metal-organic compounds

Poly[di-μ_2-acetato-diaquabis(2,2'-bipyridine)bis(μ_3-5-nitroisophthalato)-tricobalt(II)]

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The title complex, $[Co_3(C_8H_3NO_6)_2(C_2H_3O_2)_2(C_{10}H_8N_2)_2(H_2O)_2]$, was synthesized under hydrothermal conditions. 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···O hydrogen bonds.

Related literature

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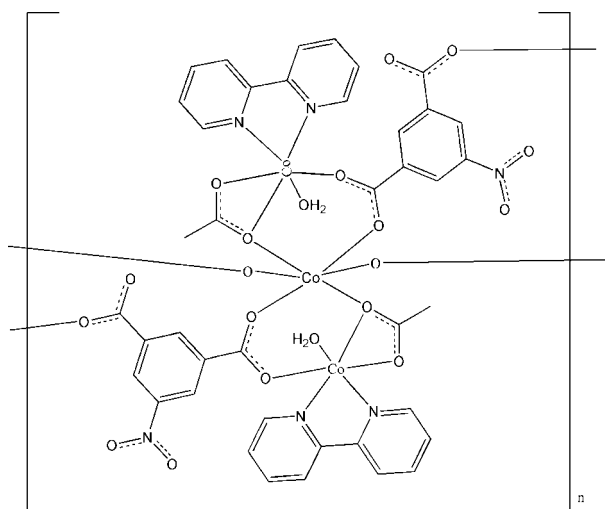
Experimental

Crystal data

$[Co_3(C_8H_3NO_6)_2(C_2H_3O_2)_2(C_{10}H_8N_2)_2(H_2O)_2]$	β = 67.685 (1)°
M_r = 1061.51	γ = 69.472 (1)°
Triclinic, $P\bar{1}$	V = 995.43 (2) Å^3
a = 10.0084 (1) Å	Z = 1
b = 10.0781 (1) Å	Mo $K\alpha$ radiation
c = 11.3941 (1) Å	μ = 1.33 mm^{-1}
α = 81.196 (1)°	T = 296 K
	0.26 × 0.13 × 0.10 mm

Data collection

Bruker SMART 1K CCD diffractometer	10424 measured reflections
Absorption correction: multi-scan (*SADABS*; Bruker, 2002)	3679 independent reflections
T_{min} = 0.724, T_{max} = 0.883	3296 reflections with $I > 2\sigma(I)$
	R_{int} = 0.020

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.030	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2)$ = 0.077	
S = 1.03	
3679 reflections	$\Delta\rho_{max}$ = 0.53 e Å^{-3}
310 parameters	$\Delta\rho_{min}$ = −0.45 e Å^{-3}
3 restraints	

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

D—H···A	D—H	H···A	D···A	D—H···A
O1W—H1WA···O3^i	0.83 (2)	1.99 (2)	2.755 (3)	154 (2)
O1W—H1WB···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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supporting information

Poly[di-*μ*₂-acetato-diaquabis(2,2′-bipyridine)bis(*μ*₃-5-nitro-isophthalato)tricobalt(II)]

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S1. 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···O hydrogen bonds (Tab. 1).

S2. Experimental

A mixture of $Co(Ac)_2.4H_2O$ (0.1240g, 0.5 mmol), 2,2′-bipyridine (0.0790g, 0.5 mmol), 5-nitroisophthalic acid (0.1050g, 0.5mmol), 8 ml H_2O 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 obsained.

S3. 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 $U_{iso}=1.2U_{eq}(C)$. 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···H distance restrained to 1.4 (1)Å.
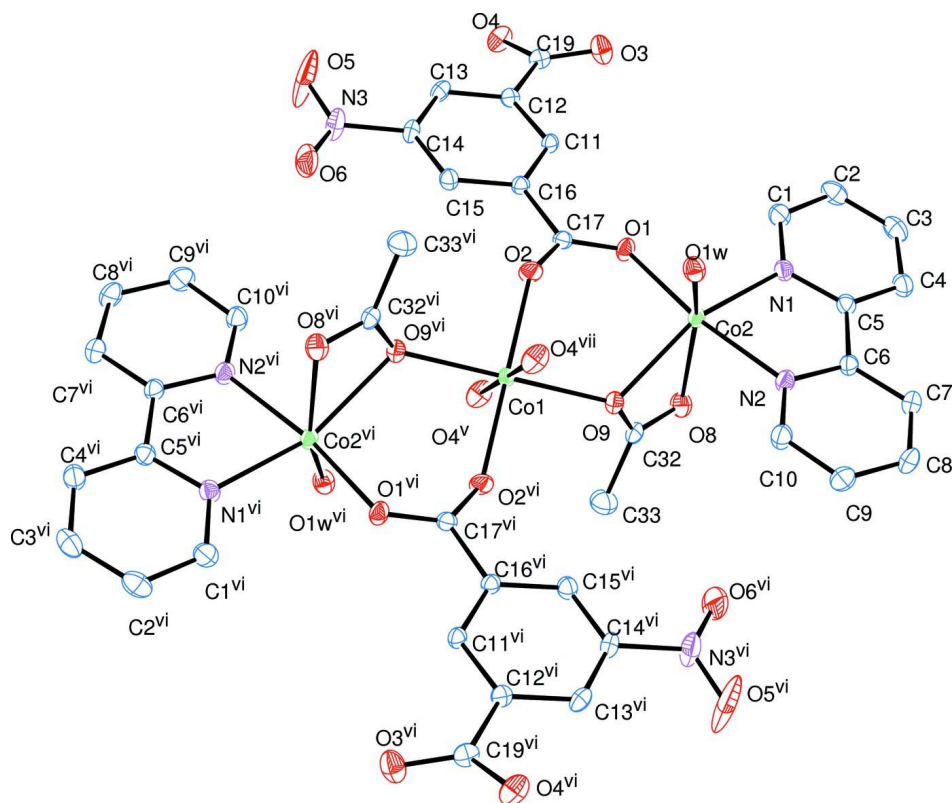
Figure 1

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-μ_2-acetato-diaquabis(2,2′-bipyridine)bis(μ_3-5-nitroisophthalato)tricobalt(II)]

Crystal data

[Co₃(C₈H₃NO₆)₂(C₂H₃O₂)₂(C₁₀H₈N₂)₂(H₂O)₂]	$Z = 1$
$M_r = 1061.51$	$F(000) = 539$
Triclinic, $P\overline{1}$	$D_x = 1.771$ Mg m⁻³
$a = 10.0084\ (1)$ Å	Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
$b = 10.0781\ (1)$ Å	Cell parameters from 10424 reflections
$c = 11.3941\ (1)$ Å	$\theta = 1.9$–25.5°
$\alpha = 81.196\ (1)°$	$\mu = 1.33$ mm⁻¹
$\beta = 67.685\ (1)°$	$T = 296$ K
$\gamma = 69.472\ (1)°$	Plate, red
$V = 995.43\ (2)$ Å³	$0.26 \times 0.13 \times 0.10$ mm

Data collection

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

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier
Least-squares matrix: full	map
$R[F^2 > 2\sigma(F^2)] = 0.030$	Hydrogen site location: inferred from
$wR(F^2) = 0.077$	neighbouring sites
$S = 1.03$	H atoms treated by a mixture of independent
3679 reflections	and constrained refinement
310 parameters	$w = 1/[\sigma^2(F_o^2) + (0.0358P)^2 + 1.058P]$
3 restraints	where $P = (F_o^2 + 2F_c^2)/3$
Primary atom site location: structure-invariant	$(\Delta/\sigma)_{max} < 0.001$
direct methods	$\Delta\rho_{max} = 0.53$ e Å^{-3}
	$\Delta\rho_{min} = -0.45$ e Å^{-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 $F^2 > 2sigma(F^2)$ 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	0.0000	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)
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 (Å²)

	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, º)

Co1—O2	2.0503 (16)	C5—C4	1.384 (3)
Co1—O2[i]	2.0503 (16)	C4—C3	1.381 (4)
Co1—O9[i]	2.1153 (15)	C4—H4A	0.9300
Co1—O9	2.1153 (15)	C14—C15	1.375 (3)
Co1—O4[ii]	2.1154 (17)	C14—C13	1.380 (4)
Co1—O4[iii]	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[iv]	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—O2ⁱ	180.0	C13—C12—C19	119.0 (2)
O2—Co1—O9ⁱ	92.58 (6)	C11—C12—C19	121.4 (2)
O2ⁱ—Co1—O9ⁱ	87.42 (6)	N1—C5—C4	121.7 (2)
O2—Co1—O9	87.42 (6)	N1—C5—C6	115.1 (2)
O2ⁱ—Co1—O9	92.58 (6)	C4—C5—C6	123.2 (2)
O9ⁱ—Co1—O9	180.000 (1)	C3—C4—C5	119.0 (2)
O2—Co1—O4ⁱⁱ	90.67 (7)	C3—C4—H4A	120.5
O2ⁱ—Co1—O4ⁱⁱ	89.33 (7)	C5—C4—H4A	120.5
O9ⁱ—Co1—O4ⁱⁱ	88.72 (7)	C15—C14—C13	123.5 (2)
O9—Co1—O4ⁱⁱ	91.28 (7)	C15—C14—N3	118.4 (2)
O2—Co1—O4ⁱⁱⁱ	89.33 (7)	C13—C14—N3	118.1 (2)
O2ⁱ—Co1—O4ⁱⁱⁱ	90.67 (7)	C14—C13—C12	118.1 (2)
O9ⁱ—Co1—O4ⁱⁱⁱ	91.28 (7)	C14—C13—H13A	120.9
O9—Co1—O4ⁱⁱⁱ	88.72 (7)	C12—C13—H13A	120.9
O4ⁱⁱ—Co1—O4ⁱⁱⁱ	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^{iv}	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, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1*W*—H1*WA*···O3[ii]	0.83 (2)	1.99 (2)	2.755 (3)	154 (2)
O1*W*—H1*WB*···O3[v]	0.83 (2)	1.96 (2)	2.762 (3)	163 (3)

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