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

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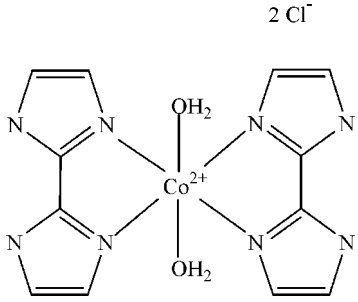
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.003 Å; R factor = 0.033; wR factor = 0.086; data-to-parameter ratio = 16.0.

There are independent cations and four chloride anions in the crystal structure of the title complex, $[Co(C_6H_6N_4)_2(H_2O)_2]Cl_2$. 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 O—H···Cl and N—H···Cl intermolecular hydrogen bonds, forming a three–dimensional supramolecular structure.

Related literature

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



Experimental

Crystal data

$[Co(C_6H_6N_4)_2(H_2O)_2]Cl_2$
M_r = 434.16
Monoclinic, $C2/m$
a = 22.037 (3) Å
b = 12.5321 (17) Å
c = 9.6421 (13) Å
β = 95.848 (2)°
V = 2649.0 (6) Å^3
Z = 6
Mo $K\alpha$ radiation
μ = 1.30 mm^{-1}
T = 298 (2) K
0.16 × 0.12 × 0.08 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2003)
T_{min} = 0.819, T_{max} = 0.903
8119 measured reflections
3205 independent reflections
2291 reflections with $I > 2\sigma(I)$
R_{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
$\Delta\rho_{max}$ = 0.29 e Å^{-3}
$\Delta\rho_{min}$ = −0.24 e Å^{-3}

Table 1
Hydrogen-bond geometry (Å, °).

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

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

Lan-Cui Zhang, Zai-Ming Zhu, Wan-Sheng You, Song Chang and En-Bo Wang

S1. Comment

The imidazole coordinated complexes have various structures and extensive uses in the field of catalysis, materials and bioactivity (Barquin *et al.*, 2003; Hirotoshi & 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 polihedron 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.

S2. 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 $CoCl_2{\cdot}6H_2O$ 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.

S3. Refinement

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

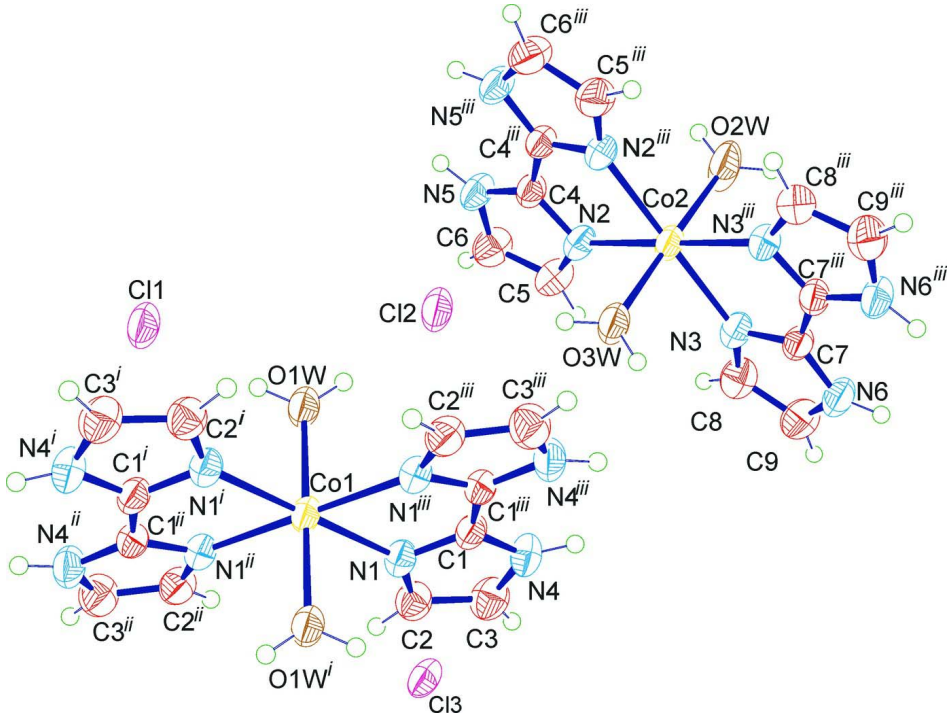

Figure 1

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.

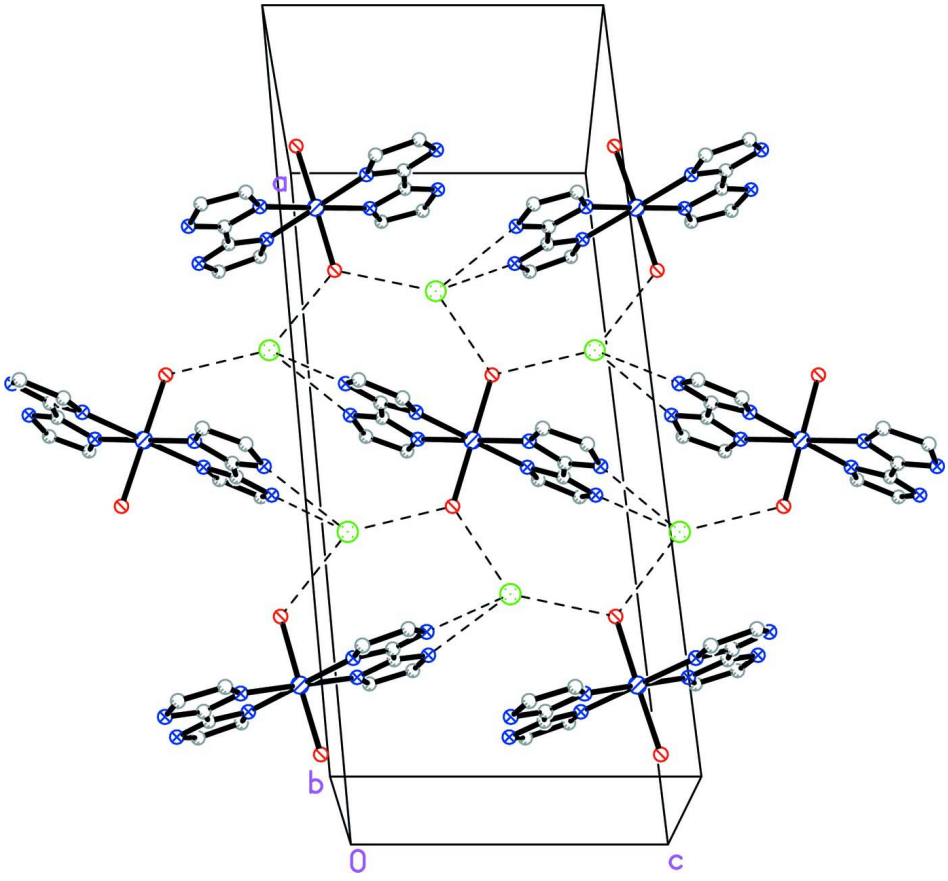

Figure 2

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

$[Co(C_6H_6N_4)_2(H_2O)_2]Cl_2$
$M_r = 434.16$
Monoclinic, *C*2/*m*
Hall symbol: -C 2y
$a = 22.037\ (3)$ Å
$b = 12.5321\ (17)$ Å
$c = 9.6421\ (13)$ Å
$\beta = 95.848\ (2)°$
$V = 2649.0\ (6)$ Å^3
$Z = 6$

$F(000) = 1326$
$D_x = 1.633$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 2062 reflections
$\theta = 2.7–26.7°$
$\mu = 1.30$ mm^{-1}
$T = 298$ K
Block, yellow
0.16 × 0.12 × 0.08 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Radiation source: fine–focus sealed tube
Graphite monochromator
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2003)
$T_{min} = 0.819$, $T_{max} = 0.903$

8119 measured reflections
3205 independent reflections
2291 reflections with $I > 2\sigma(I)$
$R_{int} = 0.026$
$\theta_{max} = 27.7°$, $\theta_{min} = 1.9°$
$h = -24\rightarrow28$
$k = -16\rightarrow15$
$l = -11\rightarrow12$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.033$
$wR(F^2) = 0.085$
$S = 1.05$
3205 reflections
200 parameters
6 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0613P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.29$ e Å^{-3}
$\Delta\rho_{min} = -0.24$ e Å^{-3}

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 (Å²)

	x	*y*	*z*	U_{iso}*/U_{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*
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 (Å²)

	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 (Å, º)

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
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 (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N4—H4*B*···Cl1^{iv}	0.86	2.40	3.213 (2)	157
N5—H5*B*···Cl3^{v}	0.86	2.42	3.2091 (19)	153
N6—H6*B*···Cl2^{iv}	0.86	2.42	3.210 (2)	154
O3*W*—H3*C*···Cl1^{iv}	0.86 (3)	2.29 (3)	3.150 (2)	175 (4)
O2*W*—H2*B*···Cl3^{vi}	0.86 (3)	2.34 (3)	3.180 (3)	166 (4)
O2*W*—H2*C*···Cl3^{vii}	0.86 (1)	2.24 (1)	3.096 (3)	178 (3)
O1*W*—H1*A*···Cl2	0.86 (1)	2.26 (1)	3.114 (2)	175 (3)
O1*W*—H1*B*···Cl1	0.86 (1)	2.29 (1)	3.139 (2)	174 (3)
O3*W*—H3*B*···Cl2	0.86 (1)	2.24 (1)	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*.