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Diaquabis(1-methyl-1*H*-imidazole-κN^3)-bis[2-(naphthalen-1-yl)acetato-κO]-cobalt(II)

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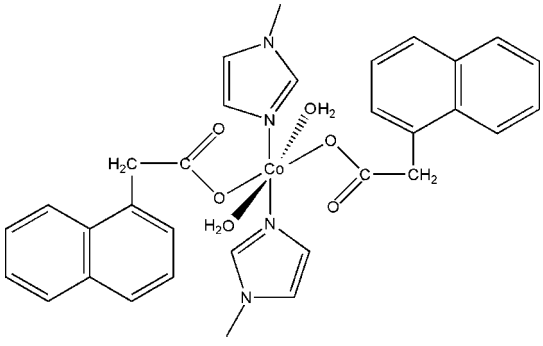
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.003 Å; R factor = 0.032; wR factor = 0.084; data-to-parameter ratio = 16.5.

In the title compound, $[Co(C_{12}H_9O_2)_2(C_4H_6N_2)_2(H_2O)_2]$, the Co^{II} ion is located on an inversion centre and displays a distorted octahedral coordination geometry. Two O atoms from two water molecules and two carboxylate O atoms from two 2-(naphthalen-1-yl)acetate ligands are in the equatorial plane and two N atoms from two 1-methyl-1*H*-imidazole ligands are in the axial positions. The structure is stabilized by intramolecular O—H···O hydrogen bonds. Intermolecular O—H···O hydrogen bonds link the complex molecules into chains along [100].

Related literature

For the structures of related complexes with 2-(naphthalen-1-yl)acetate ligands, see: Duan *et al.* (2007); Ji *et al.* (2011); Tang *et al.* (2006); Yang *et al.* (2008); Yin *et al.* (2011).



Experimental

Crystal data

$[Co(C_{12}H_9O_2)_2(C_4H_6N_2)_2(H_2O)_2]$
M_r = 629.56
Monoclinic, $P2_1/c$
a = 7.3384 (7) Å
b = 24.582 (2) Å
c = 8.8559 (8) Å
β = 111.158 (1)°
V = 1489.8 (2) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.63 mm^{-1}
T = 298 K
0.34 × 0.30 × 0.20 mm

Data collection

Bruker APEXII CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.815, T_{max} = 0.885
13335 measured reflections
3356 independent reflections
2865 reflections with $I > 2\sigma(I)$
R_{int} = 0.024

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.032
$wR(F^2)$ = 0.084
S = 1.05
3356 reflections
203 parameters
2 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.25 e Å^{-3}
$\Delta\rho_{min}$ = −0.28 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O3—H3A···O2^{i}	0.84 (2)	2.13 (2)	2.8523 (18)	144 (2)
O3—H3B···O2	0.85 (2)	1.81 (2)	2.6463 (16)	168 (2)

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

Data collection: *APEX2* (Bruker, 2007); cell refinement: *SAINT* (Bruker, 2007); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *DIAMOND* (Brandenburg, 1999); software used to prepare material for publication: *SHELXTL* (Sheldrick, 2008).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HY2522).

References

Brandenburg, K. (1999). *DIAMOND*. Crystal Impact GbR, Bonn, Germany.
Bruker (2007). *APEX2* and *SAINT*. Bruker AXS Inc., Madison, Wisconsin, USA.
Duan, J.-G., Liu, J.-W. & Wu, S. (2007). *Acta Cryst.* E**63**, m692–m694.
Ji, L.-L., Liu, J.-S. & Song, W.-D. (2011). *Acta Cryst.* E**67**, m606.
Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Tang, D.-X., Feng, L.-X. & Zhang, X.-Q. (2006). *Chin. J. Inorg. Chem.* **22**, 1891–1894.
Yang, Y.-Q., Li, C.-H., Li, W. & Kuang, Y.-F. (2008). *Chin. J. Struct. Chem.* **30**, 4524–4530.
Yin, F.-J., Han, L.-J., Yang, S.-P. & Xu, X. Y. (2011). *Acta Cryst.* E**67**, m1772.

supplementary materials

Acta Cryst. (2012). E**68**, m533 [doi:10.1107/S1600536812013505]

Diaquabis(1-methyl-1*H*-imidazole-κN^3)bis[2-(naphthalen-1-yl)acetato-κO]cobalt(II)

Hong Zhao, Fu-Jun Yin, Xing-You Xu and Li-Jun Han

Comment

In recent years 2-(naphthalen-1-yl)acetate ligand has attracted many interests in coordination chemistry due to its ability to form metal complexes (Duan *et al.*, 2007; Ji *et al.*, 2011; Tang *et al.*, 2006; Yang *et al.*, 2008; Yin *et al.*, 2011). The crystal structure of the title compound was determined as part of an ongoing study of the properties of cobalt complexes containing imidazole ligands.

In the title compound (Fig. 1), the Co^{II} ion is located on an inversion centre and displays a distorted octahedral coordination geometry. Two O atoms from two water molecules and two carboxylate O atoms from two 2-(naphthalen-1-yl)acetate ligands are in the equatorial plane and two N atoms from two N-methylimidazole ligands are in the axial positions. The structure is stabilized by intramolecular O—H···O hydrogen bonds (Table 1). In the crystal, intermolecular O—H···O hydrogen bonds link the complex molecules into chains along [100] (Fig. 2).

Experimental

The title compound was synthesized by the reaction of $CoCl_2.6H_2O$ (71.3 mg, 0.3 mmol), 2-(naphthalen-1-yl)acetic acid (93 mg, 0.5 mmol), N-methylimidazole (32.8 mg, 0.4 mmol) and NaOH (20 mg, 0.5 mmol) in 15 ml of a water-ethanol mixture (v/v 1:1) under solvothermal conditions. The starting mixture was homogenized and transferred into a sealed Teflon-lined bomb (25 ml) and heated at 140° C for three days. After cooling, red crystals of the title compound were obtained, which were washed with distilled water and absolute ethyl alcohol (yield: 26.8% based on Co).

Refinement

H atoms attached to C atoms were placed in calculated positions and refined as riding atoms, with C—H = 0.93 (CH), 0.97 (CH_2) and 0.96 (CH_3) Å and with U_{iso}(H) = 1.2(1.5 for methyl)U_{eq}(C). The water H atoms were located in a difference Fourier map and refined with a restraint of O—H = 0.85 (1) Å and with U_{iso}(H) = 1.5U_{eq}(O).

Computing details

Data collection: *APEX2* (Bruker, 2007); cell refinement: *SAINT* (Bruker, 2007); data reduction: *SAINT* (Bruker, 2007); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *DIAMOND* (Brandenburg, 1999); software used to prepare material for publication: *SHELXTL* (Sheldrick, 2008).

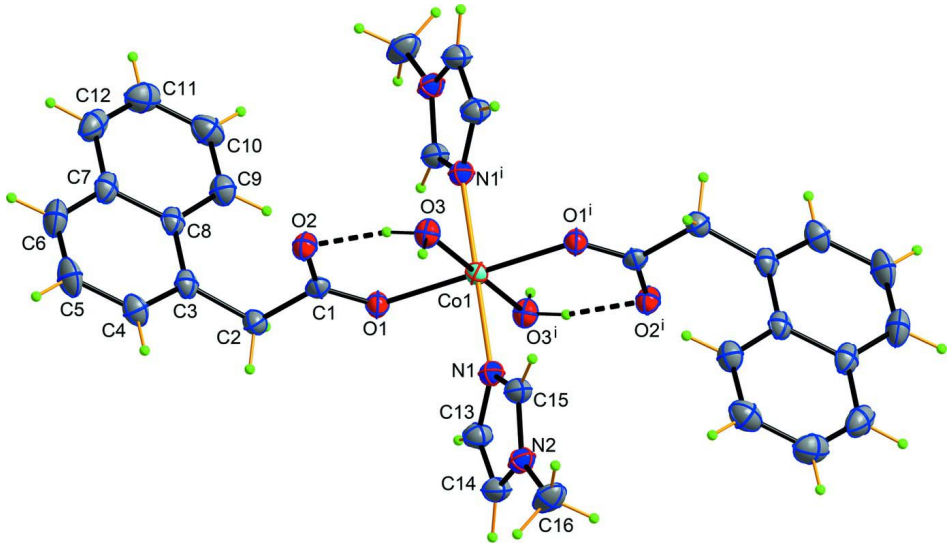

Figure 1

Molecular structure of the title compound. Displacement ellipsoids are drawn at the 30% probability level. Hydrogen bonds are shown as dashed lines. [Symmetry code: (i) -*x*+1, -*y*+1, -*z*.]

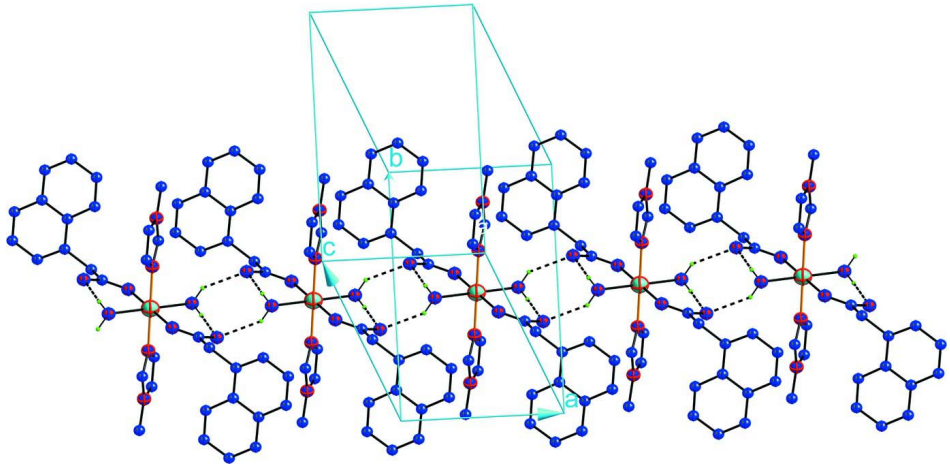

Figure 2

Part of the chain structure of the title compound. Hydrogen bonds are shown as dashed lines. H atoms not involved in hydrogen bonds are omitted for clarity.

Diaquabis(1-methyl-1*H*-imidazole-κN^3)bis[2-(naphthalen- 1-yl)acetato-κO]cobalt(II)

Crystal data

$[Co(C_{12}H_9O_2)_2(C_4H_6N_2)_2(H_2O)_2]$
$M_r = 629.56$
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
$a = 7.3384$ (7) Å
$b = 24.582$ (2) Å
$c = 8.8559$ (8) Å
$\beta = 111.158$ (1)°
$V = 1489.8$ (2) Å^3
$Z = 2$
$F(000) = 658$
$D_x = 1.403$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 3356 reflections
$\theta = 2.6$–27.3°
$\mu = 0.63$ mm^{-1}
$T = 298$ K
Block, red
0.34 × 0.30 × 0.20 mm

Data collection

Bruker APEXII CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.815, T_{max} = 0.885
13335 measured reflections
3356 independent reflections
2865 reflections with $I > 2\sigma(I)$
R_{int} = 0.024
θ_{max} = 27.3°, θ_{min} = 2.6°
h = −9→9
k = −31→30
l = −11→11

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.032
$wR(F^2)$ = 0.084
S = 1.05
3356 reflections
203 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
$w = 1/[\sigma^2(F_o^2) + (0.0408P)^2 + 0.3567P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.25 e Å^{-3}
$\Delta\rho_{min}$ = −0.28 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 $F^2 > 2$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	0.0000	0.03250 (10)
N1	0.3651 (2)	0.49725 (5)	−0.25228 (16)	0.0396 (3)
N2	0.2163 (2)	0.46891 (6)	−0.50250 (16)	0.0439 (3)
O1	0.37360 (16)	0.57809 (4)	0.00491 (14)	0.0417 (3)
O2	0.14963 (16)	0.55623 (4)	0.11124 (14)	0.0429 (3)
O3	0.26123 (16)	0.46019 (5)	0.04077 (14)	0.0414 (3)
C1	0.2365 (2)	0.58909 (6)	0.05248 (17)	0.0344 (3)
C2	0.1641 (3)	0.64816 (7)	0.0303 (2)	0.0430 (4)
H2A	0.2760	0.6720	0.0518	0.052*
H2B	0.0803	0.6533	−0.0819	0.052*
C3	0.0536 (2)	0.66527 (6)	0.1363 (2)	0.0405 (4)
C4	−0.1444 (3)	0.67227 (7)	0.0715 (2)	0.0508 (4)
H4	−0.2105	0.6649	−0.0377	0.061*
C5	−0.2506 (3)	0.69042 (8)	0.1662 (3)	0.0631 (6)
H5	−0.3851	0.6951	0.1186	0.076*
C6	−0.1594 (3)	0.70103 (8)	0.3253 (3)	0.0601 (5)

H6	−0.2311	0.7136	0.3859	0.072*
C7	0.0448 (3)	0.69323 (6)	0.4006 (2)	0.0471 (4)
C8	0.1530 (2)	0.67521 (6)	0.3049 (2)	0.0393 (3)
C9	0.3577 (3)	0.66855 (7)	0.3824 (2)	0.0494 (4)
H9	0.4314	0.6567	0.3227	0.059*
C10	0.4479 (3)	0.67927 (9)	0.5436 (3)	0.0636 (5)
H10	0.5826	0.6751	0.5918	0.076*
C11	0.3404 (4)	0.69649 (8)	0.6373 (3)	0.0686 (6)
H11	0.4038	0.7034	0.7471	0.082*
C12	0.1447 (4)	0.70302 (7)	0.5682 (3)	0.0611 (5)
H12	0.0744	0.7141	0.6317	0.073*
C13	0.3534 (3)	0.53921 (7)	−0.3573 (2)	0.0473 (4)
H13	0.4010	0.5742	−0.3270	0.057*
C14	0.2625 (3)	0.52220 (8)	−0.5115 (2)	0.0510 (4)
H14	0.2367	0.5428	−0.6051	0.061*
C15	0.2803 (2)	0.45573 (7)	−0.34511 (19)	0.0428 (4)
H15	0.2666	0.4214	−0.3062	0.051*
C16	0.1186 (3)	0.43256 (10)	−0.6383 (2)	0.0617 (5)
H16A	0.2063	0.4239	−0.6932	0.093*
H16B	0.0045	0.4502	−0.7122	0.093*
H16C	0.0810	0.3997	−0.5986	0.093*
H3A	0.161 (3)	0.4468 (11)	−0.029 (2)	0.093*
H3B	0.222 (4)	0.4886 (7)	0.074 (3)	0.093*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Co1	0.03202 (16)	0.03393 (16)	0.03224 (16)	0.00035 (11)	0.01242 (11)	−0.00172 (11)
N1	0.0412 (7)	0.0412 (7)	0.0347 (7)	0.0010 (6)	0.0119 (6)	0.0007 (6)
N2	0.0419 (7)	0.0557 (9)	0.0331 (7)	−0.0014 (6)	0.0124 (6)	−0.0032 (6)
O1	0.0423 (6)	0.0395 (6)	0.0479 (6)	0.0053 (5)	0.0220 (5)	0.0010 (5)
O2	0.0454 (6)	0.0376 (6)	0.0503 (7)	0.0003 (5)	0.0230 (5)	−0.0017 (5)
O3	0.0391 (6)	0.0393 (6)	0.0479 (7)	−0.0033 (5)	0.0183 (5)	−0.0046 (5)
C1	0.0346 (7)	0.0365 (8)	0.0287 (7)	−0.0001 (6)	0.0074 (6)	−0.0041 (6)
C2	0.0501 (9)	0.0376 (8)	0.0443 (9)	0.0055 (7)	0.0205 (7)	0.0026 (7)
C3	0.0441 (9)	0.0276 (7)	0.0532 (10)	0.0021 (6)	0.0218 (8)	0.0009 (6)
C4	0.0440 (9)	0.0412 (9)	0.0632 (12)	0.0005 (7)	0.0145 (8)	−0.0032 (8)
C5	0.0397 (10)	0.0559 (12)	0.0970 (17)	0.0036 (8)	0.0287 (11)	−0.0024 (11)
C6	0.0599 (12)	0.0485 (11)	0.0881 (16)	0.0029 (9)	0.0462 (12)	−0.0084 (10)
C7	0.0602 (11)	0.0293 (8)	0.0619 (11)	−0.0016 (7)	0.0343 (9)	−0.0039 (7)
C8	0.0457 (9)	0.0255 (7)	0.0511 (9)	−0.0002 (6)	0.0226 (7)	−0.0007 (6)
C9	0.0478 (10)	0.0444 (9)	0.0567 (11)	0.0011 (7)	0.0197 (8)	−0.0005 (8)
C10	0.0605 (12)	0.0554 (12)	0.0640 (13)	−0.0008 (9)	0.0094 (10)	0.0010 (10)
C11	0.0946 (17)	0.0521 (12)	0.0520 (12)	−0.0037 (11)	0.0180 (11)	−0.0053 (9)
C12	0.0958 (17)	0.0387 (10)	0.0614 (13)	−0.0015 (10)	0.0437 (12)	−0.0070 (9)
C13	0.0540 (10)	0.0429 (9)	0.0455 (10)	−0.0023 (8)	0.0186 (8)	0.0039 (7)
C14	0.0554 (11)	0.0575 (11)	0.0402 (9)	0.0035 (9)	0.0173 (8)	0.0105 (8)
C15	0.0467 (9)	0.0444 (9)	0.0364 (8)	−0.0006 (7)	0.0141 (7)	0.0014 (7)
C16	0.0622 (12)	0.0798 (14)	0.0396 (10)	−0.0100 (10)	0.0142 (9)	−0.0162 (9)

Geometric parameters (Å, º)

Co1—N1	2.0928 (13)	C5—H5	0.9300
Co1—O1	2.1392 (11)	C6—C7	1.416 (3)
Co1—O3	2.1483 (11)	C6—H6	0.9300
N1—C15	1.317 (2)	C7—C12	1.419 (3)
N1—C13	1.371 (2)	C7—C8	1.425 (2)
N2—C15	1.340 (2)	C8—C9	1.418 (2)
N2—C14	1.363 (2)	C9—C10	1.364 (3)
N2—C16	1.461 (2)	C9—H9	0.9300
O1—C1	1.2528 (18)	C10—C11	1.401 (3)
O2—C1	1.2525 (18)	C10—H10	0.9300
O3—H3A	0.84 (2)	C11—C12	1.352 (3)
O3—H3B	0.85 (2)	C11—H11	0.9300
C1—C2	1.534 (2)	C12—H12	0.9300
C2—C3	1.505 (2)	C13—C14	1.352 (3)
C2—H2A	0.9700	C13—H13	0.9300
C2—H2B	0.9700	C14—H14	0.9300
C3—C4	1.367 (2)	C15—H15	0.9300
C3—C8	1.427 (2)	C16—H16A	0.9600
C4—C5	1.408 (3)	C16—H16B	0.9600
C4—H4	0.9300	C16—H16C	0.9600
C5—C6	1.349 (3)		

N1—Co1—N1^{i}	180.000 (1)	C6—C5—C4	120.71 (18)
N1—Co1—O1	90.52 (5)	C6—C5—H5	119.6
N1^{i}—Co1—O1	89.48 (5)	C4—C5—H5	119.6
N1—Co1—O1^{i}	89.48 (5)	C5—C6—C7	120.51 (18)
N1^{i}—Co1—O1^{i}	90.52 (5)	C5—C6—H6	119.7
O1—Co1—O1^{i}	180.0	C7—C6—H6	119.7
N1—Co1—O3^{i}	86.31 (5)	C6—C7—C12	121.94 (18)
N1^{i}—Co1—O3^{i}	93.69 (5)	C6—C7—C8	118.93 (17)
O1—Co1—O3^{i}	88.89 (4)	C12—C7—C8	119.13 (17)
O1^{i}—Co1—O3^{i}	91.11 (4)	C9—C8—C7	117.92 (16)
N1—Co1—O3	93.69 (5)	C9—C8—C3	122.62 (15)
N1^{i}—Co1—O3	86.31 (5)	C7—C8—C3	119.46 (15)
O1—Co1—O3	91.11 (4)	C10—C9—C8	120.91 (18)
O1^{i}—Co1—O3	88.89 (4)	C10—C9—H9	119.5
O3^{i}—Co1—O3	180.00 (6)	C8—C9—H9	119.5
C15—N1—C13	105.06 (14)	C9—C10—C11	120.9 (2)
C15—N1—Co1	128.77 (11)	C9—C10—H10	119.6
C13—N1—Co1	126.13 (11)	C11—C10—H10	119.6
C15—N2—C14	106.99 (14)	C12—C11—C10	120.1 (2)
C15—N2—C16	126.28 (16)	C12—C11—H11	119.9
C14—N2—C16	126.72 (15)	C10—C11—H11	119.9
C1—O1—Co1	127.40 (10)	C11—C12—C7	121.06 (19)
Co1—O3—H3A	127.2 (18)	C11—C12—H12	119.5
Co1—O3—H3B	94.9 (19)	C7—C12—H12	119.5
H3A—O3—H3B	105 (3)	C14—C13—N1	109.88 (16)
O2—C1—O1	126.26 (14)	C14—C13—H13	125.1

O2—C1—C2	117.33 (13)	N1—C13—H13	125.1
O1—C1—C2	116.37 (14)	C13—C14—N2	106.28 (15)
C3—C2—C1	115.10 (13)	C13—C14—H14	126.9
C3—C2—H2A	108.5	N2—C14—H14	126.9
C1—C2—H2A	108.5	N1—C15—N2	111.79 (15)
C3—C2—H2B	108.5	N1—C15—H15	124.1
C1—C2—H2B	108.5	N2—C15—H15	124.1
H2A—C2—H2B	107.5	N2—C16—H16A	109.5
C4—C3—C8	118.82 (16)	N2—C16—H16B	109.5
C4—C3—C2	120.25 (16)	H16A—C16—H16B	109.5
C8—C3—C2	120.92 (14)	N2—C16—H16C	109.5
C3—C4—C5	121.53 (19)	H16A—C16—H16C	109.5
C3—C4—H4	119.2	H16B—C16—H16C	109.5
C5—C4—H4	119.2		

O1—Co1—N1—C15	−139.37 (14)	C6—C7—C8—C9	178.98 (16)
O1^{i}—Co1—N1—C15	40.63 (14)	C12—C7—C8—C9	−0.8 (2)
O3^{i}—Co1—N1—C15	131.77 (15)	C6—C7—C8—C3	−0.2 (2)
O3—Co1—N1—C15	−48.23 (15)	C12—C7—C8—C3	179.99 (15)
O1—Co1—N1—C13	43.28 (14)	C4—C3—C8—C9	179.47 (16)
O1^{i}—Co1—N1—C13	−136.72 (14)	C2—C3—C8—C9	−1.4 (2)
O3^{i}—Co1—N1—C13	−45.58 (14)	C4—C3—C8—C7	−1.3 (2)
O3—Co1—N1—C13	134.42 (14)	C2—C3—C8—C7	177.79 (14)
N1—Co1—O1—C1	107.01 (13)	C7—C8—C9—C10	−0.2 (3)
N1^{i}—Co1—O1—C1	−72.99 (13)	C3—C8—C9—C10	178.98 (17)
O3^{i}—Co1—O1—C1	−166.69 (12)	C8—C9—C10—C11	0.8 (3)
O3—Co1—O1—C1	13.31 (12)	C9—C10—C11—C12	−0.4 (3)
Co1—O1—C1—O2	2.2 (2)	C10—C11—C12—C7	−0.7 (3)
Co1—O1—C1—C2	−175.43 (10)	C6—C7—C12—C11	−178.52 (19)
O2—C1—C2—C3	22.5 (2)	C8—C7—C12—C11	1.2 (3)
O1—C1—C2—C3	−159.65 (14)	C15—N1—C13—C14	−0.2 (2)
C1—C2—C3—C4	−106.75 (18)	Co1—N1—C13—C14	177.66 (12)
C1—C2—C3—C8	74.13 (19)	N1—C13—C14—N2	0.2 (2)
C8—C3—C4—C5	1.8 (3)	C15—N2—C14—C13	−0.06 (19)
C2—C3—C4—C5	−177.34 (16)	C16—N2—C14—C13	−179.08 (17)
C3—C4—C5—C6	−0.6 (3)	C13—N1—C15—N2	0.16 (19)
C4—C5—C6—C7	−1.1 (3)	Co1—N1—C15—N2	−177.62 (10)
C5—C6—C7—C12	−178.80 (19)	C14—N2—C15—N1	−0.07 (19)
C5—C6—C7—C8	1.5 (3)	C16—N2—C15—N1	178.96 (16)

Symmetry code: (i) −*x*+1, −*y*+1, −*z*.

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O3—H3*A*···O2^{ii}	0.84 (2)	2.13 (2)	2.8523 (18)	144 (2)
O3—H3*B*···O2	0.85 (2)	1.81 (2)	2.6463 (16)	168 (2)

Symmetry code: (ii) −*x*, −*y*+1, −*z*.