

# Poly[[diaqua( $\mu$ -4,4'-bipyridine $N,N'$ -dioxide- $\kappa^2O:O'$ )( $\mu$ -terephthalato- $\kappa^2O^1:O^4$ )-cobalt(II)] 4,4'-bipyridine $N,N'$ -dioxide monosolvate]

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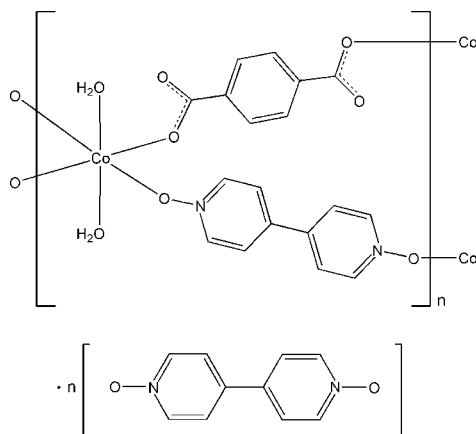
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 Key indicators: single-crystal X-ray study;  $T = 293$  K; mean  $\sigma(C-C) = 0.003$  Å;  $R$  factor = 0.031;  $wR$  factor = 0.081; data-to-parameter ratio = 12.5.

In the title compound,  $\{[Co(C_8H_4O_4)(C_{10}H_8N_2O_2)(H_2O)_2] \cdot C_{10}H_8N_2O_2\}_n$ , the  $Co^{II}$  atom, lying on an inversion center, is hexacoordinated in a distorted octahedral geometry defined by two O atoms from two terephthalate (tp) ligands, two O atoms from two 4,4'-bipyridine  $N,N'$ -dioxide (bpydo) ligands and two water molecules. The coordinated tp and bpydo ligands and uncoordinated bpydo molecule all have an inversion center. The  $Co^{II}$  atoms are connected by the tp and bpydo ligands into a layer parallel to (111). In the crystal,  $O-H \cdots O$  hydrogen bonds link the uncoordinated bpydo molecules and the layers into a three-dimensional supramolecular structure. Intralayer  $O-H \cdots O$  hydrogen bonds and  $\pi-\pi$  interactions [centroid-to-centroid distances = 3.6643 (13) and 3.8048 (13) Å] are also observed.

## Related literature

For the design of supramolecular structures containing metal ions and organic ligands, see: Liao *et al.* (2008); Wang *et al.* (2008). For a related structure, see: Su *et al.* (2009).



## Experimental

### Crystal data

$[Co(C_8H_4O_4)(C_{10}H_8N_2O_2)(H_2O)_2] \cdot C_{10}H_8N_2O_2$	$\beta = 82.200$ (2) $^\circ$
$M_r = 635.44$	$\gamma = 79.301$ (2) $^\circ$
Triclinic, $P\bar{1}$	$V = 641.92$ (15) Å <sup>3</sup>
$a = 7.3883$ (10) Å	$Z = 1$
$b = 9.1788$ (13) Å	Mo $K\alpha$ radiation
$c = 9.8054$ (13) Å	$\mu = 0.74$ mm <sup>-1</sup>
$\alpha = 81.312$ (2) $^\circ$	$T = 293$ K
	$0.27 \times 0.24 \times 0.20$ mm

### Data collection

Bruker APEXII CCD diffractometer	3574 measured reflections
Absorption correction: multi-scan (SADABS; Bruker, 2001)	2516 independent reflections
$T_{min} = 0.825$ , $T_{max} = 0.866$	2340 reflections with $I > 2\sigma(I)$
	$R_{int} = 0.017$

### Refinement

$R[F^2 > 2\sigma(F^2)] = 0.031$	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2) = 0.081$	$\Delta\rho_{max} = 0.48$ e Å <sup>-3</sup>
$S = 1.05$	$\Delta\rho_{min} = -0.33$ e Å <sup>-3</sup>
2516 reflections	
202 parameters	
2 restraints	

**Table 1**

 Hydrogen-bond geometry (Å,  $^\circ$ ).

$D-H \cdots A$	$D-H$	$H \cdots A$	$D \cdots A$	$D-H \cdots A$
$O5-H5A \cdots O2$	0.84 (2)	1.92 (2)	2.755 (2)	170 (2)
$O5-H5B \cdots O3^i$	0.85 (2)	1.85 (2)	2.660 (2)	158 (3)

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

Data collection: APEX2 (Bruker, 2007); cell refinement: SAINT (Bruker, 2007); data reduction: SAINT; program(s) used to solve structure: SHELXTL (Sheldrick, 2008); program(s) used to refine structure: SHELXTL; molecular graphics: XP in SHELXTL; 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: HY2589).

## References

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## supporting information

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**Poly[[diaqua( $\mu$ -4,4'-bipyridine *N,N'*-dioxide- $\kappa^2$ O:O')( $\mu$ -terephthalato- $\kappa^2$ O<sup>1</sup>:O<sup>4</sup>)cobalt(II)] 4,4'-bipyridine *N,N'*-dioxide monosolvate]**

**Xin Ge and Shu-Yan Song**

### S1. Comment

Much progress has been achieved in the design of supramolecular structures containing metal–organic molecules during recent years (Liao *et al.*, 2008; Wang *et al.*, 2008). Multifunctional ligands can link metal ions into one-, two- or three-dimensional structures, and in this context, aromatic carboxylates and 4,4'-bipyridine *N,N'*-dioxide have been used successfully to synthesize such materials.

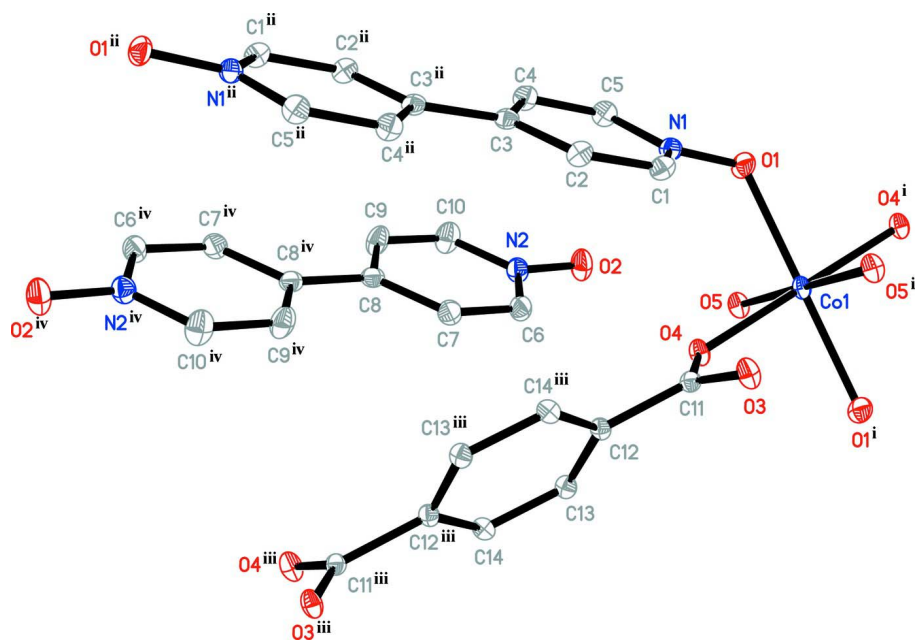
As shown in Fig. 1, the coordination environment of the Co<sup>II</sup> atom, lying on an inversion center, can be described as distorted octahedral, defined by four O atoms in the equatorial plane from two terephthalate (tp) ligands and two 4,4'-bipyridine *N,N'*-dioxide (bpydo) ligands, and two water molecules in the axial positions. The bond distances and angles are normal (Su *et al.*, 2009). The Co<sup>II</sup> atoms are connected by the tp and bpydo ligands, forming a layer structure parallel to (111). O—H $\cdots$ O hydrogen bonds (Table 1) link the uncoordinated bpydo molecules and the layers into a three-dimensional supramolecular structure (Fig. 2). Intralayer O—H $\cdots$ O hydrogen bonds and  $\pi$ – $\pi$  interactions [centroid–centroid distances = 3.6643 (13) and 3.8048 (13) Å] are also observed.

### S2. Experimental

A mixture of terephthalic acid (0.1 mmol, 0.017 g), 4,4'-bipyridine *N,N'*-dioxide (0.2 mmol, 0.038 g), cobalt nitrate (0.1 mmol, 0.030 g), H<sub>2</sub>O (5 ml) and dimethylformamide (15 ml) was stirred at 358 K for 10 min. The mixture was filtrated and pink block crystals of the title compound were isolated after evaporation of the solvent.

### S3. Refinement

H atoms on C atoms were positioned geometrically and refined as riding atoms, with C—H = 0.93 Å and with  $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$ . H atoms of water molecule were located in a difference Fourier map and refined with a restraint of O—H = 0.85 (1) Å and with  $U_{\text{iso}}(\text{H}) = 1.5U_{\text{eq}}(\text{O})$ .

**Figure 1**

The asymmetric unit of the title compound. Displacement ellipsoids are drawn at the 30% probability level. H atoms have been omitted for clarity. [Symmetry codes: (i)  $1 - x, 1 - y, 1 - z$ ; (ii)  $1 - x, 2 - y, -z$ ; (iii)  $2 - x, 1 - y, -z$ ; (iv)  $2 - x, 2 - y, -z$ .]

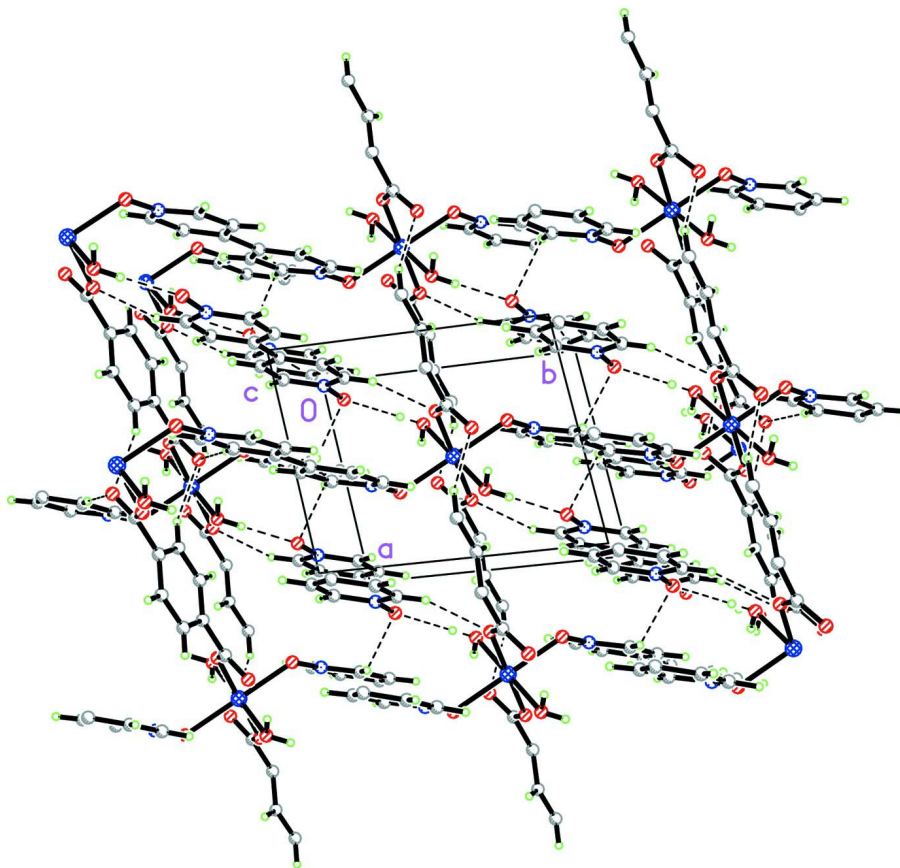


Figure 2

View of the three-dimensional structure of the title compound, built by hydrogen bonds (dashed lines).

**Poly[[diaqua( $\mu$ -4,4'-bipyridine  $N,N'$ -dioxide- $\kappa^2O:O'$ )( $\mu$ -terephthalato- $\kappa^2O^1:O^4$ )cobalt(II)] 4,4'-bipyridine  $N,N'$ -dioxide monosolvate]**

#### Crystal data

$[\text{Co}(\text{C}_8\text{H}_4\text{O}_4)(\text{C}_{10}\text{H}_8\text{N}_2\text{O}_2)(\text{H}_2\text{O})_2] \cdot \text{C}_{10}\text{H}_8\text{N}_2\text{O}_2$

$M_r = 635.44$

Triclinic,  $P\bar{1}$

Hall symbol: -P 1

$a = 7.3883$  (10) Å

$b = 9.1788$  (13) Å

$c = 9.8054$  (13) Å

$\alpha = 81.312$  (2)°

$\beta = 82.200$  (2)°

$\gamma = 79.301$  (2)°

$V = 641.92$  (15) Å<sup>3</sup>

$Z = 1$

$F(000) = 327$

$D_x = 1.644$  Mg m<sup>-3</sup>

Mo  $K\alpha$  radiation,  $\lambda = 0.71073$  Å

Cell parameters from 2899 reflections

$\theta = 2.3\text{--}26.1$ °

$\mu = 0.74$  mm<sup>-1</sup>

$T = 293$  K

Block, pink

$0.27 \times 0.24 \times 0.20$  mm

#### Data collection

Bruker APEXII CCD  
diffractometer

Radiation source: fine-focus sealed tube

Graphite monochromator

$\varphi$  and  $\omega$  scans

Absorption correction: multi-scan  
(*SADABS*; Bruker, 2001)

$T_{\min} = 0.825$ ,  $T_{\max} = 0.866$

3574 measured reflections

2516 independent reflections

2340 reflections with  $I > 2\sigma(I)$

$R_{\text{int}} = 0.017$   
 $\theta_{\text{max}} = 26.1^\circ$ ,  $\theta_{\text{min}} = 2.1^\circ$   
 $h = -8 \rightarrow 9$

$k = -10 \rightarrow 11$   
 $l = -8 \rightarrow 12$

### Refinement

Refinement on  $F^2$   
 Least-squares matrix: full  
 $R[F^2 > 2\sigma(F^2)] = 0.031$   
 $wR(F^2) = 0.081$   
 $S = 1.05$   
 2516 reflections  
 202 parameters  
 2 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  
 $w = 1/[\sigma^2(F_o^2) + (0.0389P)^2 + 0.3924P]$   
 where  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta/\sigma)_{\text{max}} < 0.001$   
 $\Delta\rho_{\text{max}} = 0.48 \text{ e } \text{\AA}^{-3}$   
 $\Delta\rho_{\text{min}} = -0.33 \text{ e } \text{\AA}^{-3}$

### Special details

**Geometry.** All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds 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 ( $\text{\AA}^2$ )

	$x$	$y$	$z$	$U_{\text{iso}}^*/U_{\text{eq}}$
Co1	0.5000	0.5000	0.5000	0.01630 (11)
C1	0.3852 (3)	0.7380 (2)	0.2083 (2)	0.0221 (4)
H1	0.3528	0.6439	0.2142	0.027*
C2	0.4275 (3)	0.8156 (2)	0.08038 (19)	0.0209 (4)
H2	0.4249	0.7727	0.0007	0.025*
C3	0.4745 (2)	0.9580 (2)	0.06822 (18)	0.0186 (4)
C4	0.4684 (3)	1.0181 (2)	0.1918 (2)	0.0233 (4)
H4	0.4925	1.1145	0.1887	0.028*
C5	0.4271 (3)	0.9365 (2)	0.3176 (2)	0.0242 (4)
H5	0.4246	0.9781	0.3988	0.029*
C6	0.8804 (3)	0.7935 (2)	0.2615 (2)	0.0270 (4)
H6	0.8534	0.6980	0.2909	0.032*
C7	0.9285 (3)	0.8359 (2)	0.1234 (2)	0.0264 (4)
H7	0.9313	0.7689	0.0606	0.032*
C8	0.9735 (3)	0.9770 (2)	0.0743 (2)	0.0217 (4)
C9	0.9655 (3)	1.0700 (2)	0.1762 (2)	0.0317 (5)
H9	0.9958	1.1649	0.1496	0.038*
C10	0.9150 (3)	1.0265 (2)	0.3131 (2)	0.0344 (5)
H10	0.9102	1.0920	0.3777	0.041*
C11	0.6942 (2)	0.44694 (19)	0.21107 (18)	0.0164 (4)
C12	0.8539 (2)	0.47312 (19)	0.10187 (18)	0.0162 (3)

C13	1.0328 (2)	0.46045 (19)	0.13839 (18)	0.0175 (4)
H13	1.0549	0.4345	0.2308	0.021*
C14	1.1778 (2)	0.4865 (2)	0.03689 (18)	0.0179 (4)
H14	1.2970	0.4770	0.0617	0.021*
N1	0.3901 (2)	0.79675 (17)	0.32562 (16)	0.0206 (3)
N2	0.8716 (2)	0.88841 (18)	0.35576 (18)	0.0254 (4)
O1	0.3567 (2)	0.71908 (15)	0.44822 (14)	0.0266 (3)
O2	0.8186 (2)	0.84874 (17)	0.48725 (15)	0.0350 (4)
O3	0.57776 (18)	0.37620 (15)	0.18300 (14)	0.0232 (3)
O4	0.68909 (17)	0.50355 (14)	0.32145 (12)	0.0194 (3)
O5	0.67652 (19)	0.59404 (15)	0.59885 (14)	0.0225 (3)
H5A	0.719 (3)	0.6689 (19)	0.555 (2)	0.034*
H5B	0.605 (3)	0.626 (3)	0.6676 (17)	0.034*

*Atomic displacement parameters (Å<sup>2</sup>)*

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
Co1	0.01820 (19)	0.02037 (19)	0.01144 (18)	−0.00652 (13)	0.00000 (13)	−0.00296 (13)
C1	0.0249 (9)	0.0193 (9)	0.0237 (10)	−0.0039 (7)	−0.0069 (8)	−0.0034 (7)
C2	0.0255 (9)	0.0216 (9)	0.0175 (9)	−0.0037 (7)	−0.0071 (7)	−0.0046 (7)
C3	0.0171 (8)	0.0206 (9)	0.0179 (9)	−0.0003 (7)	−0.0048 (7)	−0.0026 (7)
C4	0.0280 (10)	0.0213 (9)	0.0218 (10)	−0.0048 (7)	−0.0024 (8)	−0.0057 (7)
C5	0.0301 (10)	0.0250 (10)	0.0188 (9)	−0.0041 (8)	−0.0018 (8)	−0.0081 (8)
C6	0.0300 (10)	0.0204 (9)	0.0310 (11)	−0.0082 (8)	0.0042 (8)	−0.0062 (8)
C7	0.0288 (10)	0.0210 (9)	0.0302 (11)	−0.0063 (8)	0.0028 (8)	−0.0086 (8)
C8	0.0179 (9)	0.0185 (9)	0.0289 (11)	−0.0020 (7)	−0.0020 (7)	−0.0048 (7)
C9	0.0451 (13)	0.0205 (10)	0.0318 (12)	−0.0132 (9)	−0.0024 (10)	−0.0026 (8)
C10	0.0504 (14)	0.0267 (11)	0.0304 (12)	−0.0155 (10)	−0.0029 (10)	−0.0080 (9)
C11	0.0182 (8)	0.0164 (8)	0.0137 (8)	−0.0020 (6)	−0.0012 (7)	−0.0008 (7)
C12	0.0190 (8)	0.0162 (8)	0.0141 (9)	−0.0044 (6)	0.0011 (7)	−0.0055 (7)
C13	0.0218 (9)	0.0200 (8)	0.0113 (8)	−0.0042 (7)	−0.0021 (7)	−0.0028 (7)
C14	0.0166 (8)	0.0217 (9)	0.0167 (9)	−0.0039 (7)	−0.0026 (7)	−0.0051 (7)
N1	0.0212 (8)	0.0229 (8)	0.0159 (8)	−0.0011 (6)	−0.0012 (6)	−0.0009 (6)
N2	0.0265 (8)	0.0251 (8)	0.0252 (9)	−0.0074 (7)	0.0007 (7)	−0.0043 (7)
O1	0.0343 (8)	0.0249 (7)	0.0168 (7)	−0.0022 (6)	0.0022 (6)	0.0016 (5)
O2	0.0473 (9)	0.0337 (8)	0.0253 (8)	−0.0170 (7)	0.0073 (7)	−0.0058 (6)
O3	0.0241 (7)	0.0301 (7)	0.0195 (7)	−0.0133 (6)	0.0022 (5)	−0.0095 (5)
O4	0.0221 (6)	0.0259 (7)	0.0123 (6)	−0.0093 (5)	0.0018 (5)	−0.0055 (5)
O5	0.0234 (7)	0.0282 (7)	0.0181 (7)	−0.0109 (6)	0.0008 (5)	−0.0048 (6)

*Geometric parameters (Å, °)*

Co1—O4 <sup>i</sup>	2.0865 (12)	C7—H7	0.9300
Co1—O4	2.0865 (12)	C8—C9	1.398 (3)
Co1—O5	2.0975 (13)	C8—C8 <sup>iii</sup>	1.475 (4)
Co1—O5 <sup>i</sup>	2.0976 (13)	C9—C10	1.364 (3)
Co1—O1 <sup>i</sup>	2.1141 (13)	C9—H9	0.9300
Co1—O1	2.1141 (13)	C10—N2	1.356 (3)

C1—N1	1.350 (2)	C10—H10	0.9300
C1—C2	1.373 (3)	C11—O3	1.250 (2)
C1—H1	0.9300	C11—O4	1.263 (2)
C2—C3	1.397 (3)	C11—C12	1.510 (2)
C2—H2	0.9300	C12—C14 <sup>iv</sup>	1.395 (2)
C3—C4	1.398 (3)	C12—C13	1.396 (2)
C3—C3 <sup>ii</sup>	1.479 (4)	C13—C14	1.389 (3)
C4—C5	1.371 (3)	C13—H13	0.9300
C4—H4	0.9300	C14—C12 <sup>iv</sup>	1.395 (2)
C5—N1	1.349 (3)	C14—H14	0.9300
C5—H5	0.9300	N1—O1	1.319 (2)
C6—N2	1.350 (3)	N2—O2	1.312 (2)
C6—C7	1.368 (3)	O5—H5A	0.84 (2)
C6—H6	0.9300	O5—H5B	0.85 (2)
C7—C8	1.395 (3)		
O4 <sup>i</sup> —Co1—O4	180.0	C6—C7—H7	119.1
O4 <sup>i</sup> —Co1—O5	90.46 (5)	C8—C7—H7	119.1
O4—Co1—O5	89.54 (5)	C7—C8—C9	115.04 (18)
O4 <sup>i</sup> —Co1—O5 <sup>i</sup>	89.54 (5)	C7—C8—C8 <sup>iii</sup>	122.1 (2)
O4—Co1—O5 <sup>i</sup>	90.46 (5)	C9—C8—C8 <sup>iii</sup>	122.9 (2)
O5—Co1—O5 <sup>i</sup>	180.00 (6)	C10—C9—C8	122.32 (19)
O4 <sup>i</sup> —Co1—O1 <sup>i</sup>	95.05 (5)	C10—C9—H9	118.8
O4—Co1—O1 <sup>i</sup>	84.95 (5)	C8—C9—H9	118.8
O5—Co1—O1 <sup>i</sup>	92.31 (6)	N2—C10—C9	120.4 (2)
O5 <sup>i</sup> —Co1—O1 <sup>i</sup>	87.69 (6)	N2—C10—H10	119.8
O4 <sup>i</sup> —Co1—O1	84.95 (5)	C9—C10—H10	119.8
O4—Co1—O1	95.05 (5)	O3—C11—O4	126.25 (16)
O5—Co1—O1	87.69 (6)	O3—C11—C12	117.81 (15)
O5 <sup>i</sup> —Co1—O1	92.31 (6)	O4—C11—C12	115.90 (15)
O1 <sup>i</sup> —Co1—O1	180.0	C14 <sup>iv</sup> —C12—C13	119.39 (16)
N1—C1—C2	120.77 (17)	C14 <sup>iv</sup> —C12—C11	119.82 (15)
N1—C1—H1	119.6	C13—C12—C11	120.77 (15)
C2—C1—H1	119.6	C14—C13—C12	120.09 (16)
C1—C2—C3	120.92 (17)	C14—C13—H13	120.0
C1—C2—H2	119.5	C12—C13—H13	120.0
C3—C2—H2	119.5	C13—C14—C12 <sup>iv</sup>	120.52 (16)
C2—C3—C4	116.56 (17)	C13—C14—H14	119.7
C2—C3—C3 <sup>ii</sup>	121.9 (2)	C12 <sup>iv</sup> —C14—H14	119.7
C4—C3—C3 <sup>ii</sup>	121.5 (2)	O1—N1—C5	119.74 (16)
C5—C4—C3	120.68 (18)	O1—N1—C1	120.43 (16)
C5—C4—H4	119.7	C5—N1—C1	119.82 (16)
C3—C4—H4	119.7	O2—N2—C6	120.49 (16)
N1—C5—C4	121.11 (17)	O2—N2—C10	120.07 (17)
N1—C5—H5	119.4	C6—N2—C10	119.44 (18)
C4—C5—H5	119.4	N1—O1—Co1	121.82 (11)
N2—C6—C7	120.93 (18)	C11—O4—Co1	130.60 (11)
N2—C6—H6	119.5	Co1—O5—H5A	117.3 (17)

C7—C6—H6	119.5	Co1—O5—H5B	102.4 (17)
C6—C7—C8	121.82 (19)	H5A—O5—H5B	106 (2)
N1—C1—C2—C3	-0.8 (3)	C4—C5—N1—C1	-3.0 (3)
C1—C2—C3—C4	-2.5 (3)	C2—C1—N1—O1	-177.21 (16)
C1—C2—C3—C3 <sup>ii</sup>	178.3 (2)	C2—C1—N1—C5	3.6 (3)
C2—C3—C4—C5	3.1 (3)	C7—C6—N2—O2	177.42 (19)
C3 <sup>ii</sup> —C3—C4—C5	-177.7 (2)	C7—C6—N2—C10	-1.4 (3)
C3—C4—C5—N1	-0.5 (3)	C9—C10—N2—O2	-178.3 (2)
N2—C6—C7—C8	1.1 (3)	C9—C10—N2—C6	0.5 (3)
C6—C7—C8—C9	0.0 (3)	C5—N1—O1—Co1	-128.29 (15)
C6—C7—C8—C8 <sup>iii</sup>	179.6 (2)	C1—N1—O1—Co1	52.5 (2)
C7—C8—C9—C10	-0.9 (3)	O4 <sup>i</sup> —Co1—O1—N1	-171.81 (14)
C8 <sup>iii</sup> —C8—C9—C10	179.5 (2)	O4—Co1—O1—N1	8.19 (14)
C8—C9—C10—N2	0.6 (4)	O5—Co1—O1—N1	97.52 (14)
O3—C11—C12—C14 <sup>iv</sup>	42.0 (2)	O5 <sup>i</sup> —Co1—O1—N1	-82.48 (14)
O4—C11—C12—C14 <sup>iv</sup>	-135.93 (17)	O3—C11—O4—Co1	2.1 (3)
O3—C11—C12—C13	-139.35 (17)	C12—C11—O4—Co1	179.77 (11)
O4—C11—C12—C13	42.7 (2)	O5—Co1—O4—C11	170.87 (15)
C14 <sup>iv</sup> —C12—C13—C14	-0.6 (3)	O5 <sup>i</sup> —Co1—O4—C11	-9.13 (15)
C11—C12—C13—C14	-179.28 (16)	O1 <sup>i</sup> —Co1—O4—C11	78.51 (15)
C12—C13—C14—C12 <sup>iv</sup>	0.6 (3)	O1—Co1—O4—C11	-101.49 (15)
C4—C5—N1—O1	177.84 (17)		

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

*Hydrogen-bond geometry* ( $\text{\AA}$ ,  $^\circ$ )

<i>D</i> —H $\cdots$ <i>A</i>	<i>D</i> —H	H $\cdots$ <i>A</i>	<i>D</i> $\cdots$ <i>A</i>	<i>D</i> —H $\cdots$ <i>A</i>
O5—H5A $\cdots$ O2	0.84 (2)	1.92 (2)	2.755 (2)	170 (2)
O5—H5B $\cdots$ O3 <sup>i</sup>	0.85 (2)	1.85 (2)	2.660 (2)	158 (3)

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