

Diaquabis(2,2'-biimidazole)cobalt(II) dichloride

Lan-Cui Zhang,^{a,b} Zai-Ming Zhu,^b Wan-Sheng You,^c Song Chang^a and En-Bo Wang^{a*}

^aKey Laboratory of Polyoxometalate Science of the Ministry of Education, Faculty of Chemistry, Institute of Polyoxometalate Chemistry, Northeast Normal University, Ren Min Street No. 5268, Changchun, Jilin 130024, People's Republic of China, ^bCollege of Chemistry and Chemical Engineering, Liaoning Normal University, Dalian 116029, People's Republic of China, and ^cInstitute of Chemistry for Functionalized Materials, College of Chemistry and Chemical Engineering, Liaoning Normal University, Dalian 116029, People's Republic of China
Correspondence e-mail: wangenbo@public.cc.jl.cn

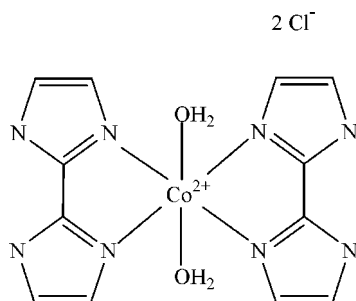
Received 4 November 2007; accepted 24 December 2007

Key indicators: single-crystal X-ray study; $T = 298$ K; mean $\sigma(\text{C}-\text{C}) = 0.003$ Å; R factor = 0.033; wR factor = 0.086; data-to-parameter ratio = 16.0.

There are independent cations and four chloride anions in the crystal structure of the title complex, $[\text{Co}(\text{C}_6\text{H}_6\text{N}_4)_2(\text{H}_2\text{O})_2]\text{Cl}_2$. In each cation, the Co^{II} cation is coordinated by four N atoms from two biimidazole and two O atoms of two water molecules; one Co atom is at a position of site symmetry m , the other at a position of site symmetry $2/m$. All Cl^- ions and water molecules are also located on the mirror plane. Each structural unit is connected through $\text{O}-\text{H}\cdots\text{Cl}$ and $\text{N}-\text{H}\cdots\text{Cl}$ intermolecular hydrogen bonds, forming a three-dimensional supramolecular structure.

Related literature

For related literature, see: Barquin *et al.* (2003); Hirotsoshi & Eisaku (2005); Tadokoro & Nakasuji (2000; Roth *et al.* (2000); Fieselmann *et al.* (1978).



Experimental

Crystal data

$[\text{Co}(\text{C}_6\text{H}_6\text{N}_4)_2(\text{H}_2\text{O})_2]\text{Cl}_2$
 $M_r = 434.16$

Monoclinic, $C2/m$
 $a = 22.037$ (3) Å

$b = 12.5321$ (17) Å
 $c = 9.6421$ (13) Å
 $\beta = 95.848$ (2)°
 $V = 2649.0$ (6) Å³
 $Z = 6$

Mo $K\alpha$ radiation
 $\mu = 1.30$ mm⁻¹
 $T = 298$ (2) K
 $0.16 \times 0.12 \times 0.08$ mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2003)
 $T_{\text{min}} = 0.819$, $T_{\text{max}} = 0.903$

8119 measured reflections
3205 independent reflections
2291 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.026$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.033$
 $wR(F^2) = 0.085$
 $S = 1.04$
3205 reflections
200 parameters
6 restraints

H atoms treated by a mixture of independent and constrained refinement
 $\Delta\rho_{\text{max}} = 0.29$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.24$ e Å⁻³

Table 1

Hydrogen-bond geometry (Å, °).

$D-\text{H}\cdots A$	$D-\text{H}$	$\text{H}\cdots A$	$D\cdots A$	$D-\text{H}\cdots A$
$\text{N4}-\text{H4B}\cdots\text{Cl1}^{\text{i}}$	0.86	2.40	3.213 (2)	157
$\text{N5}-\text{H5B}\cdots\text{Cl3}^{\text{ii}}$	0.86	2.42	3.2091 (19)	153
$\text{N6}-\text{H6B}\cdots\text{Cl2}^{\text{i}}$	0.86	2.42	3.210 (2)	154
$\text{O3W}-\text{H3C}\cdots\text{Cl1}^{\text{i}}$	0.86 (3)	2.29 (3)	3.150 (2)	175 (4)
$\text{O2W}-\text{H2B}\cdots\text{Cl3}^{\text{iii}}$	0.86 (3)	2.34 (3)	3.180 (3)	166 (4)
$\text{O2W}-\text{H2C}\cdots\text{Cl3}^{\text{iv}}$	0.860 (10)	2.236 (11)	3.096 (3)	178 (3)
$\text{O1W}-\text{H1A}\cdots\text{Cl2}$	0.857 (10)	2.259 (11)	3.114 (2)	175 (3)
$\text{O1W}-\text{H1B}\cdots\text{Cl1}$	0.857 (10)	2.285 (11)	3.139 (2)	174 (3)
$\text{O3W}-\text{H3B}\cdots\text{Cl2}$	0.859 (10)	2.239 (11)	3.096 (2)	177 (3)

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

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINT* (Bruker, 2001); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Bruker, 1997); software used to prepare material for publication: *SHELXTL*.

The authors are grateful to Professor Guang-Ning Zhang for his selfless help with our work.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: RK2059).

References

- Barquin, M., Gonzalez Garmendia, M. J. & Bellido, V. (2003). *Transition Met. Chem.* **28**, 356–360.
Bruker (1997). *SHELXTL*. Version 5.10. Bruker AXS inc., Madison, Wisconsin, USA.
Bruker (2001). *SAINT* and *SMART*. Bruker AXS inc., Madison, Wisconsin, USA.
Fieselmann, B. F., Hendrickson, D. N. & Stucky, G. D. (1978). *Inorg. Chem.* **17**, 333–334.
Hirotsoshi, M. & Eisaku, M. (2005). *J. Theor. Cancer Chem.* **4**, 2078–2084.
Roth, J. P., Lovell, S. & Mayer, J. M. (2000). *J. Am. Chem. Soc.* **122**, 5486–5498.
Sheldrick, G. M. (2003). *SADABS*. University of Göttingen, Germany.
Sheldrick, G. M. (2008). *Acta Cryst.* **A64**, 112–122.
Tadokoro, M. & Nakasuji, K. (2000). *Coord. Chem. Rev.* **198**, 205–218.

supplementary materials

Acta Cryst. (2008). E64, m308 [doi:10.1107/S160053680706833X]

Diaquabis(2,2'-biimidazole)cobalt(II) dichloride

L.-C. Zhang, Z.-M. Zhu, W.-S. You, S. Chang and E.-B. Wang

Comment

The imidazole coordinated complexes have various structures and extensive uses in the field of catalysis, materials and bio-activity (Barquin *et al.*, 2003; Hirotohi & Eisaku, 2005). The bis(2,2'-biimidazole)dihydrate cobalt dichloride was synthesized. The 2,2'-biimidazole is an interesting dicyclo-ligand of containing four N atoms: the two N atoms forming coordinate bonds and the other two - uncoordinated N atoms of biimidazole form N—H...Cl hydrogen bonds. This crystal structure are constructed by intermolecular hydrogen bonds (Tadokoro & Nakasuji, 2000; Roth *et al.*, 2000).

The average bond distance Co—N is of 2.1563 (18) Å, the average bond angle N—Co—N is 101.50 (8)°, the average bond distance Co—O is 2.091 (2) Å. These parameters show, that the polyhedron configuration is distorted octahedron (Fig. 1.). The biimidazole moieties and Cl atoms are linked by N—H...Cl and the water molecules and Cl atoms are linked by O—H...Cl hydrogen bonds, which shown on Fig. 2.

Experimental

The 2,2'-biimidazole was prepared according to (Fieselmann *et al.*, 1978). 2,2'-Biimidazole (0.1 mmol) was mixed with 0.1 mmol CoCl₂·6H₂O in solution. After 10 min of stirring, the precipitate was filtered off, the resulting clear solution was allowed to stand at room temperature, after a few days yellow block-shaped crystals were obtained.

Refinement

H atoms of water molecules are located in a difference map and refined with distance restraints of O—H = 0.86 (1) Å.

Figures

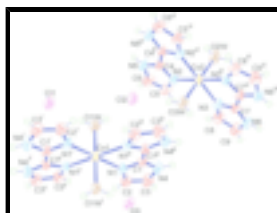


Fig. 1. The molecular structure of the title complex with the atom labeling scheme. Displacement ellipsoids are drawn at 50% probability level. H atoms are presented as small spheres of arbitrary radius.

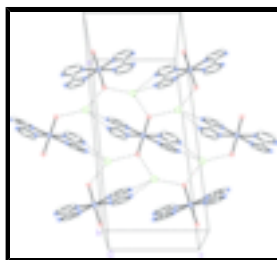


Fig. 2. The packing diagram of title complex - viewed down the *b* axis. Dashed lines show hydrogen bonds.

Diaquabis(2,2'-biimidazole)cobalt(II) dichloride

Crystal data

$[\text{Co}(\text{C}_6\text{H}_6\text{N}_4)_2(\text{H}_2\text{O})_2]\text{Cl}_2$	$F_{000} = 1326$
$M_r = 434.16$	$D_x = 1.633 \text{ Mg m}^{-3}$
Monoclinic, $C2/m$	Mo $K\alpha$ radiation
Hall symbol: $-C 2y$	$\lambda = 0.71073 \text{ \AA}$
$a = 22.037 (3) \text{ \AA}$	Cell parameters from 2062 reflections
$b = 12.5321 (17) \text{ \AA}$	$\theta = 2.7\text{--}26.7^\circ$
$c = 9.6421 (13) \text{ \AA}$	$\mu = 1.30 \text{ mm}^{-1}$
$\beta = 95.848 (2)^\circ$	$T = 298 (2) \text{ K}$
$V = 2649.0 (6) \text{ \AA}^3$	Block, yellow
$Z = 6$	$0.16 \times 0.12 \times 0.08 \text{ mm}$

Data collection

Bruker SMART CCD area-detector diffractometer	3205 independent reflections
Radiation source: fine-focus sealed tube	2291 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{\text{int}} = 0.026$
$T = 298(2) \text{ K}$	$\theta_{\text{max}} = 27.7^\circ$
φ and ω scans	$\theta_{\text{min}} = 1.9^\circ$
Absorption correction: multi-scan (SADABS; Sheldrick, 2003)	$h = -24 \rightarrow 28$
$T_{\text{min}} = 0.819$, $T_{\text{max}} = 0.903$	$k = -16 \rightarrow 15$
8119 measured reflections	$l = -11 \rightarrow 12$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.033$	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2) = 0.085$	$w = 1/[\sigma^2(F_o^2) + (0.0613P)^2]$
$S = 1.05$	where $P = (F_o^2 + 2F_c^2)/3$
3205 reflections	$(\Delta/\sigma)_{\text{max}} = 0.001$
200 parameters	$\Delta\rho_{\text{max}} = 0.29 \text{ e \AA}^{-3}$
6 restraints	$\Delta\rho_{\text{min}} = -0.24 \text{ e \AA}^{-3}$
Primary atom site location: structure-invariant direct methods	Extinction correction: none

Special details

Geometry. All s.u.'s (except the s.u.'s in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell s.u.'s are taken into account individually in the estimation of s.u.'s in distances, angles and torsion angles; correlations between s.u.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell s.u.'s is used for estimating s.u.'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 $F^2 > 2\sigma(F^2)$ 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)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
Co1	0.0000	0.0000	0.5000	0.03508 (16)
Co2	0.332770 (17)	0.0000	0.08867 (4)	0.03888 (14)
O1W	0.09155 (10)	0.0000	0.5815 (2)	0.0493 (6)
H1A	0.1231 (9)	0.0000	0.536 (3)	0.049 (10)*
H1B	0.0984 (16)	0.0000	0.6706 (11)	0.071 (12)*
O2W	0.42387 (11)	0.0000	0.0446 (2)	0.0836 (10)
H2B	0.4517 (13)	0.0000	0.114 (3)	0.090 (14)*
H2C	0.4321 (16)	0.0000	-0.0407 (16)	0.074 (12)*
O3W	0.24136 (10)	0.0000	0.1289 (2)	0.0544 (6)
H3B	0.2314 (15)	0.0000	0.2127 (16)	0.065 (12)*
H3C	0.2115 (12)	0.0000	0.064 (3)	0.083 (13)*
N1	0.01986 (7)	0.10903 (15)	0.33535 (16)	0.0378 (4)
N2	0.35622 (8)	0.10868 (16)	0.25695 (16)	0.0413 (4)
N3	0.30994 (8)	0.10867 (16)	-0.07959 (16)	0.0420 (4)
N4	0.05671 (8)	0.12463 (16)	0.13273 (17)	0.0458 (5)
H4B	0.0719	0.1074	0.0571	0.055*
N5	0.38823 (8)	0.12580 (16)	0.47968 (18)	0.0471 (5)
H5B	0.4007	0.1093	0.5644	0.056*
N6	0.27788 (8)	0.12601 (17)	-0.30166 (17)	0.0494 (5)
H6B	0.2653	0.1097	-0.3864	0.059*
C1	0.04173 (8)	0.05762 (17)	0.23184 (19)	0.0363 (5)
C2	0.02053 (10)	0.2150 (2)	0.2986 (2)	0.0446 (5)
H2A	0.0073	0.2710	0.3511	0.054*
C3	0.04345 (11)	0.2251 (2)	0.1741 (2)	0.0516 (6)
H3A	0.0490	0.2883	0.1264	0.062*
C4	0.37410 (9)	0.05749 (18)	0.37374 (19)	0.0379 (5)
C5	0.35969 (10)	0.2148 (2)	0.2901 (2)	0.0509 (6)
H5A	0.3502	0.2704	0.2277	0.061*
C6	0.37892 (11)	0.2268 (2)	0.4267 (2)	0.0546 (6)
H6A	0.3847	0.2907	0.4752	0.066*
C7	0.29209 (9)	0.05720 (19)	-0.19698 (19)	0.0397 (5)
C8	0.30664 (10)	0.2147 (2)	-0.1125 (2)	0.0526 (6)
H8A	0.3164	0.2702	-0.0501	0.063*

supplementary materials

C9	0.28699 (10)	0.2271 (2)	-0.2492 (3)	0.0564 (6)
H9A	0.2809	0.2910	-0.2976	0.068*
Cl1	0.12670 (4)	0.0000	0.90521 (8)	0.0602 (3)
Cl2	0.21127 (4)	0.0000	0.43563 (7)	0.0551 (2)
Cl3	0.04319 (4)	0.5000	0.25997 (7)	0.0501 (2)

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Co1	0.0382 (3)	0.0427 (4)	0.0243 (3)	0.000	0.0025 (2)	0.000
Co2	0.0385 (2)	0.0531 (3)	0.0243 (2)	0.000	-0.00013 (16)	0.000
O1W	0.0386 (13)	0.0814 (19)	0.0279 (12)	0.000	0.0031 (10)	0.000
O2W	0.0386 (14)	0.181 (3)	0.0307 (14)	0.000	0.0011 (11)	0.000
O3W	0.0406 (13)	0.093 (2)	0.0289 (12)	0.000	0.0017 (10)	0.000
N1	0.0417 (10)	0.0429 (12)	0.0285 (8)	-0.0017 (8)	0.0025 (7)	-0.0009 (8)
N2	0.0435 (10)	0.0495 (13)	0.0293 (9)	-0.0028 (9)	-0.0034 (7)	0.0027 (8)
N3	0.0447 (10)	0.0503 (13)	0.0304 (9)	-0.0030 (9)	0.0008 (7)	0.0019 (8)
N4	0.0582 (12)	0.0493 (13)	0.0309 (9)	-0.0039 (10)	0.0096 (8)	0.0030 (8)
N5	0.0574 (12)	0.0506 (13)	0.0307 (9)	-0.0015 (10)	-0.0080 (8)	-0.0006 (9)
N6	0.0546 (12)	0.0630 (15)	0.0296 (9)	-0.0007 (10)	-0.0002 (8)	0.0054 (9)
C1	0.0365 (11)	0.0453 (13)	0.0265 (10)	-0.0024 (9)	0.0003 (8)	0.0024 (9)
C2	0.0488 (13)	0.0448 (15)	0.0397 (12)	-0.0014 (11)	0.0018 (9)	-0.0037 (10)
C3	0.0629 (15)	0.0451 (16)	0.0468 (14)	-0.0034 (13)	0.0055 (11)	0.0066 (11)
C4	0.0372 (11)	0.0476 (13)	0.0283 (10)	-0.0022 (10)	-0.0003 (8)	-0.0015 (9)
C5	0.0551 (14)	0.0509 (16)	0.0445 (13)	-0.0044 (12)	-0.0059 (10)	0.0076 (11)
C6	0.0637 (15)	0.0473 (16)	0.0504 (14)	-0.0053 (13)	-0.0066 (11)	-0.0051 (12)
C7	0.0364 (11)	0.0540 (14)	0.0287 (10)	0.0006 (10)	0.0030 (8)	0.0037 (9)
C8	0.0546 (14)	0.0570 (18)	0.0459 (13)	-0.0091 (12)	0.0040 (11)	0.0014 (12)
C9	0.0639 (16)	0.0559 (18)	0.0489 (14)	-0.0009 (13)	0.0032 (12)	0.0097 (12)
Cl1	0.0536 (5)	0.0994 (8)	0.0274 (4)	0.000	0.0029 (3)	0.000
Cl2	0.0528 (5)	0.0848 (7)	0.0280 (4)	0.000	0.0056 (3)	0.000
Cl3	0.0622 (5)	0.0554 (6)	0.0305 (4)	0.000	-0.0065 (3)	0.000

Geometric parameters (\AA , $^\circ$)

Co1—O1W	2.089 (2)	N3—C8	1.366 (3)
Co1—O1W ⁱ	2.089 (2)	N4—C1	1.338 (3)
Co1—N1 ⁱⁱ	2.1727 (17)	N4—C3	1.362 (3)
Co1—N1 ⁱ	2.1727 (17)	N4—H4B	0.8600
Co1—N1 ⁱⁱⁱ	2.1727 (17)	N5—C4	1.345 (3)
Co1—N1	2.1727 (17)	N5—C6	1.372 (3)
Co2—O3W	2.090 (2)	N5—H5B	0.8600
Co2—O2W	2.094 (2)	N6—C7	1.340 (3)
Co2—N3 ⁱⁱⁱ	2.1386 (18)	N6—C9	1.371 (3)
Co2—N3	2.1386 (18)	N6—H6B	0.8600
Co2—N2	2.1410 (18)	C1—C1 ⁱⁱⁱ	1.444 (4)
Co2—N2 ⁱⁱⁱ	2.1410 (18)	C2—C3	1.355 (3)

O1W—H1A	0.857 (10)	C2—H2A	0.9300
O1W—H1B	0.857 (10)	C3—H3A	0.9300
O2W—H2B	0.86 (3)	C4—C4 ⁱⁱⁱ	1.441 (4)
O2W—H2C	0.860 (10)	C5—C6	1.351 (3)
O3W—H3B	0.859 (10)	C5—H5A	0.9300
O3W—H3C	0.86 (3)	C6—H6A	0.9300
N1—C1	1.320 (2)	C7—C7 ⁱⁱⁱ	1.434 (5)
N1—C2	1.374 (3)	C8—C9	1.354 (3)
N2—C4	1.321 (3)	C8—H8A	0.9300
N2—C5	1.368 (3)	C9—H9A	0.9300
N3—C7	1.327 (3)		
O1W—Co1—O1W ⁱ	180.00 (4)	C4—N2—C5	105.57 (17)
O1W—Co1—N1 ⁱⁱ	89.08 (6)	C4—N2—Co2	111.42 (15)
O1W ⁱ —Co1—N1 ⁱⁱ	90.92 (6)	C5—N2—Co2	143.01 (14)
O1W—Co1—N1 ⁱ	89.08 (6)	C7—N3—C8	105.70 (18)
O1W ⁱ —Co1—N1 ⁱ	90.92 (6)	C7—N3—Co2	111.34 (16)
N1 ⁱⁱ —Co1—N1 ⁱ	77.93 (9)	C8—N3—Co2	142.96 (15)
O1W—Co1—N1 ⁱⁱⁱ	90.92 (6)	C1—N4—C3	107.16 (18)
O1W ⁱ —Co1—N1 ⁱⁱⁱ	89.08 (6)	C1—N4—H4B	126.4
N1 ⁱⁱ —Co1—N1 ⁱⁱⁱ	180.0	C3—N4—H4B	126.4
N1 ⁱ —Co1—N1 ⁱⁱⁱ	102.07 (9)	C4—N5—C6	106.87 (18)
O1W—Co1—N1	90.92 (6)	C4—N5—H5B	126.6
O1W ⁱ —Co1—N1	89.08 (6)	C6—N5—H5B	126.6
N1 ⁱⁱ —Co1—N1	102.07 (9)	C7—N6—C9	107.62 (19)
N1 ⁱ —Co1—N1	180.0	C7—N6—H6B	126.2
N1 ⁱⁱⁱ —Co1—N1	77.93 (9)	C9—N6—H6B	126.2
O3W—Co2—O2W	179.00 (9)	N1—C1—N4	111.7 (2)
O3W—Co2—N3 ⁱⁱⁱ	89.09 (6)	N1—C1—C1 ⁱⁱⁱ	119.22 (12)
O2W—Co2—N3 ⁱⁱⁱ	90.14 (7)	N4—C1—C1 ⁱⁱⁱ	128.86 (12)
O3W—Co2—N3	89.09 (6)	C3—C2—N1	109.5 (2)
O2W—Co2—N3	90.14 (7)	C3—C2—H2A	125.2
N3 ⁱⁱⁱ —Co2—N3	79.11 (10)	N1—C2—H2A	125.2
O3W—Co2—N2	91.27 (7)	C2—C3—N4	106.4 (2)
O2W—Co2—N2	89.50 (7)	C2—C3—H3A	126.8
N3 ⁱⁱⁱ —Co2—N2	179.64 (7)	N4—C3—H3A	126.8
N3—Co2—N2	100.94 (7)	N2—C4—N5	111.4 (2)
O3W—Co2—N2 ⁱⁱⁱ	91.27 (7)	N2—C4—C4 ⁱⁱⁱ	119.06 (12)
O2W—Co2—N2 ⁱⁱⁱ	89.50 (7)	N5—C4—C4 ⁱⁱⁱ	129.54 (12)
N3 ⁱⁱⁱ —Co2—N2 ⁱⁱⁱ	100.94 (7)	C6—C5—N2	109.9 (2)
N3—Co2—N2 ⁱⁱⁱ	179.64 (7)	C6—C5—H5A	125.0
N2—Co2—N2 ⁱⁱⁱ	79.01 (10)	N2—C5—H5A	125.0
Co1—O1W—H1A	128 (2)	C5—C6—N5	106.3 (2)
Co1—O1W—H1B	116 (2)	C5—C6—H6A	126.9
H1A—O1W—H1B	116 (3)	N5—C6—H6A	126.9

supplementary materials

Co2—O2W—H2B	118 (3)	N3—C7—N6	110.8 (2)
Co2—O2W—H2C	120 (2)	N3—C7—C7 ⁱⁱⁱ	119.08 (13)
H2B—O2W—H2C	123 (4)	N6—C7—C7 ⁱⁱⁱ	130.05 (13)
Co2—O3W—H3B	121 (2)	C9—C8—N3	110.0 (2)
Co2—O3W—H3C	123 (3)	C9—C8—H8A	125.0
H3B—O3W—H3C	116 (3)	N3—C8—H8A	125.0
C1—N1—C2	105.19 (17)	C8—C9—N6	105.8 (2)
C1—N1—Co1	111.22 (14)	C8—C9—H9A	127.1
C2—N1—Co1	143.52 (14)	N6—C9—H9A	127.1

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

Hydrogen-bond geometry ($\text{\AA}, ^\circ$)

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
N4—H4B \cdots C11 ^{iv}	0.86	2.40	3.213 (2)	157
N5—H5B \cdots Cl3 ^v	0.86	2.42	3.2091 (19)	153
N6—H6B \cdots Cl2 ^{iv}	0.86	2.42	3.210 (2)	154
O3W—H3C \cdots C11 ^{iv}	0.86 (3)	2.29 (3)	3.150 (2)	175 (4)
O2W—H2B \cdots Cl3 ^{vi}	0.86 (3)	2.34 (3)	3.180 (3)	166 (4)
O2W—H2C \cdots Cl3 ^{vii}	0.860 (10)	2.236 (11)	3.096 (3)	178 (3)
O1W—H1A \cdots Cl2	0.857 (10)	2.259 (11)	3.114 (2)	175 (3)
O1W—H1B \cdots Cl1	0.857 (10)	2.285 (11)	3.139 (2)	174 (3)
O3W—H3B \cdots Cl2	0.859 (10)	2.239 (11)	3.096 (2)	177 (3)

Symmetry codes: (iv) $x, y, z-1$; (v) $-x+1/2, -y+1/2, -z+1$; (vi) $x+1/2, y-1/2, z$; (vii) $-x+1/2, -y+1/2, -z$.

Fig. 1

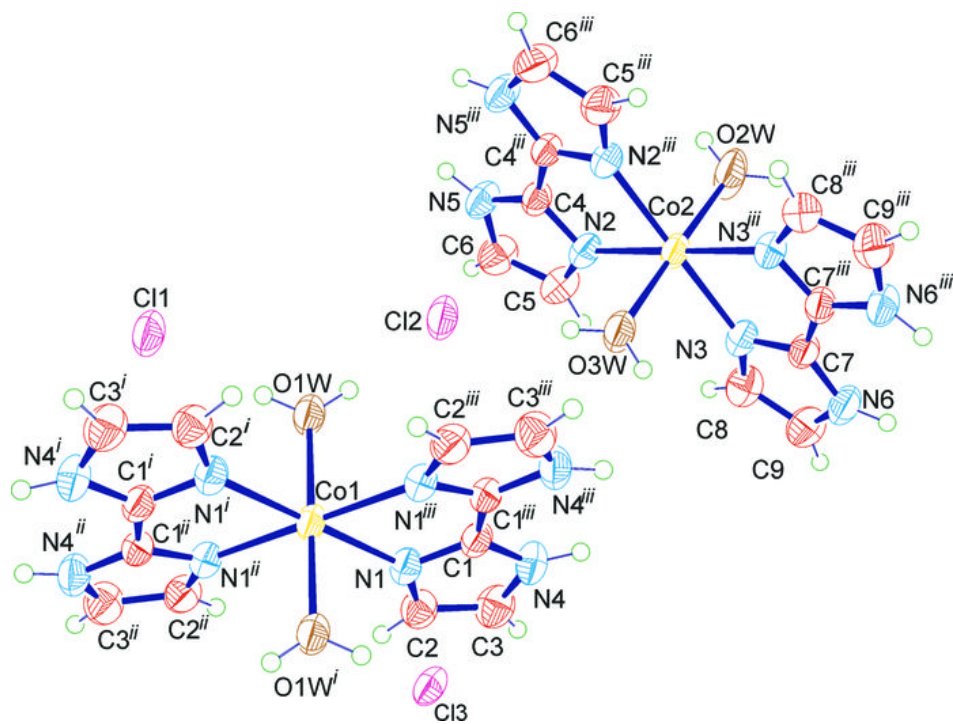


Fig. 2

