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# Synthesis, Characterization and Structural Analysis of Cobaloximes Complexes

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A series of bioactive cobalt(III) complexes were synthesized with bidentate ligand have been investigated as vitamin $B_{12}$ models. The experiment was two pot snythesis, in the first part was green microcrystalline dihalo(dimethylglyoximato)cobalt(III) and second part was brown microcrystalline halo(pyridine based ligand) cobaloximes. Final part of synthesized complexes was characterized by IR, electronic and NMR spectral studies. Infrared spectra of metal complexes indicated the formation of Co-N axial bond and Co-N equatorial bond. Thermal analysis revealed that the Co(III) complexes were stable up to 350 ºC. The experimental results of antimicrobial were showed good zone of inhibition towards selected microbes.

**Keywords: Cobaloximes, Vitamin $B_{12}$, Antimicrobial activities.**

## INTRODUCTION

Metal complexes with oximes has become more attention for their interesting physico-chemical properties, reaction mechanism and potential applications in the areas of bioorganic systems, catalysis, molecular modelling, drug designing, electrochemical and electro optical sensors [1]. The metallo-drugs have more attention due to their role in cellular regulation and signaling. Cobaloximes have been widely described as structural and functional mimics for the coenzyme vitamin $B_{12}$ [2]. The development of cobaloximes complexes in the past few years, for their promising hydrogen-evolving catalytic capability at their reduced Co(I) state because of their low-cost, high activity and direct synthesis methodology [3-5].

The most common octahedral cobaloximes, Co(III) were synthesized with a chemical composition of $XCo(dmgH)_2L$, where the equatorial dmgH ligands are monoanions of dimethylglyoxime ($dmgH_2$) and the axial ligands are nitrogen based ligands. Each model possess strong equatorial ligand field strength [6,7]. Herein, we report the synthesis, characterization and antimicrobial activities of a series of Co(III) glyoximato complexes using two different dioxime ligands ($dmgH_2$ and $dpgH_2$) and five different axial ligands (pyridine, pyrazine, 2-methylpyrazine, pyrazine carboxylic acid and pyrimidine). Various characterization techniques such as $^1$H NMR, FT-IR, UV-Vis and thermal analysis were employed for understanding of the structural properties of the synthesized complexes.

## EXPERIMENTAL

Two types of cobalt(III) complexes containing pyrazine based axial ligands with two different dioxime networks *viz.* dimethylglyoxime ($dmgH_2$) and diphenylglyoxime ($dpgH_2$). Type-1: $[Co(dmgH)_2LX]$ and Type-2: $[Co(dpgH)_2LX]$, where X = $Cl^-$ or $Br^-$; L = pyridine (Py), pyrazine (Pyz), 2-methyl pyrazine (MPyz), pyrimidine (Pym) and pyrazinecarboxylic acid (PyzC). The analytical grade chemicals were used for the synthetic process. The UV-visible spectra of the complexes of suitable concentrations in aqueous ethanol were obtained from Double Beam spectrophotometer using 1 cm matched quartz cells. The complexes were subjected to IR analysis using Shimadzu IR spectrophotometer in KBr disc. The proton NMR spectra of the complexes were characterized by Joel- 500 MHz NMR spectrophotometer at SAIF IIT Madras, Chennai, India. The TGA curves of the complexes were obtained using SII TG-DTA 6300 Exstar at Avinashilingam University, Coimbatore, India. The antimicrobial studies were carried out by diffusion method and ciprofloxacin was used as standard.

**Synthesis of *trans*-hydrogendihalobisdimethylglyoximatocobaltate(III) {$H[Co(dmgH)_2Cl_2]$/$H[Co(dmgH)_2Br_2]$}:**

Exactly 0.01 mol of cobalt (II) chloride hexahydrate/cobalt (II) bromide was dissolved in 50 mL of acetone in a 250 mL iodine flask and stirred using magnetic stirrer for about 15 min. A dark blue coloured solution was obtained. To this, 0.02 mol of dimethylglyoxime was added and the solution was stirred for about 1 h under aerobic condition. The blue coloured solution turned light green and then to dark green. The green coloured mass was filtered by acetone and then ether finally dried over vacuum desiccator (yield: 60%).

**Synthesis of complexes: *trans*-Pyrazinechlorobisdimethylglyoximatocobalt(III) {[Co(dmgH)$_2$(Pyz)Cl]}:** The green coloured dichloro complex, H[Co(dmgH)$_2$Cl$_2$] (0.01 mol) was placed in 50 mL of ethanol. The slurry was stirred for 10 min and mixed with 0.01 mol of pyrazine [8]. The reactants were stirred for about 1 h at 60 ºC. The green colour turned into pale brown indicating the completion of the reaction. It was allowed to stand for an hour and then filtered through sintered crucible. The light brown colour complex formed, which was filtered and dried over vacuum desiccator and yield was about 60%. Similarly, other *trans*-pyrazine(axial ligands)halo*bis*-dimethylglyoximatocobalt (III), [Co(dmgH)$_2$LX] were also synthesized.

**Synthesis of complexes: *trans*-Pyrazinechloro*bis*diphenylglyoximatocobalt(III) [Co(dpgH)$_2$(Pyz)Cl]:** Exactly 0.01 mol of $CoCl_2 \cdot 6H_2O$ was dissolved in 75 mL of ethanol in a 250 mL iodine flask and stirred using magnetic stirrer for about 15 min. A dark blue coloured solution was obtained. To this, 0.02 mol of diphenylglyoxime was added and the solution was stirred for about 60 min under aerobic condition. The blue coloured solution turned light green and then to dark green. Exactly, 0.01 mol of pyrazine was added to the green coloured dichloro complex solution, H[Co(dpgH)$_2$Cl$_2$]. The reaction mixture was stirred at 60 ºC for about 1 h. The green coloured turned into pale brown indicating the completion of the reaction. It was allowed to stand for an hour and filtered through sintered crucible. The light brown colour complex formed and then washed with solvent and dried [9]. Similarly, other *trans*-pyrazine(axial ligands)halobisdiphenylglyoximatocobalt(III), [Co(dpgH)$_2$LX] were also synthesized.

## RESULTS AND DISCUSSION

**FTIR studies:** In the IR spectra of the synthesized metal complexes indicates that the electron density around the metal is increased due to nitrogen of glyoximate moeities, which facilitates back-donation from cobalt(III), thereby the electron density increase in C=N and N–O bonds. The N–O stretching vibrations shift to higher frequency because of increase in electron density of which leads to stronger hydrogen bridges of O–H…O. The IR spectra of Co(III) complexes of type [Co(dmgH)$_2$LX] revealed that the C=N stretching frequency ranging from 1600 to 1560 cm$^{-1}$ may be ascribed to dimethylglyoxime moiety in its complex. A strong peak in 1150-1080 cm$^{-1}$ region may be recognized the -N-O stretching frequency of dimethylglyoxime moitety. Appearance of the peaks at 450 cm$^{-1}$ and 550 cm$^{-1}$ indicated the formation of Co-N axial bond and Co-N equatorial bond, respectively. The band around 1050 cm$^{-1}$ indicated the presence of O-H stretching in the metal complexes. The band ranges from 1430-1390 cm$^{-1}$ indicating the presence of C- H stretching of $sp^3$ hybridization (Table-1).

The IR spectra of the metal complexes of type [Co(dpgH)$_2$-LX] described the band around 610 cm$^{-1}$ is assignable to Co-N stretching of diphenylglyoxime moiety and central metal atom. The stretching frequency at the range of 460-440 cm$^{-1}$ attributed to Co-N bond of axial pyrazine based moiety and central metal atom. The peaks around 880 cm$^{-1}$ and 2900-2800 cm$^{-1}$ may be attributed to the presence of phenyl ring in the complex *i.e.* phenyl ring in the equatorial diphenylglyoxime moiety and the C=N stretching of the axial pyrazine based moieties, respectively (Table-1).

**$^1$H NMR studies:** The proton NMR spectra of complexes of type [Co(dmgH)$_2$LX] revealed that a sharp singlet at around δ 2.404 ppm corresponds to the twelve methyl protons of equatorial dimethylglyoxime moiety [9], which shows the chemical equivalence of four methyl groups. The -OH proton of oxime resonates above 8 ppm for all the complexes [10]. The substituted axial pyrazine moiety appeared as multiplet in the range δ 8.0-8.5 ppm. A singlet appeared at δ 2.503 ppm correspond to methyl proton of methyl pyrazine which is an axial ligand.

The $^1$H NMR spectra of the metal complexes of type [Co(dpgH)$_2$LX] The peak appeared in downfield around δ 7.5-8.5ppm is due to the aromatic nature of the equatorial ligand. The oxime proton appeared as singlet above δ 8.5 ppm. The -OH proton of oxime resonates above around 7 ppm for all the complexes [10]. The pyrimidine and pyrazine ring appeared as multiplet in the range δ 7-8 ppm supporting the presence of the axial ligands [11]. The peak positions and multiplicity of the some synthesized complexes are listed in Table-2.

TABLE-1
IR SPECTRAL DATA (cm$^{-1}$) OF COMPLEXES OF THE TYPE [Co(dmgH/dpgH)$_2$LX]

| | Dimethylglyoxime moiety | | | | | M-N (#Axial ligand) | | Axial ligands | |
|---|---|---|---|---|---|---|---|---|---|
| (dmgH)$_2$ complex | ν(CH$_3$) | ν(C=N) | ν(N-O) | ν(O-H) | ν(C=N-O) | ν(Co-N) | ν(Co-N)$^{\#}$ | ν(C=N) | ν(C-N) |
| PyzC | 1382 | 1594 | 1170 | 1058 | 730 | 520 | 446 | 3333 | 1240 |
| MPyz | 1437 | 1559 | 1086 | 1030 | 734 | 550 | 440 | 2370 | 1241 |
| (Py)Cl | 1373 | 1558 | 1095 | 1095 | 740 | 509 | 424 | 2368 | 1242 |
| (Pym)Cl | 1373 | 1558 | 1087 | 1087 | 740 | 509 | 447 | 2376 | 1242 |
| (Pyz)Br | 1381 | 1558 | 1087 | 1087 | 740 | 516 | 432 | 2376 | 1242 |
| (Pym)Br | 1373 | 1558 | 1087 | 1087 | 709 | 509 | 447 | 2276 | 1242 |
| (dpgH)$_2$ complex | ν(C$_6$H$_5$) | ν(C=N) | ν(N-O) | ν(O-H) | ν(C=N-O) | ν(Co-N) | ν(Co-N)$^{\#}$ | ν(C=N) | ν(-N-H) |
| MPyz | 879 | 1489 | 1010 | 1140 | 732 | 609 | 439 | 2862 | 3433 |

TABLE-2
$^1$H NMR SPECTRA (ppm) OF COMPLEXES
OF THE TYPE [Co(DH)$_2$LX]

| [Co(DH)$_2$LX] | Equatorial ligands | | Axial ligands |
|---|---|---|---|
| | -CH$_3$ | -OH | H |
| [Co(dmgH)$_2$(MPyz)Br] | 2.4 (12 H, s) | 8.01 (1H, s) | 8-8.5 (m) |
| [Co(dmgH)$_2$(Pyz)Br] | 2.5 (12 H, s) | 7 (1H, s) | 7-8 (m) |
| [Co(dmgH)$_2$(pym)Cl] | 2.5 (12 H, s) | 7 | 7-8 (m) |
| [Co(dpgH)$_2$(PyzC)Cl] | – | 8.79 (1H, s) | 7.1-7.4 (m) |

**Thermal analysis:** Thermal analysis revealed that the complexes are stable up to 350 ºC and follow a three stage decomposition pattern depending up on the configuration finally to give $Co_3O_4$ as residue [12]. Thermal analysis of complexes of the [Co(dmgH)$_2$LX] and [Co(dpgH)$_2$LX] showed three stage decomposition pattern (Fig. 1). In the first stage, weight loss occurred at 160-200 ºC corresponds to the removal of axial halide ligand. The second stage weight loss at 320-350 ºC corresponds to the leaving of pyrazine based moieties. The residual complex *viz.* [Co(dmgH)$_2$]$^+$ and [Co(dpgH)$_2$]$^+$ seems to be stable up to 350 ºC after which, it decomposed without any sharp change in the mass to leave $Co_2O_3$ as the final residue [13].

**Electronic spectra:** Electronic spectra of complexes of type [Co(dmgH)$_2$LX] showed an absorption band in the range 200-230 nm, which may be due to $\pi\rightarrow\pi^*$ transition of the heterocyclic moiety [14]. This absorption band remains unaltered in their complexes. The moderately intense band around 250-280 nm, which may be ascribed to $\pi\rightarrow\pi^*$ [15] of the dmgH$_2$, also remain unaltered in the complexes [16]. A shoulder around 280-310 nm may be due to the ligand to metal charge transfer (LMCT) transition [17]. The weak absorption at around 370 nm may be due to the spin allowed *d-d* transition *viz.* $^1A_{1g} \rightarrow {}^1T_{2g}$. The electronic spectra of the type [Co(dpgH)$_2$LX] revealed that the diphenylglyoxime complexes showed a similar trend, with dimethylglyoxime complexes. The slight shift in absorption maximum of these complexes may be attributed to the presence of the phenyl ring in the system. Fig. 2 showed the electronic spectra of some dimethylglyoxime and diphenylglyoxime complexes. The electronic spectral data of these complexes are given in Table-3.

**Antimicrobial activity:** The cobalt complexes showed good antimicrobial activity against various pathogens due to the chelation effect.

**Antibacterial activity:** The antibacterial activity of cobalt complexes of type [Co(dmgH)$_2$LX]showed fairly good level of zone of inhibition towards the tested microbes. The complex containing pyrazine carboxylic acid as the axial ligand showed good activity than all the other synthesized complexes when compared with the standard ciproflaxcin. The presence of axial pyrazine based ligands has much influence on the activity against pathogens in chloro complexes whereas the presence of axial moiety has not much influence on the activity in bromo complexes.

The antibacterial activity of type [Co(dpgH)$_2$LX] showed moderate actitivity when compared to dimethylgloxime complex

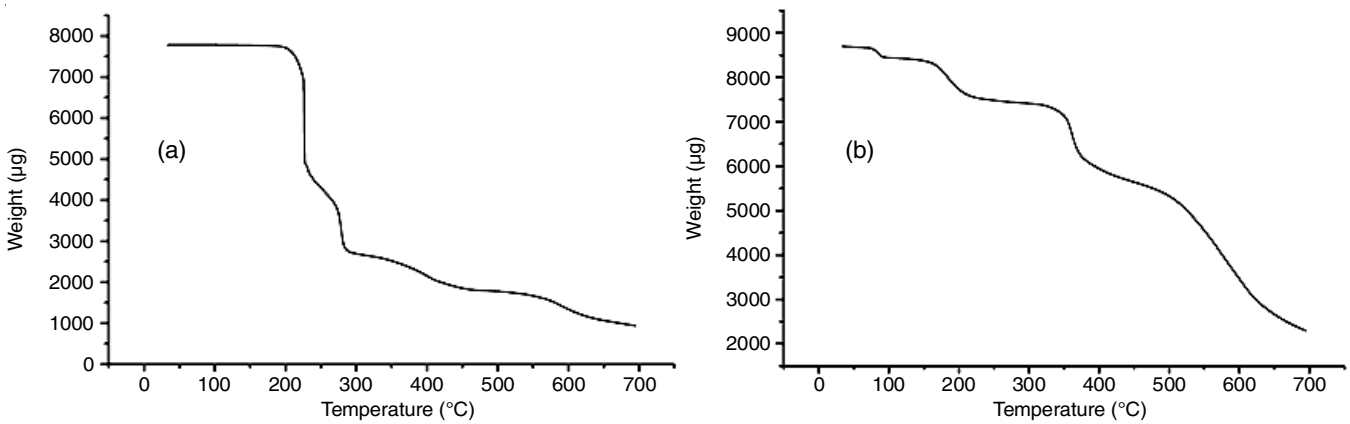


Fig. 1. (a) TGA curve of [Co(dmgH)$_2$(PyzC)Cl] (b) TGA curve of [Co(dpgH)$_2$(MPyz)Cl]

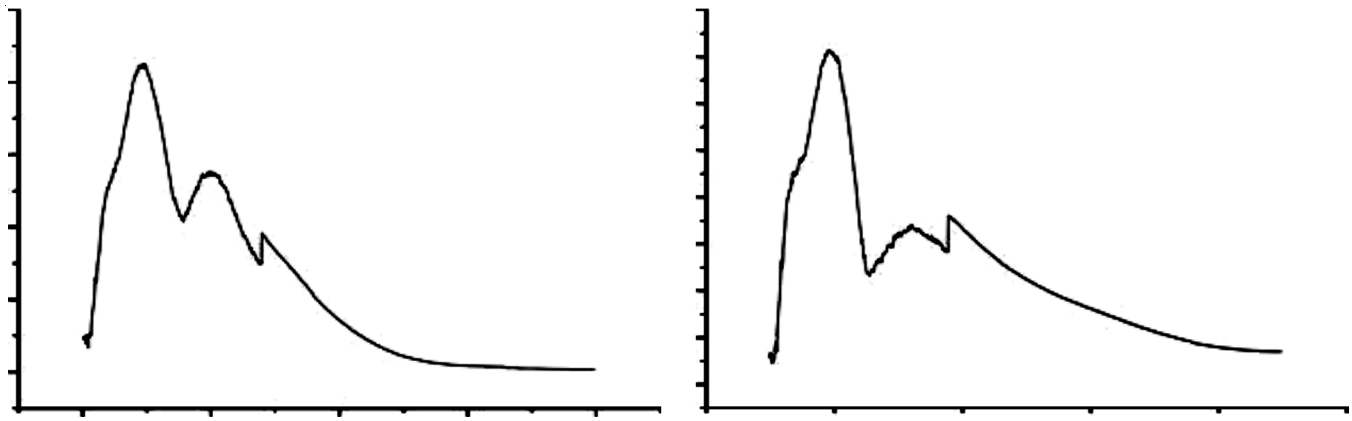

Fig. 2. Electronic spectrum of the complex 1 × 10$^{-5}$ M [Co(dmgH)$_2$(MPyz)Br] and [Co(dpgH)$_2$(Pyz)Br]

TABLE-3
UV DATA OF THE $1 \times 10^{-5}$ M
$[Co(dmgH/dpgH)_2(L)X]$ IN ETHANOL

| $[Co(dmgH/dpgH)_2(L)X]$ | $\lambda_{max}$ (nm) | | | |
|---|---|---|---|---|
| | $\pi \rightarrow \pi^*$ of pyridine based ligand | $\pi \rightarrow \pi^*$ of (dmgH/ dpgH) | LMCT | *d–d* transition |
| $[Co(dmgH)_2(Py)Cl]$ | 230 | 261 | 312 | – |
| $[Co(dmgH)_2(Pyz)Cl]$ | 206 | 237 | 261 | 370 |
| $[Co(dmgH)_2(MPyz)Cl]$ | 203 | 223 | 246 | 340 |
| $[Co(dmgH)_2(PyzC)Cl]$ | 220 | 250 | 300 | 380 |
| $[Co(dmgH)_2(Pym)Cl]$ | 226 | 258 | 359 | – |
| $[Co(dmgH)_2(Py)Br]$ | 219 | 292 | 272 | 320 |
| $[Co(dmgH)_2(Pyz)Br]$ | 237 | 262 | 293 | 339 |
| $[Co(dmgH)_2(MPyz)Br]$ | 224 | 246 | 301 | 340 |
| $[Co(dmgH)_2$ (Pym)Br] | 218 | 234 | 293 | – |
| $[Co(dpgH)_2(Pyz)Cl]$ | 225 | 246 | – | 343 |
| $[Co(dpgH)_2(MPyz)Cl]$ | 210 | 253 | – | 339 |
| $[Co(dpgH)_2(PyzC)Cl]$ | 217 | 247 | – | 340 |
| $[Co(dpgH)_2(Pyz)Br]$ | 220 | 246 | – | 340 |
| $[Co(dpgH)_2(MPyz)Br]$ | 226 | 245 | – | 341 |

against the tested microbes. All the diphenylglyoxime complexes showed greater activity against gram negative bacterium *viz. Escherichia coli* when compared with the Gram positive bacterium *Staphylococcus aureus*. In these complexes presence of different axial pyrazine based and halide moieties have not much influence on the activity of complexes against tested microbes. The zone of inhibition of both diphenylgloxime and dimethylglyoxime complexes with different microbes are listed in Table-4.

**Single crystal XRD studies:** This cobaloxime crystallizes in orthorhombic system with space group, $P2_12_12_1$. The asymmetric unit contains one complex molecule and there are four complex molecules present per unit cell (Tables 5-7). The coordination geometry around cobalt is slightly distorted octahedron with the four nitrogen atoms of dimethyl glyoximato ligand forming an approximate square plane. The axially coordinating bromide and methylpyridine nitrogen [N(5)-Co(1)-Br(1) =178.67(7)] are perpendicular to the equatorial plane composed by the four N atoms of two dimethyl glyoxime moieties. The bond length between central metal ion and the bromine Co(1)-Br(1) = 2.3739(4) Å. The two glyoximate moieties are linked by strong internal O-H···O hydrogen bonds (Table-8). The structure is further stabilized through van der Waals interaction.

TABLE-4
ANTIMICROBIAL ACTIVITY OF
THE $[Co(DH)_2LX]$ COMPLEXES

| $[Co(DH)_2(L)X]$ | Zone of inhibition (mm) | | |
|---|---|---|---|
| | Bacterial | | Fungi |
| | *S. aureus* | *E. coli* | *A. niger* |
| $[Co(dmgH)_2(Pyz)Cl]$ | 12 | 20 | 14 |
| $[Co(dmgH)_2(MPyz)Cl]$ | 20 | 20 | 16 |
| $[Co(dmgH)_2(PyzC)Cl]$ | 21 | 22 | 20 |
| $[Co(dmgH)_2(Pyz)Br]$ | 20 | 18 | 15 |
| $[Co(dmgH)_2(MPyz)Br]$ | 19 | 18 | 13 |
| $[Co(dpgH)_2(Pyz)Cl]$ | 10 | 16 | 15 |
| $[Co(dpgH)_2(MPyz)Cl]$ | 13 | 14 | 14 |
| $[Co(dpgH)_2(PyzC)Cl]$ | 13 | 15 | 21 |
| $[Co(dpgH)_2(Pyz)Br]$ | 12 | 12 | 14 |
| $[Co(dpgH)_2(MPyz)Br]$ | 13 | 18 | 15 |
| Ciproflaxcin | 30 | 33 | – |
| Flucanazole | – | – | 23 |

TABLE-5
CRYSTAL DATA AND REFINEMENT OF
STRUCTURE FOR $[Co(dmgH)_2(MP)Br]$

| | |
|---|---|
| Empirical formula | $C_{14}H_{21}BrCoN_5O_{4.50}$ |
| Formula weight | 470.20 |
| Temperature | 293(2) K |
| Wavelength | 0.71073 Å |
| Crystal system, space group Orthorhombic | $P2_12_12_1$ |
| Unit cell dimensions | a = 8.3670(3) Å, α = 90°<br>b = 14.3325(6) Å, β = 90°<br>c = 15.9336(6) Å, γ = 90° |
| Volume | 1910.76(13) $A^3$ |
| Z, Calculated density | 4, 1.634 $Mg/m^3$ |
| Absorption coefficient | 3.020 $mm^{-1}$ |
| F(000) | 952 |
| Crystal size | 0.30 × 0.25 × 0.25 mm |
| θ range for data collection | 2.56 to 29.75° |
| Limiting indices | -11<= h <=11, -18<= k <=20, -22<= l <=21 |
| Reflections collected/unique | 13618/5426 [R(int) = 0.0334] |
| Completeness to θ | 29.75 99.8% |
| Absorption correction semi-empirical from equivalents max. and min. transmission | 0.5189 and 0.4644 |
| Refinement method full-matrix least-squares on $F^2$ data/restraints/parameters | 5426/2/243 |
| Goodness-of-fit on $F^2$ | 0.987 |
| Final R indices [I>2σ(I)] | R1 = 0.0346, wR2 = 0.0682 |
| R indices (all data) | R1 = 0.0567, wR2 = 0.0744 |
| Absolute structure parameter | 0.033(9) |
| Largest diff. peak and hole | 0.357 and -0.475 $e.A^{-3}$ |

TABLE-6
ATOMIC COORDINATES (× $10^4$) AND EQUIVALENT ISOTROPIC DISPLACEMENT PARAMETERS ($A^2 \times 10^3$) FOR $[Co(dmgH)_2(MP)Br]$

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| C(1) | 2603(3) | 3850(3) | 2493(2) | 40(1) | C(14) | 8326(5) | 2597(3) | 5132(2) | 63(1) |
| C(2) | 2893(4) | 4779(2) | 2824(2) | 40(1) | N(1) | 3735(3) | 3552(2) | 2010(2) | 32(1) |
| C(3) | 8403(3) | 4878(2) | 1260(2) | 41(1) | N(2) | 4253(3) | 5127(2) | 2572(1) | 35(1) |
| C(4) | 8109(4) | 3950(3) | 931(2) | 44(1) | N(3) | 7252(3) | 5179(2) | 1723(2) | 35(1) |
| C(5) | 1133(4) | 3296(3) | 2683(3) | 60(1) | N(4) | 6772(3) | 3607(2) | 1161(2) | 37(1) |
| C(6) | 1782(5) | 5304(3) | 3380(3) | 71(1) | N(5) | 6506(3) | 3819(2) | 2875(1) | 28(1) |
| C(7) | 9866(4) | 5434(3) | 1084(3) | 68(1) | O(1) | 4714(3) | 5976(2) | 2810(1) | 48(1) |
| C(8) | 9283(5) | 3454(3) | 371(3) | 79(1) | O(2) | 3656(3) | 2727(2) | 1640(2) | 47(1) |
| C(9) | 6575(3) | 2891(2) | 2975(2) | 34(1) | O(3) | 6303(3) | 2767(2) | 900(2) | 54(1) |
| C(10) | 7159(4) | 2492(2) | 3687(2) | 41(1) | O(4) | 7307(3) | 6033(2) | 2063(2) | 50(1) |
| C(11) | 7724(3) | 3027(2) | 4339(2) | 40(1) | Co(1) | 5502(1) | 4361(1) | 1879(1) | 26(1) |
| C(12) | 7690(4) | 3983(2) | 4221(2) | 40(1) | Br(1) | 4231(1) | 4996(1) | 675(1) | 45(1) |
| C(13) | 7075(4) | 4347(2) | 3495(2) | 35(1) | O(1W) | 1424(9) | 1387(5) | 990(4) | 102(2) |

TABLE-7
BOND LENGTHS (Å) AND BOND ANGLES (°) FOR [Co(dmgH$_2$)(MP)Br]

| Bond length (Å) | | Bond angles (°) | | | |
|---|---|---|---|---|---|
| N(1)-Co(1) | 1.891(2) | C(1)-N(1)-Co(1) | 115.8(2) | N(1)-Co(1)-N(3) | 178.72(11) |
| N(2)-Co(1) | 1.875(2) | O(2)-N(1)-Co(1) | 122.54(18) | N(2)-Co(1)-N(4) | 178.82(11) |
| N(3)-Co(1) | 1.893(2) | C(2)-N(2)-O(1) | 120.9(3) | N(1)-Co(1)-N(4) | 98.93(11) |
| N(4)-Co(1) | 1.899(2) | C(2)-N(2)-Co(1) | 116.4(2) | N(3)-Co(1)-N(4) | 80.85(11) |
| N(5)-Co(1) | 1.957(2) | O(1)-N(2)-Co(1) | 122.8(2) | N(2)-Co(1)-N(5) | 89.66(9) |
| Co(1)-Br(1) | 2.3739(4) | C(3)-N(3)-Co(1) | 116.4(2) | N(1)-Co(1)-N(5) | 90.13(10) |
| | | O(4)-N(3)-Co(1) | 122.70(19) | N(3)-Co(1)-N(5) | 91.14(10) |
| | | C(4)-N(4)-Co(1) | 116.4(2) | N(4)-Co(1)-N(5) | 91.25(10) |
| | | O(3)-N(4)-Co(1) | 122.5(2) | N(2)-Co(1)-Br(1) | 90.10(7) |
| | | C(13)-N(5)-Co(1) | 122.0(2) | N(1)-Co(1)-Br(1) | 88.54(7) |
| | | C(9)-N(5)-Co(1) | 120.64(18) | N(3)-Co(1)-Br(1) | 90.19(7) |
| | | N(2)-Co(1)-N(1) | 81.83(10) | N(4)-Co(1)-Br(1) | 89.01(8) |
| | | N(2)-Co(1)-N(3) | 98.38(11) | N(5)-Co(1)-Br(1) | 178.67(7) |

TABLE-8
HYDROGEN BONDS FOR [Co(dmgH$_2$)(MP)Br]

| D-H···A | d(D-H) | d(H···A) | d(D···A) | ∠(DHA) |
|---|---|---|---|---|
| O(3)-H(3A)···O(2) | 0.903(10) | 1.619(13) | 2.510(3) | 169(4) |
| O(4)-H(4A)···O(1) | 0.906(10) | 1.587(14) | 2.476(3) | 166(4) |

Fig. 3a gives ortep representation of the molecule with the atom numbering scheme. Atoms are represented as 50% probability ellipsoids. Fig. 3b gives packing of the molecules in the unit cell.

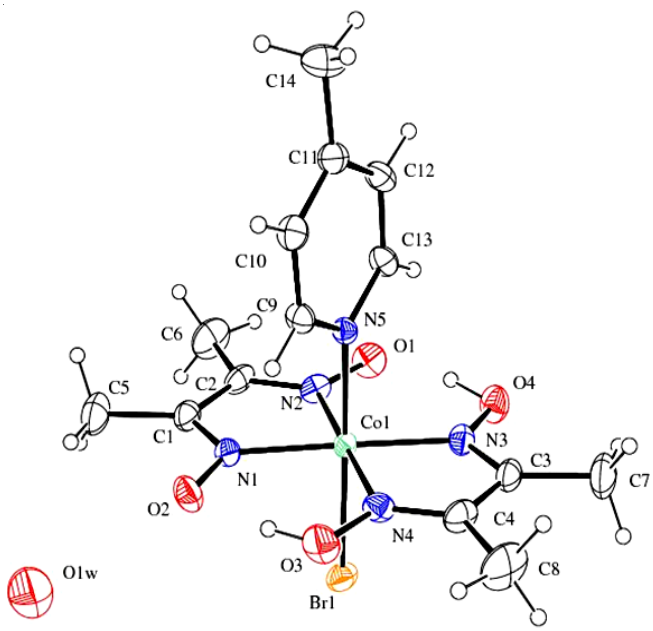


Fig. 3a. ORTEP of [Co(dmgH)$_2$(MP)(Br)]

## Conclusion

Few cobaloximes were synthesized and spectroscopically characterized. The yield of mononuclear octahedral cobalt complexes was found to be in the range from 60-70% and all the spectral data were in agreement with the expected results. All the metal complexes are thermally stable at room temperature. All the synthesized complexes showed good results against selected pathogens when compared to standard. The XRD data clearly represents the molecular structure of cobaloximes.

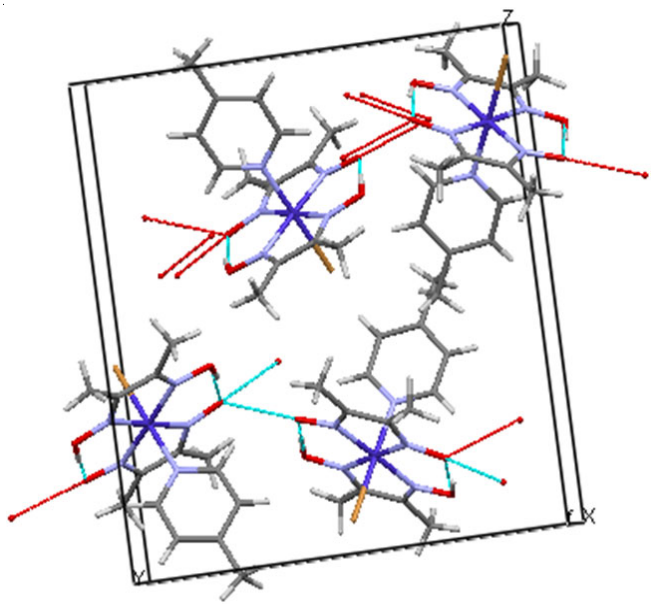


Fig. 3b. Packing of [Co(dmgH)$_2$(MP)Br] [dotted lines indicate hydrogen bonds]

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## CONFLICT OF INTEREST

The authors declare that there is no conflict of interests regarding the publication of this article.

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