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Aqua[2,2′-(propane-1,3-diyl)bis(5-carboxy-1*H*-imidazole-4-carboxylato)-$\kappa^4N^3,O^4:N^{3'},O^{4'}$](pyridine-$\kappa N$)-cobalt(II)–4,4′-bipyridine (1/1)

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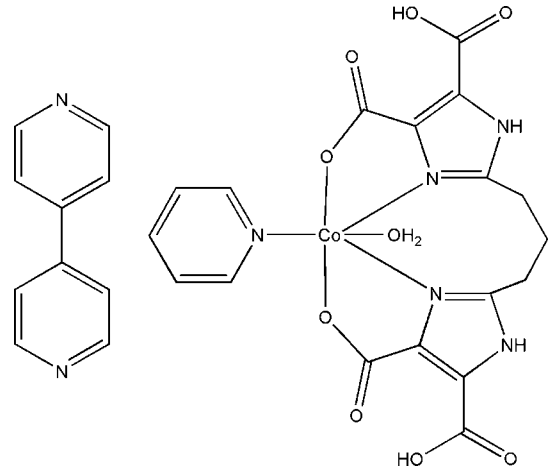
Key indicators: single-crystal X-ray study; T = 296 K; mean σ(C–C) = 0.003 Å; disorder in main residue; R factor = 0.043; wR factor = 0.105; data-to-parameter ratio = 15.7.

In the title compound, $[Co(C_{13}H_{10}N_4O_8)(C_5H_5N)(H_2O)]\cdot C_{10}H_8N_2$, the asymmetric unit comprises half a Co^{II} complex located on a mirror plane and half a cocrystallized molecule of 4,4′-bipyridine located on an inversion center. The Co^{II} ion is six coordinate, with distorted octahedral geometry, ligated by two N atoms and two O atoms from a 2,2′-(propane-1,3-diyl)bis(5-carboxy-1*H*-imidazole-4-carboxylate) dianion, one N atom from a pyridine molecule and one coordinating water molecule. The Co—O bond lengths range from 2.076 (2) to 2.1441 (15) Å, while the Co—N bond lengths are 2.138 (3) and 2.1515 (17) Å. A two-dimensional network of N—H···O and O—H···N hydrogen bonds stabilizes the crystal packing. There are π–π interactions between the bipyridine and imidazole rings [centroid–centroid distance = 3.7694 (4) Å]. The propane-1,3-diyl group is disordered over two conformations, with refined occupancies of 0.755 (8) and 0.245 (8).

Related literature

For complexes based on substituted 4,5-imidazoledicarboxylic acids, see: Zhu *et al.* (2010, 2011); Lu *et al.* (2010); Song *et al.* (2010); Zhang *et al.* (2010); Wang *et al.* (2008); Feng *et al.* (2010); Liu *et al.* (2010); Zheng *et al.* (2011); Li *et al.* (2009, 2010).



Experimental

Crystal data

$[Co(C_{13}H_{10}N_4O_8)(C_5H_5N)(H_2O)]\cdot C_{10}H_8N_2$
M_r = 661.47
Monoclinic, $P2_1/m$
a = 7.9733 (10) Å
b = 20.738 (3) Å
c = 8.2987 (11) Å
β = 91.350 (2)°
V = 1371.8 (3) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.70 mm^{-1}
T = 296 K
0.22 × 0.18 × 0.11 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2001)
T_{min} = 0.862, T_{max} = 0.927
11480 measured reflections
3443 independent reflections
2633 reflections with $I > 2\sigma(I)$
R_{int} = 0.033

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.043
$wR(F^2)$ = 0.105
S = 1.05
3443 reflections
219 parameters
1 restraint
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.43 e Å^{-3}
$\Delta\rho_{min}$ = −0.34 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O3—H3···O2	0.82	1.65	2.473 (2)	177
O5—H1W···N4^{i}	0.82	1.95	2.727 (3)	157
N2—H2···O4^{ii}	0.86	1.93	2.763 (3)	162

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

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINT* (Bruker, 2001); data reduction: *SAINT*; 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: PK2422).

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supplementary materials

Acta Cryst. (2012). E**68**, m1109–m1110 [doi:10.1107/S1600536812029856]

Aqua[2,2′-(propane-1,3-diyl)bis(5-carboxy-1*H*-imidazole-4-carboxylato)-$\kappa^4N^3,O^4:N^{3'},O^{4'}$](pyridine-$\kappa N$)cobalt(II)–4,4′-bipyridine (1/1)

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Comment

It is well known that aromatic polycarboxylates, especially the N-heterocyclic carboxylates, are excellent candidates for preparing novel MOFs, because of their versatile coordination modes and potential hydrogen-bonding donors and acceptors. Recently, 4,5-imidazoledicarboxylic acid (Zhu *et al.*, 2010; Lu *et al.*, 2010) and its 2-position substituent derivatives, such as 2-methyl-1*H*-imidazole-4,5-dicarboxylic acid (Song *et al.*, 2010), 2-ethyl-1*H*-imidazole-4,5-dicarboxylic acid (Zhang *et al.*, 2010; Wang *et al.*, 2008), 2-propyl-1*H*-imidazole-4,5-dicarboxylic acid (Feng *et al.*, 2010; Liu *et al.*, 2010), 2-(hydroxymethyl)-1*H*-imidazole-4,5-dicarboxylic acid (Zheng *et al.*, 2011), 2-phenyl-1*H*-imidazole-4,5-dicarboxylic acid (Zhu *et al.*, 2011) and 2-pyridyl-1*H*-imidazole-4,5-dicarboxylic acid (Li *et al.*, 2009; Li *et al.*, 2010) have attracted great attention in the field of coordination chemistry. Now, our group has strong interest in adopting another imidazole dicarboxylate ligand, 1,3-bis-(1*H*-imidazole-4,5-dicarboxylate acid) propane to prepare various coordination compounds.

As shown in Fig. 1, the molecule is a discrete neutral monomer, in which the asymmetric unit comprises half a CoII complex located on a mirror plane and half a co-crystallized molecule of 4,4′-bipyridine located on an inversion center. The Co^{II} ion is six coordinate and has a distorted octahedral geometry. It is ligated by two nitrogen atoms and two oxygen atoms from a 1,3-bis-(1*H*-imidazole-4,5-dicarboxylate) propane dianion, one nitrogen atom from a pyridine molecule and one oxygen atom from a coordinated water molecule. The Co—O distances range from 2.076 (2) to 2.1441 (15) Å, while Co—N distances are 2.138 (3) and 2.1515 (17) Å, respectively. A two-dimensional network of N—H···O and O—H···N hydrogen bonds help to stabilize the crystal packing. Aromatic π-π interactions between bipyridine rings and imidazole rings [centroid—centroid distance = 3.7694 (4) Å] are also observed.

Experimental

A mixture of cobalt chloride hexahydrate (0.0238 g, 0.1 mmol), 1,3-bis-(1*H*-imidazole-4,5-dicarboxylate acid) propane (0.0352 g, 0.1 mmol), 4,4′-bipyridine (0.0198 g, 0.1 mmol), pyridine (0.8 ml) and H_2O (10 ml) was sealed in a Teflon-lined stainless autoclave and heated at 413 K for 3 days. The bomb was allowed to cool to room temperature gradually and red prismatic crystals were obtained.

Refinement

H atoms attached to N and O atoms were located in a difference Fourier maps and refined as riding in their as-found relative positions, with U_{iso}(H) = 1.5U_{eq}(O, N). Other H atoms were positioned geometrically with C—H = 0.93 and 0.97 Å for aromatic and methylene H, and constrained to ride on their parent atoms with U_{iso}(H) = 1.2U_{eq}(C).

Computing details

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINT* (Bruker, 2001); data reduction: *SAINT* (Bruker, 2001); 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* (Sheldrick, 2008).

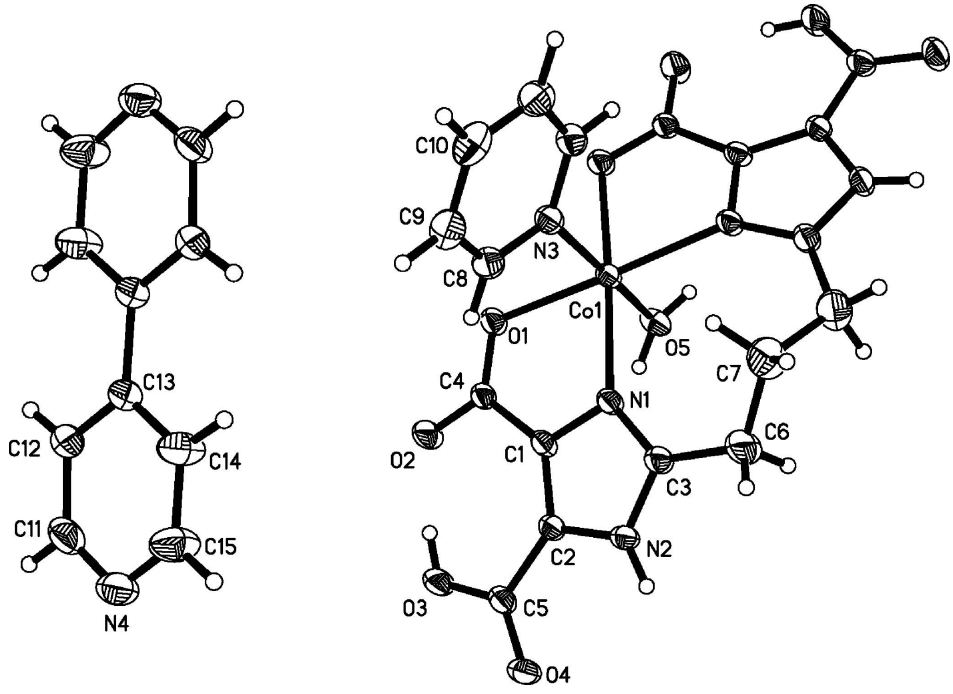

Figure 1

The molecular structure of the title compound, showing 30% probability displacement ellipsoids. Unlabelled atoms are related to labelled atoms by the symmetry operations (x, -y+1/2, z for CoII complex; 1-x, 1-y, 1-z for 4,4-bipy).

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Crystal data

$[Co(C_{13}H_{10}N_4O_8)(C_5H_5N)(H_2O)]\cdot C_{10}H_8N_2$
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Monoclinic, $P2_1/m$
Hall symbol: -P 2yb
a = 7.9733 (10) Å
b = 20.738 (3) Å
c = 8.2987 (11) Å
β = 91.350 (2)°
V = 1371.8 (3) Å^3
Z = 2
$F(000)$ = 680
D_x = 1.601 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 2701 reflections
θ = 2.6–28.3°
μ = 0.70 mm^{-1}
T = 296 K
Prismatic, red
0.22 × 0.18 × 0.11 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2001)
T_{min} = 0.862, T_{max} = 0.927

11480 measured reflections
3443 independent reflections
2633 reflections with $I > 2\sigma(I)$
$R_{int} = 0.033$
$\theta_{max} = 28.3°$, $\theta_{min} = 2.6°$
$h = -10 \rightarrow 10$
$k = -27 \rightarrow 27$
$l = -11 \rightarrow 10$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.043$
$wR(F^2) = 0.105$
$S = 1.05$
3443 reflections
219 parameters
1 restraint
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0442P)^2 + 0.5516P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.43$ e Å^{-3}
$\Delta\rho_{min} = -0.34$ 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}	Occ. (<1)
Co1	1.06603 (5)	0.2500	0.45178 (5)	0.03122 (13)	
O1	1.1510 (2)	0.32701 (7)	0.60553 (18)	0.0383 (4)	
O2	1.2252 (2)	0.43073 (8)	0.6011 (2)	0.0522 (5)	
O3	1.2037 (3)	0.52310 (8)	0.4133 (2)	0.0529 (5)	
H3	1.2128	0.4918	0.4734	0.079*	
O4	1.1130 (3)	0.54174 (8)	0.1645 (2)	0.0529 (5)	
O5	1.3034 (3)	0.2500	0.3543 (3)	0.0427 (6)	
H1W	1.3294	0.2130	0.3301	0.064*	0.50
N1	1.0110 (2)	0.33325 (8)	0.3051 (2)	0.0333 (4)	
N2	0.9918 (2)	0.41425 (8)	0.1356 (2)	0.0376 (4)	
H2	0.9680	0.4358	0.0494	0.045*	
N3	0.8291 (3)	0.2500	0.5671 (3)	0.0362 (6)	
N4	0.5482 (3)	0.64535 (11)	0.7813 (3)	0.0581 (6)	
C1	1.0812 (3)	0.38718 (10)	0.3751 (3)	0.0323 (5)	
C2	1.0707 (3)	0.43808 (10)	0.2707 (3)	0.0339 (5)	
C3	0.9574 (3)	0.35140 (10)	0.1597 (3)	0.0391 (5)	
C4	1.1577 (3)	0.38108 (10)	0.5396 (3)	0.0352 (5)	
C5	1.1307 (3)	0.50565 (11)	0.2790 (3)	0.0389 (5)	
C6	0.8845 (10)	0.3117 (3)	0.0277 (8)	0.077 (2)	0.755 (8)
H6A	0.9736	0.2990	−0.0432	0.092*	0.755 (8)
H6B	0.8060	0.3380	−0.0347	0.092*	0.755 (8)
C7	0.7919 (6)	0.2500	0.0846 (6)	0.0417 (13)	0.755 (8)

H7A	0.6779	0.2500	0.0411	0.050*	0.755 (8)
H7B	0.7867	0.2500	0.2012	0.050*	0.755 (8)
C8	0.7494 (3)	0.30506 (12)	0.6012 (3)	0.0432 (6)	
H8	0.8032	0.3439	0.5807	0.052*	
C9	0.5915 (3)	0.30676 (14)	0.6651 (3)	0.0531 (7)	
H9	0.5404	0.3460	0.6869	0.064*	
C10	0.5108 (5)	0.2500	0.6959 (5)	0.0564 (10)	
H10	0.4033	0.2500	0.7371	0.068*	
C11	0.6117 (4)	0.63819 (13)	0.9295 (4)	0.0565 (7)	
H11	0.6701	0.6727	0.9751	0.068*	
C12	0.5967 (3)	0.58259 (12)	1.0209 (3)	0.0467 (6)	
H12	0.6442	0.5802	1.1241	0.056*	
C13	0.5101 (3)	0.53088 (11)	0.9558 (3)	0.0378 (5)	
C14	0.4429 (4)	0.53878 (13)	0.8010 (4)	0.0604 (8)	
H14	0.3829	0.5054	0.7520	0.072*	
C15	0.4649 (4)	0.59541 (15)	0.7211 (4)	0.0681 (9)	
H15	0.4183	0.5992	0.6177	0.082*	
C7′	0.9726 (4)	0.25000 (15)	−0.0032 (4)	0.048 (4)*	0.245 (8)
H7′1	0.9962	0.2500	−0.1173	0.057*	0.245 (8)
H7′2	1.0762	0.2500	0.0604	0.057*	0.245 (8)
C6′	0.841 (2)	0.3086 (7)	0.049 (2)	0.034 (3)*	0.245 (8)
H6′1	0.8001	0.3323	−0.0446	0.041*	0.245 (8)
H6′2	0.7470	0.2917	0.1074	0.041*	0.245 (8)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Co1	0.0391 (2)	0.0229 (2)	0.0313 (2)	0.000	−0.00719 (16)	0.000
O1	0.0514 (10)	0.0286 (8)	0.0344 (9)	−0.0005 (7)	−0.0105 (7)	−0.0007 (7)
O2	0.0784 (13)	0.0338 (9)	0.0434 (10)	−0.0142 (8)	−0.0229 (9)	−0.0026 (7)
O3	0.0842 (14)	0.0277 (9)	0.0458 (11)	−0.0100 (8)	−0.0171 (9)	−0.0005 (7)
O4	0.0819 (13)	0.0294 (9)	0.0466 (11)	−0.0079 (8)	−0.0133 (9)	0.0070 (8)
O5	0.0451 (13)	0.0284 (11)	0.0549 (15)	0.000	0.0038 (11)	0.000
N1	0.0417 (10)	0.0235 (8)	0.0342 (10)	−0.0004 (7)	−0.0091 (8)	−0.0011 (7)
N2	0.0518 (11)	0.0257 (9)	0.0349 (10)	−0.0025 (8)	−0.0109 (8)	0.0041 (8)
N3	0.0409 (15)	0.0319 (14)	0.0356 (15)	0.000	−0.0052 (11)	0.000
N4	0.0629 (15)	0.0422 (13)	0.0696 (17)	0.0037 (11)	0.0090 (12)	0.0145 (11)
C1	0.0381 (11)	0.0237 (10)	0.0349 (12)	0.0008 (9)	−0.0056 (9)	−0.0030 (8)
C2	0.0414 (12)	0.0268 (10)	0.0333 (12)	0.0016 (9)	−0.0040 (9)	−0.0017 (9)
C3	0.0533 (14)	0.0280 (11)	0.0354 (13)	−0.0024 (10)	−0.0111 (10)	0.0007 (9)
C4	0.0427 (12)	0.0288 (11)	0.0336 (12)	0.0000 (9)	−0.0074 (9)	−0.0031 (9)
C5	0.0497 (14)	0.0275 (11)	0.0394 (13)	−0.0007 (10)	−0.0042 (10)	−0.0029 (10)
C6	0.127 (6)	0.053 (3)	0.049 (3)	−0.053 (3)	−0.024 (4)	0.005 (2)
C7	0.049 (3)	0.033 (2)	0.042 (3)	0.000	−0.020 (2)	0.000
C8	0.0486 (14)	0.0405 (13)	0.0402 (14)	0.0048 (11)	−0.0044 (10)	0.0007 (11)
C9	0.0528 (16)	0.0609 (18)	0.0456 (15)	0.0178 (13)	−0.0006 (12)	0.0010 (13)
C10	0.043 (2)	0.084 (3)	0.042 (2)	0.000	−0.0003 (16)	0.000
C11	0.0655 (18)	0.0355 (14)	0.069 (2)	−0.0091 (12)	0.0129 (15)	−0.0069 (13)
C12	0.0578 (16)	0.0388 (13)	0.0433 (14)	−0.0068 (11)	0.0000 (11)	−0.0039 (11)

C13	0.0384 (12)	0.0330 (12)	0.0419 (13)	−0.0018 (9)	−0.0019 (10)	0.0015 (10)
C14	0.076 (2)	0.0456 (15)	0.0580 (18)	−0.0175 (14)	−0.0252 (15)	0.0147 (13)
C15	0.083 (2)	0.0592 (19)	0.061 (2)	−0.0065 (16)	−0.0203 (16)	0.0207 (16)

Geometric parameters (Å, º)

Co1—O5	2.076 (2)	C6—H6A	0.9700
Co1—N3	2.138 (3)	C6—H6B	0.9700
Co1—O1	2.1441 (15)	C7—C6^{i}	1.557 (6)
Co1—O1^{i}	2.1441 (15)	C7—H7A	0.9700
Co1—N1^{i}	2.1515 (17)	C7—H7B	0.9700
Co1—N1	2.1515 (17)	C8—C9	1.378 (4)
O1—C4	1.249 (3)	C8—H8	0.9300
O2—C4	1.264 (3)	C9—C10	1.369 (3)
O3—C5	1.297 (3)	C9—H9	0.9300
O3—H3	0.8200	C10—C9^{i}	1.369 (3)
O4—C5	1.215 (3)	C10—H10	0.9300
O5—H1W	0.8200	C11—C12	1.387 (4)
N1—C3	1.326 (3)	C11—H11	0.9300
N1—C1	1.374 (3)	C12—C13	1.378 (3)
N2—C3	1.348 (3)	C12—H12	0.9300
N2—C2	1.366 (3)	C13—C14	1.390 (3)
N2—H2	0.8600	C13—C13^{ii}	1.486 (4)
N3—C8	1.340 (3)	C14—C15	1.362 (4)
N3—C8^{i}	1.340 (3)	C14—H14	0.9300
N4—C15	1.322 (4)	C15—H15	0.9300
N4—C11	1.327 (4)	C7′—C6′^{i}	1.667 (13)
C1—C2	1.367 (3)	C7′—C6′	1.667 (13)
C1—C4	1.487 (3)	C7′—H7′1	0.9700
C2—C5	1.482 (3)	C7′—H7′2	0.9700
C3—C6	1.478 (6)	C6′—H6′1	0.9700
C3—C6′	1.565 (19)	C6′—H6′2	0.9700
C6—C7	1.557 (6)		

O5—Co1—N3	176.35 (10)	C3—C6—H6A	108.6
O5—Co1—O1	87.35 (7)	C7—C6—H6A	108.6
N3—Co1—O1	90.22 (7)	C3—C6—H6B	108.6
O5—Co1—O1^{i}	87.35 (7)	C7—C6—H6B	108.6
N3—Co1—O1^{i}	90.22 (7)	H6A—C6—H6B	107.6
O1—Co1—O1^{i}	96.30 (8)	C6—C7—C6^{i}	110.7 (7)
O5—Co1—N1^{i}	87.43 (7)	C6—C7—H7A	109.5
N3—Co1—N1^{i}	94.74 (7)	C6^{i}—C7—H7A	109.5
O1—Co1—N1^{i}	172.62 (6)	C6—C7—H7B	109.5
O1^{i}—Co1—N1^{i}	78.25 (6)	C6^{i}—C7—H7B	109.5
O5—Co1—N1	87.43 (7)	H7A—C7—H7B	108.1
N3—Co1—N1	94.74 (7)	N3—C8—C9	123.0 (2)
O1—Co1—N1	78.25 (6)	N3—C8—H8	118.5
O1^{i}—Co1—N1	172.62 (6)	C9—C8—H8	118.5
N1^{i}—Co1—N1	106.72 (9)	C10—C9—C8	119.2 (3)
C4—O1—Co1	115.09 (14)	C10—C9—H9	120.4

C5—O3—H3	109.5	C8—C9—H9	120.4
Co1—O5—H1W	109.5	C9—C10—C9^{i}	118.7 (4)
C3—N1—C1	105.87 (18)	C9—C10—H10	120.7
C3—N1—Co1	143.14 (15)	C9^{i}—C10—H10	120.7
C1—N1—Co1	109.78 (13)	N4—C11—C12	124.3 (3)
C3—N2—C2	108.63 (18)	N4—C11—H11	117.8
C3—N2—H2	125.7	C12—C11—H11	117.8
C2—N2—H2	125.7	C13—C12—C11	118.8 (3)
C8—N3—C8^{i}	116.9 (3)	C13—C12—H12	120.6
C8—N3—Co1	121.51 (15)	C11—C12—H12	120.6
C8^{i}—N3—Co1	121.51 (15)	C12—C13—C14	116.7 (2)
C15—N4—C11	116.1 (2)	C12—C13—C13^{ii}	122.5 (3)
C2—C1—N1	110.02 (19)	C14—C13—C13^{ii}	120.9 (3)
C2—C1—C4	131.70 (19)	C15—C14—C13	120.0 (3)
N1—C1—C4	118.24 (18)	C15—C14—H14	120.0
N2—C2—C1	105.15 (18)	C13—C14—H14	120.0
N2—C2—C5	121.5 (2)	N4—C15—C14	124.1 (3)
C1—C2—C5	133.3 (2)	N4—C15—H15	118.0
N1—C3—N2	110.33 (19)	C14—C15—H15	118.0
N1—C3—C6	129.0 (3)	C6′^{i}—C7′—C6′	93.5 (12)
N2—C3—C6	120.4 (3)	C6′^{i}—C7′—H7′1	113.0
N1—C3—C6′	123.2 (7)	C6′—C7′—H7′1	113.0
N2—C3—C6′	125.5 (6)	C6′^{i}—C7′—H7′2	113.0
C6—C3—C6′	14.6 (7)	C6′—C7′—H7′2	113.0
O1—C4—O2	125.2 (2)	H7′1—C7′—H7′2	110.4
O1—C4—C1	117.23 (18)	C3—C6′—C7′	101.5 (9)
O2—C4—C1	117.59 (19)	C3—C6′—H6′1	111.5
O4—C5—O3	122.8 (2)	C7′—C6′—H6′1	111.5
O4—C5—C2	121.0 (2)	C3—C6′—H6′2	111.5
O3—C5—C2	116.2 (2)	C7′—C6′—H6′2	111.5
C3—C6—C7	114.5 (5)	H6′1—C6′—H6′2	109.3
O5—Co1—O1—C4	77.25 (17)	C1—N1—C3—C6	174.5 (5)
N3—Co1—O1—C4	−105.47 (17)	Co1—N1—C3—C6	9.5 (6)
O1^{i}—Co1—O1—C4	164.28 (13)	C1—N1—C3—C6′	−169.0 (6)
N1^{i}—Co1—O1—C4	122.3 (5)	Co1—N1—C3—C6′	26.1 (7)
N1—Co1—O1—C4	−10.68 (16)	C2—N2—C3—N1	−0.1 (3)
O5—Co1—N1—C3	86.0 (3)	C2—N2—C3—C6	−174.9 (4)
N3—Co1—N1—C3	−96.9 (3)	C2—N2—C3—C6′	168.9 (7)
O1—Co1—N1—C3	173.8 (3)	Co1—O1—C4—O2	−169.8 (2)
O1^{i}—Co1—N1—C3	131.0 (5)	Co1—O1—C4—C1	9.7 (3)
N1^{i}—Co1—N1—C3	−0.5 (3)	C2—C1—C4—O1	−178.4 (2)
O5—Co1—N1—C1	−78.58 (15)	N1—C1—C4—O1	−1.1 (3)
N3—Co1—N1—C1	98.49 (15)	C2—C1—C4—O2	1.1 (4)
O1—Co1—N1—C1	9.25 (14)	N1—C1—C4—O2	178.5 (2)
O1^{i}—Co1—N1—C1	−33.6 (6)	N2—C2—C5—O4	−0.9 (4)
N1^{i}—Co1—N1—C1	−165.12 (11)	C1—C2—C5—O4	176.1 (2)
O5—Co1—N3—C8	91.7 (2)	N2—C2—C5—O3	180.0 (2)
O1—Co1—N3—C8	43.6 (2)	C1—C2—C5—O3	−3.1 (4)

O1^{i}—Co1—N3—C8	139.9 (2)	N1—C3—C6—C7	27.9 (8)
N1^{i}—Co1—N3—C8	−141.9 (2)	N2—C3—C6—C7	−158.5 (4)
N1—Co1—N3—C8	−34.6 (2)	C6′—C3—C6—C7	−44 (3)
O5—Co1—N3—C8^{i}	−91.7 (2)	C3—C6—C7—C6^{i}	−114.7 (5)
O1—Co1—N3—C8^{i}	−139.9 (2)	C8^{i}—N3—C8—C9	−1.4 (5)
O1^{i}—Co1—N3—C8^{i}	−43.6 (2)	Co1—N3—C8—C9	175.34 (19)
N1^{i}—Co1—N3—C8^{i}	34.6 (2)	N3—C8—C9—C10	0.1 (4)
N1—Co1—N3—C8^{i}	141.9 (2)	C8—C9—C10—C9^{i}	1.3 (5)
C3—N1—C1—C2	−0.4 (3)	C15—N4—C11—C12	0.6 (4)
Co1—N1—C1—C2	170.09 (15)	N4—C11—C12—C13	−0.2 (4)
C3—N1—C1—C4	−178.2 (2)	C11—C12—C13—C14	−0.2 (4)
Co1—N1—C1—C4	−7.8 (2)	C11—C12—C13—C13^{ii}	179.1 (3)
C3—N2—C2—C1	−0.1 (3)	C12—C13—C14—C15	0.3 (4)
C3—N2—C2—C5	177.6 (2)	C13^{ii}—C13—C14—C15	−179.0 (3)
N1—C1—C2—N2	0.3 (2)	C11—N4—C15—C14	−0.4 (5)
C4—C1—C2—N2	177.8 (2)	C13—C14—C15—N4	0.0 (5)
N1—C1—C2—C5	−177.0 (2)	N1—C3—C6′—C7′	−70.7 (10)
C4—C1—C2—C5	0.5 (4)	N2—C3—C6′—C7′	121.7 (6)
C1—N1—C3—N2	0.3 (3)	C6—C3—C6′—C7′	48 (2)
Co1—N1—C3—N2	−164.64 (19)	C6′^{i}—C7′—C6′—C3	129.0 (6)

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

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O3—H3···O2	0.82	1.65	2.473 (2)	177
O5—H1*W*···N4^{iii}	0.82	1.95	2.727 (3)	157
N2—H2···O4^{iv}	0.86	1.93	2.763 (3)	162

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