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Diaquabis[2-(2-hydroxyethyl)pyridine- κ^2N,O]cobalt(II) dichloride

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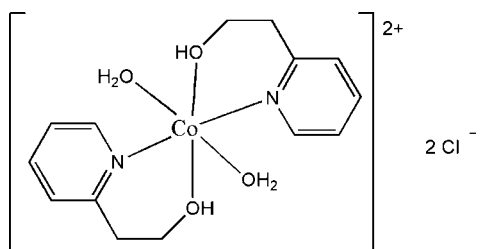
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 Key indicators: single-crystal X-ray study; $T = 293$ K; mean $\sigma(\text{C}-\text{C}) = 0.003$ Å; R factor = 0.020; wR factor = 0.056; data-to-parameter ratio = 13.3.

In the title salt, $[\text{Co}(\text{C}_7\text{H}_9\text{NO})_2(\text{H}_2\text{O})_2]\text{Cl}_2$, the Co^{II} cation, located on an inversion center, is N,O -chelated by two hydroxyethylpyridine ligands and coordinated by two water molecules in a distorted O_4N_2 octahedral geometry. In the crystal, the Cl^- anions link with the complex cations *via* $\text{O}-\text{H}\cdots\text{Cl}$ hydrogen bonds, forming a three-dimensional supra-molecular architecture. $\pi-\pi$ stacking is observed between the pyridine rings of adjacent molecules [centroid-centroid distance = 3.5810 (11) Å].

Related literature

For applications of pyridine derivatives in the synthesis of coordination polymers, see: Sanudo *et al.* (2003); Boskovic *et al.* (2002). For related complexes containing a 2(2-hydroxyethyl)pyridine ligand, see: Kong *et al.* (2009); Mobin *et al.* (2010). For hydrogen-bond motifs, see: Bernstein *et al.* (1995).



Experimental

Crystal data

$[\text{Co}(\text{C}_7\text{H}_9\text{NO})_2(\text{H}_2\text{O})_2]\text{Cl}_2$	$V = 1741.44$ (7) Å ³
$M_r = 412.17$	$Z = 4$
Orthorhombic, <i>Pbcn</i>	Mo $K\alpha$ radiation
$a = 12.8911$ (3) Å	$\mu = 1.31$ mm ⁻¹
$b = 8.0049$ (2) Å	$T = 293$ K
$c = 16.8757$ (4) Å	$0.3 \times 0.2 \times 0.2$ mm

Data collection

Bruker APEXII diffractometer	1419 reflections with $I > 2\sigma(I)$
9407 measured reflections	$R_{\text{int}} = 0.015$
1535 independent reflections	

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.020$	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2) = 0.056$	
$S = 1.04$	
1535 reflections	$\Delta\rho_{\text{max}} = 0.21$ e Å ⁻³
115 parameters	$\Delta\rho_{\text{min}} = -0.22$ e Å ⁻³

Table 1

Selected bond lengths (Å).

Co1—O1	2.1210 (13)	Co1—N1	2.1537 (14)
Co1—O1W	2.0715 (13)		

Table 2

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
O1—H1 \cdots Cl ⁱ	0.84 (2)	2.26 (2)	3.0625 (13)	162 (2)
O1W—H1W \cdots Cl ⁱⁱ	0.932 (11)	2.145 (12)	3.0738 (13)	174.6 (19)
O1W—H2W \cdots Cl ⁱⁱⁱ	0.835 (16)	2.285 (16)	3.1121 (14)	170.4 (15)

 Symmetry codes: (i) $x, -y, z - \frac{1}{2}$; (ii) $-x + 1, y, -z + \frac{1}{2}$; (iii) $x + \frac{1}{2}, y + \frac{1}{2}, -z + \frac{1}{2}$

Data collection: APEX2 (Bruker, 2006); cell refinement: SAINT (Bruker, 2006); data reduction: SAINT; program(s) used to solve structure: SIR2002 (Burla *et al.*, 2005); program(s) used to refine structure: SHELXL97 (Sheldrick, 2008); molecular graphics: ORTEP-3 for Windows (Farrugia, 2012); software used to prepare material for publication: WinGX (Farrugia, 2012), Mercury (Macrae *et al.*, 2006) and POV-RAY (Persistence of Vision Team, 2004).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: XU5717).

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Diaquabis[2-(2-hydroxyethyl)pyridine- κ^2N,O]cobalt(II) dichloride

Ouahida Zeghouan, Fatiha Guenifa, Nasreddine Hadjadj, Lamia Bendjeddou and Hocine Merazig

S1. Comment

Pyridine derivatives ligands have the potential to be used in the synthesis of supramolecular materials, particularly transition metal coordination polymers (Sanudo *et al.*, 2003; Boskovic *et al.*, 2002). A few complexes containing *L* (*L* = 2-(2-hydroxyethyl)pyridine) have been studied for years, because this ligand has a versatile coordination activities and bridging function (Kong *et al.*, 2009; Mobin *et al.*, 2010). We report here the synthesis and crystal structure of the title compound.

The complex comprises two *L* (*L* = 2-(2-hydroxyethyl)pyridine) ligands, one Co^{II} ion, two aqua ligands and uncoordinated Cl anions (Fig. 1). The coordination geometry around the Co center is octahedral with a CoN₂O₄ ligand set (Table 1). The bis *L* ligands coordinate to the Co(II) ions through the nitrogen atom of pyridine ring and the oxygen atom of hydroxyl group, creating a chelate ring. The octahedral geometries are completed by two *trans* aqua ligands at axial positions.

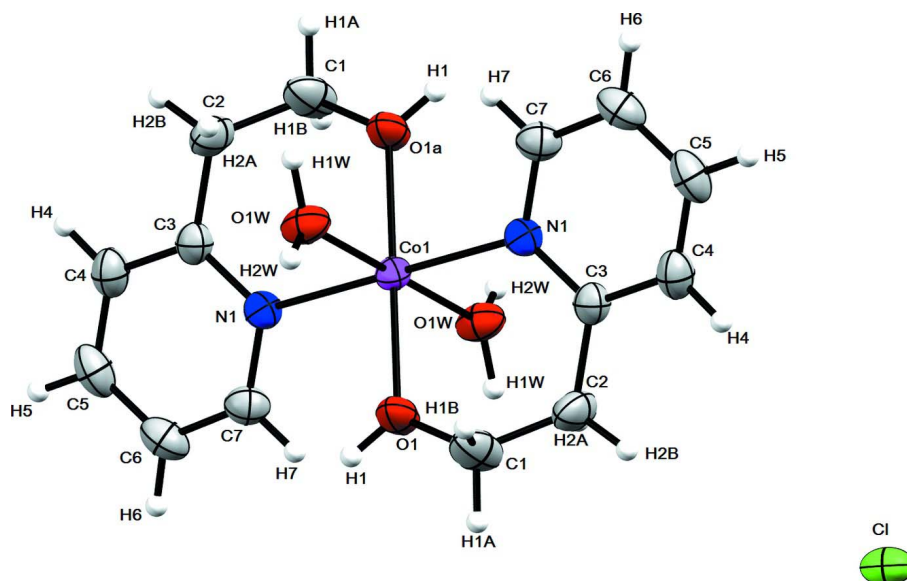
The complex cations are connected *via* O—H...Cl hydrogen bonds (Fig. 2), forming a centrosymmetric and a noncentrosymmetric rings, in two dimensionel network, which can be described by the graph set $R^2_4(12)$ and $R^2_4(10)$, respectively (Bernstein *et al.*, 1995). π - π stacking between the pyridine rings [centroid-centroid distance = 3.5810 (11) Å] is also present (Fig. 3).

S2. Experimental

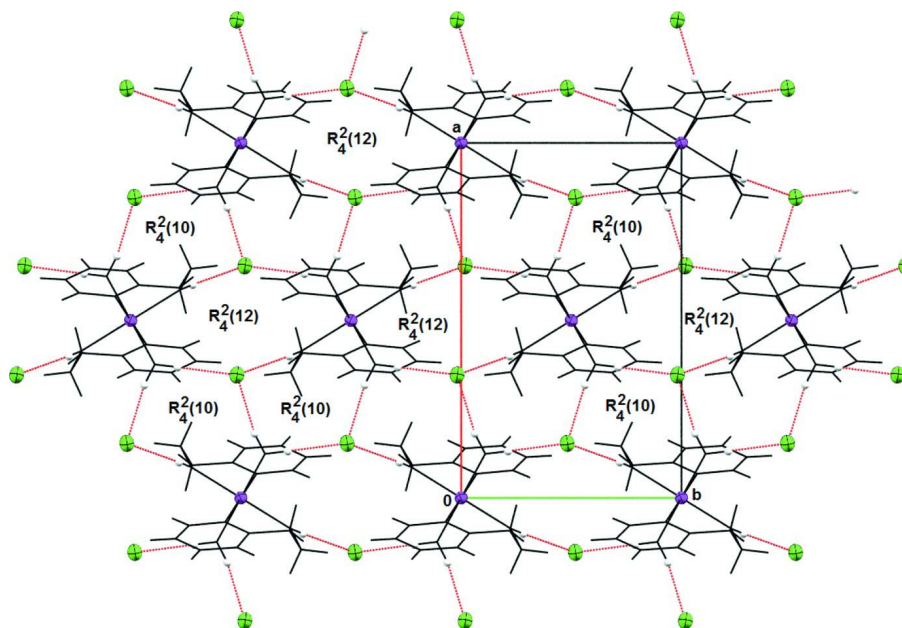
The title compound was prepared by reaction of 2 (2-hydroxyethyl)pyridine (10.0 mmol, 1.67 g) in a mixture of ethanol–water (V/V = 1:1) and CoCl₂·6H₂O (10.0 mmol, 2.50 g), the solution was maintained at 313 K under agitation during 24 h at room temperature. Pink crystals were obtained by slow evaporation of the solvents within 3 weeks.

S3. Refinement

H atoms were placed at calculated positions with C—H = 0.93 Å (aromatic H atoms) and 0.97 Å (methylene H atoms), and refined in riding mode with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$. The O-bound H-atoms was located in a Fourier map and refined with O—H restraint of 0.85 (1) Å, $U_{\text{iso}}(\text{H}) = 1.5U_{\text{eq}}(\text{O})$.

**Figure 1**

The asymmetric unit of the title structure with the atom numbering scheme. Displacement ellipsoids are drawn at the 50% probability level and H atoms are represented as small spheres of arbitrary radii.

**Figure 2**

Part of the crystal structure, showing the aggregation of $R_4^2(12)$ and $R_4^2(10)$ hydrogen-bonding motifs.

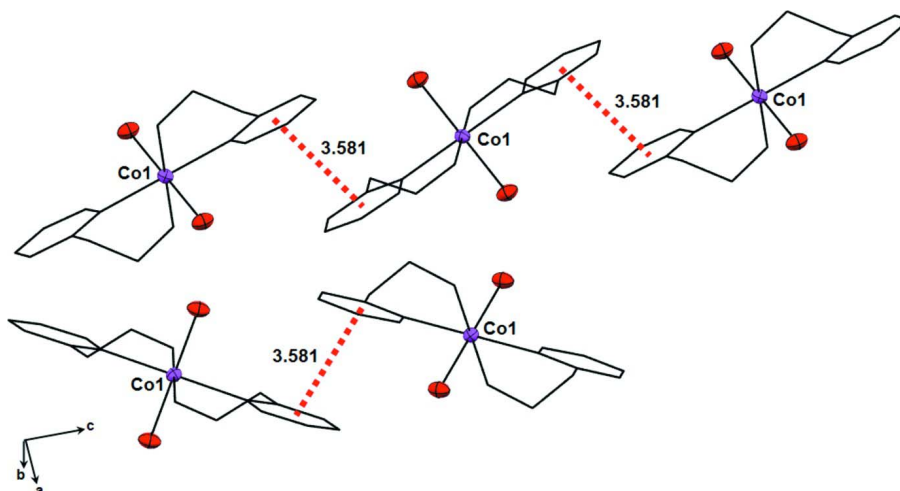


Figure 3

A part of the crystal packing showing π - π stacking interactions between the pyridine rings (dashed lines).

Diaquabis[2-(2-hydroxyethyl)pyridine- κ^2 N,O]cobalt(II) dichloride

Crystal data

$[\text{Co}(\text{C}_7\text{H}_9\text{NO})_2(\text{H}_2\text{O})_2]\text{Cl}_2$

$M_r = 412.17$

Orthorhombic, *Pbcn*

Hall symbol: -P 2n 2ab

$a = 12.8911$ (3) Å

$b = 8.0049$ (2) Å

$c = 16.8757$ (4) Å

$V = 1741.44$ (7) Å³

$Z = 4$

$F(000) = 852$

$D_x = 1.572$ Mg m⁻³

Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å

Cell parameters from 1536 reflections

$\theta = 3.2$ – 25.1°

$\mu = 1.31$ mm⁻¹

$T = 293$ K

Prism, pink

$0.3 \times 0.2 \times 0.2$ mm

Data collection

Bruker APEXII

diffractometer

Radiation source: fine-focus sealed tube

Graphite monochromator

φ scans

9407 measured reflections

1535 independent reflections

1419 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.015$

$\theta_{\text{max}} = 25.1^\circ$, $\theta_{\text{min}} = 3.9^\circ$

$h = -14 \rightarrow 15$

$k = -9 \rightarrow 9$

$l = -19 \rightarrow 20$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.020$

$wR(F^2) = 0.056$

$S = 1.04$

1535 reflections

115 parameters

0 restraints

H atoms treated by a mixture of independent and constrained refinement

$w = 1/[\sigma^2(F_o^2) + (0.0293P)^2 + 0.7255P]$

where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{\text{max}} < 0.001$

$\Delta\rho_{\text{max}} = 0.21$ e Å⁻³

$\Delta\rho_{\text{min}} = -0.22$ e Å⁻³

Special details

Geometry. Bond distances, angles *etc.* have been calculated using the rounded fractional coordinates. All su's are estimated from the variances of the (full) variance-covariance matrix. The cell e.s.d.'s are taken into account in the estimation of distances, angles and torsion angles

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 $F^2 > \sigma(F^2)$ 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 (\AA^2)

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
Co1	0.50000	0.50000	0.00000	0.0229 (1)
O1	0.41357 (11)	0.27513 (16)	0.00777 (7)	0.0360 (4)
O1W	0.62402 (10)	0.39039 (16)	0.05822 (8)	0.0360 (4)
N1	0.43197 (11)	0.57142 (18)	0.11153 (8)	0.0272 (4)
C1	0.35447 (17)	0.2261 (3)	0.07500 (12)	0.0476 (7)
C2	0.40794 (17)	0.2792 (2)	0.15026 (11)	0.0413 (6)
C3	0.40051 (14)	0.4625 (2)	0.16765 (10)	0.0288 (5)
C4	0.36041 (17)	0.5176 (2)	0.23920 (11)	0.0367 (6)
C5	0.35342 (16)	0.6852 (3)	0.25479 (11)	0.0417 (6)
C6	0.38502 (15)	0.7962 (2)	0.19758 (12)	0.0404 (6)
C7	0.42246 (14)	0.7350 (2)	0.12727 (11)	0.0331 (6)
Cl	0.34635 (4)	0.01817 (5)	0.40317 (3)	0.0402 (2)
H1	0.3978 (18)	0.211 (3)	-0.0294 (11)	0.0540*
H1A	0.34570	0.10570	0.07490	0.0570*
H1B	0.28620	0.27680	0.07240	0.0570*
H1W	0.6327 (17)	0.2761 (13)	0.0664 (13)	0.0540*
H2A	0.48060	0.24860	0.14680	0.0500*
H2B	0.37800	0.21780	0.19420	0.0500*
H2W	0.6813 (12)	0.436 (2)	0.0664 (14)	0.0540*
H4	0.33820	0.44050	0.27680	0.0440*
H5	0.32780	0.72310	0.30310	0.0500*
H6	0.38110	0.91080	0.20640	0.0490*
H7	0.44230	0.81090	0.08840	0.0400*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Co1	0.0221 (2)	0.0221 (2)	0.0245 (2)	0.0002 (1)	0.0017 (1)	0.0009 (1)
O1	0.0429 (8)	0.0315 (7)	0.0337 (7)	-0.0128 (6)	0.0066 (6)	-0.0041 (5)
O1W	0.0293 (7)	0.0295 (7)	0.0491 (8)	0.0000 (5)	-0.0083 (6)	0.0071 (6)
N1	0.0259 (7)	0.0276 (7)	0.0280 (7)	0.0020 (6)	0.0025 (6)	-0.0007 (6)
C1	0.0534 (13)	0.0401 (11)	0.0492 (12)	-0.0200 (10)	0.0219 (10)	-0.0088 (9)
C2	0.0564 (13)	0.0310 (10)	0.0365 (10)	-0.0006 (9)	0.0159 (9)	0.0067 (8)
C3	0.0263 (9)	0.0336 (9)	0.0266 (9)	-0.0003 (7)	0.0004 (7)	0.0003 (7)
C4	0.0353 (11)	0.0479 (12)	0.0270 (9)	-0.0029 (8)	0.0034 (8)	-0.0003 (8)
C5	0.0381 (11)	0.0547 (12)	0.0324 (10)	0.0017 (10)	0.0038 (8)	-0.0152 (9)

C6	0.0395 (11)	0.0354 (10)	0.0463 (11)	0.0033 (9)	0.0010 (9)	-0.0134 (9)
C7	0.0306 (10)	0.0297 (9)	0.0389 (10)	0.0004 (7)	0.0022 (8)	-0.0013 (7)
C1	0.0376 (3)	0.0269 (2)	0.0561 (3)	-0.0017 (2)	-0.0020 (2)	0.0015 (2)

Geometric parameters (Å, °)

Co1—O1	2.1210 (13)	C2—C3	1.499 (2)
Co1—O1W	2.0715 (13)	C3—C4	1.386 (3)
Co1—N1	2.1537 (14)	C4—C5	1.370 (3)
Co1—O1 ⁱ	2.1210 (13)	C5—C6	1.374 (3)
Co1—O1W ⁱ	2.0715 (13)	C6—C7	1.371 (3)
Co1—N1 ⁱ	2.1537 (14)	C1—H1A	0.9704
O1—C1	1.422 (2)	C1—H1B	0.9701
O1—H1	0.84 (2)	C2—H2A	0.9699
O1W—H2W	0.835 (16)	C2—H2B	0.9697
O1W—H1W	0.932 (11)	C4—H4	0.9303
N1—C3	1.350 (2)	C5—H5	0.9305
N1—C7	1.342 (2)	C6—H6	0.9307
C1—C2	1.506 (3)	C7—H7	0.9300
O1—Co1—O1W	90.95 (5)	N1—C3—C4	121.20 (15)
O1—Co1—N1	87.56 (5)	C2—C3—C4	120.39 (15)
O1—Co1—O1 ⁱ	180.00	N1—C3—C2	118.40 (15)
O1—Co1—O1W ⁱ	89.05 (5)	C3—C4—C5	120.24 (17)
O1—Co1—N1 ⁱ	92.44 (5)	C4—C5—C6	118.61 (18)
O1W—Co1—N1	90.70 (5)	C5—C6—C7	118.77 (16)
O1 ⁱ —Co1—O1W	89.05 (5)	N1—C7—C6	123.51 (16)
O1W—Co1—O1W ⁱ	180.00	O1—C1—H1A	109.58
O1W—Co1—N1 ⁱ	89.30 (5)	O1—C1—H1B	109.54
O1 ⁱ —Co1—N1	92.44 (5)	C2—C1—H1A	109.58
O1W ⁱ —Co1—N1	89.30 (5)	C2—C1—H1B	109.59
N1—Co1—N1 ⁱ	180.00	H1A—C1—H1B	108.04
O1 ⁱ —Co1—O1W ⁱ	90.95 (5)	C1—C2—H2A	108.66
O1 ⁱ —Co1—N1 ⁱ	87.56 (5)	C1—C2—H2B	108.64
O1W ⁱ —Co1—N1 ⁱ	90.70 (5)	C3—C2—H2A	108.70
Co1—O1—C1	124.41 (12)	C3—C2—H2B	108.72
C1—O1—H1	107.4 (15)	H2A—C2—H2B	107.60
Co1—O1—H1	127.1 (15)	C3—C4—H4	119.87
H1W—O1W—H2W	107.4 (17)	C5—C4—H4	119.89
Co1—O1W—H2W	125.1 (12)	C4—C5—H5	120.72
Co1—O1W—H1W	125.4 (13)	C6—C5—H5	120.67
C3—N1—C7	117.65 (14)	C5—C6—H6	120.60
Co1—N1—C7	117.99 (11)	C7—C6—H6	120.63
Co1—N1—C3	124.34 (11)	N1—C7—H7	118.22
O1—C1—C2	110.47 (17)	C6—C7—H7	118.27
C1—C2—C3	114.33 (16)		

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

Hydrogen-bond geometry (Å, °)

<i>D</i> —H \cdots <i>A</i>	<i>D</i> —H	H \cdots <i>A</i>	<i>D</i> \cdots <i>A</i>	<i>D</i> —H \cdots <i>A</i>
O1—H1 \cdots Cl ⁱⁱ	0.84 (2)	2.26 (2)	3.0625 (13)	162 (2)
O1 <i>W</i> —H1 <i>W</i> \cdots Cl ⁱⁱⁱ	0.932 (11)	2.145 (12)	3.0738 (13)	174.6 (19)
O1 <i>W</i> —H2 <i>W</i> \cdots Cl ^{iv}	0.835 (16)	2.285 (16)	3.1121 (14)	170.4 (15)

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