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Crystal structure of bis[*N*,*N*-bis(2-hydroxyethyl)glycinato-κ^3O^1,N,O^2]-cobalt(II) monohydrate

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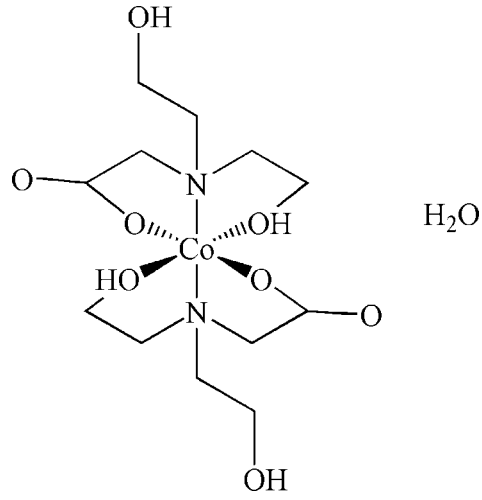
The title compound, $[Co(C_6H_{12}O_4)_2]\cdot H_2O$, was prepared by mild heating of an aqueous solution. The Co^{II} ion has a slightly distorted octahedral coordination environment which is defined by two N atoms occupying the apical position, while the equatorial plane is furnished by two hydroxy O atoms and two carboxylate O atoms. The four hydroxy O atoms from two distinct *N*,*N*-bis(2-hydroxyethyl)glycine ($bicH_2^-$) ligands act as hydrogen-bond donors with two carboxylate O atoms as acceptors to form O—H···O hydrogen-bonded layers extending parallel to (100). In addition, the guest water molecule acts as both a hydrogen-bond donor and acceptor, so that each $Co(bicH_2)_2$ molecule is connected simultaneously to six neighbouring $Co(bicH_2)_2$ and two guest water molecules by hydrogen bonding.

Keywords: crystal structure; *N*,*N*-bis(2-hydroxyethyl)glycine; hydrogen bond.

CCDC reference: 1431271

1. Related literature

For *N*,*N*-bis(2-hydroxyethyl)glycine complexes with transition metals, see: Graham *et al.* (2009); Katsoulakou *et al.* (2011); Liu *et al.* (2013); Inomata *et al.* (2001); Messimeri *et al.* (2002). Iminodiacetic acid (Cui *et al.*, 2008; Kong *et al.*, 2008), nitrilotriacetic acid (Ma *et al.*, 2009) and *N*-(2-carbamoylmethyl)iminodiacetic acid (Bugella-Altamirano *et al.*, 2003) are also known to be effective ligands for transition metal ions.



2. Experimental

2.1. Crystal data

$[Co(C_6H_{12}NO_4)_2]\cdot H_2O$
M_r = 401.28
Monoclinic, $P2_1/c$
a = 19.274 (3) Å
b = 12.0033 (17) Å
c = 7.196 (1) Å
β = 100.081 (2)°
V = 1639.1 (4) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 1.10 mm^{-1}
T = 296 K
0.20 × 0.20 × 0.20 mm

2.2. Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2012)
T_{min} = 0.810, T_{max} = 0.810
9415 measured reflections
3685 independent reflections
2982 reflections with $I > 2\sigma(I)$
R_{int} = 0.031

2.3. Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.037
$wR(F^2)$ = 0.108
S = 1.04
3685 reflections
229 parameters
7 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 1.22 e Å^{-3}
$\Delta\rho_{min}$ = −0.51 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O3—H3*AA*···O6^{i}	0.81 (2)	1.79 (2)	2.591 (2)	169 (3)
O4—H4*AA*···O2^{ii}	0.76 (2)	1.98 (2)	2.733 (2)	171 (3)
O7—H7*AA*···O2^{iii}	0.82 (2)	1.83 (2)	2.648 (2)	178 (3)
O8—H8*AA*···O9^{iv}	0.82 (2)	1.89 (2)	2.687 (3)	162 (3)
O9—H9*AA*···O6^{v}	0.82 (2)	1.99 (2)	2.796 (2)	171 (3)
O9—H9*BB*···O8^{iii}	0.81 (2)	1.95 (2)	2.759 (3)	176 (3)

Symmetry codes: (i) $x, -y+\frac{3}{2}, z+\frac{1}{2}$; (ii) $-x, y+\frac{1}{2}, -z+\frac{1}{2}$; (iii) $x, -y+\frac{1}{2}, z-\frac{1}{2}$; (iv) $x, y, z+1$; (v) $-x+1, y-\frac{1}{2}, -z+\frac{1}{2}$.

Data collection: *SMART* (Bruker, 2012); cell refinement: *SAINT* (Bruker, 2012); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 2012); software used to prepare material for publication: *SHELXTL* (Sheldrick, 2008).

Acknowledgements

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Supporting information for this paper is available from the IUCr electronic archives (Reference: BQ2401).

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Crystal structure of bis[*N*,*N*-bis(2-hydroxyethyl)glycinato-κ^3O^1,N,O^2]cobalt(II) monohydrate

Yang Liu, Dan Zhou, Hai-Hui Liu and Chen-Cong He

S1. Comment

The design and synthesis of transition metal coordination complexes based on those multi-dentate flexible carboxylate ligands have attracted significant attention due to their structural diversity and utility in supramolecular chemistry and crystal engineering. Iminodiacetic acid (Cui *et al.*, 2008; Kong *et al.*, 2008), nitrilotriacetic acid (Ma *et al.*, 2009) and N-(2-carbamoylmethyl)iminodiacetic acid (Bugella-Altamirano *et al.*, 2003) have been known as effective ligands for transition metal ions. As an analogous ligand, N,N-bis(2-hydroxyethyl) glycine is a widely used buffer in many biochemical studies. However, transition metal complexes with N,N-bis(2-hydroxyethyl) glycine has been less extensively studied, and only a few reports describing N,N-bis(2-hydroxyethyl) glycine complexes have appeared (Graham *et al.*, 2009; Katsoulakou *et al.*, 2011; Liu *et al*., 2013; Inomata *et al.*, 2001; Messimeri *et al.*, 2002). In the present report, we describe the synthesis and structure of title compound.

Single-crystal X-ray diffraction analysis shows that the title compound crystallizes in the monoclinic space group $P2_1/c$ and its asymmetric unit contains one Co (II) ion, two distinct deprotonated N,N-bis(2-hydroxyethyl) glycine ($bicH_2^-$) anions and one water molecule. As showed in Fig. 1, Co^{II} ion has a six-coordinated octahedral geometry which is defined by two nitrogen atoms occupying the apical position, while the equatorial plane are furnished by two hydroxyl oxygen atoms and two carboxylate atoms. The Co—O (Co1—O1 = 2.0544 (14) Å; Co1—O3 = 2.1093 Å; Co1—O5 = 2.0853 (15) Å; Co1—O7 = 2.1006 (7) Å) and Co—N (Co1—N1 = 2.1641 Å; Co1—N2 = 2.1881 Å) bond lengths are fall in the usual range. The crystal structure of the title compound is stabilized by hydrogen bonds. A packing diagram of the complex showing hydrogen bonding interactions is shown in Fig. 2. The hydroxyl oxygen atoms (O3, O4, O7, O8) from the N,N-bis(2-hydroxyethyl)glycine ligands act as donors, while the carboxylate oxygen atoms (O2 and O6) are the acceptors. The hydrogen bonding interactions around one molecule are shown in Fig. 3. The hydrogen bonding parameters are tabulated in Table 1.

S2. Experimental

A mixture of $CoCl_2·6H_2O$ (0.237g, 1mmol) and N,N-bis(2-hydroxyethyl) glycine; (0.16g, 1mmol) was dissolved in water (20mL) and then drop of ethlylene diamine was added, and the mixture was stirred vigorously for 1h at 60 °C. Slow evaporation of the clear solution resulted in the separation of blue block crystals.

S3. Refinement

All H atoms were positioned geometrically and treated as riding on their parent atoms [C—H =0.97 Å and *U*iso = 1.2Ueq (C) for CH_2 H atoms].

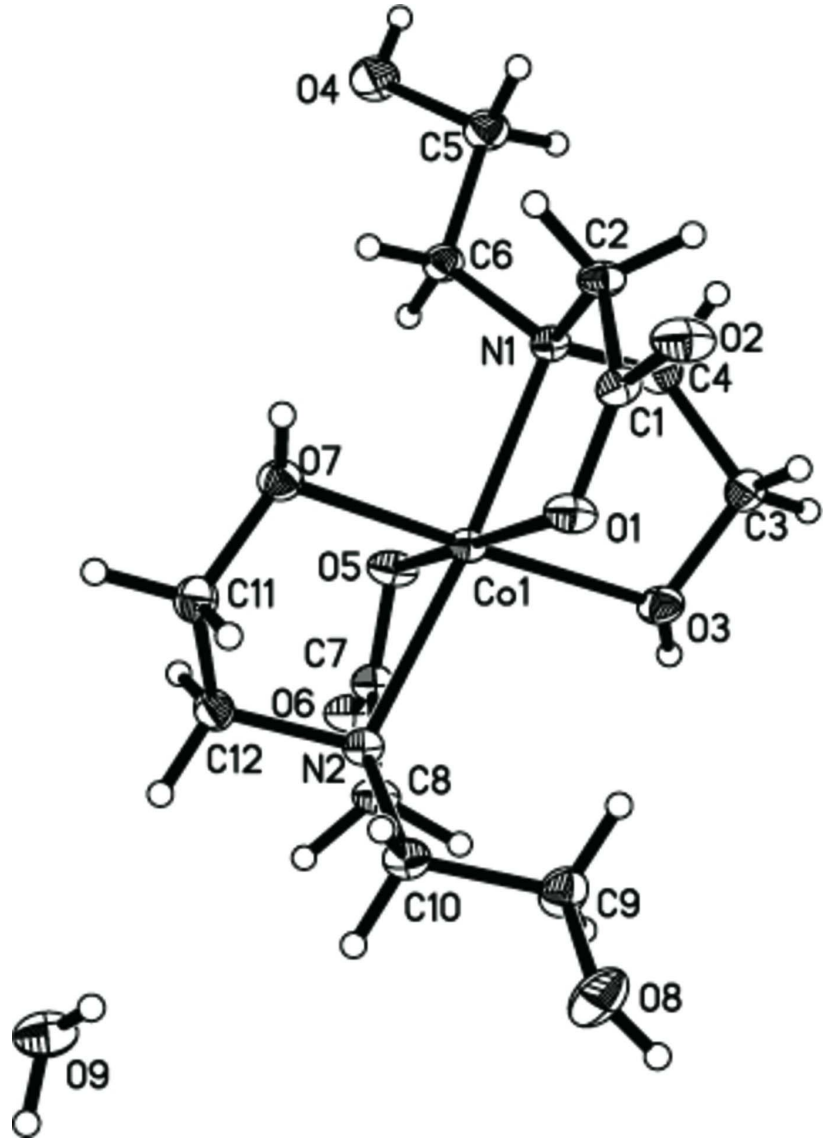

Figure 1

The structure of the title complex, showing 30% probability displacement ellipsoids and the atom-numbering scheme. H atoms have been omitted for clarity.

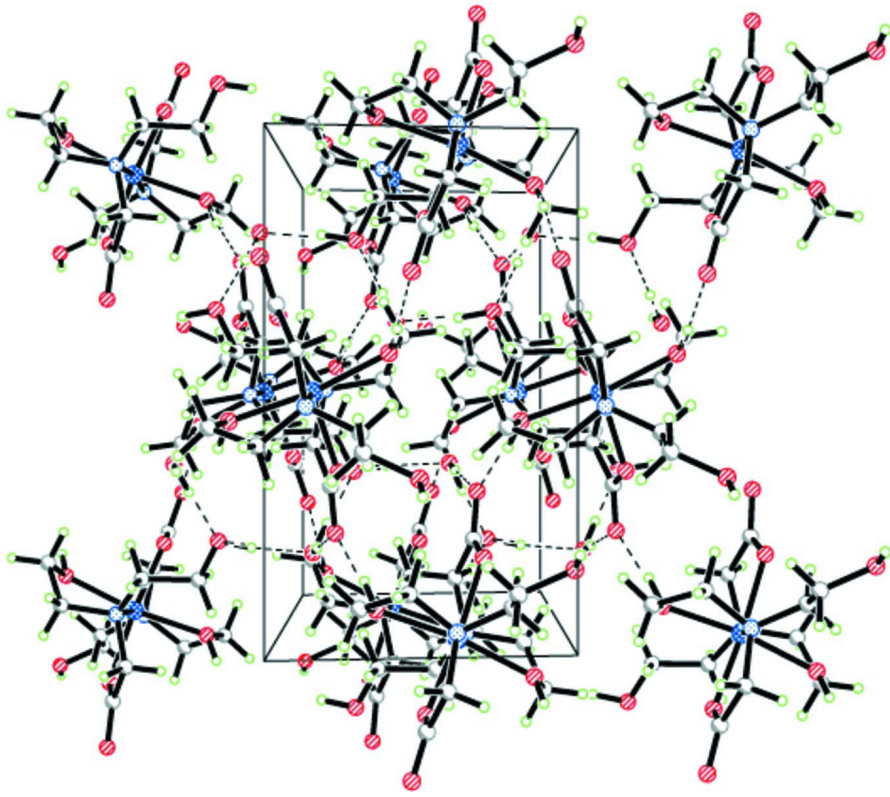

Figure 2

A partial view along the *c* axis of the crystal packing of the title compound.

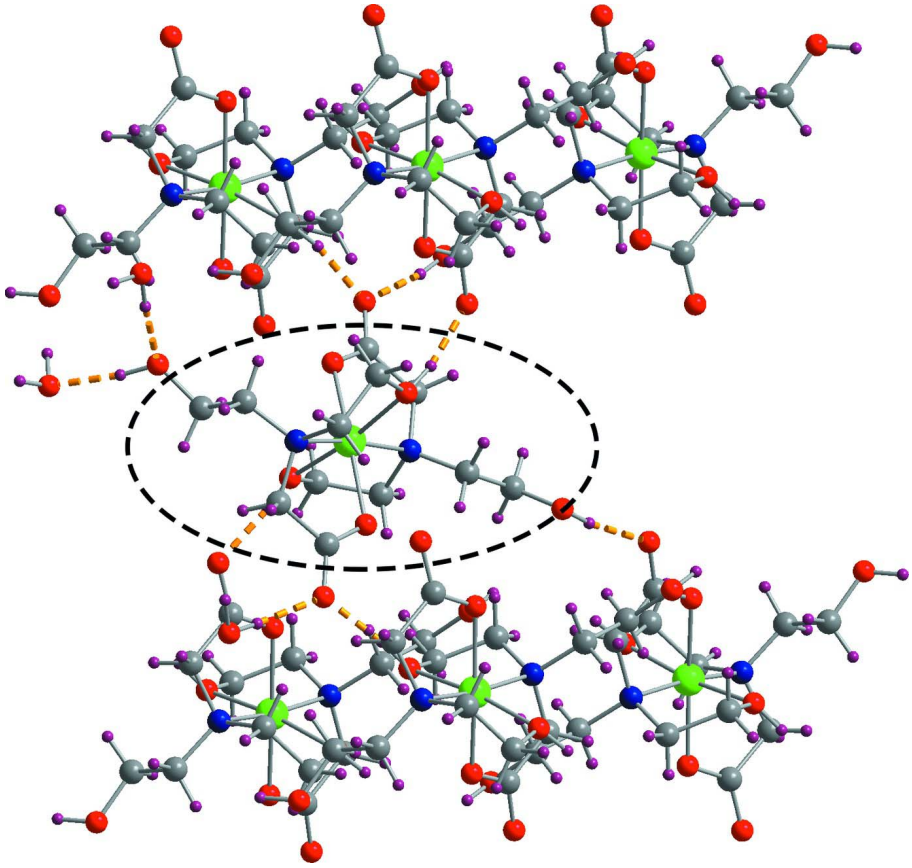

Figure 3

View of the hydrogen-bonding interactions for the title compound.

Bis[*N*,*N*-bis(2-hydroxyethyl)glycinato-κ^3O^1,*N*,O^2]cobalt(II) monohydrate

Crystal data

$[Co(C_6H_{12}NO_4)_2]\cdot H_2O$
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$c = 7.196$ (1) Å
$\beta = 100.081$ (2)°
$V = 1639.1$ (4) Å^3
$Z = 4$
$F(000) = 844$
$D_x = 1.626$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 4351 reflections
$\theta = 2.7$–27.4°
$\mu = 1.10$ mm^{-1}
$T = 296$ K
Block, red
0.20 × 0.20 × 0.20 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
phi and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2012)
$T_{min} = 0.810$, $T_{max} = 0.810$
9415 measured reflections
3685 independent reflections
2982 reflections with $I > 2\sigma(I)$
$R_{int} = 0.031$
$\theta_{max} = 27.5°$, $\theta_{min} = 1.1°$
$h = -25\rightarrow24$
$k = -14\rightarrow15$
$l = -7\rightarrow9$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.037$
$wR(F^2) = 0.108$
$S = 1.04$
3685 reflections
229 parameters
7 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
$w = 1/[\sigma^2(F_o^2) + (0.0683P)^2 + 0.2267P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 1.22$ e Å^{-3}
$\Delta\rho_{min} = -0.51$ e Å^{-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 (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
C1	0.15613 (10)	0.32888 (16)	0.4861 (3)	0.0250 (4)
C2	0.10124 (10)	0.41726 (16)	0.4166 (3)	0.0257 (4)
H2A	0.0728	0.3921	0.2995	0.031*
H2B	0.0703	0.4255	0.5086	0.031*
C3	0.18533 (11)	0.56936 (19)	0.7134 (3)	0.0317 (5)
H3A	0.1877	0.6247	0.8125	0.038*
H3B	0.1715	0.4989	0.7620	0.038*
C4	0.13146 (11)	0.60422 (18)	0.5450 (3)	0.0292 (5)
H4A	0.0850	0.6048	0.5794	0.035*
H4B	0.1419	0.6792	0.5075	0.035*
C5	0.02221 (11)	0.61413 (19)	0.1906 (3)	0.0323 (5)
H5A	−0.0073	0.5502	0.2042	0.039*
H5B	0.0177	0.6676	0.2889	0.039*
C6	0.09822 (6)	0.57870 (9)	0.20355 (17)	0.0258 (4)
H6A	0.1008	0.5260	0.1029	0.031*
H6B	0.1256	0.6436	0.1812	0.031*
C7	0.32255 (6)	0.69375 (9)	0.32133 (17)	0.0248 (4)
C8	0.37980 (6)	0.60795 (9)	0.38576 (17)	0.0260 (4)
H8A	0.4193	0.6211	0.3217	0.031*
H8B	0.3964	0.6158	0.5204	0.031*
C9	0.40241 (13)	0.41472 (19)	0.6612 (3)	0.0364 (5)
H9A	0.4220	0.4849	0.7126	0.044*
H9B	0.3550	0.4077	0.6882	0.044*
C10	0.40096 (11)	0.41103 (16)	0.4523 (3)	0.0264 (4)

H10A	0.4483	0.4236	0.4281	0.032*
H10B	0.3865	0.3371	0.4064	0.032*
C11	0.29542 (11)	0.38393 (18)	0.0716 (3)	0.0304 (5)
H11A	0.2917	0.3727	−0.0633	0.036*
H11B	0.3093	0.3141	0.1353	0.036*
C12	0.34855 (5)	0.47358 (8)	0.13899 (15)	0.0273 (4)
H12A	0.3944	0.4512	0.1144	0.033*
H12B	0.3352	0.5418	0.0698	0.033*
N1	0.13172 (5)	0.52733 (8)	0.38473 (15)	0.0212 (3)
N2	0.35292 (5)	0.49430 (8)	0.34461 (15)	0.0211 (4)
O1	0.21990 (7)	0.34960 (12)	0.4875 (2)	0.0277 (3)
O2	0.13358 (8)	0.23761 (12)	0.5359 (2)	0.0371 (4)
O3	0.25265 (7)	0.55828 (13)	0.6590 (2)	0.0301 (3)
O4	0.00231 (8)	0.66298 (18)	0.0101 (2)	0.0420 (5)
O5	0.25988 (7)	0.66233 (12)	0.2898 (2)	0.0300 (3)
O6	0.34269 (8)	0.79245 (11)	0.3073 (2)	0.0345 (4)
O7	0.22955 (8)	0.42119 (12)	0.1150 (2)	0.0287 (3)
O8	0.44467 (10)	0.32506 (15)	0.7424 (3)	0.0462 (5)
O9	0.51436 (10)	0.34647 (15)	0.0981 (3)	0.0430 (4)
Co1	0.242384 (13)	0.500933 (18)	0.37854 (4)	0.01991 (11)
H3AA	0.2766 (14)	0.6113 (19)	0.700 (4)	0.051 (9)*
H4AA	−0.0348 (10)	0.685 (2)	0.010 (4)	0.047 (8)*
H7AA	0.1993 (14)	0.373 (2)	0.091 (5)	0.067 (10)*
H8AA	0.4681 (15)	0.345 (3)	0.843 (3)	0.056 (9)*
H9AA	0.5568 (9)	0.336 (2)	0.118 (4)	0.049 (8)*
H9BB	0.4938 (13)	0.298 (2)	0.145 (4)	0.064 (11)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0250 (10)	0.0219 (10)	0.0260 (10)	−0.0018 (8)	−0.0013 (8)	0.0019 (8)
C2	0.0209 (9)	0.0212 (10)	0.0333 (11)	−0.0024 (7)	0.0001 (8)	0.0042 (8)
C3	0.0303 (11)	0.0378 (12)	0.0264 (11)	−0.0023 (9)	0.0031 (8)	−0.0051 (9)
C4	0.0304 (11)	0.0256 (10)	0.0310 (11)	0.0031 (8)	0.0035 (9)	−0.0044 (9)
C5	0.0271 (11)	0.0337 (12)	0.0352 (12)	0.0057 (9)	0.0023 (9)	0.0055 (9)
C6	0.0234 (10)	0.0268 (10)	0.0262 (10)	0.0030 (8)	0.0016 (8)	0.0048 (8)
C7	0.0250 (10)	0.0187 (9)	0.0299 (10)	0.0005 (7)	0.0027 (8)	0.0034 (8)
C8	0.0215 (9)	0.0172 (9)	0.0380 (12)	−0.0020 (7)	0.0020 (8)	0.0013 (8)
C9	0.0405 (13)	0.0335 (12)	0.0339 (12)	0.0120 (10)	0.0029 (10)	0.0063 (9)
C10	0.0261 (10)	0.0194 (9)	0.0328 (11)	0.0056 (8)	0.0024 (8)	0.0013 (8)
C11	0.0316 (11)	0.0303 (11)	0.0291 (11)	0.0000 (9)	0.0049 (9)	−0.0059 (9)
C12	0.0259 (10)	0.0297 (10)	0.0270 (10)	0.0009 (8)	0.0069 (8)	0.0025 (8)
N1	0.0209 (8)	0.0174 (7)	0.0246 (8)	0.0018 (6)	0.0019 (6)	0.0010 (6)
N2	0.0216 (9)	0.0155 (8)	0.0254 (9)	0.0008 (6)	0.0025 (7)	0.0007 (6)
O1	0.0212 (7)	0.0206 (7)	0.0403 (8)	−0.0010 (5)	0.0021 (6)	0.0058 (6)
O2	0.0274 (8)	0.0254 (8)	0.0553 (10)	−0.0057 (6)	−0.0015 (7)	0.0155 (7)
O3	0.0254 (8)	0.0305 (9)	0.0324 (8)	−0.0043 (6)	−0.0006 (6)	−0.0082 (6)
O4	0.0300 (9)	0.0542 (12)	0.0399 (10)	0.0163 (8)	0.0011 (8)	0.0155 (7)

O5	0.0218 (7)	0.0213 (7)	0.0459 (9)	0.0004 (5)	0.0030 (6)	0.0069 (6)
O6	0.0283 (8)	0.0177 (7)	0.0546 (10)	−0.0021 (6)	−0.0012 (7)	0.0092 (6)
O7	0.0258 (8)	0.0288 (8)	0.0310 (8)	−0.0031 (6)	0.0035 (6)	−0.0057 (6)
O8	0.0596 (12)	0.0354 (9)	0.0381 (10)	0.0159 (8)	−0.0070 (8)	0.0072 (8)
O9	0.0337 (10)	0.0388 (10)	0.0527 (11)	0.0051 (8)	−0.0032 (8)	0.0065 (9)
Co1	0.01819 (17)	0.01581 (17)	0.02525 (18)	−0.00122 (8)	0.00248 (11)	0.00056 (9)

Geometric parameters (Å, º)

C1—O1	1.252 (2)	C9—O8	1.413 (3)
C1—O2	1.254 (2)	C9—C10	1.499 (3)
C1—C2	1.520 (3)	C9—H9A	0.9700
C2—N1	1.480 (2)	C9—H9B	0.9700
C2—H2A	0.9700	C10—N2	1.485 (2)
C2—H2B	0.9700	C10—H10A	0.9700
C3—O3	1.426 (3)	C10—H10B	0.9700
C3—C4	1.510 (3)	C11—O7	1.431 (3)
C3—H3A	0.9700	C11—C12	1.506 (2)
C3—H3B	0.9700	C11—H11A	0.9700
C4—N1	1.478 (2)	C11—H11B	0.9700
C4—H4A	0.9700	C12—N2	1.4882
C4—H4B	0.9700	C12—H12A	0.9700
C5—O4	1.416 (3)	C12—H12B	0.9700
C5—C6	1.513 (2)	N1—Co1	2.1644
C5—H5A	0.9700	N2—Co1	2.1878
C5—H5B	0.9700	O1—Co1	2.0544 (14)
C6—N1	1.4840 (15)	O3—Co1	2.1083 (15)
C6—H6A	0.9700	O3—H3AA	0.811 (17)
C6—H6B	0.9700	O4—H4AA	0.761 (17)
C7—O5	1.2476 (17)	O5—Co1	2.0858 (14)
C7—O6	1.2562 (17)	O7—Co1	2.1000 (15)
C7—C8	1.5212	O7—H7AA	0.820 (18)
C8—N2	1.4709 (15)	O8—H8AA	0.822 (17)
C8—H8A	0.9700	O9—H9AA	0.815 (16)
C8—H8B	0.9700	O9—H9BB	0.810 (16)
O1—C1—O2	124.06 (18)	C9—C10—H10B	108.8
O1—C1—C2	119.33 (17)	H10A—C10—H10B	107.7
O2—C1—C2	116.60 (17)	O7—C11—C12	106.59 (15)
N1—C2—C1	113.69 (15)	O7—C11—H11A	110.4
N1—C2—H2A	108.8	C12—C11—H11A	110.4
C1—C2—H2A	108.8	O7—C11—H11B	110.4
N1—C2—H2B	108.8	C12—C11—H11B	110.4
C1—C2—H2B	108.8	H11A—C11—H11B	108.6
H2A—C2—H2B	107.7	N2—C12—C11	110.89 (9)
O3—C3—C4	109.65 (17)	N2—C12—H12A	109.5
O3—C3—H3A	109.7	C11—C12—H12A	109.5
C4—C3—H3A	109.7	N2—C12—H12B	109.5

O3—C3—H3B	109.7	C11—C12—H12B	109.5
C4—C3—H3B	109.7	H12A—C12—H12B	108.0
H3A—C3—H3B	108.2	C4—N1—C2	112.38 (14)
N1—C4—C3	110.93 (16)	C4—N1—C6	111.45 (11)
N1—C4—H4A	109.5	C2—N1—C6	112.57 (11)
C3—C4—H4A	109.5	C4—N1—Co1	104.21 (10)
N1—C4—H4B	109.5	C2—N1—Co1	106.97 (9)
C3—C4—H4B	109.5	C6—N1—Co1	108.76 (7)
H4A—C4—H4B	108.0	C8—N2—C10	110.71 (11)
O4—C5—C6	106.08 (16)	C8—N2—C12	108.16 (6)
O4—C5—H5A	110.5	C10—N2—C12	109.15 (9)
C6—C5—H5A	110.5	C8—N2—Co1	105.03 (7)
O4—C5—H5B	110.5	C10—N2—Co1	119.78 (10)
C6—C5—H5B	110.5	C12—N2—Co1	103.31 (3)
H5A—C5—H5B	108.7	C1—O1—Co1	116.41 (12)
N1—C6—C5	116.02 (12)	C3—O3—Co1	110.85 (11)
N1—C6—H6A	108.3	C3—O3—H3AA	108 (2)
C5—C6—H6A	108.3	Co1—O3—H3AA	124 (2)
N1—C6—H6B	108.3	C5—O4—H4AA	104 (2)
C5—C6—H6B	108.3	C7—O5—Co1	115.36 (10)
H6A—C6—H6B	107.4	C11—O7—Co1	111.77 (12)
O5—C7—O6	124.99 (13)	C11—O7—H7AA	111 (2)
O5—C7—C8	118.57 (8)	Co1—O7—H7AA	119 (2)
O6—C7—C8	116.43 (8)	C9—O8—H8AA	109 (2)
N2—C8—C7	110.82 (6)	H9AA—O9—H9BB	111 (2)
N2—C8—H8A	109.5	O1—Co1—O5	173.89 (6)
C7—C8—H8A	109.5	O1—Co1—O7	86.68 (6)
N2—C8—H8B	109.5	O5—Co1—O7	98.43 (6)
C7—C8—H8B	109.5	O1—Co1—O3	85.08 (6)
H8A—C8—H8B	108.1	O5—Co1—O3	89.81 (6)
O8—C9—C10	107.49 (18)	O7—Co1—O3	171.76 (6)
O8—C9—H9A	110.2	O1—Co1—N1	81.21 (5)
C10—C9—H9A	110.2	O5—Co1—N1	94.77 (5)
O8—C9—H9B	110.2	O7—Co1—N1	97.16 (5)
C10—C9—H9B	110.2	O3—Co1—N1	81.97 (5)
H9A—C9—H9B	108.5	O1—Co1—N2	106.55 (5)
N2—C10—C9	113.81 (16)	O5—Co1—N2	77.69 (5)
N2—C10—H10A	108.8	O7—Co1—N2	81.12 (5)
C9—C10—H10A	108.8	O3—Co1—N2	100.87 (5)
N2—C10—H10B	108.8	N1—Co1—N2	171.86 (5)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O3—H3*AA*···O6^{i}	0.81 (2)	1.79 (2)	2.591 (2)	169 (3)
O4—H4*AA*···O2^{ii}	0.76 (2)	1.98 (2)	2.733 (2)	171 (3)
O7—H7*AA*···O2^{iii}	0.82 (2)	1.83 (2)	2.648 (2)	178 (3)
O8—H8*AA*···O9^{iv}	0.82 (2)	1.89 (2)	2.687 (3)	162 (3)

O9—H9*AA*···O6^{v}	0.82 (2)	1.99 (2)	2.796 (2)	171 (3)
O9—H9*BB*···O8^{iii}	0.81 (2)	1.95 (2)	2.759 (3)	176 (3)

Symmetry codes: (i) x, $-y+3/2$, $z+1/2$; (ii) $-x$, $y+1/2$, $-z+1/2$; (iii) x, $-y+1/2$, $z-1/2$; (iv) x, y, $z+1$; (v) $-x+1$, $y-1/2$, $-z+1/2$.