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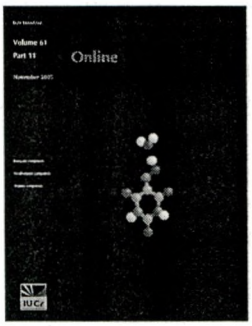

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Aquachloridobis(diphenylglyoximato-κ^2N,N')cobalt(III) dihydrate

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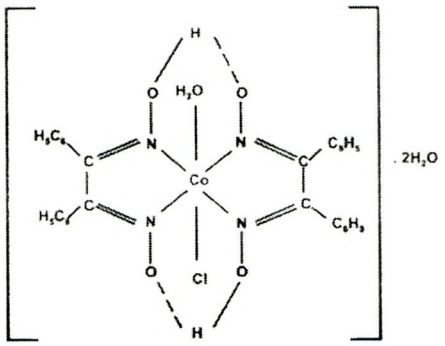
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.007 Å; H-atom completeness 79%; disorder in main residue; R factor = 0.062; wR factor = 0.199; data-to-parameter ratio = 12.5.

The asymmetric unit of the title complex, $[Co(C_{14}H_{11}N_2O_2)_2Cl(H_2O)]\cdot 2H_2O$ or $[Co(dpgH)_2Cl(H_2O)]\cdot 2H_2O$, where $dpgH^-$ is diphenyl glyoximate, consists of one-half of a $[Co(dpgH)_2Cl(H_2O)]$ complex and one solvent water molecule. The complex is completed through inversion symmetry, with the Co^{III} atom situated at the centre of symmetry. The coordination geometry around the Co^{III} atom is distorted octahedral with the four N atoms of the two $dpgH^-$ ligands forming an approximate square plane with N—Co—N bite angles of 81.13 (14) and 98.87 (14)°. The Cl^- ligand and the water molecule are disordered in a 1:1 ratio and are in the axial positions, almost perpendicular to the plane of the glyoximate ligands [O—Co—Cl = 175.3 (10)°]. The two glyoximate ligands are linked by strong intramolecular O—H···O hydrogen bonds. In addition, O—H···O interactions involving the solvent water molecules and O—H···N hydrogen-bonding interactions are also observed. The solvent water molecule is disordered over five positions with different occupancies.

Related literature

For related complexes, see: Gupta *et al.* (2003); Randaccio (1999); Brown & Satyanarayana (1992); Gilaberte *et al.* (1988). For the nature of equatorial ligands, see: Varhelyi *et al.* (1999). For similar structures, see: Meera *et al.* (2009). For details of the synthesis, see: Toscano *et al.* (1983); Gupta *et al.* (2001). For spectroscopic studies related to the complex, see: Gupta *et al.* (2004); Lopez *et al.* (1992); Silverstein & Bassler (1984); Mandal & Gupta (2005).



Experimental

Crystal data

$[Co(C_{14}H_{11}N_2O_2)_2Cl(H_2O)]\cdot 2H_2O$
M_r = 626.92
Monoclinic, $P2_1/n$
a = 12.0709 (4) Å
b = 5.9689 (2) Å
c = 21.9224 (5) Å
β = 104.770 (1)°
V = 1527.32 (8) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.70 mm^{-1}
T = 293 K
0.30 × 0.20 × 0.20 mm

Data collection

Bruker APEXII CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 1999)
T_{min} = 0.761, T_{max} = 0.861
13610 measured reflections
2682 independent reflections
2431 reflections with $I > 2\sigma(I)$
R_{int} = 0.030

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.062
$wR(F^2)$ = 0.199
S = 1.25
2682 reflections
215 parameters
1 restraint
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.92 e Å^{-3}
$\Delta\rho_{min}$ = −0.53 e Å^{-3}

Table 1
Selected bond lengths (Å).

Co1—N2^i	1.891 (3)	Co1—O3	1.95 (3)
Co1—N1^i	1.894 (3)	Co1—Cl1	2.214 (11)

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

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

D—H···A	D—H	H···A	D···A	D—H···A
O2—H2A···O1^i	0.82	1.68	2.477 (4)	162
O2—H2A···N1^i	0.82	2.40	2.999 (4)	130
O4A···O3^{ii}			2.592 (4)	

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

Data collection: *APEX2* (Bruker, 2004); cell refinement: *SAINT* (Bruker, 2004); data reduction: *SAINT*; program(s) used to solve structure: *SIR92* (Altomare *et al.*, 1993); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3* (Farrugia, 1997) and *Mercury* (Macrae *et al.*, 2008); soft-

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ware used to prepare material for publication: *PLATON* (Spek, 2009).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: WM2477).

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supplementary materials

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Aquachloridobis(diphenylglyoximato-κ^2N,N')cobalt(III) dihydrate

P. Meera, M. A. Selvi and A. Dayalan

Comment

The dioxime complexes of cobalt(III), known as cobaloximes, and their derivatives have been found to mimic vitamin-B_{12} coenzyme. The studies on steric and electronic effects of cobaloximes helped in the successful design of novel derivatives with desired properties (Gupta *et al.*, 2003; Randaccio, 1999; Brown & Satyanarayana, 1992; Gilaberte *et al.*, 1988). Among the stereoisomeric benzildioximes (*syn*, *amphi*, *anti*), only the *anti* isomer shows chelation properties towards transition metal ions (Varhelyi *et al.*, 1999).

In the structure of the title compound, $[Co(C_{14}H_{11}N_2O_2)_2Cl(H_2O)]\cdot 2H_2O$, or $[Co(dpgH)_2Cl(H_2O)]\cdot 2H_2O$, where $dpgH^-$ = diphenyl glyoximate, two halves of the complex molecule are related through inversion symmetry with Co^{III} situated at the centre of symmetry. The coordination geometry around Co^{III} is a slightly distorted octahedron (Fig. 1) with the four N atoms of the $dpgH^-$ ligand forming an approximate square plane. The bite angles N1—Co—N2 of the equatorial ligands are 81.13 (14) and 98.87 (14)°, respectively. The Cl^- ligand and the water molecule are in axial positions and are disordered in a 1:1 ratio. They are almost perpendicular to the plane containing the equatorial $dpgH^-$ ligand (O3—Co1—Cl1 = 175.3 (10)°). The two glyoximate ligands are linked by strong intramolecular O—H···O hydrogen bonds. In addition, O1—H1···N2 hydrogen bonding interaction is also observed (Fig. 2). A similar interaction was observed for a related complex (Meera *et al.*, 2009). The lattice water molecule (O4) is disordered over five positions with different occupancies. Although the H positions of the disordered water molecules could not be located, close O···O interactions suggest likewise an involvement in hydrogen bonding (Table 2).

Experimental

Cobalt(II) chloride hexahydrate was thoroughly ground and mixed with diphenylglyoxime in a 1:2 molar ratio in an aqueous solution of acetone. The reaction mixture was stirred for five hours at an elevated temperature (Toscano *et al.*, 1983; Gupta *et al.*, 2001). The resulting brown mass was filtered, washed with acetone, ether and dried in a desiccator. Brown coloured crystals appeared in two to three days on slow evaporation of the saturated solution of the complex in ethanol. Elemental analysis, obtained by analytical method, agreed well with the theoretical data expected for the formula of the complex, $C_{28}H_{28}N_4O_7ClCo$. Anal., % (calc., %): C 53.97 (53.58); H 4.94 (4.47); N 9.05 (8.93). The C=N stretching vibration of oxime in its complex was observed at 1385 cm^{-1} and the intramolecular hydrogen bonded –OH around 3140 cm^{-1}. A moderate peak around 1090 cm^{-1} may be assigned to the C=N—O stretching of the oxime. The band around 540 cm^{-1} could be attributed to cobalt(III)-nitrogen stretching. The ^1H NMR spectrum of the complex in acetone-d_6 shows three different signals corresponding to the three different aromatic protons of the diphenylglyoximate (Gupta *et al.*, 2004; Lopez *et al.*, 1992). The H atoms in the second and the sixth position of the benzene ring of the diphenylglyoximate show a doublet at 7.2 p.p.m., while the third and fifth H atoms show a triplet at 7.4 p.p.m.. Similarly, the fourth one gives a triplet at 7.3 p.p.m..The

oxime –OH protons resonate at 9.1 p.p.m.. A singlet around 8.5 p.p.m. represents the protons of the –OH group of the aqua ligand (Silverstein & Bassler, 1984; Mandal & Gupta, 2005).

Refinement

The O atom of the solvent water molecule in the lattice is disordered over five positions O4A, O4B, O4C, O4D, O4E with different site occupancy factor. The refinement of occupancy by means of free variable in each case is 0.302, 0.250, 0.131, 0.198 and 0.119 for O4A, O4B, O4C, O4D and O4E, respectively. The O atoms of water were refined anisotropically with equal anisotropic displacement parameters. The disordered chloride (Cl1) and oxygen (O3) atom sharing the axial position were refined with equal site occupancies of 1:1. The H atoms bound to aromatic carbon were constrained to ride on their parent atom with d(C—H) = 0.93Å and U_{iso}(H) =1.2U_{equ}(C). The position of the H atom bound to the hydroxyl group was identified from the difference in the electron density map and constrained to a distance of d(O2—H2) = 0.92 (1) Å. H positions of the positionally disordered lattice water molecules could not be found from difference maps and were eventually omitted from refinement.

Figures

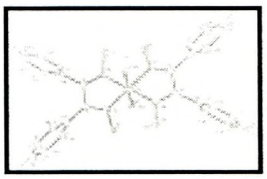

Fig. 1. *ORTEP* representation of the complex drawn at the 30% probability level with the atom labelling scheme. [Symmetry Code: (i) 1-*x*, -*y*, -*z*].

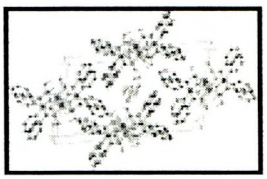

Fig. 2. Packing of the complex in the unit cell with the disordered water occupying the intermolecular voids. The hydrogen atoms bound to aromatic carbons have been omitted for clarity.

Aquachloridobis(diphenylglyoximato-κ^2N,N')cobalt(III) dihydrate

Crystal data

$[Co(C_{14}H_{11}N_2O_2)_2Cl(H_2O)]\cdot 2H_2O$	$F(000)$ = 648
M_r = 626.92	D_x = 1.363 Mg m^{-3}
Monoclinic, $P2_1/n$	Mo $K\alpha$ radiation, λ = 0.71073 Å
Hall symbol: -P 2yn	Cell parameters from 2441 reflections
a = 12.0709 (4) Å	θ = 2.8–25.0°
b = 5.9689 (2) Å	μ = 0.70 mm^{-1}
c = 21.9224 (5) Å	T = 293 K
β = 104.770 (1)°	Block, brown
V = 1527.32 (8) Å^3	0.30 × 0.20 × 0.20 mm
Z = 2	

Data collection

Bruker APEXII CCD diffractometer	2682 independent reflections
Radiation source: fine-focus sealed tube	2431 reflections with $I > 2\sigma(I)$
graphite	$R_{int} = 0.030$
ω and φ scan	$\theta_{max} = 25.0°$, $\theta_{min} = 1.8°$
Absorption correction: multi-scan (*SADABS*; Bruker, 1999)	$h = -14 \rightarrow 14$
$T_{min} = 0.761$, $T_{max} = 0.861$	$k = -7 \rightarrow 7$
13610 measured reflections	$l = -25 \rightarrow 26$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.062$	H-atom parameters constrained
$wR(F^2) = 0.199$	$w = 1/[\sigma^2(F_o^2) + (0.1021P)^2 + 2.2574P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.25$	$(\Delta/\sigma)_{max} < 0.001$
2682 reflections	$\Delta\rho_{max} = 0.92$ e Å^{-3}
215 parameters	$\Delta\rho_{min} = -0.53$ e Å^{-3}
1 restraint	Extinction correction: *SHELXL97* (Sheldrick, 2008), $Fc^* = kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Primary atom site location: structure-invariant direct methods	Extinction coefficient: 0.025 (3)

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 (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
C1	0.3917 (4)	0.0079 (7)	0.0955 (2)	0.0349 (9)	
C2	0.5064 (3)	0.0989 (7)	0.12232 (19)	0.0342 (9)	
C3	0.3003 (4)	0.0027 (8)	0.1290 (2)	0.0404 (11)	
C4	0.2296 (4)	−0.1819 (9)	0.1254 (2)	0.0519 (12)	

H4	0.2423	−0.3092	0.1037	0.062*	
C5	0.1405 (5)	−0.1770 (12)	0.1539 (3)	0.0668 (16)	
H5	0.0927	−0.3009	0.1508	0.080*	
C6	0.1215 (5)	0.0054 (12)	0.1864 (3)	0.0677 (18)	
H6	0.0610	0.0062	0.2055	0.081*	
C7	0.1911 (5)	0.1880 (11)	0.1913 (3)	0.0619 (15)	
H7	0.1784	0.3131	0.2139	0.074*	
C8	0.2809 (4)	0.1867 (9)	0.1625 (2)	0.0482 (11)	
H8	0.3284	0.3112	0.1660	0.058*	
C9	0.5534 (3)	0.1512 (8)	0.19009 (18)	0.0353 (9)	
C10	0.5471 (4)	−0.0079 (8)	0.2349 (2)	0.0457 (11)	
H10	0.5078	−0.1412	0.2227	0.055*	
C11	0.5994 (5)	0.0313 (11)	0.2977 (2)	0.0576 (14)	
H11	0.5969	−0.0767	0.3279	0.069*	
C12	0.6550 (4)	0.2299 (11)	0.3153 (2)	0.0604 (16)	
H12	0.6900	0.2559	0.3576	0.073*	
C13	0.6600 (4)	0.3909 (10)	0.2718 (2)	0.0519 (13)	
H13	0.6972	0.5259	0.2844	0.062*	
C14	0.6092 (4)	0.3513 (8)	0.2090 (2)	0.0432 (11)	
H14	0.6125	0.4599	0.1791	0.052*	
N1	0.3780 (3)	−0.0578 (6)	0.03761 (16)	0.0335 (8)	
N2	0.5663 (3)	0.1165 (6)	0.08134 (15)	0.0325 (8)	
O1	0.2790 (2)	−0.1374 (6)	0.00398 (14)	0.0455 (8)	
O2	0.6748 (2)	0.1866 (6)	0.09899 (14)	0.0416 (8)	
H2A	0.7025	0.1849	0.0685	0.10 (3)*	
Co1	0.5000	0.0000	0.0000	0.0294 (3)	
Cl1	0.5813 (10)	−0.3227 (16)	0.0360 (5)	0.0429 (13)	0.50
O3	0.564 (2)	−0.296 (4)	0.0254 (12)	0.044 (7)	0.50
O4A	0.7645 (12)	0.624 (3)	0.0072 (7)	0.084 (3)	0.302 (9)
O4B	0.9669 (16)	0.417 (4)	0.0424 (9)	0.084 (3)	0.250 (10)
O4C	0.875 (3)	0.618 (7)	0.0176 (17)	0.084 (3)	0.131 (9)
O4D	1.023 (2)	0.437 (5)	−0.0007 (13)	0.084 (3)	0.198 (9)
O4E	1.002 (3)	0.295 (9)	0.028 (2)	0.084 (3)	0.119 (10)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.033 (2)	0.038 (2)	0.034 (2)	−0.0038 (17)	0.0086 (17)	−0.0021 (16)
C2	0.031 (2)	0.037 (2)	0.034 (2)	−0.0015 (17)	0.0082 (17)	0.0000 (17)
C3	0.033 (2)	0.054 (3)	0.033 (2)	−0.0056 (19)	0.0075 (18)	−0.0005 (18)
C4	0.054 (3)	0.059 (3)	0.046 (3)	−0.016 (2)	0.019 (2)	−0.004 (2)
C5	0.054 (3)	0.087 (4)	0.064 (3)	−0.030 (3)	0.023 (3)	0.003 (3)
C6	0.045 (3)	0.109 (5)	0.057 (3)	−0.008 (3)	0.027 (3)	−0.003 (3)
C7	0.049 (3)	0.083 (4)	0.058 (3)	0.010 (3)	0.022 (2)	−0.009 (3)
C8	0.039 (2)	0.058 (3)	0.050 (3)	−0.002 (2)	0.015 (2)	−0.005 (2)
C9	0.0275 (19)	0.046 (2)	0.033 (2)	0.0019 (18)	0.0090 (16)	−0.0058 (18)
C10	0.041 (3)	0.057 (3)	0.041 (2)	0.002 (2)	0.013 (2)	−0.001 (2)
C11	0.053 (3)	0.083 (4)	0.036 (3)	0.013 (3)	0.011 (2)	0.009 (2)

C12	0.038 (3)	0.104 (5)	0.035 (2)	0.008 (3)	0.002 (2)	−0.020 (3)
C13	0.038 (2)	0.067 (3)	0.050 (3)	−0.003 (2)	0.011 (2)	−0.023 (3)
C14	0.035 (2)	0.053 (3)	0.043 (2)	−0.005 (2)	0.0112 (18)	−0.008 (2)
N1	0.0282 (17)	0.0370 (18)	0.0344 (18)	−0.0050 (14)	0.0061 (14)	−0.0023 (15)
N2	0.0278 (17)	0.0378 (19)	0.0312 (16)	−0.0044 (14)	0.0061 (13)	−0.0015 (14)
O1	0.0311 (15)	0.065 (2)	0.0411 (16)	−0.0167 (15)	0.0101 (13)	−0.0096 (15)
O2	0.0272 (15)	0.060 (2)	0.0369 (15)	−0.0128 (14)	0.0064 (12)	−0.0088 (14)
Co1	0.0256 (5)	0.0331 (5)	0.0286 (5)	−0.0046 (3)	0.0054 (3)	−0.0011 (3)
Cl1	0.044 (3)	0.0374 (18)	0.041 (3)	0.0015 (18)	−0.001 (3)	0.004 (2)
O3	0.027 (8)	0.064 (12)	0.031 (8)	−0.003 (7)	−0.012 (5)	0.016 (5)
O4A	0.062 (6)	0.103 (9)	0.087 (7)	0.019 (6)	0.021 (5)	0.004 (6)
O4B	0.062 (6)	0.103 (9)	0.087 (7)	0.019 (6)	0.021 (5)	0.004 (6)
O4C	0.062 (6)	0.103 (9)	0.087 (7)	0.019 (6)	0.021 (5)	0.004 (6)
O4D	0.062 (6)	0.103 (9)	0.087 (7)	0.019 (6)	0.021 (5)	0.004 (6)
O4E	0.062 (6)	0.103 (9)	0.087 (7)	0.019 (6)	0.021 (5)	0.004 (6)

Geometric parameters (Å, °)

C1—N1	1.298 (6)	C11—C12	1.368 (9)
C1—C2	1.463 (6)	C11—H11	0.9300
C1—C3	1.473 (6)	C12—C13	1.366 (8)
C2—N2	1.294 (5)	C12—H12	0.9300
C2—C9	1.482 (6)	C13—C14	1.377 (6)
C3—C8	1.375 (7)	C13—H13	0.9300
C3—C4	1.383 (7)	C14—H14	0.9300
C4—C5	1.375 (7)	N1—O1	1.323 (4)
C4—H4	0.9300	N1—Co1	1.894 (3)
C5—C6	1.353 (9)	N2—O2	1.334 (4)
C5—H5	0.9300	N2—Co1	1.891 (3)
C6—C7	1.363 (9)	O2—H2A	0.8200
C6—H6	0.9300	Co1—N2^{i}	1.891 (3)
C7—C8	1.386 (7)	Co1—N1^{i}	1.894 (3)
C7—H7	0.9300	Co1—O3	1.95 (3)
C8—H8	0.9300	Co1—O3^{i}	1.95 (3)
C9—C14	1.382 (6)	Co1—Cl1	2.214 (11)
C9—C10	1.382 (6)	Co1—Cl1^{i}	2.214 (11)
C10—C11	1.381 (7)	O4D—O4D^{ii}	0.94 (4)
C10—H10	0.9300		
O4A···O3^{iii}	2.592 (4)	O4A···CL1^{iii}	2.470 (2)
O4A···O1^{i}	2.951 (2)		
N1—C1—C2	112.1 (4)	C13—C14—C9	120.5 (5)
N1—C1—C3	123.8 (4)	C13—C14—H14	119.8
C2—C1—C3	124.0 (4)	C9—C14—H14	119.8
N2—C2—C1	113.0 (4)	C1—N1—O1	121.7 (3)
N2—C2—C9	122.6 (4)	C1—N1—Co1	116.8 (3)
C1—C2—C9	124.2 (4)	O1—N1—Co1	121.0 (3)
C8—C3—C4	118.7 (4)	C2—N2—O2	120.4 (3)

C8—C3—C1	120.1 (4)	C2—N2—Co1	116.6 (3)
C4—C3—C1	121.2 (4)	O2—N2—Co1	122.5 (2)
C5—C4—C3	120.0 (5)	N2—O2—H2A	109.5
C5—C4—H4	120.0	N2—Co1—N2^{i}	179.998 (1)
C3—C4—H4	120.0	N2—Co1—N1	81.13 (14)
C6—C5—C4	120.9 (5)	N2^{i}—Co1—N1	98.87 (14)
C6—C5—H5	119.5	N2—Co1—N1^{i}	98.87 (14)
C4—C5—H5	119.5	N2^{i}—Co1—N1^{i}	81.13 (14)
C5—C6—C7	120.1 (5)	N1—Co1—N1^{i}	180.00 (17)
C5—C6—H6	120.0	N2—Co1—O3	91.3 (7)
C7—C6—H6	120.0	N2^{i}—Co1—O3	88.7 (7)
C6—C7—C8	119.8 (5)	N1—Co1—O3	90.4 (9)
C6—C7—H7	120.1	N1^{i}—Co1—O3	89.6 (9)
C8—C7—H7	120.1	N2—Co1—O3^{i}	88.7 (7)
C3—C8—C7	120.5 (5)	N2^{i}—Co1—O3^{i}	91.3 (7)
C3—C8—H8	119.7	N1—Co1—O3^{i}	89.6 (9)
C7—C8—H8	119.7	N1^{i}—Co1—O3^{i}	90.4 (9)
C14—C9—C10	119.5 (4)	O3—Co1—O3^{i}	179.999 (2)
C14—C9—C2	121.0 (4)	N2—Co1—Cl1	86.6 (3)
C10—C9—C2	119.4 (4)	N2^{i}—Co1—Cl1	93.4 (3)
C11—C10—C9	119.9 (5)	N1—Co1—Cl1	90.6 (3)
C11—C10—H10	120.1	N1^{i}—Co1—Cl1	89.4 (3)
C9—C10—H10	120.1	O3—Co1—Cl1	4.7 (10)
C12—C11—C10	119.6 (5)	O3^{i}—Co1—Cl1	175.3 (10)
C12—C11—H11	120.2	N2—Co1—Cl1^{i}	93.4 (3)
C10—C11—H11	120.2	N2^{i}—Co1—Cl1^{i}	86.6 (3)
C13—C12—C11	121.3 (4)	N1—Co1—Cl1^{i}	89.4 (3)
C13—C12—H12	119.4	N1^{i}—Co1—Cl1^{i}	90.6 (3)
C11—C12—H12	119.4	O3—Co1—Cl1^{i}	175.3 (10)
C12—C13—C14	119.3 (5)	O3^{i}—Co1—Cl1^{i}	4.7 (10)
C12—C13—H13	120.3	Cl1—Co1—Cl1^{i}	179.999 (1)
C14—C13—H13	120.3		
N1—C1—C2—N2	6.6 (5)	C1—C2—N2—O2	−176.8 (3)
C3—C1—C2—N2	−170.3 (4)	C9—C2—N2—O2	−0.8 (6)
N1—C1—C2—C9	−169.3 (4)	C1—C2—N2—Co1	−5.3 (5)
C3—C1—C2—C9	13.8 (7)	C9—C2—N2—Co1	170.7 (3)
N1—C1—C3—C8	−132.9 (5)	C2—N2—Co1—N2^{i}	164 (6)
C2—C1—C3—C8	43.6 (6)	O2—N2—Co1—N2^{i}	−25 (6)
N1—C1—C3—C4	44.5 (7)	C2—N2—Co1—N1	2.1 (3)
C2—C1—C3—C4	−139.0 (5)	O2—N2—Co1—N1	173.5 (3)
C8—C3—C4—C5	1.4 (7)	C2—N2—Co1—N1^{i}	−177.9 (3)
C1—C3—C4—C5	−176.0 (5)	O2—N2—Co1—N1^{i}	−6.5 (3)
C3—C4—C5—C6	−0.9 (8)	C2—N2—Co1—O3	−88.1 (10)

C4—C5—C6—C7	0.0 (9)	O2—N2—Co1—O3	83.2 (10)
C5—C6—C7—C8	0.4 (9)	C2—N2—Co1—O3^{i}	91.9 (10)
C4—C3—C8—C7	−1.0 (7)	O2—N2—Co1—O3^{i}	−96.8 (10)
C1—C3—C8—C7	176.4 (4)	C2—N2—Co1—Cl1	−89.0 (4)
C6—C7—C8—C3	0.1 (8)	O2—N2—Co1—Cl1	82.4 (4)
N2—C2—C9—C14	50.7 (6)	C2—N2—Co1—Cl1^{i}	91.0 (4)
C1—C2—C9—C14	−133.8 (4)	O2—N2—Co1—Cl1^{i}	−97.6 (4)
N2—C2—C9—C10	−125.5 (5)	C1—N1—Co1—N2	2.0 (3)
C1—C2—C9—C10	50.0 (6)	O1—N1—Co1—N2	174.3 (3)
C14—C9—C10—C11	−1.9 (7)	C1—N1—Co1—N2^{i}	−178.0 (3)
C2—C9—C10—C11	174.4 (4)	O1—N1—Co1—N2^{i}	−5.7 (3)
C9—C10—C11—C12	1.4 (7)	C1—N1—Co1—N1^{i}	−133 (100)
C10—C11—C12—C13	−0.1 (8)	O1—N1—Co1—N1^{i}	39 (100)
C11—C12—C13—C14	−0.8 (7)	C1—N1—Co1—O3	93.2 (8)
C12—C13—C14—C9	0.2 (7)	O1—N1—Co1—O3	−94.5 (8)
C10—C9—C14—C13	1.1 (6)	C1—N1—Co1—O3^{i}	−86.8 (8)
C2—C9—C14—C13	−175.1 (4)	O1—N1—Co1—O3^{i}	85.5 (8)
C2—C1—N1—O1	−177.4 (4)	C1—N1—Co1—Cl1	88.4 (4)
C3—C1—N1—O1	−0.5 (6)	O1—N1—Co1—Cl1	−99.2 (4)
C2—C1—N1—Co1	−5.1 (5)	C1—N1—Co1—Cl1^{i}	−91.6 (4)
C3—C1—N1—Co1	171.8 (3)	O1—N1—Co1—Cl1^{i}	80.8 (4)

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

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O2—H2A···O1^{i}	0.82	1.68	2.477 (4)	162.
O2—H2A···N1^{i}	0.82	2.40	2.999 (4)	130.
O4A—···.O3^{iii}	.	.	2.592 (4)	.

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

Fig. 1

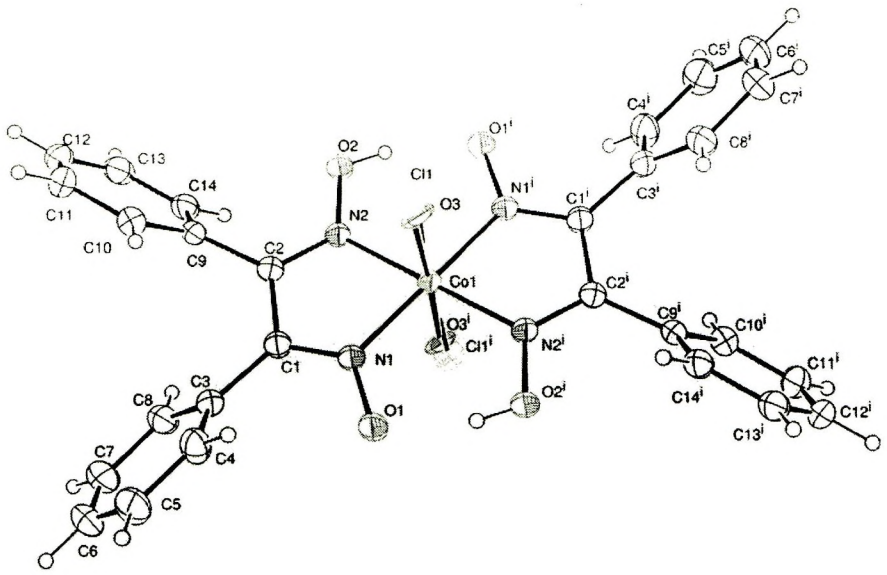

Fig. 2