

## Dichlorido(dimethylglyoximato- $\kappa^2N,N'$ )-(dimethylglyoxime- $\kappa^2N,N'$ )cobalt(III)

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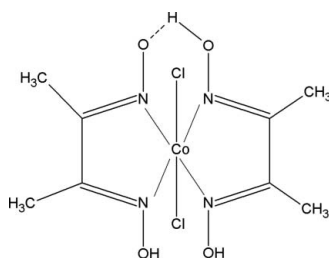
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Key indicators: single-crystal X-ray study;  $T = 293$  K; mean  $\sigma(C-C) = 0.002$  Å;  $R$  factor = 0.025;  $wR$  factor = 0.058; data-to-parameter ratio = 29.5.

In the title compound,  $[Co(C_4H_7N_2O_2)Cl_2(C_4H_8N_2O_2)]$ , the  $Co^{III}$  ion has a distorted octahedral coordination environment. The equatorial plane consists of four N atoms, two each from the dimethylglyoxime and dimethylglyoximate ligands, while the two axial positions are occupied by two chloride ions. Strong intramolecular  $O-H \cdots O$  hydrogen bonds are observed between the dimethylglyoxime and dimethylglyoximate ligands. Molecules are linked into a chain running along the  $[101]$  direction by  $O-H \cdots O$  and  $C-H \cdots Cl$  hydrogen bonds. The chains are cross-linked through intermolecular  $C-H \cdots Cl$  hydrogen bonds.

### Related literature

For related literature, see: Dayalan & Vijayaraghavan (2001); Lee *et al.* (2007); Gupta *et al.* (2000, 2001, 2004); Ohkubo & Fukuzumi (2005); Razavelt *et al.* (2005). Trommel *et al.* (2001).



### Experimental

#### Crystal data

$[Co(C_4H_7N_2O_2)Cl_2(C_4H_8N_2O_2)]$

$M_r = 361.07$

Monoclinic,  $Pn$

$a = 8.1901$  (2) Å

$b = 8.1261$  (2) Å

$c = 10.4463$  (3) Å

$\beta = 102.007$  (1)°

$V = 680.03$  (3) Å<sup>3</sup>

$Z = 2$

Mo  $K\alpha$  radiation

$\mu = 1.67$  mm<sup>-1</sup>

$T = 293$  (2) K

0.20 × 0.12 × 0.12 mm

#### Data collection

Bruker–Nonius Kappa-APEXII

CCD diffractometer

Absorption correction: multi-scan

(*SADABS*; Bruker, 1999)

$T_{min} = 0.786$ ,  $T_{max} = 0.819$

10990 measured reflections

5284 independent reflections

4711 reflections with  $I > 2\sigma(I)$

$R_{int} = 0.021$

#### Refinement

$R[F^2 > 2\sigma(F^2)] = 0.025$

$wR(F^2) = 0.057$

$S = 0.99$

5284 reflections

179 parameters

2 restraints

H-atom parameters constrained

$\Delta\rho_{max} = 0.56$  e Å<sup>-3</sup>

$\Delta\rho_{min} = -0.29$  e Å<sup>-3</sup>

Absolute structure: Flack (1983),

2067 Friedel pairs

Flack parameter: 0.008 (7)

**Table 1**

Selected bond lengths (Å).

Cl1—Co	2.2292 (4)	Co—N3	1.9048 (13)
Cl2—Co	2.2261 (4)	Co—N1	1.9051 (12)
Co—N2	1.8870 (12)	Co—N4	1.9181 (12)

**Table 2**

Hydrogen-bond geometry (Å, °).

$D-H \cdots A$	$D-H$	$H \cdots A$	$D \cdots A$	$D-H \cdots A$
O3—H3 $\cdots$ O1	0.82	1.81	2.5875 (16)	158
O4—H4 $\cdots$ O2	0.82	1.89	2.6604 (18)	156
O2—H2 $\cdots$ O1 <sup>i</sup>	0.82	1.73	2.5297 (17)	163
C4—H4C $\cdots$ Cl1 <sup>i</sup>	0.96	2.73	3.6473 (19)	160
C5—H5A $\cdots$ Cl1 <sup>ii</sup>	0.96	2.67	3.6317 (18)	175

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

Data collection: *APEX2* (Bruker–Nonius, 2004); cell refinement: *APEX2*; data reduction: *SAINT* (Bruker–Nonius, 2004); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3* (Farrugia, 1997); software used to prepare material for publication: *SHELXL97* and *PLATON* (Spek, 2003).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: CI2517).

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**supplementary materials**

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## Dichlorido(dimethylglyoximato- $\kappa^2N,N'$ )(dimethylglyoxime- $\kappa^2N,N'$ )cobalt(III)

P. Ramesh, A. SubbiahPandi, P. Jothi, C. Revathi and A. Dayalan

### Comment

Dimethylglyoximato-cobalt(III) complexes, generally known as cobaloximes, have been studied extensively as model compounds for vitamin-B<sub>12</sub> (Trommel *et al.*, 2001; Ohkubo & Fukuzumi, 2005). Most of the work on cobaloximes include electron-transfer reactions (Dayalan & Vijayaraghavan, 2001) and catalytic activity (Razavelt *et al.*, 2005) in solution. There are few literature evidences relating the structural aspects of cobaloximes (Gupta *et al.*, 2000; Gupta *et al.*, 2001; Gupta *et al.*, 2004). We report here the synthesis and X-ray crystal structure of the title compound.

The coordination geometry around the Co<sup>III</sup> ion can be described as a slightly distorted octahedron. The axial positions are occupied by the chloride ions. The glyoxime moieties are individually planar. The Co<sup>III</sup> ion and the four N atoms of dimethylglyoxime ligands are approximately coplanar. The Co—N and Co—Cl bond lengths are normal (Table 1), and are comparable with the corresponding values observed in a related complex (Lee *et al.*, 2007).

Strong intramolecular O—H $\cdots$ O hydrogen bonds are observed between the dimethylglyoxime and dimethylglyoximate ligands (Table 2). The crystal packing is stabilized by O—H $\cdots$ O and C—H $\cdots$ Cl hydrogen bonds. Atoms O2 and C4 of the molecule at (*x*, *y*, *z*) act as donors to atoms O1 and Cl1, respectively, of the molecule at (-1/2 + *x*, -*y*, -1/2 + *z*). These two hydrogen bonds form a chain running along the [1 0 1] direction. The chains are cross-linked through C—H $\cdots$ Cl intermolecular hydrogen bonds.

### Experimental

Cobalt(II) chloride hexahydrate was thoroughly grinded and exposed to microwave for 30 s. Dehydrated cobalt(II) chloride (1.3 g) was mixed with dimethyl glyoxime (2.32 g). The mixture was intimately grinded and made into a paste using acetone and exposed to microwave radiation for 60 s. The microwave treated reaction mixture was exposed to atmosphere, till it became green. The green coloured product was recrystallized from acetone. Single crystals were obtained by slow evaporation of the acetone solution.

### Refinement

All H atoms were fixed geometrically (O—H = 0.82 Å and C—H = 0.96 Å) and allowed to ride on their parent atoms, with  $U_{\text{iso}}(\text{H}) = 1.5U_{\text{eq}}(\text{C}, \text{O})$ .

## Figures

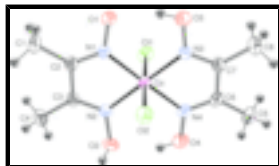


Fig. 1. The structure of the title complex. Displacement ellipsoids are drawn at the 50% probability level and H atoms are shown as small spheres of arbitrary radii.

## Dichlorido(dimethylglyoximato- $\kappa^2N,N'$ )(dimethylglyoxime- $\kappa^2N,N'$ )cobalt(III)

### Crystal data

[Co(C<sub>4</sub>H<sub>7</sub>N<sub>2</sub>O<sub>2</sub>)Cl<sub>2</sub>(C<sub>4</sub>H<sub>8</sub>N<sub>2</sub>O<sub>2</sub>)]

$M_r = 361.07$

Monoclinic,  $Pn$

Hall symbol: P -2yac

$a = 8.1901$  (2) Å

$b = 8.1261$  (2) Å

$c = 10.4463$  (3) Å

$\beta = 102.007$  (1)°

$V = 680.03$  (3) Å<sup>3</sup>

$Z = 2$

$F_{000} = 368$

$D_x = 1.763$  Mg m<sup>-3</sup>

Mo  $K\alpha$  radiation

$\lambda = 0.71073$  Å

Cell parameters from 3586 reflections

$\theta = 2.8$ – $37.2$ °

$\mu = 1.67$  mm<sup>-1</sup>

$T = 293$  (2) K

Plate, green

$0.20 \times 0.12 \times 0.12$  mm

### Data collection

Bruker–Nonius Kappa APEXII CCD diffractometer

Radiation source: fine-focus sealed tube

Monochromator: graphite

$T = 293$ (2) K

$\omega$  and  $\varphi$  scans

Absorption correction: multi-scan (SADABS; Bruker, 1999)

$T_{\min} = 0.786$ ,  $T_{\max} = 0.819$

10990 measured reflections

5284 independent reflections

4711 reflections with  $I > 2\sigma(I)$

$R_{\text{int}} = 0.021$

$\theta_{\max} = 37.2$ °

$\theta_{\min} = 2.9$ °

$h = -12$ → $13$

$k = -13$ → $13$

$l = -17$ → $17$

### Refinement

Refinement on  $F^2$

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.025$

$wR(F^2) = 0.057$

$S = 0.99$

5284 reflections

Hydrogen site location: inferred from neighbouring sites

H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0235P)^2]$

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

$(\Delta/\sigma)_{\max} = 0.023$

$\Delta\rho_{\max} = 0.56$  e Å<sup>-3</sup>

$\Delta\rho_{\min} = -0.29$  e Å<sup>-3</sup>

179 parameters  
 2 restraints  
 Primary atom site location: structure-invariant direct methods  
 Secondary atom site location: difference Fourier map  
 Extinction correction: none  
 Absolute structure: Flack (1983), 2067 Friedel pairs  
 Flack parameter: 0.008 (7)

*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  $F^2 > \sigma(F^2)$  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 ( $\text{\AA}^2$ )*

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
C1	0.2744 (2)	-0.2411 (2)	0.7384 (2)	0.0354 (4)
H1A	0.3762	-0.3016	0.7436	0.053*
H1B	0.1848	-0.2974	0.6812	0.053*
H1C	0.2497	-0.2325	0.8241	0.053*
C2	0.29345 (19)	-0.07336 (17)	0.68614 (15)	0.0255 (3)
C3	0.15626 (19)	0.01410 (18)	0.60187 (15)	0.0259 (3)
C4	-0.0162 (2)	-0.0517 (2)	0.56788 (19)	0.0362 (4)
H4A	-0.0912	0.0339	0.5290	0.054*
H4B	-0.0486	-0.0908	0.6457	0.054*
H4C	-0.0207	-0.1408	0.5069	0.054*
C5	0.5786 (2)	0.6808 (2)	0.5132 (2)	0.0353 (4)
H5A	0.6540	0.6827	0.4541	0.053*
H5B	0.6213	0.7497	0.5873	0.053*
H5C	0.4712	0.7208	0.4691	0.053*
C6	0.5617 (2)	0.50905 (17)	0.55842 (15)	0.0264 (3)
C7	0.70180 (19)	0.41674 (18)	0.63553 (16)	0.0266 (3)
C8	0.8762 (2)	0.4804 (2)	0.6649 (2)	0.0411 (4)
H8A	0.8866	0.5647	0.7305	0.062*
H8B	0.9027	0.5253	0.5867	0.062*
H8C	0.9518	0.3921	0.6966	0.062*
Cl1	0.36969 (5)	0.33736 (5)	0.79458 (4)	0.03361 (8)
Cl2	0.48754 (5)	0.09885 (5)	0.44061 (4)	0.03422 (9)
Co	0.42858 (2)	0.21491 (2)	0.618650 (19)	0.02055 (4)
N1	0.43373 (15)	0.00641 (15)	0.70278 (13)	0.0232 (2)
N2	0.20367 (15)	0.15171 (15)	0.56038 (12)	0.0242 (2)
N3	0.65689 (16)	0.27610 (14)	0.67399 (13)	0.0249 (2)
N4	0.42440 (16)	0.42760 (15)	0.53841 (13)	0.0257 (2)
O1	0.57344 (14)	-0.05436 (13)	0.77384 (12)	0.0303 (2)

## supplementary materials

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O2	0.09198 (16)	0.24162 (15)	0.46980 (13)	0.0301 (2)
H2	0.0688	0.1904	0.4008	0.045*
O3	0.77626 (15)	0.18097 (16)	0.74654 (14)	0.0362 (3)
H3	0.7352	0.0934	0.7628	0.054*
O4	0.28559 (16)	0.50431 (15)	0.46882 (14)	0.0378 (3)
H4	0.2091	0.4377	0.4506	0.057*

### Atomic displacement parameters ( $\text{\AA}^2$ )

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
C1	0.0400 (9)	0.0242 (7)	0.0421 (10)	-0.0089 (7)	0.0088 (8)	0.0041 (7)
C2	0.0304 (7)	0.0209 (5)	0.0252 (7)	-0.0042 (5)	0.0061 (6)	-0.0010 (5)
C3	0.0278 (7)	0.0254 (6)	0.0247 (7)	-0.0041 (5)	0.0061 (5)	-0.0038 (5)
C4	0.0295 (8)	0.0382 (8)	0.0401 (9)	-0.0097 (7)	0.0052 (6)	-0.0017 (7)
C5	0.0420 (10)	0.0239 (6)	0.0423 (10)	-0.0035 (7)	0.0138 (8)	0.0061 (7)
C6	0.0352 (7)	0.0208 (5)	0.0250 (7)	-0.0012 (5)	0.0108 (6)	0.0010 (5)
C7	0.0266 (7)	0.0249 (6)	0.0284 (7)	-0.0044 (5)	0.0060 (6)	-0.0009 (6)
C8	0.0336 (8)	0.0405 (9)	0.0493 (11)	-0.0137 (7)	0.0085 (7)	0.0027 (8)
Cl1	0.0474 (2)	0.02841 (16)	0.02782 (18)	0.00147 (15)	0.01415 (16)	-0.00198 (14)
Cl2	0.0435 (2)	0.03213 (17)	0.02942 (18)	-0.00460 (16)	0.01298 (16)	-0.00663 (15)
Co	0.02324 (7)	0.01784 (6)	0.02009 (7)	-0.00196 (6)	0.00338 (5)	0.00024 (6)
N1	0.0265 (6)	0.0198 (5)	0.0229 (6)	-0.0016 (4)	0.0040 (4)	0.0001 (4)
N2	0.0249 (6)	0.0231 (5)	0.0229 (6)	-0.0003 (5)	0.0011 (4)	-0.0002 (5)
N3	0.0257 (5)	0.0213 (5)	0.0265 (6)	-0.0010 (4)	0.0028 (5)	0.0003 (5)
N4	0.0313 (6)	0.0225 (5)	0.0231 (6)	0.0021 (5)	0.0050 (5)	0.0031 (4)
O1	0.0290 (5)	0.0268 (5)	0.0320 (6)	0.0008 (4)	-0.0010 (4)	0.0085 (4)
O2	0.0293 (6)	0.0312 (5)	0.0260 (5)	0.0023 (4)	-0.0027 (4)	-0.0016 (4)
O3	0.0286 (6)	0.0295 (5)	0.0462 (8)	0.0009 (5)	-0.0020 (5)	0.0101 (5)
O4	0.0339 (6)	0.0338 (6)	0.0420 (7)	0.0040 (5)	-0.0002 (5)	0.0115 (6)

### Geometric parameters ( $\text{\AA}$ , $^\circ$ )

C1—C2	1.489 (2)	C7—C8	1.490 (2)
C1—H1A	0.96	C8—H8A	0.96
C1—H1B	0.96	C8—H8B	0.96
C1—H1C	0.96	C8—H8C	0.96
C2—N1	1.2990 (19)	Cl1—Co	2.2292 (4)
C2—C3	1.460 (2)	Cl2—Co	2.2261 (4)
C3—N2	1.2881 (18)	Co—N2	1.8870 (12)
C3—C4	1.483 (2)	Co—N3	1.9048 (13)
C4—H4A	0.96	Co—N1	1.9051 (12)
C4—H4B	0.96	Co—N4	1.9181 (12)
C4—H4C	0.96	N1—O1	1.3231 (17)
C5—C6	1.489 (2)	N1—O1	1.3231 (17)
C5—H5A	0.96	N2—O2	1.3805 (17)
C5—H5B	0.96	N3—O3	1.3489 (17)
C5—H5C	0.96	N4—O4	1.3659 (17)
C6—N4	1.284 (2)	O2—H2	0.82
C6—C7	1.464 (2)	O3—H3	0.82

C7—N3	1.2901 (18)	O4—H4	0.82
C2—C1—H1A	109.5	H8A—C8—H8C	109.5
C2—C1—H1B	109.5	H8B—C8—H8C	109.5
H1A—C1—H1B	109.5	N2—Co—N3	178.64 (6)
C2—C1—H1C	109.5	N2—Co—N1	80.40 (5)
H1A—C1—H1C	109.5	N3—Co—N1	99.56 (5)
H1B—C1—H1C	109.5	N2—Co—N4	100.18 (5)
N1—C2—C3	112.72 (13)	N3—Co—N4	79.90 (5)
N1—C2—C1	124.42 (15)	N1—Co—N4	178.48 (6)
C3—C2—C1	122.72 (13)	N2—Co—Cl2	88.97 (4)
N2—C3—C2	112.18 (13)	N3—Co—Cl2	89.67 (4)
N2—C3—C4	124.84 (15)	N1—Co—Cl2	91.19 (4)
C2—C3—C4	122.98 (13)	N4—Co—Cl2	90.23 (4)
C3—C4—H4A	109.5	N2—Co—Cl1	91.34 (4)
C3—C4—H4B	109.5	N3—Co—Cl1	90.02 (4)
H4A—C4—H4B	109.5	N1—Co—Cl1	90.26 (4)
C3—C4—H4C	109.5	N4—Co—Cl1	88.33 (4)
H4A—C4—H4C	109.5	Cl2—Co—Cl1	178.550 (17)
H4B—C4—H4C	109.5	C2—N1—O1	121.76 (12)
C6—C5—H5A	109.5	C2—N1—O1	121.76 (12)
C6—C5—H5B	109.5	C2—N1—Co	116.61 (11)
H5A—C5—H5B	109.5	O1—N1—Co	121.62 (9)
C6—C5—H5C	109.5	O1—N1—Co	121.62 (9)
H5A—C5—H5C	109.5	C3—N2—O2	119.14 (12)
H5B—C5—H5C	109.5	C3—N2—Co	118.04 (11)
N4—C6—C7	112.65 (13)	O2—N2—Co	122.70 (9)
N4—C6—C5	124.55 (16)	C7—N3—O3	117.54 (13)
C7—C6—C5	122.77 (14)	C7—N3—Co	117.53 (11)
N3—C7—C6	112.57 (13)	O3—N3—Co	124.89 (9)
N3—C7—C8	124.50 (15)	C6—N4—O4	117.09 (12)
C6—C7—C8	122.93 (14)	C6—N4—Co	117.25 (11)
C7—C8—H8A	109.5	O4—N4—Co	125.52 (9)
C7—C8—H8B	109.5	N2—O2—H2	109.5
H8A—C8—H8B	109.5	N3—O3—H3	109.5
C7—C8—H8C	109.5	N4—O4—H4	109.5
N1—C2—C3—N2	0.71 (19)	N4—Co—N2—C3	-176.40 (11)
C1—C2—C3—N2	-175.17 (14)	Cl2—Co—N2—C3	93.56 (11)
N1—C2—C3—C4	179.90 (14)	Cl1—Co—N2—C3	-87.86 (11)
C1—C2—C3—C4	4.0 (2)	N1—Co—N2—O2	-173.82 (12)
N4—C6—C7—N3	-3.70 (19)	N4—Co—N2—O2	7.61 (12)
C5—C6—C7—N3	174.29 (15)	Cl2—Co—N2—O2	-82.44 (11)
N4—C6—C7—C8	176.17 (15)	Cl1—Co—N2—O2	96.15 (11)
C5—C6—C7—C8	-5.8 (2)	C6—C7—N3—O3	-179.68 (13)
C3—C2—N1—O1	-178.56 (13)	C8—C7—N3—O3	0.5 (2)
C1—C2—N1—O1	-2.8 (2)	C6—C7—N3—Co	2.60 (17)
C3—C2—N1—O1	-178.56 (13)	C8—C7—N3—Co	-177.27 (13)
C1—C2—N1—O1	-2.8 (2)	N1—Co—N3—C7	-179.35 (11)
C3—C2—N1—Co	1.02 (16)	N4—Co—N3—C7	-0.79 (11)



## supplementary materials

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C1—C2—N1—Co	176.83 (13)	Cl2—Co—N3—C7	89.50 (11)
N2—Co—N1—C2	-1.70 (11)	Cl1—Co—N3—C7	-89.08 (11)
N3—Co—N1—C2	179.68 (11)	N1—Co—N3—O3	3.11 (13)
Cl2—Co—N1—C2	-90.45 (11)	N4—Co—N3—O3	-178.33 (13)
Cl1—Co—N1—C2	89.61 (10)	Cl2—Co—N3—O3	-88.04 (12)
N2—Co—N1—O1	177.89 (12)	Cl1—Co—N3—O3	93.37 (12)
N3—Co—N1—O1	-0.74 (12)	C7—C6—N4—O4	179.09 (13)
Cl2—Co—N1—O1	89.14 (11)	C5—C6—N4—O4	1.1 (2)
Cl1—Co—N1—O1	-90.80 (11)	C7—C6—N4—Co	3.19 (17)
N2—Co—N1—O1	177.89 (12)	C5—C6—N4—Co	-174.76 (13)
N3—Co—N1—O1	-0.74 (12)	N2—Co—N4—C6	179.87 (11)
Cl2—Co—N1—O1	89.14 (11)	N3—Co—N4—C6	-1.51 (11)
Cl1—Co—N1—O1	-90.80 (11)	Cl2—Co—N4—C6	-91.14 (11)
C2—C3—N2—O2	173.96 (13)	Cl1—Co—N4—C6	88.81 (11)
C4—C3—N2—O2	-5.2 (2)	N2—Co—N4—O4	4.35 (13)
C2—C3—N2—Co	-2.17 (17)	N3—Co—N4—O4	-177.02 (13)
C4—C3—N2—Co	178.66 (12)	Cl2—Co—N4—O4	93.35 (12)
N1—Co—N2—C3	2.17 (11)	Cl1—Co—N4—O4	-86.70 (12)

### Hydrogen-bond geometry (Å, °)

<i>D</i> —H... <i>A</i>	<i>D</i> —H	H... <i>A</i>	<i>D</i> ... <i>A</i>	<i>D</i> —H... <i>A</i>
O3—H3...O1	0.82	1.81	2.5875 (16)	158
O4—H4...O2	0.82	1.89	2.6604 (18)	156
O2—H2...O1 <sup>i</sup>	0.82	1.73	2.5297 (17)	163
C4—H4C...Cl1 <sup>i</sup>	0.96	2.73	3.6473 (19)	160
C5—H5A...Cl1 <sup>ii</sup>	0.96	2.67	3.6317 (18)	175

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

Fig. 1

