substituted salicylaldehyde have yielded a new Schiff bases having potential binding sites towards metal ions to form six member chelates. Schiff base acts as bidentate ligand by coordinating through azomethine nitrogen and phenolic oxygen. It forms octahedral complexes with Cu(II), Co(II), Ni(II), Zn(II), Cd(II) and Hg(II) ions. Thermal studies support the presence of coordinated water in these complexes.

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Table 1: Elemental Analysis, Color, Melting Point and Conductance Data for Ligands and Metal Complexes

| S.N. | Ligand / complex | Mol.Wt. | Analysis % | | | | M.P | Color | Molar | |
|------|--|---------|------------|--------|-------------|---------|--------|-------|-------------|---|
| | | | | Fou | nd (Calcula | nted) | | °C | | Conductance |
| | | | C | Н | Ν | S | М | | | Ω^{-1} Cm ² Mol ⁻² |
| 01 | C ₁₄ H ₈ N ₂ OSFCl (CFBIMP) | 306.50 | 54.38 | 2.59 | 9.16 | 10.40 | | 175 | Pale yellow | 10 |
| | | | (54.81) | (2.61) | (9.13) | (10.44) | - | | | |
| 02 | C ₁₅ H ₁₀ N ₂ OSFCl (CFBIMMP) | 320.50 | 56.08 | 3.07 | 8.80 | 9.96 | - | 204 | Yellow | 13 |
| | | | (56.16) | (3.12) | (8.73) | (9.98) | | | | |
| 03 | C ₁₄ H ₇ N ₂ OSFCl ₂ (CCFBIMP) | 341.00 | 49.27 | 1.99 | 8.23 | 9.40 | - | 165 | Yellow | 11 |
| | | | (49.20) | (2.05) | (8.21) | (9.38) | | | | |
| 04 | $[Co(CFBIMP)_2 (H_2O)_2]$ | 703.93 | 47.75 | 2.22 | 7.98 | 9.07 | 8.43 | 215 | Dark brown | 17 |
| | | | (47.73) | (2.27) | (7.95) | (9.09) | (8.37) | | | |
| 05 | $[Co(CFBIMMP)_2(H_2O)_2]$ | 731.93 | 49.13 | 2.16 | 7.69 | 8.77 | 7.97 | 222 | Dark brown | 29 |
| | | | (49.18) | (2.18) | (7.65) | (8.74) | (8.05) | | | |
| 06 | $[Co(CCFBIMP)_2 (H_2O)_2]$ | 772.93 | 43.48 | 1.80 | 7.29 | 8.30 | 7.74 | 235 | Brown | 24 |
| | | | (43.47) | (1.81) | (7.24) | (8.28) | (7.62) | | | |
| 07 | $[Ni(CFBIMP)_2 (H_2O)_2]$ | 703.69 | 47.77 | 2.32 | 7.90 | 9.06 | 8.59 | 200 | Pale green | 41 |
| | | | (47.74) | (2.27) | (7.95) | (9.09) | (8.34) | | | |
| 08 | [Ni(CFBIMMP) ₂ (H ₂ O) ₂] | 731.69 | 49.13 | 2.78 | 7.60 | 8.76 | 7.99 | 220 | Pale yellow | 26 |
| | | | (49.20) | (2.73) | (7.65) | (8.74) | (8.02) | | | |
| 09 | $[Ni(CCFBIMP)_2 (H_2O)_2]$ | 772.69 | 43.53 | 1.78 | 7.19 | 8.25 | (7.55) | >300 | Pale green | 37 |
| | | | (43.48) | (1.81) | (7.24) | (8.28) | (7.59) | | | |
| 10 | $[Cu(CFBIMP)_2 (H_2O)_2]$ | 708.54 | 47.48 | 2.20 | 8.02 | 9.05 | 9.05 | 280 | Brown | 18 |
| | | | (47.42) | (2.25) | (7.90) | (9.03) | (8.96) | | | |
| 11 | $[Cu(CFBIMMP)_2(H_2O)_2]$ | 736.54 | 48.90 | 2.76 | 7.63 | 8.65 | 8.56 | 205 | Brown | 35 |
| | | | (48.87) | (2.71) | (7.60) | (8.68) | (8.62) | | | |
| 12 | $[Cu(CCFBIMP)_2 (H_2O)_2]$ | 777.54 | 43.16 | 1.80 | 7.28 | 8.28 | 8.30 | 250 | Brown | 23 |
| | | | (43.21) | (1.80) | (7.20) | (8.23) | (8.17) | | | |
| 13 | $[Zn(CFBIMP)_2 (H_2O)_2]$ | 710.39 | 47.31 | 2.22 | 7.90 | 9.04 | 9.29 | 210 | Yellow | 37 |
| | | | (47.29) | (2.25) | (7.88) | (9.00) | (9.20) | | | |
| 14 | [Zn(CFBIMMP) ₂ (H ₂ O) ₂] | 738.39 | 48.79 | 2.73 | 7.69 | 8.61 | 9.01 | 216 | Yellow | 19 |
| | | | (48.75) | (2.70) | (7.58) | (8.66) | (8.85) | | | |
| 15 | [Zn(CCFBIMP)2 (H2O)2] | 779.39 | 43.20 | 1.80 | 7.13 | 8.24 | 8.44 | 225 | Yellow | 26 |
| | | | (43.11) | (1.79) | (7.18) | (8.21) | (8.38) | | | |
| 16 | [Cd(CFBIMP)2 (H2O)2] | 757.41 | 44.32 | 2.07 | 7.40 | 8.40 | 14.92 | 215 | Pale yellow | 15 |

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| | | | (44.36) | (2.11) | (7.39) | (8.44) | (14.84) | | | |
|----|----------------------|--------|---------|--------|--------|--------|---------|-----|-------------|----|
| 17 | [Cd(CFBIMMP)2(H2O)2] | 785.41 | 45.88 | 2.58 | 7.19 | 8.17 | 14.37 | 216 | Pale yellow | 32 |
| | | | (45.83) | (2.54) | (7.13) | (8.14) | (14.31) | | | |
| 18 | [Cd(CCFBIMP)2(H2O)2] | 826.41 | 40.59 | 1.70 | 6.80 | 7.70 | 13.79 | 252 | Pale yellow | 33 |
| | | | (40.65) | (1.69) | (6.77) | (7.74) | (13.60) | | | |
| 19 | [Hg(CFBIMP)2 (H2O)2] | 845.59 | 39.75 | 1.93 | 6.55 | 7.51 | 23.86 | 235 | White | 17 |
| | | | (39.73) | (1.89) | (6.62) | (7.56) | (23.72) | | | |
| 20 | [Hg(CFBIMMP)2(H2O)2] | 873.59 | 41.25 | 2.31 | 6.44 | 7.37 | 23.08 | 209 | Gray | 21 |
| | | | (41.20) | (2.28) | (6.41) | (7.32) | (22.96) | | | |
| 21 | [Hg(CCFBIMP)2(H2O)2] | 914.59 | 36.67 | 1.59 | 6.09 | 7.04 | 22.08 | 242 | White | 31 |
| | | | (36.73) | (1.53) | (6.12) | (6.99) | (21.93) | | | |

Table 2: Important IR Frequencies of Ligands, Complexes and Their Assignments

| S.N. | Ligand/ Complex | H-bonded -OH | v(H ₂ O) | v (C-O) | v (C=N) in thiazole | v (C=N) in azomethine | v(C-S-C) | v(M- H ₂ O) | v(M-N) | v(M-O) |
|------|--|-----------------|---------------------|---------|---------------------------|--------------------------|----------|------------------------|--------|--------|
| 01 | C ₁₄ H ₈ N ₂ OSFCl (CFBIMP) | | | | | | | | | |
| | | 2735 | - | 1287 | 1612 | 1572 | 730 | - | - | - |
| 02 | C ₁₅ H ₁₀ N ₂ OSFCl (CFBIMMP) | 2800 | - | 1290 | 1663 | 1582 | 694 | - | - | - |
| 03 | C ₁₄ H ₇ N ₂ OSFCl ₂ (CCFBIMP) | 2731 | - | 1297 | 1660 | 1594 | 723 | - | - | - |
| 04 | $[Co(CFBIMP)_2 (H_2O)_2]$ | - | 3442 | 1307 | 1664 | 1558 | 731 | 846 | 596 | 462 |
| 05 | $[Co(CFBIMMP)_2(H_2O)_2]$ | - | 3481 | 1327 | 1663 | 1558 | 692 | 837 | 558 | 442 |
| 06 | $[Co(CCFBIMP)_2(H_2O)_2]$ | - | 3470 | 1307 | 1660 | 1558 | 724 | 846 | 596 | 452 |
| 07 | $[Ni(CFBIMP)_2 (H_2O)_2]$ | - | 3477 | 1306 | 1616 | 1528 | 735 | 833 | 556 | 450 |
| 08 | [Ni(CFBIMMP) ₂ (H ₂ O) ₂] | - | 3481 | 1327 | 1664 | 1558 | 692 | 808 | 587 | 449 |
| 09 | [Ni(CCFBIMP) ₂ (H ₂ O) ₂] | - | 3495 | 1306 | 1667 | 1550 | 722 | 833 | 550 | 449 |
| 10 | $[Cu(CFBIMP)_2 (H_2O)_2]$ | - | 3480 | 1308 | 1615 | 1539 | 731 | 826 | 590 | 442 |
| 11 | $[Cu(CFBIMMP)_2(H_2O)_2]$ | - | 3480 | 1320 | 1660 | 1540 | 680 | 850 | 563 | 440 |
| 12 | $[Cu(CCFBIMP)_2(H_2O)_2]$ | - | 3490 | 1320 | 1660 | 1540 | 720 | 840 | 536 | 470 |
| 13 | $[Zn(CFBIMP)_2 (H_2O)_2]$ | - | 3480 | 1320 | 1619 | 1550 | 730 | 800 | 540 | 445 |
| 14 | $[Zn(CFBIMMP)_2(H_2O)_2]$ | - | 3451 | 1346 | 1663 | 1538 | 692 | 842 | 588 | 457 |
| 15 | $[Zn(CCFBIMP)_2(H_2O)_2]$ | - | 3480 | 1320 | 1665 | 1580 | 720 | 800 | 540 | 440 |
| 16 | $[Cd(CFBIMP)_2(H_2O)_2]$ | - | 3527 | 1311 | 1615 | 1568 | 730 | 858 | 596 | 460 |
| 17 | $[Cd(CFBIMMP)_2(H_2O)_2]$ | - | 3460 | 1307 | 1615 | 1558 | 731 | 846 | 570 | 458 |

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| 18 | [Cd(CCFBIMP) ₂ (H ₂ O) ₂] | - | 3460 | 1311 | 1659 | 1568 | 721 | 858 | 534 | 460 |
|----|---|---|------|------|------|------|-----|-----|-----|-----|
| 19 | $[Hg(CFBIMP)_2 (H_2O)_2]$ | - | 3486 | 1327 | 1615 | 1558 | 731 | 857 | 595 | 442 |
| 20 | $[Hg(CFBIMMP)_2(H_2O)_2]$ | - | 3463 | 1333 | 1663 | 1546 | 685 | 870 | 565 | 448 |
| 21 | [Hg(CCFBIMP) ₂ (H ₂ O) ₂] | - | 3460 | 1333 | 1662 | 1546 | 723 | 870 | 565 | 446 |

| S.N. | Name of the complex | Bands in cm ⁻¹ | Electronic spectral assignments | Magnetic moment (µeff B.M) |
|------|---|----------------------------------|---|-------------------------------|
| 01 | [Co(CFBIMP) ₂ (H ₂ O) ₂] | 23255.81 17857.14 10416.66 | $\label{eq:1.1} \begin{array}{rcl} {}^{4}T_{1g}(F) \ \to \ {}^{4}T_{2g}\left(F\right) \\ \\ {}^{4}T_{1g}(F) \ \to \ {}^{4}A_{2g}\left(F\right) \ {}^{4}T_{1g}(F) \ \to \ {}^{4}T_{1g}(P) \end{array}$ | 4.65 |
| 02 | [Co(CFBIMMP) ₂ (H ₂ O) ₂] | 23640.66 18115.94 10438.41 | ${}^{4}T_{1g}(F) \rightarrow {}^{4}T_{2g}(F)$ ${}^{4}T_{1g}(F) \rightarrow {}^{4}A_{2g}(F) {}^{4}T_{1g}(F) \rightarrow {}^{4}T_{1g}(P)$ | 4.88 |
| 03 | [Co(CCFBIMP) ₂ (H ₂ O) ₂] | 22988.50 17667.84 10341.26 | ${}^{4}T_{1g}(F) \rightarrow {}^{4}T_{2g}(F)$ ${}^{4}T_{1g}(F) \rightarrow {}^{4}A_{2g}(F) {}^{4}T_{1g}(F) \rightarrow {}^{4}T_{1g}(P)$ | 4.58 |
| 04 | [Ni(CFBIMP) ₂ (H ₂ O) ₂] | 24096.38 15384.61 10869.56 | ${}^{4}T_{1g}(F) \rightarrow {}^{4}T_{2g}(F)$ ${}^{4}T_{1g}(F) \rightarrow {}^{4}A_{2g}(F) {}^{4}T_{1g}(F) \rightarrow {}^{4}T_{1g}(P)$ | 4.42 |
| 05 | [Ni(CFBIMMP)2(H2O)2] | 23809.52 15151.51 11111.11 | ${}^{3}A_{2g}(F) \rightarrow {}^{3}T_{2g}(F)$ ${}^{3}A_{2g}(P) \rightarrow {}^{3}T_{1g}(F) {}^{3}A_{2g}(F) \rightarrow {}^{3}T_{1g}(P)$ | 3.33 |
| 06 | [Ni(CCFBIMP) ₂ (H ₂ O) ₂] | 24390.24 15408.32 | ${}^{3}A_{2g}(F) \rightarrow {}^{3}T_{2g}(F)$ ${}^{3}A_{2g}(P) \rightarrow {}^{3}T_{1g}(F) {}^{3}A_{2g}(F) \rightarrow {}^{3}T_{1g}(P)$ | 3.36 |

Table 3: Electronic Spectra and Magnetic Susceptibility Measurements Data

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| | | 10917.03 | | |
|----|---|----------|---|------|
| | | | | |
| 07 | $[C_{-}(CEDIMD), (U, O)]$ | 22800 52 | ² D 2D | 1.00 |
| 07 | $[Cu(CFBINP)_2(H_2O)_2]$ | 25809.52 | ${}^{-}\mathbf{D}_{1g} \rightarrow {}^{-}\mathbf{D}_{2g}$ | 1.90 |
| | | 15974.44 | $^{2}\mathrm{B}_{1\mathrm{g}} \rightarrow ^{2}\mathrm{E}_{2\mathrm{g}}$ | |
| | | | | |
| | | | | |
| 08 | [Cu(CFBIMMP) ₂ (H ₂ O) ₂] | 24390.24 | $^{2}\mathrm{B}_{1\mathrm{g}} \rightarrow ^{2}\mathrm{B}_{2\mathrm{g}}$ | 1.75 |
| | | 15873.01 | $^{2}B_{1g} \rightarrow ^{2}E_{2g}$ | |
| | | | | |
| | | | | |
| 09 | [Cu(CCFBIMP) ₂ (H ₂ O) ₂] | 24038.46 | ${}^{2}\mathrm{B}_{1g} \rightarrow {}^{2}\mathrm{B}_{2g}$ | 1.86 |
| | | 16155.08 | $^{2}B_{1g} \rightarrow ^{2}E_{2g}$ | |

Table 4: Powder XRD Data of Complex

| Complex | Peak No. | 20 | θ | Sinθ | Sin ² 0 | h k l | d observed |
|---|----------|--------|---------|----------|--------------------|------------|------------|
| | 1 | 6.260 | 2.19 | 0.04002 | 0.00240 | 200 | 12.00/4 |
| | 1 | 6.360 | 3.18 | 0.04993 | 0.00249 | 200 | 13.8864 |
| $[Cu (CFBIMMP)_2 (H_2O)_2]$ | 2 | 11.402 | 5.701 | 0.089431 | 0.00799 | 211 | 7.7539 |
| | 3 | 14.319 | 7.1595 | 0.112242 | 0.01259 | 220 | 6.1803 |
| | 4 | 15.620 | 7.81 | 0.122371 | 0.01497 | 300 | 5.6686 |
| | 5 | 16.821 | 8.4105 | 0.131727 | 0.01735 | 311 | 5.2663 |
| | 6 | 23.960 | 11.69 | 0.182595 | 0.03334 | 222 | 3.7110 |
| | 7 | 27.380 | 13.69 | 0.213388 | 0.04553 | 321 | 3.2570 |
| | 8 | 31.081 | 15.5405 | 0.241692 | 0.05841 | 420 | 2.8272 |
| | | | | | | | |
| [Cu (CFBIMP) ₂ (H ₂ O) ₂] | 1 | 5.802 | 2.901 | 0.04555 | 0.0020750 | (100) | 12.659 |
| | 2 | 15.586 | 7.793 | 0.12210 | 0.014910 | (111) | 7.551 |
| | 3 | 15.640 | 7.82 | 0.12252 | 0.015013 | (200) | 6.357 |
| | 4 | 22.522 | 11.261 | 0.17596 | 0.030964 | (210) | 5.666 |
| | 6 | 24.039 | 12.0195 | 0.18768 | 0.035224 | (300, 221) | 4.243 |
| | 7 | 24.961 | 12.4805 | 0.194789 | 0.037943 | (310) | 3.958 |

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| 8 | 27.161 | 13.585 | 0.211707 | 0.044820 | (400) | 3.189 |
|----|--------|--------|----------|----------|------------|-------|
| 9 | 27.420 | 13.71 | 0.21369 | 0.045665 | (410, 322) | 3.081 |
| 10 | 30.180 | 15.09 | 0.234819 | 0.055140 | (420) | 2.824 |

Table 5: Antibacterial and Antifungal Activity Results of Ligands and Metal Complexes

| S.N. | Ligand/Complex | Antibac (i | terial activity n mm) | Antifu (| ingal activity in mm) |
|------|--|---------------|--------------------------|-------------|--------------------------|
| | | E. coli | S. aureus | A. niger | F. oxysporum |
| 01 | C ₁₄ H ₈ N ₂ OSFC1 (CFBIMP) | 11 | 11 | 17 | 17 |
| 02 | C ₁₅ H ₁₀ N ₂ OSFC1 (CFBIMMP) | 13 | 14 | 16 | 18 |
| 03 | C ₁₄ H ₇ N ₂ OSFCl ₂ (CCFBIMP) | 13 | 15 | 17 | 16 |
| 04 | $[Co(CFBIMP)_2 (H_2O)_2]$ | 16 | 15 | 14 | 19 |
| 05 | [Co(CFBIMMP) ₂ (H ₂ O) ₂] | 15 | 16 | 18 | 20 |
| 06 | [Co(CCFBIMP) ₂ (H ₂ O) ₂] | 16 | 14 | 12 | 16 |
| 07 | [Ni(CFBIMP) ₂ (H ₂ O) ₂] | 18 | 15 | 19 | 14 |
| 08 | [Ni(CFBIMMP) ₂ (H ₂ O) ₂] | 14 | 15 | 12 | 15 |
| 09 | [Ni(CCFBIMP) ₂ (H ₂ O) ₂] | 16 | 17 | 16 | 18 |
| 10 | $[Cu(CFBIMP)_2 (H_2O)_2]$ | 13 | 12 | 13 | 13 |
| 11 | [Cu(CFBIMMP) ₂ (H ₂ O) ₂] | 17 | 11 | 14 | 12 |
| 12 | [Cu(CCFBIMP) ₂ (H ₂ O) ₂] | 12 | 11 | 15 | 14 |
| 13 | $[Zn(CFBIMP)_2 (H_2O)_2]$ | 15 | 17 | 17 | 19 |
| 14 | $[Zn(CFBIMMP)_2(H_2O)_2]$ | 16 | 17 | 16 | 17 |
| 15 | $[Zn(CCFBIMP)_2(H_2O)_2]$ | 14 | 18 | 15 | 15 |
| 16 | $[Cd(CFBIMP)_2(H_2O)_2]$ | 17 | 19 | 13 | 18 |
| 17 | [Cd(CFBIMMP) ₂ (H ₂ O) ₂] | 19 | 20 | 14 | 15 |
| 18 | [Cd(CCFBIMP) ₂ (H ₂ O) ₂] | 20 | 20 | 16 | 18 |
| 19 | $[Hg(CFBIMP)_2 (H_2O)_2]$ | 17 | 18 | 18 | 17 |
| 20 | [Hg(CFBIMMP) ₂ (H ₂ O) ₂] | 19 | 20 | 19 | 21 |
| 21 | [Hg(CCFBIMP) ₂ (H ₂ O) ₂] | 21 | 20 | 20 | 19 |
| | Ciproflaxacin | 24 | 22 | - | - |
| | (Standard) | | | | |
| | Grisofulvin | - | - | 24 | 23 |
| | (Standard) | | | | |
| | DMF(Control) | 0 | 0 | 0 | 0 |

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