Acta Crystallographica Section E
**Structure Reports Online**
ISSN 1600-5368

# Diaquabis(5-*n*-butylpyridine-2-carboxylato)cobalt(II)

**Run-Zhen Fan, Wen-Dong Song* and Xiao-Min Hao**

College of Science, Guang Dong Ocean University, Zhan Jiang 524088, People's Republic of China
Correspondence e-mail: songwd60@126.com

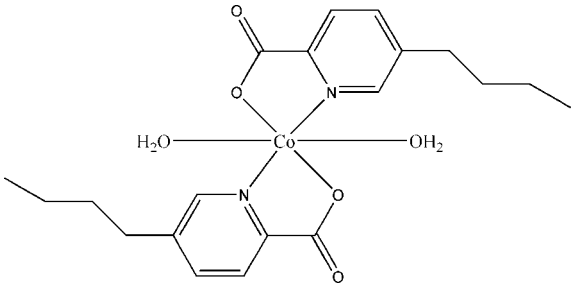
Received 17 July 2007; accepted 18 July 2007

Key indicators: single-crystal X-ray study; $T$ = 223 K; mean $\sigma$(C–C) = 0.005 Å; $R$ factor = 0.049; $wR$ factor = 0.109; data-to-parameter ratio = 17.9.

The title complex, $[Co(C_{10}H_{12}NO_2)_2(H_2O)_2]$, a neutral mononuclear molecule, consists of a $Co^{II}$ ion, two 5-*n*-butylpyridine-2-carboxylate ligands and two water molecules. The $Co^{II}$ atom, located on a centre of symmetry, displays a distorted octahedral coordination geometry. Intermolecular O—H···O hydrogen bonds form a supramolecular network structure.

## Related literature

For related literature, see: Okabe, Wada *et al.* (2002); Okabe, Muranishi *et al.* (2002).




## Experimental

*Crystal data*

$[Co(C_{10}H_{12}NO_2)_2(H_2O)_2]$
$M_r$ = 451.37
Monoclinic, $P2_1/c$
$a$ = 5.1378 (1) Å
$b$ = 34.0034 (9) Å
$c$ = 7.5922 (2) Å
$\beta$ = 124.181 (2)°
$V$ = 1097.27 (5) Å$^3$
$Z$ = 2
Mo $K\alpha$ radiation
$\mu$ = 0.82 mm$^{-1}$
$T$ = 223 (2) K
0.25 × 0.12 × 0.10 mm

*Data collection*

Bruker APEXII area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min}$ = 0.822, $T_{max}$ = 0.923
9237 measured reflections
2511 independent reflections
1528 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.056

*Refinement*

$R[F^2 > 2\sigma(F^2)]$ = 0.049
$wR(F^2)$ = 0.109
$S$ = 1.01
2511 reflections
140 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.31 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.70 e Å$^{-3}$

**Table 1**
Selected geometric parameters (Å, °).

| | | | |
|---|---|---|---|
| Co1—O1 | 2.0641 (18) | Co1—N1 | 2.123 (2) |
| Co1—O1*W* | 2.076 (2) | | |
| O1—Co1—O1*W*$^{i}$ | 88.28 (8) | O1—Co1—N1 | 79.04 (8) |
| O1—Co1—O1*W* | 91.72 (9) | O1*W*$^{i}$—Co1—N1 | 87.27 (9) |
| O1$^{i}$—Co1—N1 | 100.96 (8) | O1*W*—Co1—N1 | 92.73 (9) |

Symmetry code: (i) $-x+1, -y+2, -z+2$.

**Table 2**
Hydrogen-bond geometry (Å, °).

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| O1*W*—H2*W*···O2$^{ii}$ | 0.80 (3) | 1.90 (3) | 2.688 (3) | 170 (3) |
| O1*W*—H1*W*···O1$^{iii}$ | 0.76 (3) | 1.97 (3) | 2.712 (3) | 165 (3) |

Symmetry codes: (ii) $x-1, y, z-1$; (iii) $-x+2, -y+2, -z+2$.

Data collection: *APEX2* (Bruker, 2004); cell refinement: *SAINT* (Bruker, 2004); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 2004); software used to prepare material for publication: *SHELXTL*.

The authors acknowledge the Scientific and Technical Key Leading Project of Guangdong Province of China (grant No. B05119) and the Foundation for Excellent Person over Introduction of Zhanjiang and Guangdong Ocean University.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: ZL2048).

## References

Bruker (2004). *APEX2* (Version 5.62) and *SAINT* (Version 7.23a) and *SHELXTL* (Version 6.10). Bruker AXS Inc., Madison, Wisconsin, USA.
Okabe, N., Muranishi, Y. & Wada, Y. (2002). *Acta Cryst.* C**58**, m511–m513.
Okabe, N., Wada, Y. & Muranishi, Y. (2002). *Acta Cryst.* E**58**, m372–m374.
Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.
Sheldrick, G. M. (1997). *SHELXL97* and *SHELXS97*. University of Göttingen, Germany.

  doi:10.1107/S1600536807035295 

# supplementary materials

*Acta Cryst.* (2007). E**63**, m2214 [ **doi:10.1107/S1600536807035295** ]

# Diaquabis(5-*n*-butylpyridine-2-carboxylato)cobalt(II)

**R.-Z. Fan, W.-D. Song and X.-M. Hao**

## Comment

Some structures of transition metal complexes containing the 5-butyl-pyridyl-2-carboxylic acid (fusaric acid) ligand have been reported. In the structural investigation of these complexes, it has been found that the fusaric acid functions as a multidentate ligand (Okabe, Wada *et al.*, 2002; Okabe, Muranishi *et al.*, 2002), with versatile binding and coordination modes. In this paper, we report the crystal structure of the title compound, (I), a new Co complex obtained by the reaction of fusaric acid with cobalt chloride in aqueous solution.

As illustrated in Fig. 1, the $Co^{II}$ atom, which is a neutral mononuclear molecule, lies on a centre of symmetry and has a distorted octahedral geometry with six coordinating atoms being two carboxyl O and two N atoms from two different fusaric acid ligands and two water molecules (Table 1). The coordinating O and N atoms and $Co^{II}$ atom are coplanar. The structural components are connected through O—H···O hydrogen bonding involving the coordinating water molecules as donors and the carboxyl O atoms as acceptors, forming neutral layers perpendicular to *b* axis (Fig. 2; Table 2).

## Experimental

The title complex was prepared by the addition of a stoichiometric amount of cobalt chloride (20 mmol) to a hot aqueous solution (25 ml) of 5-butyl-pyridyl-2-carboxylic acid (fusaric acid, 30 mmol). The pH was then adjusted to 7.0–8.0 with NaOH (30 mmol). The resulting solution was filtered, and red crystals were obtained at room temperature on slow evaporation of the solvent over several days.

## Refinement

Carbon-bound H atoms were placed at calculated positions and were treated as riding on the parent C atoms with C—H = 0.93–0.97 Å, and with $U_{iso}$(H) = 1.2 or 1.5 $U_{eq}$(C). Water H atoms were tentatively located in difference Fourier maps and were refined with distance restraints of O–H = 0.82 Å and H···H = 1.29 Å, each within a standard deviation of 0.01 Å; other H-atoms with $U_{iso}$(H) = 1.2 $U_{eq}$(O).

## Figures

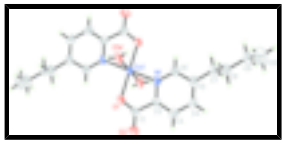


Fig. 1. The structure of (I), showing the atom-numbering scheme and displacement ellipsoids drawn at the 30% probability level. Unlabelled atoms are related to the labelled atoms by the symmetry operator (1 − *x*, 2 − *y*, 2 − *z*).

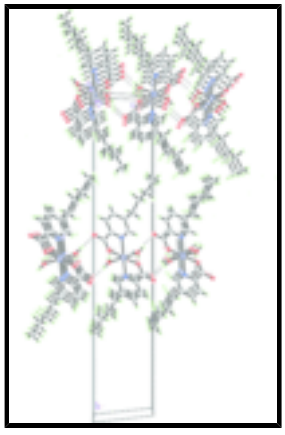


Fig. 2. A packing view of (I), showing the intermolecular hydrogen bonding interactions as broken lines.

**Diaquabis(5-n-butylpyridine-2-carboxylato)cobalt(II)**

*Crystal data*

| | |
|---|---|
| $[Co(C_{10}H_{12}NO_2)_2(H_2O)_2]$ | $F_{000}$ = 474 |
| $M_r$ = 451.37 | $D_x$ = 1.366 Mg m$^{-3}$ |
| Monoclinic, $P2_1/c$ | Mo $K\alpha$ radiation<br>λ = 0.71073 Å |
| Hall symbol: -P 2ybc | Cell parameters from 2500 reflections |
| $a$ = 5.13780 (10) Å | θ = 1.4–28.0º |
| $b$ = 34.0034 (9) Å | μ = 0.82 mm$^{-1}$ |
| $c$ = 7.5922 (2) Å | $T$ = 223 (2) K |
| β = 124.181 (2)º | Lamellar, red |
| $V$ = 1097.27 (5) Å$^3$ | 0.25 × 0.12 × 0.10 mm |
| $Z$ = 2 | |

*Data collection*

| | |
|---|---|
| Bruker APEXII area-detector diffractometer | 2511 independent reflections |
| Radiation source: fine-focus sealed tube | 1528 reflections with $I > 2\sigma(I)$ |
| Monochromator: graphite | $R_{int}$ = 0.056 |
| $T$ = 223(2) K | $\theta_{max}$ = 27.5º |
| φ and ω scans | $\theta_{min}$ = 2.4º |
| Absorption correction: multi-scan (SADABS; Sheldrick, 1996) | $h$ = −6→6 |
| $T_{min}$ = 0.822, $T_{max}$ = 0.923 | $k$ = −43→32 |
| 9237 measured reflections | $l$ = −9→9 |

*Refinement*

| | |
|---|---|
| Refinement on $F^2$ | Secondary atom site location: difference Fourier map |
| Least-squares matrix: full | Hydrogen site location: inferred from neighbouring sites |
| $R[F^2 > 2\sigma(F^2)]$ = 0.049 | H atoms treated by a mixture of |

| | |
|---|---|
| | independent and constrained refinement |
| $wR(F^2) = 0.109$ | $w = 1/[\sigma^2(F_o^2) + (0.0454P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$ |
| $S = 1.02$ | $(\Delta/\sigma)_{max} < 0.001$ |
| 2511 reflections | $\Delta\rho_{max} = 0.31$ e Å$^{-3}$ |
| 140 parameters | $\Delta\rho_{min} = -0.70$ e Å$^{-3}$ |
| Primary atom site location: structure-invariant direct methods | Extinction correction: none |

*Special details*

**Geometry**. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

**Refinement**. Refinement of $F^2$ against ALL reflections. The weighted *R*-factor *wR* and goodness of fit S are based on $F^2$, conventional *R*-factors *R* are based on F, with F set to zero for negative $F^2$. The threshold expression of $F^2 > 2\text{sigma}(F^2)$ is used only for calculating *R*-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. *R*-factors based on $F^2$ are statistically about twice as large as those based on F, and R– factors based on ALL data will be even larger.

*Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å$^2$)*

| | *x* | *y* | *z* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| Co1 | 0.5000 | 1.0000 | 1.0000 | 0.03057 (19) |
| O1 | 0.9434 (4) | 0.98064 (6) | 1.2377 (3) | 0.0348 (5) |
| O1W | 0.5780 (5) | 0.98681 (7) | 0.7663 (4) | 0.0454 (6) |
| H1W | 0.698 (8) | 0.9997 (9) | 0.764 (6) | 0.068* |
| H2W | 0.480 (8) | 0.9701 (10) | 0.680 (5) | 0.068* |
| O2 | 1.1879 (4) | 0.93289 (6) | 1.4790 (3) | 0.0448 (6) |
| N1 | 0.4053 (5) | 0.94044 (6) | 1.0289 (4) | 0.0321 (6) |
| C1 | 0.9548 (6) | 0.94757 (9) | 1.3189 (5) | 0.0336 (7) |
| C2 | 0.6498 (6) | 0.92409 (8) | 1.2061 (4) | 0.0316 (7) |
| C3 | 0.6270 (6) | 0.88849 (8) | 1.2802 (5) | 0.0427 (8) |
| H3 | 0.8022 | 0.8776 | 1.4047 | 0.051* |
| C4 | 0.3432 (7) | 0.86867 (8) | 1.1698 (5) | 0.0458 (8) |
| H4 | 0.3234 | 0.8445 | 1.2209 | 0.055* |
| C5 | 0.0877 (6) | 0.88440 (8) | 0.9838 (5) | 0.0370 (7) |
| C6 | 0.1329 (6) | 0.92054 (8) | 0.9207 (5) | 0.0354 (7) |
| H6 | −0.0371 | 0.9318 | 0.7949 | 0.043* |
| C7 | −0.2300 (7) | 0.86463 (8) | 0.8580 (5) | 0.0457 (8) |
| H7A | −0.3810 | 0.8825 | 0.7444 | 0.055* |
| H7B | −0.3010 | 0.8601 | 0.9521 | 0.055* |
| C8 | −0.2326 (6) | 0.82584 (8) | 0.7594 (5) | 0.0446 (8) |
| H8A | −0.1665 | 0.8303 | 0.6624 | 0.054* |
| H8B | −0.0795 | 0.8081 | 0.8722 | 0.054* |
| C9 | −0.5523 (7) | 0.80628 (10) | 0.6378 (5) | 0.0581 (10) |
| H9A | −0.7079 | 0.8248 | 0.5314 | 0.070* |

| | | | | |
|---|---|---|---|---|
| H9B | −0.6120 | 0.8003 | 0.7368 | 0.070* |
| C10 | −0.5619 (10) | 0.76872 (12) | 0.5266 (7) | 0.0948 (14) |
| H10A | −0.5030 | 0.7744 | 0.4282 | 0.142* |
| H10B | −0.7731 | 0.7579 | 0.4488 | 0.142* |
| H10C | −0.4158 | 0.7498 | 0.6316 | 0.142* |

*Atomic displacement parameters (Å$^2$)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| Co1 | 0.0264 (3) | 0.0264 (3) | 0.0351 (3) | −0.0030 (2) | 0.0149 (2) | −0.0004 (3) |
| O1 | 0.0269 (10) | 0.0321 (12) | 0.0398 (12) | −0.0050 (9) | 0.0153 (9) | 0.0012 (10) |
| O1W | 0.0395 (13) | 0.0501 (16) | 0.0516 (16) | −0.0185 (10) | 0.0287 (12) | −0.0153 (11) |
| O2 | 0.0362 (11) | 0.0369 (13) | 0.0387 (13) | 0.0003 (9) | 0.0073 (10) | 0.0002 (10) |
| N1 | 0.0286 (12) | 0.0266 (14) | 0.0389 (14) | −0.0026 (10) | 0.0176 (12) | −0.0008 (11) |
| C1 | 0.0320 (15) | 0.0300 (17) | 0.0370 (18) | −0.0024 (13) | 0.0183 (15) | −0.0058 (14) |
| C2 | 0.0320 (15) | 0.0258 (16) | 0.0330 (17) | −0.0007 (12) | 0.0160 (14) | −0.0014 (13) |
| C3 | 0.0431 (18) | 0.0366 (19) | 0.0394 (19) | −0.0018 (15) | 0.0178 (16) | 0.0057 (15) |
| C4 | 0.053 (2) | 0.0317 (18) | 0.053 (2) | −0.0074 (16) | 0.0297 (18) | 0.0084 (16) |
| C5 | 0.0409 (17) | 0.0249 (17) | 0.050 (2) | −0.0058 (13) | 0.0286 (16) | −0.0048 (14) |
| C6 | 0.0320 (15) | 0.0266 (17) | 0.0444 (19) | −0.0028 (13) | 0.0194 (14) | −0.0041 (14) |
| C7 | 0.0408 (17) | 0.0341 (18) | 0.064 (2) | −0.0085 (14) | 0.0308 (18) | −0.0058 (16) |
| C8 | 0.0434 (17) | 0.0375 (19) | 0.052 (2) | −0.0067 (15) | 0.0261 (16) | −0.0041 (16) |
| C9 | 0.055 (2) | 0.046 (2) | 0.070 (3) | −0.0183 (17) | 0.033 (2) | −0.0118 (19) |
| C10 | 0.106 (3) | 0.057 (3) | 0.099 (4) | −0.027 (2) | 0.044 (3) | −0.032 (2) |

*Geometric parameters (Å, °)*

| | | | |
|---|---|---|---|
| Co1—O1$^{i}$ | 2.0641 (18) | C4—H4 | 0.9400 |
| Co1—O1 | 2.0641 (18) | C5—C6 | 1.385 (4) |
| Co1—O1W$^{i}$ | 2.076 (2) | C5—C7 | 1.509 (4) |
| Co1—O1W | 2.076 (2) | C6—H6 | 0.9400 |
| Co1—N1$^{i}$ | 2.123 (2) | C7—C8 | 1.513 (4) |
| Co1—N1 | 2.123 (2) | C7—H7A | 0.9800 |
| O1—C1 | 1.268 (3) | C7—H7B | 0.9800 |
| O1W—H1W | 0.76 (3) | C8—C9 | 1.513 (4) |
| O1W—H2W | 0.80 (3) | C8—H8A | 0.9800 |
| O2—C1 | 1.235 (3) | C8—H8B | 0.9800 |
| N1—C2 | 1.341 (3) | C9—C10 | 1.517 (5) |
| N1—C6 | 1.342 (3) | C9—H9A | 0.9800 |
| C1—C2 | 1.523 (4) | C9—H9B | 0.9800 |
| C2—C3 | 1.367 (4) | C10—H10A | 0.9700 |
| C3—C4 | 1.382 (4) | C10—H10B | 0.9700 |
| C3—H3 | 0.9400 | C10—H10C | 0.9700 |
| C4—C5 | 1.386 (4) | | |
| O1$^{i}$—Co1—O1 | 180.000 (1) | C3—C4—H4 | 119.9 |
| O1$^{i}$—Co1—O1W$^{i}$ | 91.72 (9) | C5—C4—H4 | 119.9 |
| O1—Co1—O1W$^{i}$ | 88.28 (8) | C6—C5—C4 | 116.6 (3) |

| | | | |
|---|---|---|---|
| O1$^{i}$—Co1—O1W | 88.28 (8) | C6—C5—C7 | 120.5 (3) |
| O1—Co1—O1W | 91.72 (9) | C4—C5—C7 | 122.8 (3) |
| O1W$^{i}$—Co1—O1W | 180.000 (2) | N1—C6—C5 | 123.8 (3) |
| O1$^{i}$—Co1—N1$^{i}$ | 79.04 (8) | N1—C6—H6 | 118.1 |
| O1—Co1—N1$^{i}$ | 100.96 (8) | C5—C6—H6 | 118.1 |
| O1W$^{i}$—Co1—N1$^{i}$ | 92.73 (9) | C5—C7—C8 | 114.0 (2) |
| O1W—Co1—N1$^{i}$ | 87.27 (9) | C5—C7—H7A | 108.7 |
| O1$^{i}$—Co1—N1 | 100.96 (8) | C8—C7—H7A | 108.7 |
| O1—Co1—N1 | 79.04 (8) | C5—C7—H7B | 108.7 |
| O1W$^{i}$—Co1—N1 | 87.27 (9) | C8—C7—H7B | 108.7 |
| O1W—Co1—N1 | 92.73 (9) | H7A—C7—H7B | 107.6 |
| N1$^{i}$—Co1—N1 | 180.000 (1) | C9—C8—C7 | 112.9 (2) |
| C1—O1—Co1 | 115.76 (16) | C9—C8—H8A | 109.0 |
| Co1—O1W—H1W | 116 (3) | C7—C8—H8A | 109.0 |
| Co1—O1W—H2W | 121 (3) | C9—C8—H8B | 109.0 |
| H1W—O1W—H2W | 122 (4) | C7—C8—H8B | 109.0 |
| C2—N1—C6 | 118.2 (2) | H8A—C8—H8B | 107.8 |
| C2—N1—Co1 | 111.06 (17) | C8—C9—C10 | 113.2 (3) |
| C6—N1—Co1 | 129.70 (18) | C8—C9—H9A | 108.9 |
| O2—C1—O1 | 126.2 (3) | C10—C9—H9A | 108.9 |
| O2—C1—C2 | 117.7 (3) | C8—C9—H9B | 108.9 |
| O1—C1—C2 | 116.1 (2) | C10—C9—H9B | 108.9 |
| N1—C2—C3 | 122.1 (2) | H9A—C9—H9B | 107.7 |
| N1—C2—C1 | 115.8 (2) | C9—C10—H10A | 109.5 |
| C3—C2—C1 | 122.1 (3) | C9—C10—H10B | 109.5 |
| C2—C3—C4 | 119.2 (3) | H10A—C10—H10B | 109.5 |
| C2—C3—H3 | 120.4 | C9—C10—H10C | 109.5 |
| C4—C3—H3 | 120.4 | H10A—C10—H10C | 109.5 |
| C3—C4—C5 | 120.2 (3) | H10B—C10—H10C | 109.5 |

Symmetry codes: (i) −*x*+1, −*y*+2, −*z*+2.

*Hydrogen-bond geometry (Å, °)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| O1W—H2W···O2$^{ii}$ | 0.80 (3) | 1.90 (3) | 2.688 (3) | 170 (3) |
| O1W—H1W···O1$^{iii}$ | 0.76 (3) | 1.97 (3) | 2.712 (3) | 165 (3) |

Symmetry codes: (ii) *x*−1, *y*, *z*−1; (iii) −*x*+2, −*y*+2, −*z*+2.

**Fig. 1**

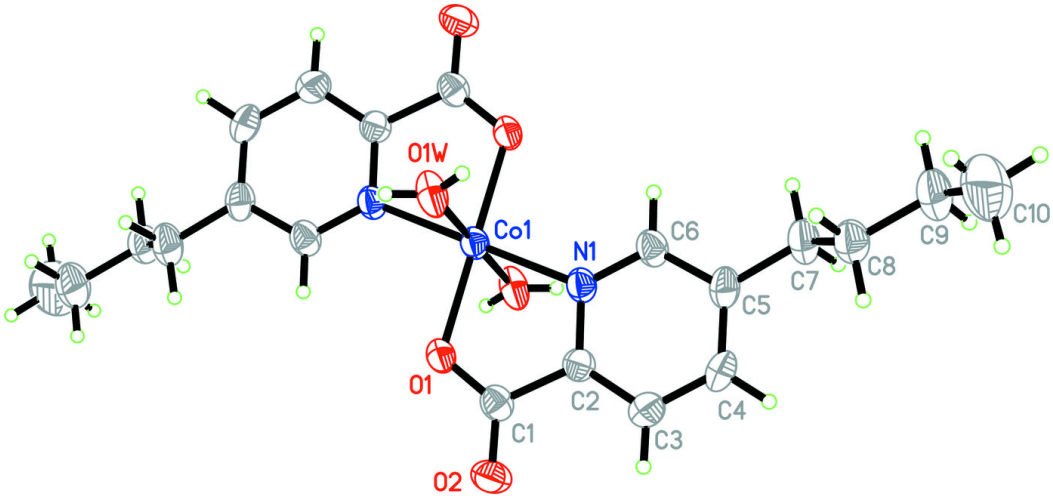


**Fig. 2**