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Diaquabis(2,2′-biimidazole)cobalt(II) 4,4′-dicarboxybiphenyl-3,3′-dicarboxylate

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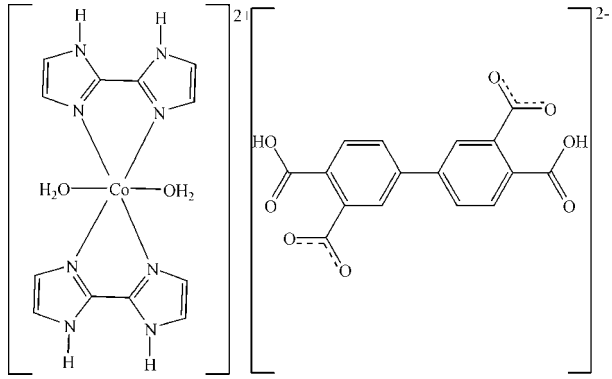
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.003 Å; R factor = 0.033; wR factor = 0.087; data-to-parameter ratio = 11.5.

In the title compound, $[Co(C_6H_6N_4)_2(H_2O)_2](C_{16}H_8O_8)$, the Co^{II} cation and the organic anion occupy different crystallographic inversion centres and, as a consequence, the asymmetric unit comprises two half-molecules. The benzene groups are coplanar. The four coordinating N atoms of the two bidentate biimidazole ligands define the equatorial plane of a slightly distorted octahedral CoO_2N_4 geometry, and the water O atoms lie in the axial coordination sites. Translational (a,$\bar{b}$) and inversion-related symmetry operations link the Co complex molecules and the negatively charged carboxylate anions *via* intermolecular N—H···O and O—H···O hydrogen bonds into sheets parallel to ($\bar{1}$01). The coordinated water molecules connect the sheets through O—H···O hydrogen bonds, forming a three-dimensional framework. In addition, two intramolecular O—H···O hydrogen bonds are observed between the carboxyl and carboxylate groups.

Related literature

For a review on organic–inorganic hybrid materials, see: Hagrman *et al.* (1999). For a tetranuclear cobalt complex with a 1,2,4-benzenetricarboxylate linker, see: Jia *et al.* (2007). For a highly porous metal-organic framework with a benzenedicarboxylate linker, see: Li *et al.* (1999). For coordination polymers of Ag(I), Cd(II) and Zn(II) with the flexible 2-(1*H*-imidazole-1-yl)acetic acid linker, see: Wang *et al.* (2007). For the structure of 1,1′-biphenyl-2,3,3′,4′-tetracarboxylic acid monohydrate and related structures cited therein, see: Jiang *et al.* (2008).



Experimental

Crystal data

$[Co(C_6H_6N_4)_2(H_2O)_2](C_{16}H_8O_8)$
M_r = 691.48
Triclinic, $P\bar{1}$
a = 8.2272 (16) Å
b = 9.772 (2) Å
c = 10.484 (2) Å
α = 63.81 (3)°
β = 67.93 (3)°
γ = 84.03 (3)°
V = 699.0 (2) Å^3
Z = 1
Mo $K\alpha$ radiation
μ = 0.69 mm^{-1}
T = 293 K
0.42 × 0.26 × 0.20 mm

Data collection

Bruker APEXII CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2001)
T_{min} = 0.760, T_{max} = 0.874
4982 measured reflections
2603 independent reflections
2527 reflections with $I > 2\sigma(I)$
R_{int} = 0.022

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.033
$wR(F^2)$ = 0.087
S = 1.01
2603 reflections
227 parameters
5 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.31 e Å^{-3}
$\Delta\rho_{min}$ = −0.21 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Co1—O5	2.0882 (19)	Co1—N3	2.1579 (16)
Co1—N1	2.1412 (16)		
O5—Co1—N1	88.32 (7)	O5—Co1—N3	87.82 (7)
N1—Co1—N3^{i}	100.77 (6)		

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

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

D—H···A	D—H	H···A	D···A	D—H···A
N2—H2A···O1^{ii}	0.92 (2)	1.87 (2)	2.791 (3)	178.8 (18)
N4—H4A···O2^{ii}	0.920 (18)	1.897 (19)	2.808 (3)	170.3 (19)
O5—H1W···O1^{iii}	0.82 (2)	1.93 (2)	2.739 (3)	169 (2)
O5—H2W···O4^{i}	0.81 (2)	1.88 (2)	2.673 (3)	163 (2)
O3—H3···O2	0.82	1.62	2.432 (3)	172

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

Data collection: *APEX2* (Bruker, 2004); cell refinement: *SAINT-Plus* (Bruker, 2001); data reduction: *SAINT-Plus*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: SI2153).

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supporting information

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Diaquabis(2,2′-biimidazole)cobalt(II) 4,4′-dicarboxybiphenyl-3,3′-dicarboxylate

Jie Kang, Chang-Cang Huang, Lai-Sheng Zhai, Xiao-Huan Qin and Zhong-Qian Liu

S1. Comment

Design and construction of metal-organic frameworks (MOFs) have attracted considerable attention in recent years, not only for their intriguing structural motifs (Wang *et al.* 2007), but also for their potential applications, e. g. as organic-inorganic hybrid materials (Hagrman *et al.*, 1999), highly porous metal-organic framework (Li *et al.*, 1999), magnetochemistry (Jia *et al.*, 2007). In contrast, the two ionic components of the title structure interact with N—H···O and O—H···O hydrogen bonds to form a three-dimensional framework.

As shown in Fig. 1, the Co atom (site symmetry $\bar{1}$) is bonded to two aqua and two bidentate biimidizole ligands, to result in a slightly distorterd octahedral CoO_2N_4 geometry for the central metal. The Co^{II} cation and the organic anion occupy different crystallographic inversion centres, and as a consequence the asymmetric unit of the cell comprises two half molecules (Z′ = 1/2), and the benzene groups are co-planar. The four nitrogen atoms belonging to two biimidizole ligands lie in the equatorial plane and the two aqua oxygen atoms lie in the axial coordination sites. Selected bond lengths and angles around Co are listed in Table 1. The 1,1′-biphenyl-3,3′-dicarboxylate-4,4′-dicarboxylic acid acts as a negative electron balance. With three kinds of hydrogen bonds (Table 2) of N2—H2A···O1, N4—H4A···O2, and O5—H1W···O1, two-dimensional planes are formed. Furthermore, a three-dimensional framework (Fig. 2) is generated with the intermolecular hydrogen bonding contact O5—H2W···O4 along the [-1 0 1] direction. The organic anion has two intramolecular O3—H3···O2 hydrogen bonds between the carboxylic acid units and the carboxylate acceptors (Table 2). In contrast to the co-planar biphenyl group of the title compound, a dihedral angle of 42.30 (11)° between the two benzene rings was observed in the structure of 1,1′-biphenyl-2,3,3′,4′-tetracarboxylic acid monohydrate (Jiang *et al.* 2008).

S2. Experimental

All chemicals and Teflon-lined stainless steel autoclave were purchased from Jinan Henghua Sci. & Tec. Co. Ltd. A mixture of 3,3′,4,4′-biphenyl tetracarboxylic acid (0.1 mmoL), cobalt(II) acetate (0.1 mmoL), and diimdazole (0.1 mmoL) in 10 ml distilled water sealed in a 25 ml Teflon-lined stainless steel autoclave was kept at 433 K for three days. Yellow crystals suitable for the X-ray experiment were obtained.

S3. Refinement

The H atoms of the water molecule were located from difference density maps and were refined with distance restraints of d(H–H) = 1.38 (2) Å, d(O–H) = 0.88 (2) Å, and with a fixed U_{iso} of 0.056 Å^2. All other H atoms were placed in calculated positions with a C—H bond distance of 0.93 Å and U_{iso}(H) = 1.2U_{eq} of the carrier atom.

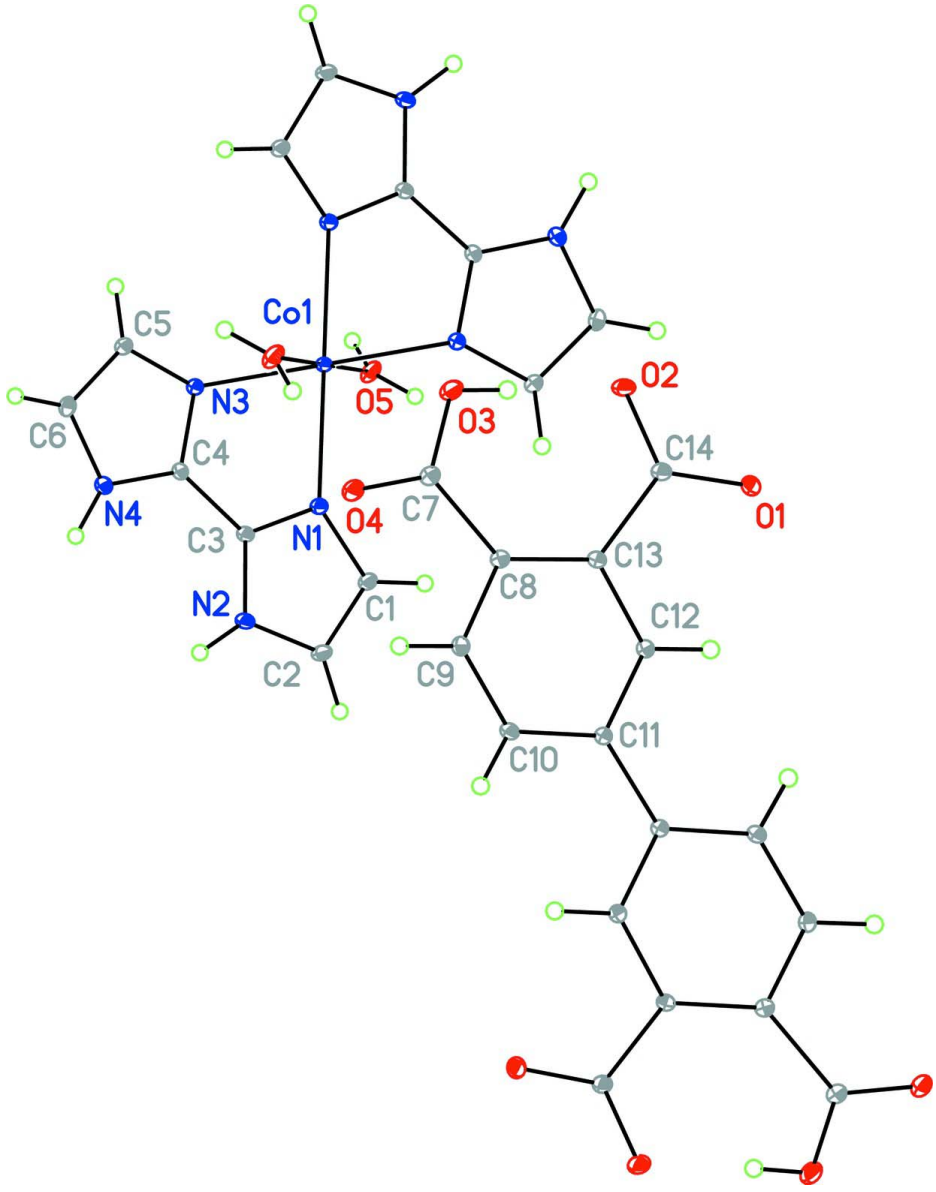

Figure 1

The molecular structure of the title compound with displacement ellipsoids drawn at the 10% probability level. Symmetry-related atoms are unlabelled. Symmetry code for the Co-complex: (1 - *x*, 1 - *y*, 1 - *z*); symmetry code for the organic anion: (1 - *x*, 2 - *y*, 2 - *z*).

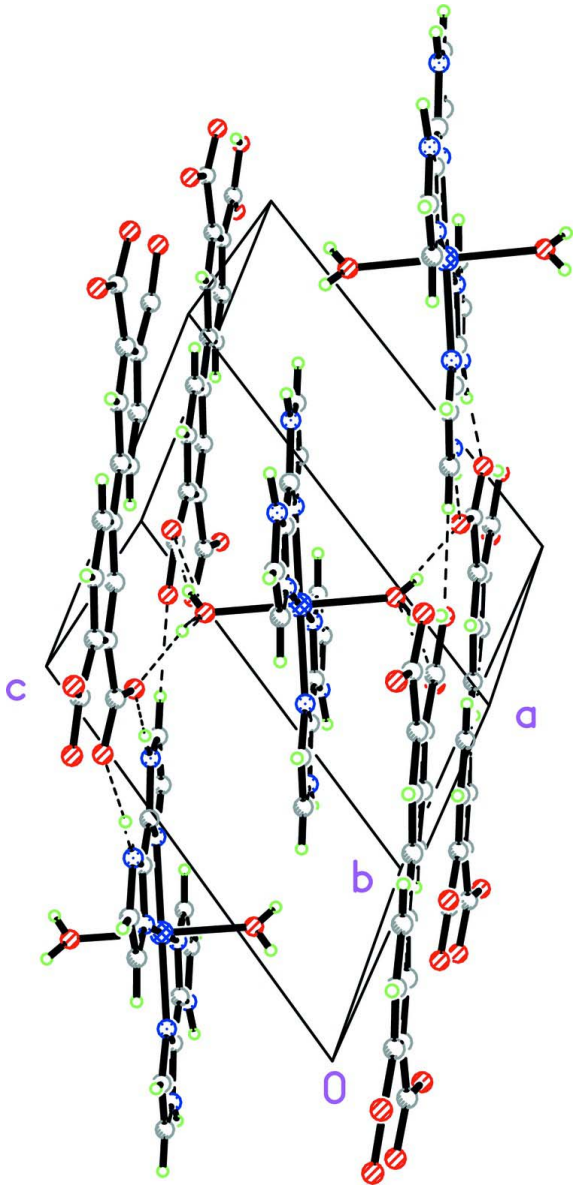

Figure 2

A packing view of the title compound. Hydrogen bonds are marked by dashed lines.

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Crystal data

$[Co(C_6H_6N_4)_2(H_2O)_2](C_{16}H_8O_8)$
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Triclinic, $P\overline{1}$
Hall symbol: -P 1
$a = 8.2272$ (16) Å
$b = 9.772$ (2) Å
$c = 10.484$ (2) Å
$\alpha = 63.81$ (3)°
$\beta = 67.93$ (3)°
$\gamma = 84.03$ (3)°
$V = 699.0$ (2) Å^3
$Z = 1$
$F(000) = 355$
$D_x = 1.643$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 2603 reflections
$\theta = 3.1$–25.8°
$\mu = 0.69$ mm^{-1}

T = 293 K
Block, colorless

0.42 × 0.26 × 0.20 mm

Data collection

Bruker APEXII CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2001)
T_{min} = 0.760, T_{max} = 0.874

4982 measured reflections
2603 independent reflections
2527 reflections with $I > 2\sigma(I)$
R_{int} = 0.022
θ_{max} = 25.8°, θ_{min} = 3.1°
h = −10→9
k = −11→11
l = −12→12

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.033
$wR(F^2)$ = 0.087
S = 1.01
2603 reflections
227 parameters
5 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
$w = 1/[\sigma^2(F_o^2) + (0.045P)^2 + 0.376P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.31 e Å^{-3}
$\Delta\rho_{min}$ = −0.21 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 (Å^2)

	x	y	z	U_{iso}*/U_{eq}
Co1	0.5000	0.5000	0.5000	0.03059 (13)
C1	0.7400 (3)	0.5910 (2)	0.6513 (3)	0.0388 (5)
H1	0.7036	0.6865	0.6446	0.047*
C2	0.8671 (3)	0.5187 (2)	0.7049 (3)	0.0403 (5)
H2	0.9323	0.5542	0.7415	0.048*
C3	0.7617 (2)	0.3779 (2)	0.6368 (2)	0.0303 (4)
C4	0.7231 (2)	0.2591 (2)	0.6037 (2)	0.0305 (4)
C5	0.5986 (3)	0.1500 (2)	0.5229 (3)	0.0396 (5)
H5	0.5266	0.1311	0.4812	0.047*
C6	0.7143 (3)	0.0532 (2)	0.5751 (3)	0.0428 (5)
H6	0.7355	−0.0425	0.5762	0.051*
C7	0.2215 (3)	0.6649 (2)	0.8670 (2)	0.0355 (4)
C8	0.2957 (2)	0.7806 (2)	0.8950 (2)	0.0300 (4)

C9	0.4327 (3)	0.7276 (2)	0.9485 (2)	0.0372 (5)
H9	0.4710	0.6319	0.9577	0.045*
C10	0.5135 (3)	0.8106 (2)	0.9882 (3)	0.0383 (5)
H10	0.6051	0.7708	1.0222	0.046*
C11	0.4595 (2)	0.9535 (2)	0.9779 (2)	0.0289 (4)
C12	0.3260 (2)	1.0084 (2)	0.9211 (2)	0.0301 (4)
H12	0.2894	1.1046	0.9116	0.036*
C13	0.2436 (2)	0.9278 (2)	0.8777 (2)	0.0279 (4)
C14	0.1084 (2)	1.0170 (2)	0.8107 (2)	0.0330 (4)
N1	0.6735 (2)	0.50249 (18)	0.60857 (19)	0.0340 (4)
N2	0.8799 (2)	0.3839 (2)	0.6943 (2)	0.0365 (4)
H2A	0.951 (3)	0.307 (2)	0.726 (2)	0.044*
N3	0.6043 (2)	0.27901 (17)	0.54115 (19)	0.0335 (4)
N4	0.7934 (2)	0.12422 (19)	0.6258 (2)	0.0371 (4)
H4A	0.869 (2)	0.078 (2)	0.676 (2)	0.045*
O1	0.0983 (2)	1.15279 (16)	0.7860 (2)	0.0492 (4)
O2	0.0097 (2)	0.95144 (19)	0.7838 (2)	0.0552 (5)
O3	0.0823 (2)	0.68970 (19)	0.8329 (2)	0.0546 (4)
H3	0.0513	0.7749	0.8241	0.082*
O4	0.2931 (2)	0.54625 (18)	0.8800 (2)	0.0500 (4)
O5	0.7116 (2)	0.58986 (18)	0.29083 (18)	0.0469 (4)
H1W	0.763 (3)	0.6721 (18)	0.259 (3)	0.056*
H2W	0.730 (3)	0.557 (2)	0.228 (2)	0.056*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Co1	0.0353 (2)	0.0244 (2)	0.0457 (2)	0.00797 (14)	−0.02832 (17)	−0.01710 (17)
C1	0.0454 (11)	0.0331 (11)	0.0579 (13)	0.0098 (9)	−0.0324 (10)	−0.0271 (10)
C2	0.0445 (11)	0.0408 (12)	0.0564 (13)	0.0074 (9)	−0.0326 (10)	−0.0281 (10)
C3	0.0306 (9)	0.0293 (10)	0.0390 (10)	0.0070 (7)	−0.0211 (8)	−0.0158 (8)
C4	0.0343 (10)	0.0251 (9)	0.0380 (10)	0.0072 (7)	−0.0206 (8)	−0.0140 (8)
C5	0.0514 (12)	0.0301 (10)	0.0528 (12)	0.0054 (9)	−0.0327 (10)	−0.0206 (9)
C6	0.0559 (13)	0.0272 (10)	0.0599 (13)	0.0106 (9)	−0.0321 (11)	−0.0240 (10)
C7	0.0417 (11)	0.0327 (11)	0.0414 (11)	0.0038 (8)	−0.0214 (9)	−0.0194 (9)
C8	0.0341 (9)	0.0292 (10)	0.0327 (9)	0.0033 (7)	−0.0170 (8)	−0.0150 (8)
C9	0.0479 (11)	0.0277 (10)	0.0519 (12)	0.0141 (8)	−0.0317 (10)	−0.0222 (9)
C10	0.0468 (11)	0.0320 (10)	0.0561 (12)	0.0159 (9)	−0.0388 (10)	−0.0227 (9)
C11	0.0341 (9)	0.0250 (9)	0.0348 (9)	0.0058 (7)	−0.0202 (8)	−0.0139 (8)
C12	0.0337 (9)	0.0254 (9)	0.0389 (10)	0.0071 (7)	−0.0210 (8)	−0.0153 (8)
C13	0.0286 (9)	0.0276 (9)	0.0326 (9)	0.0043 (7)	−0.0176 (7)	−0.0126 (8)
C14	0.0321 (10)	0.0332 (11)	0.0443 (11)	0.0072 (8)	−0.0229 (8)	−0.0197 (9)
N1	0.0382 (9)	0.0291 (9)	0.0491 (10)	0.0093 (7)	−0.0287 (8)	−0.0205 (8)
N2	0.0371 (9)	0.0364 (9)	0.0505 (10)	0.0116 (7)	−0.0303 (8)	−0.0215 (8)
N3	0.0399 (9)	0.0260 (8)	0.0451 (9)	0.0066 (7)	−0.0273 (8)	−0.0159 (7)
N4	0.0416 (9)	0.0299 (9)	0.0503 (10)	0.0115 (7)	−0.0286 (8)	−0.0187 (8)
O1	0.0495 (9)	0.0308 (8)	0.0865 (12)	0.0132 (7)	−0.0501 (9)	−0.0234 (8)
O2	0.0614 (10)	0.0485 (9)	0.0989 (13)	0.0239 (8)	−0.0639 (10)	−0.0445 (9)

O3	0.0583 (10)	0.0429 (9)	0.0953 (13)	0.0131 (7)	−0.0519 (10)	−0.0402 (10)
O4	0.0654 (10)	0.0392 (9)	0.0746 (11)	0.0165 (7)	−0.0444 (9)	−0.0368 (8)
O5	0.0579 (10)	0.0382 (9)	0.0516 (9)	−0.0085 (7)	−0.0184 (8)	−0.0244 (7)

Geometric parameters (Å, º)

Co1—O5^{i}	2.0882 (19)	C7—O4	1.220 (3)
Co1—O5	2.0882 (19)	C7—O3	1.293 (2)
Co1—N1	2.1412 (16)	C7—C8	1.519 (3)
Co1—N1^{i}	2.1412 (16)	C8—C9	1.397 (3)
Co1—N3^{i}	2.1579 (16)	C8—C13	1.410 (3)
Co1—N3	2.1579 (16)	C9—C10	1.375 (3)
C1—C2	1.359 (3)	C9—H9	0.9300
C1—N1	1.369 (2)	C10—C11	1.390 (3)
C1—H1	0.9300	C10—H10	0.9300
C2—N2	1.360 (3)	C11—C12	1.391 (3)
C2—H2	0.9300	C11—C11^{ii}	1.490 (3)
C3—N1	1.325 (2)	C12—C13	1.395 (3)
C3—N2	1.340 (2)	C12—H12	0.9300
C3—C4	1.444 (3)	C13—C14	1.528 (3)
C4—N3	1.324 (2)	C14—O1	1.235 (2)
C4—N4	1.341 (2)	C14—O2	1.261 (2)
C5—C6	1.360 (3)	N2—H2A	0.921 (10)
C5—N3	1.364 (2)	N4—H4A	0.918 (10)
C5—H5	0.9300	O3—H3	0.8200
C6—N4	1.366 (3)	O5—H1W	0.82 (2)
C6—H6	0.9300	O5—H2W	0.81 (2)

O5^{i}—Co1—O5	180	C13—C8—C7	129.44 (17)
O5^{i}—Co1—N1	91.68 (7)	C10—C9—C8	122.91 (18)
O5—Co1—N1	88.32 (7)	C10—C9—H9	118.5
O5^{i}—Co1—N1^{i}	88.32 (7)	C8—C9—H9	118.5
N1—Co1—N1^{i}	180	C9—C10—C11	120.56 (18)
O5^{i}—Co1—N3^{i}	87.82 (7)	C9—C10—H10	119.7
O5—Co1—N3^{i}	92.18 (7)	C11—C10—H10	119.7
N1—Co1—N3^{i}	100.77 (6)	C10—C11—C12	116.73 (17)
N1^{i}—Co1—N3^{i}	79.23 (6)	C10—C11—C11^{ii}	122.6 (2)
O5^{i}—Co1—N3	92.18 (7)	C12—C11—C11^{ii}	120.7 (2)
O5—Co1—N3	87.82 (7)	C11—C12—C13	123.93 (17)
N1—Co1—N3	79.23 (6)	C11—C12—H12	118.0
N3^{i}—Co1—N3	180	C13—C12—H12	118.0
C2—C1—N1	109.90 (17)	C12—C13—C8	118.32 (16)
C2—C1—H1	125.0	C12—C13—C14	113.67 (16)
N1—C1—H1	125.0	C8—C13—C14	127.98 (16)
N2—C2—C1	106.11 (17)	O1—C14—O2	121.81 (18)
N2—C2—H2	126.9	O1—C14—C13	118.10 (17)
C1—C2—H2	126.9	O2—C14—C13	120.09 (17)
N1—C3—N2	111.51 (17)	C3—N1—C1	105.05 (16)

N1—C3—C4	119.29 (16)	C3—N1—Co1	111.21 (12)
N2—C3—C4	129.20 (17)	C1—N1—Co1	143.48 (13)
N3—C4—N4	111.61 (17)	C3—N2—C2	107.42 (17)
N3—C4—C3	119.34 (16)	C3—N2—H2A	125.3 (15)
N4—C4—C3	129.05 (17)	C2—N2—H2A	127.2 (15)
C6—C5—N3	109.48 (18)	C4—N3—C5	105.57 (16)
C6—C5—H5	125.3	C4—N3—Co1	110.75 (12)
N3—C5—H5	125.3	C5—N3—Co1	143.64 (14)
C5—C6—N4	106.57 (17)	C4—N4—C6	106.77 (17)
C5—C6—H6	126.7	C4—N4—H4A	129.4 (15)
N4—C6—H6	126.7	C6—N4—H4A	123.4 (15)
O4—C7—O3	120.13 (18)	C7—O3—H3	109.5
O4—C7—C8	119.10 (18)	Co1—O5—H1W	121.0 (16)
O3—C7—C8	120.75 (17)	Co1—O5—H2W	121.0 (16)
C9—C8—C13	117.47 (17)	H1W—O5—H2W	116.1 (17)
C9—C8—C7	113.08 (16)		

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

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2—H2*A*···O1^{iii}	0.92 (2)	1.87 (2)	2.791 (3)	179 (2)
N4—H4*A*···O2^{iii}	0.92 (2)	1.90 (2)	2.808 (3)	170 (2)
O5—H1*W*···O1^{iv}	0.82 (2)	1.93 (2)	2.739 (3)	169 (2)
O5—H2*W*···O4^{i}	0.81 (2)	1.88 (2)	2.673 (3)	163 (2)
O3—H3···O2	0.82	1.62	2.432 (3)	172

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