

Acta Crystallographica Section E

## Structure Reports

Online

ISSN 1600-5368

# Poly[di- $\mu_2$ -acetato-diaquabis(2,2'-bipyridine)bis( $\mu_3$ -5-nitroisophthalato)-tricobalt(II)]

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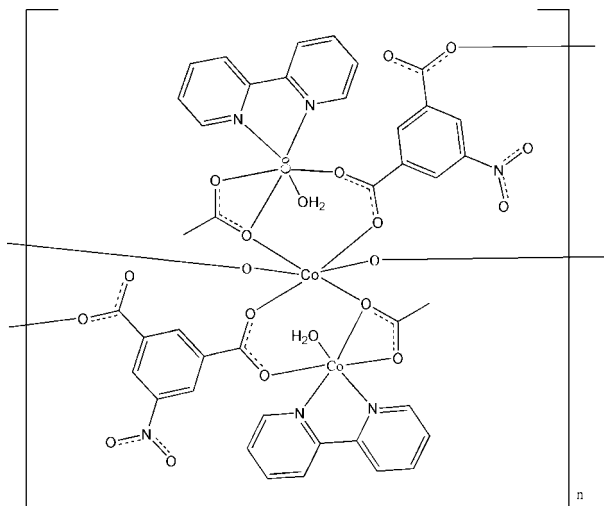
Received 1 April 2009; accepted 3 April 2009

Key indicators: single-crystal X-ray study;  $T = 296$  K; mean  $\sigma(\text{C}-\text{C}) = 0.004$  Å;  $R$  factor = 0.030;  $wR$  factor = 0.077; data-to-parameter ratio = 11.9.

The title complex,  $[\text{Co}_3(\text{C}_8\text{H}_3\text{NO}_6)_2(\text{C}_2\text{H}_3\text{O}_2)_2(\text{C}_{10}\text{H}_8\text{N}_2)_2(\text{H}_2\text{O})_2]$ , was synthesized under hydrothermal conditions. The structure features a centrosymmetric complex with three  $\text{Co}^{\text{II}}$  centres, one of which is located on a centre of inversion. The Co centres are coordinated in a distorted octahedral geometry. The bipyridine ligands are bonded to just one Co centre in a chelating mode, whereas the 5-nitroisophthalate and acetate ions are bonded to two different Co atoms. The crystal structure is stabilized by  $\text{O}-\text{H}\cdots\text{O}$  hydrogen bonds.

## Related literature

For related structures, see: He *et al.* (2004, 2005); Zhang *et al.* (2006).



## Experimental

## Crystal data

$[\text{Co}_3(\text{C}_8\text{H}_3\text{NO}_6)_2(\text{C}_2\text{H}_3\text{O}_2)_2(\text{C}_{10}\text{H}_8\text{N}_2)_2(\text{H}_2\text{O})_2]$   
 $M_r = 1061.51$   
 Triclinic,  $P\bar{1}$   
 $a = 10.0084$  (1) Å  
 $b = 10.0781$  (1) Å  
 $c = 11.3941$  (1) Å  
 $\alpha = 81.196$  (1)°

$\beta = 67.685$  (1)°  
 $\gamma = 69.472$  (1)°  
 $V = 995.43$  (2) Å<sup>3</sup>  
 $Z = 1$   
 Mo  $K\alpha$  radiation  
 $\mu = 1.33$  mm<sup>-1</sup>  
 $T = 296$  K  
 $0.26 \times 0.13 \times 0.10$  mm

## Data collection

Bruker SMART 1K CCD diffractometer  
 Absorption correction: multi-scan (SADABS; Bruker, 2002)  
 $T_{\text{min}} = 0.724$ ,  $T_{\text{max}} = 0.883$

10424 measured reflections  
 3679 independent reflections  
 3296 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.020$

## Refinement

$R[F^2 > 2\sigma(F^2)] = 0.030$   
 $wR(F^2) = 0.077$   
 $S = 1.03$   
 3679 reflections  
 310 parameters  
 3 restraints

H atoms treated by a mixture of independent and constrained refinement  
 $\Delta\rho_{\text{max}} = 0.53$  e Å<sup>-3</sup>  
 $\Delta\rho_{\text{min}} = -0.45$  e Å<sup>-3</sup>

Table 1

Hydrogen-bond geometry (Å, °).

$D-\text{H}\cdots A$	$D-\text{H}$	$\text{H}\cdots A$	$D\cdots A$	$D-\text{H}\cdots A$
$\text{O1W}-\text{H1WA}\cdots\text{O3}^i$	0.83 (2)	1.99 (2)	2.755 (3)	154 (2)
$\text{O1W}-\text{H1WB}\cdots\text{O3}^{ii}$	0.826 (18)	1.96 (2)	2.762 (3)	163 (3)

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

Data collection: SMART (Bruker, 2002); cell refinement: SAINT (Bruker, 2002); 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, 1997); software used to prepare material for publication: PLATON (Spek, 2009).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BT2923).

## References

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**supplementary materials**

*Acta Cryst.* (2009). E65, m510 [ doi:10.1107/S1600536809012562 ]

**Poly[di- $\mu_2$ -acetato-diaquabis(2,2'-bipyridine)bis( $\mu_3$ -5-nitroisophthalato)tricobalt(II)]**

**H.-D. Wang, M.-M. Li and H.-Y. He**

**Comment**

Recently, we were interested in polymers formed by isophthalate ligands and the complexes the form with transition metals because of their diverse topologies and potential applications as functional materials (He *et al.*, 2004, 2005, Zhang *et al.*, 2006).

The structure features a centrosymmetric complex with three Co(II) centres, one of which is located on a centre of inversion. The Co centres are coordinated in a distorted octahedral geometry. The bipyridine ligands are bonded to just one Co centre in a chelating mode, whereas the 5-nitroisophthalate and acetate ions are bonded to two different Co atoms. The crystal structure is stabilized by O-H $\cdots$ O hydrogen bonds (Tab. 1).

**Experimental**

A mixture of Co(Ac)<sub>2</sub>·4H<sub>2</sub>O (0.1240g, 0.5 mmol), 2,2'-bipyridine (0.0790g, 0.5 mmol), 5-nitroisophthalic acid (0.1050g, 0.5mmol), 8 ml H<sub>2</sub>O and 8ml EtOH was heated at 413 K for three days in a 20 ml Teflon-lined stainless-steel autoclave. After cooling, a red plate shaped crystals of the title compound were obtained.

**Refinement**

The H atoms of aromatic and methyl group were positioned geometrically, and included in the refinement in the riding model approximation with C-H = 0.93 Å for aromatic H atoms and C-H = 0.96 Å for H atoms of methyl groups and U<sub>iso</sub> = 1.2U<sub>eq</sub>(C). The H atoms of the water molecule were found in a difference Fourier map and refined isotropically with the O-H bonds restrained to 0.82 (1)Å and the H $\cdots$ H distance restrained to 1.4 (1)Å.

**Figures**

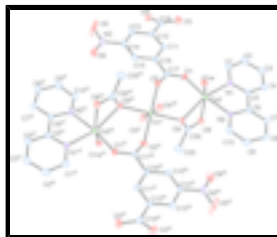


Fig. 1. View of the title complex view. Displacement ellipsoids are drawn at the 30% probability level. H atoms are omitted for clarity. Symmetry codes for generating equivalent atoms: (v) x-1, y, z. (vi) x, -y, 1-z. (vii) 1-x, 2-y, 1-z.

**Poly[di- $\mu_2$ -acetato-diaquabis(2,2'-bipyridine)bis( $\mu_3$ -5-nitroisophthalato)tricobalt(II)]**

*Crystal data*

[Co<sub>3</sub>(C<sub>8</sub>H<sub>3</sub>NO<sub>6</sub>)<sub>2</sub>(C<sub>2</sub>H<sub>3</sub>O<sub>2</sub>)<sub>2</sub>(C<sub>10</sub>H<sub>8</sub>N<sub>2</sub>)<sub>2</sub>(H<sub>2</sub>O)<sub>2</sub>] Z = 1

# supplementary materials

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$M_r = 1061.51$	$F_{000} = 539$
Triclinic, $P\bar{1}$	$D_x = 1.771 \text{ Mg m}^{-3}$
$a = 10.0084 (1) \text{ \AA}$	Mo $K\alpha$ radiation
$b = 10.0781 (1) \text{ \AA}$	$\lambda = 0.71073 \text{ \AA}$
$c = 11.3941 (1) \text{ \AA}$	Cell parameters from 10424 reflections
$\alpha = 81.196 (1)^\circ$	$\theta = 1.9\text{--}25.5^\circ$
$\beta = 67.685 (1)^\circ$	$\mu = 1.33 \text{ mm}^{-1}$
$\gamma = 69.472 (1)^\circ$	$T = 296 \text{ K}$
$V = 995.430 (17) \text{ \AA}^3$	Plate, red
	$0.26 \times 0.13 \times 0.10 \text{ mm}$

## Data collection

Bruker SMART 1K CCD diffractometer	3679 independent reflections
Radiation source: fine-focus sealed tube	3296 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{\text{int}} = 0.020$
$T = 296 \text{ K}$	$\theta_{\text{max}} = 25.5^\circ$
phi/ $\omega$ scans	$\theta_{\text{min}} = 1.9^\circ$
Absorption correction: multi-scan (SADABS; Bruker, 2002)	$h = -12 \rightarrow 12$
$T_{\text{min}} = 0.724$ , $T_{\text{max}} = 0.883$	$k = -12 \rightarrow 12$
10424 measured reflections	$l = -13 \rightarrow 13$

## Refinement

Refinement on $F^2$	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.030$	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2) = 0.077$	$w = 1/[\sigma^2(F_o^2) + (0.0358P)^2 + 1.058P]$
$S = 1.03$	where $P = (F_o^2 + 2F_c^2)/3$
3679 reflections	$(\Delta/\sigma)_{\text{max}} < 0.001$
310 parameters	$\Delta\rho_{\text{max}} = 0.53 \text{ e \AA}^{-3}$
3 restraints	$\Delta\rho_{\text{min}} = -0.45 \text{ e \AA}^{-3}$
Primary atom site location: structure-invariant direct methods	Extinction correction: none

## 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	$U_{iso}^*/U_{eq}$
Co1	0.0000	1.0000	0.5000	0.02056 (11)
Co2	0.29863 (3)	0.66172 (3)	0.34001 (3)	0.02348 (10)
N1	0.5014 (2)	0.4947 (2)	0.26205 (19)	0.0264 (4)
N2	0.2395 (2)	0.5533 (2)	0.23098 (19)	0.0271 (4)
C6	0.3533 (3)	0.4463 (2)	0.1610 (2)	0.0259 (5)
O1	0.38924 (18)	0.74188 (17)	0.43457 (16)	0.0283 (4)
O9	0.10814 (18)	0.86327 (17)	0.34394 (15)	0.0263 (4)
C11	0.5544 (3)	0.8074 (2)	0.5603 (2)	0.0218 (5)
H11A	0.6088	0.7353	0.5017	0.026*
C17	0.3124 (3)	0.8272 (2)	0.5243 (2)	0.0233 (5)
C16	0.3980 (3)	0.8686 (2)	0.5891 (2)	0.0219 (5)
C19	0.8024 (3)	0.7950 (3)	0.5801 (2)	0.0269 (5)
C12	0.6310 (3)	0.8526 (2)	0.6180 (2)	0.0233 (5)
O3	0.8695 (2)	0.67757 (19)	0.5289 (2)	0.0414 (5)
C5	0.5033 (3)	0.4180 (2)	0.1738 (2)	0.0256 (5)
C4	0.6363 (3)	0.3199 (3)	0.1018 (2)	0.0337 (6)
H4A	0.6361	0.2703	0.0395	0.040*
C14	0.3935 (3)	1.0141 (2)	0.7364 (2)	0.0273 (5)
C13	0.5491 (3)	0.9578 (3)	0.7079 (2)	0.0272 (5)
H13A	0.5977	0.9894	0.7478	0.033*
C15	0.3160 (3)	0.9740 (2)	0.6786 (2)	0.0262 (5)
H15A	0.2114	1.0163	0.6989	0.031*
C9	0.0689 (3)	0.5133 (3)	0.1519 (3)	0.0382 (6)
H9A	-0.0288	0.5389	0.1495	0.046*
C7	0.3293 (3)	0.3687 (3)	0.0849 (3)	0.0352 (6)
H7A	0.4092	0.2951	0.0369	0.042*
C10	0.1008 (3)	0.5858 (3)	0.2260 (3)	0.0328 (6)
H10A	0.0225	0.6601	0.2742	0.039*
C1	0.6309 (3)	0.4698 (3)	0.2832 (3)	0.0327 (6)
H1A	0.6295	0.5217	0.3447	0.039*
C8	0.1844 (3)	0.4028 (3)	0.0818 (3)	0.0406 (7)
H8A	0.1652	0.3512	0.0324	0.049*
C2	0.7661 (3)	0.3707 (3)	0.2180 (3)	0.0379 (6)
H2A	0.8533	0.3539	0.2369	0.046*
N3	0.3069 (3)	1.1250 (3)	0.8321 (2)	0.0462 (6)
C3	0.7690 (3)	0.2970 (3)	0.1241 (3)	0.0392 (6)
H3A	0.8598	0.2323	0.0761	0.047*
O6	0.1710 (3)	1.1769 (3)	0.8577 (3)	0.0776 (9)
O2	0.17072 (18)	0.88101 (19)	0.56665 (16)	0.0318 (4)
O4	0.8652 (2)	0.8704 (2)	0.60355 (17)	0.0369 (4)

## supplementary materials

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O5	0.3732 (3)	1.1514 (4)	0.8890 (3)	0.1161 (15)
O1W	0.17349 (19)	0.56964 (19)	0.50084 (18)	0.0318 (4)
H1WA	0.0831 (15)	0.620 (2)	0.523 (3)	0.048*
H1WB	0.180 (3)	0.4895 (15)	0.486 (3)	0.048*
O8	0.31763 (19)	0.80788 (18)	0.17845 (16)	0.0334 (4)
C32	0.1871 (3)	0.8911 (2)	0.2305 (2)	0.0263 (5)
C33	0.1213 (4)	1.0190 (3)	0.1602 (3)	0.0468 (7)
H33A	0.1949	1.0239	0.0772	0.070*
H33B	0.0952	1.1025	0.2056	0.070*
H33C	0.0314	1.0129	0.1524	0.070*

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

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
Co1	0.0155 (2)	0.0220 (2)	0.0263 (2)	-0.00532 (16)	-0.00810 (17)	-0.00619 (17)
Co2	0.02330 (17)	0.02240 (17)	0.02775 (18)	-0.00702 (13)	-0.01024 (13)	-0.00655 (13)
N1	0.0258 (10)	0.0226 (10)	0.0315 (11)	-0.0068 (8)	-0.0108 (8)	-0.0030 (8)
N2	0.0270 (10)	0.0274 (10)	0.0295 (11)	-0.0090 (8)	-0.0106 (9)	-0.0057 (8)
C6	0.0327 (13)	0.0215 (11)	0.0249 (12)	-0.0087 (10)	-0.0114 (10)	-0.0010 (9)
O1	0.0230 (8)	0.0311 (9)	0.0350 (9)	-0.0075 (7)	-0.0115 (7)	-0.0123 (7)
O9	0.0279 (9)	0.0240 (8)	0.0270 (9)	-0.0078 (7)	-0.0085 (7)	-0.0052 (7)
C11	0.0251 (11)	0.0195 (11)	0.0236 (11)	-0.0089 (9)	-0.0092 (9)	-0.0022 (9)
C17	0.0251 (12)	0.0214 (11)	0.0255 (12)	-0.0074 (9)	-0.0121 (9)	0.0016 (9)
C16	0.0243 (11)	0.0212 (11)	0.0221 (11)	-0.0085 (9)	-0.0093 (9)	-0.0001 (9)
C19	0.0258 (12)	0.0310 (13)	0.0279 (12)	-0.0145 (10)	-0.0099 (10)	0.0027 (10)
C12	0.0256 (12)	0.0219 (11)	0.0256 (11)	-0.0115 (9)	-0.0099 (9)	0.0020 (9)
O3	0.0261 (9)	0.0334 (10)	0.0636 (13)	-0.0083 (8)	-0.0114 (9)	-0.0124 (9)
C5	0.0301 (12)	0.0213 (11)	0.0248 (12)	-0.0083 (10)	-0.0093 (10)	0.0005 (9)
C4	0.0369 (14)	0.0273 (13)	0.0303 (13)	-0.0046 (11)	-0.0087 (11)	-0.0040 (10)
C14	0.0327 (13)	0.0255 (12)	0.0241 (12)	-0.0113 (10)	-0.0063 (10)	-0.0070 (10)
C13	0.0337 (13)	0.0317 (13)	0.0246 (12)	-0.0182 (11)	-0.0113 (10)	-0.0029 (10)
C15	0.0239 (12)	0.0250 (12)	0.0274 (12)	-0.0058 (9)	-0.0073 (9)	-0.0040 (10)
C9	0.0380 (15)	0.0400 (15)	0.0478 (16)	-0.0155 (12)	-0.0235 (13)	-0.0031 (13)
C7	0.0434 (15)	0.0287 (13)	0.0365 (14)	-0.0074 (11)	-0.0180 (12)	-0.0090 (11)
C10	0.0288 (13)	0.0325 (13)	0.0387 (14)	-0.0082 (11)	-0.0117 (11)	-0.0098 (11)
C1	0.0318 (13)	0.0284 (13)	0.0433 (15)	-0.0104 (11)	-0.0180 (11)	-0.0015 (11)
C8	0.0552 (18)	0.0359 (15)	0.0451 (16)	-0.0165 (13)	-0.0280 (14)	-0.0090 (12)
C2	0.0274 (13)	0.0329 (14)	0.0530 (17)	-0.0102 (11)	-0.0160 (12)	0.0063 (13)
N3	0.0444 (15)	0.0481 (14)	0.0441 (14)	-0.0132 (12)	-0.0057 (11)	-0.0256 (12)
C3	0.0300 (14)	0.0309 (14)	0.0419 (15)	-0.0007 (11)	-0.0053 (12)	-0.0006 (12)
O6	0.0595 (16)	0.0778 (18)	0.0809 (18)	0.0265 (13)	-0.0342 (14)	-0.0527 (15)
O2	0.0200 (8)	0.0421 (10)	0.0341 (9)	-0.0035 (7)	-0.0137 (7)	-0.0073 (8)
O4	0.0339 (10)	0.0497 (11)	0.0392 (10)	-0.0286 (9)	-0.0109 (8)	-0.0037 (9)
O5	0.0539 (16)	0.176 (3)	0.130 (3)	-0.0378 (19)	0.0024 (16)	-0.128 (3)
O1W	0.0276 (9)	0.0288 (9)	0.0382 (10)	-0.0091 (7)	-0.0093 (8)	-0.0044 (8)
O8	0.0297 (9)	0.0333 (9)	0.0322 (9)	-0.0078 (8)	-0.0055 (8)	-0.0059 (8)
C32	0.0309 (13)	0.0255 (12)	0.0277 (12)	-0.0107 (10)	-0.0125 (10)	-0.0058 (10)
C33	0.0542 (18)	0.0416 (16)	0.0379 (16)	-0.0079 (14)	-0.0182 (14)	0.0054 (13)

Geometric parameters (Å, °)

Co1—O2	2.0503 (16)	C5—C4	1.384 (3)
Co1—O2 <sup>i</sup>	2.0503 (16)	C4—C3	1.381 (4)
Co1—O9 <sup>i</sup>	2.1153 (15)	C4—H4A	0.9300
Co1—O9	2.1153 (15)	C14—C15	1.375 (3)
Co1—O4 <sup>ii</sup>	2.1154 (17)	C14—C13	1.380 (4)
Co1—O4 <sup>iii</sup>	2.1154 (17)	C14—N3	1.471 (3)
Co2—O1	2.0392 (15)	C13—H13A	0.9300
Co2—O1W	2.0831 (18)	C15—H15A	0.9300
Co2—N1	2.1053 (19)	C9—C8	1.372 (4)
Co2—N2	2.1249 (19)	C9—C10	1.380 (4)
Co2—O8	2.1668 (18)	C9—H9A	0.9300
Co2—O9	2.2382 (16)	C7—C8	1.382 (4)
N1—C1	1.338 (3)	C7—H7A	0.9300
N1—C5	1.350 (3)	C10—H10A	0.9300
N2—C10	1.331 (3)	C1—C2	1.377 (4)
N2—C6	1.345 (3)	C1—H1A	0.9300
C6—C7	1.385 (3)	C8—H8A	0.9300
C6—C5	1.487 (3)	C2—C3	1.380 (4)
O1—C17	1.259 (3)	C2—H2A	0.9300
O9—C32	1.281 (3)	N3—O5	1.199 (3)
C11—C16	1.391 (3)	N3—O6	1.206 (3)
C11—C12	1.395 (3)	C3—H3A	0.9300
C11—H11A	0.9300	O4—Co1 <sup>iv</sup>	2.1154 (17)
C17—O2	1.248 (3)	O1W—H1WA	0.826 (10)
C17—C16	1.508 (3)	O1W—H1WB	0.824 (10)
C16—C15	1.388 (3)	O8—C32	1.248 (3)
C19—O3	1.244 (3)	C32—C33	1.493 (4)
C19—O4	1.252 (3)	C33—H33A	0.9600
C19—C12	1.510 (3)	C33—H33B	0.9600
C12—C13	1.390 (3)	C33—H33C	0.9600
O2—Co1—O2 <sup>i</sup>	180.0	C13—C12—C19	119.0 (2)
O2—Co1—O9 <sup>i</sup>	92.58 (6)	C11—C12—C19	121.4 (2)
O2 <sup>i</sup> —Co1—O9 <sup>i</sup>	87.42 (6)	N1—C5—C4	121.7 (2)
O2—Co1—O9	87.42 (6)	N1—C5—C6	115.1 (2)
O2 <sup>i</sup> —Co1—O9	92.58 (6)	C4—C5—C6	123.2 (2)
O9 <sup>i</sup> —Co1—O9	180.000 (1)	C3—C4—C5	119.0 (2)
O2—Co1—O4 <sup>ii</sup>	90.67 (7)	C3—C4—H4A	120.5
O2 <sup>i</sup> —Co1—O4 <sup>ii</sup>	89.33 (7)	C5—C4—H4A	120.5
O9 <sup>i</sup> —Co1—O4 <sup>ii</sup>	88.72 (7)	C15—C14—C13	123.5 (2)
O9—Co1—O4 <sup>ii</sup>	91.28 (7)	C15—C14—N3	118.4 (2)
O2—Co1—O4 <sup>iii</sup>	89.33 (7)	C13—C14—N3	118.1 (2)
O2 <sup>i</sup> —Co1—O4 <sup>iii</sup>	90.67 (7)	C14—C13—C12	118.1 (2)

## supplementary materials

O9 <sup>i</sup> —Co1—O4 <sup>iii</sup>	91.28 (7)	C14—C13—H13A	120.9
O9—Co1—O4 <sup>iii</sup>	88.72 (7)	C12—C13—H13A	120.9
O4 <sup>ii</sup> —Co1—O4 <sup>iii</sup>	180.0	C14—C15—C16	118.3 (2)
O1—Co2—O1W	94.98 (7)	C14—C15—H15A	120.9
O1—Co2—N1	94.01 (7)	C16—C15—H15A	120.9
O1W—Co2—N1	103.72 (7)	C8—C9—C10	118.6 (2)
O1—Co2—N2	170.78 (7)	C8—C9—H9A	120.7
O1W—Co2—N2	87.41 (7)	C10—C9—H9A	120.7
N1—Co2—N2	76.77 (7)	C8—C7—C6	118.7 (2)
O1—Co2—O8	98.32 (7)	C8—C7—H7A	120.7
O1W—Co2—O8	152.53 (7)	C6—C7—H7A	120.7
N1—Co2—O8	99.22 (7)	N2—C10—C9	122.5 (2)
N2—Co2—O8	83.29 (7)	N2—C10—H10A	118.8
O1—Co2—O9	94.50 (6)	C9—C10—H10A	118.8
O1W—Co2—O9	95.80 (7)	N1—C1—C2	123.0 (2)
N1—Co2—O9	157.91 (7)	N1—C1—H1A	118.5
N2—Co2—O9	94.12 (7)	C2—C1—H1A	118.5
O8—Co2—O9	59.37 (6)	C9—C8—C7	119.6 (2)
C1—N1—C5	118.4 (2)	C9—C8—H8A	120.2
C1—N1—Co2	124.99 (16)	C7—C8—H8A	120.2
C5—N1—Co2	116.21 (15)	C1—C2—C3	118.4 (2)
C10—N2—C6	119.0 (2)	C1—C2—H2A	120.8
C10—N2—Co2	124.78 (16)	C3—C2—H2A	120.8
C6—N2—Co2	116.22 (15)	O5—N3—O6	122.5 (3)
N2—C6—C7	121.6 (2)	O5—N3—C14	117.9 (3)
N2—C6—C5	114.8 (2)	O6—N3—C14	119.3 (2)
C7—C6—C5	123.6 (2)	C2—C3—C4	119.5 (2)
C17—O1—Co2	124.66 (14)	C2—C3—H3A	120.3
C32—O9—Co1	126.76 (14)	C4—C3—H3A	120.3
C32—O9—Co2	88.61 (13)	C17—O2—Co1	138.15 (16)
Co1—O9—Co2	121.97 (8)	C19—O4—Co1 <sup>iv</sup>	137.23 (17)
C16—C11—C12	121.0 (2)	Co2—O1W—H1WA	109 (2)
C16—C11—H11A	119.5	Co2—O1W—H1WB	111 (2)
C12—C11—H11A	119.5	H1WA—O1W—H1WB	109 (2)
O2—C17—O1	126.4 (2)	C32—O8—Co2	92.74 (15)
O2—C17—C16	116.0 (2)	O8—C32—O9	119.2 (2)
O1—C17—C16	117.6 (2)	O8—C32—C33	120.5 (2)
C15—C16—C11	119.6 (2)	O9—C32—C33	120.2 (2)
C15—C16—C17	117.9 (2)	C32—C33—H33A	109.5
C11—C16—C17	122.5 (2)	C32—C33—H33B	109.5
O3—C19—O4	125.4 (2)	H33A—C33—H33B	109.5
O3—C19—C12	118.0 (2)	C32—C33—H33C	109.5
O4—C19—C12	116.6 (2)	H33A—C33—H33C	109.5
C13—C12—C11	119.5 (2)	H33B—C33—H33C	109.5

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

*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>
O1W—H1WA···O3 <sup>ii</sup>	0.83 (2)	1.99 (2)	2.755 (3)	154 (2)
O1W—H1WB···O3 <sup>v</sup>	0.826 (18)	1.96 (2)	2.762 (3)	163 (3)

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

