Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

Diaquabis(4-carboxy-2-propyl-1*H*-imidazole-5-carboxylato-κ^2N^3,O^4)-cobalt(II) *N*,*N*-dimethylformamide disolvate

Shi-Jie Li,[a] Li-Li Ji,[a] Wen-Dong Song,[b]* Shi-Wei Hu[a] and Pei-Wen Qin[c]

[a]College of Food Science and Technology, Guangdong Ocean University, Zhanjiang 524088, People's Republic of China, [b]College of Science, Guangdong Ocean University, Zhanjiang 524088, People's Republic of China, and [c]College of Agriculture, Guang Dong Ocean University, Zhanjiang 524088, People's Republic of China
Correspondence e-mail: songwd60@163.com

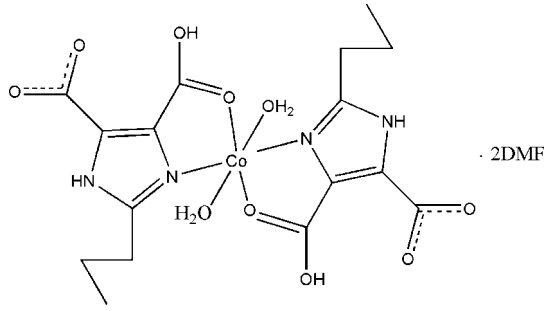
Received 4 October 2010; accepted 17 October 2010

Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.005 Å; R factor = 0.046; wR factor = 0.120; data-to-parameter ratio = 12.5.

In the title complex, $[Co(C_8H_9N_2O_4)_2(H_2O)_2]\cdot 2C_3H_7NO$, the Co^{II} cation (site symmetry $\overline{1}$) is six-coordinated by two 5-carboxy-2-propyl-1*H*-imidazole-4-carboxylate ligands and two water molecules in a distorted octahedral environment. In the crystal structure, the complex molecules and dimethylformamide solvent molecules are linked by extensive O—H···O and N—H···O hydrogen bonding into sheets lying parallel to $(21\overline{1})$.

Related literature

For our past work based on the 2-propyl-1*H*-imidazole-4,5-carboxylate (H_3pimda) ligand, see: Yan *et al.* (2010); Li *et al.* (2010*a*,*b*,*c*,*d*); Song *et al.* (2010); He *et al.* (2010); Fan *et al.* (2010). For Co complexes of a similar ligand, see: Lu *et al.* (2008); Wang *et al.* (2004).



Experimental

Crystal data

$[Co(C_8H_9N_2O_4)_2(H_2O)_2]\cdot 2C_3H_7NO$
M_r = 635.50
Triclinic, $P\overline{1}$
a = 7.3325 (7) Å
b = 9.330 (1) Å
c = 11.2255 (12) Å
α = 76.930 (1)°
β = 87.564 (2)°
γ = 68.857 (1)°
V = 697.06 (12) Å^3
Z = 1
Mo $K\alpha$ radiation
μ = 0.69 mm^{-1}
T = 298 K
0.28 × 0.16 × 0.12 mm

Data collection

Bruker SMART 1000 CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2007)
T_{min} = 0.831, T_{max} = 0.922
3602 measured reflections
2393 independent reflections
1785 reflections with $I > 2\sigma(I)$
R_{int} = 0.025

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.046
$wR(F^2)$ = 0.120
S = 1.06
2393 reflections
191 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.37 e Å^{-3}
$\Delta\rho_{min}$ = −0.52 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O5—H5D···O4^{i}	0.83	2.12	2.946 (3)	174
O5—H5C···O4^{ii}	0.83	1.94	2.773 (3)	175
O2—H2A···O3	0.82	1.66	2.478 (3)	177
N2—H2···O6^{iii}	0.86	1.84	2.685 (4)	166

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

Data collection: *SMART* (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: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL*.

The work was supported by the Nonprofit Industry Foundation of the National Ocean Administration of China (grant No. 2000905021), the Guangdong Oceanic Fisheries Technology Promotion Project [grant No. A2009003–018(*c*)], the Guangdong Chinese Academy of Science comprehensive strategic cooperation project (grant No. 2009B091300121), the Guangdong Province key project in the field of social development [grant No. A2009011–007(*c*)], the Science and Technology Department of Guangdong Province Project (grant No. 00087061110314018) and the Guangdong Natural Science Fundation (No. 9252408801000002)

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: JH2216).

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supporting information

Acta Cryst. (2010). E**66**, m1443–m1444 [https://doi.org/10.1107/S1600536810042054]

Diaquabis(4-carboxy-2-propyl-1*H*-imidazole-5-carboxylato-κ^2N^3,O^4)cobalt(II) *N*,*N*-dimethylformamide disolvate

Shi-Jie Li, Li-Li Ji, Wen-Dong Song, Shi-Wei Hu and Pei-Wen Qin

S1. Comment

Design of a metal-organic framework *via* deliberate selection of metals and multifunctional ligands is one of the most attractive topics because of the fascinating structural diversity and potential applications in catalysis, chirality, conductivity, luminescence, magnetism, sensors, nonlinear optics, and porosity. 2-propyl-1*H*-imidazole-4,5-carboxylate(H_3pimda) ligand as one derivative of H_3IDC with efficient N,*O*-donors has been used to obtain new metal-organic complexes by our research group, such as poly[diaquabis(5-carboxy-2-propyl-1*H*-imidazole-4-carboxylato-k^3 N^3, O^4,*O*^{5})calcium(II)](Song *et al.*, 2010), [diaquabis(5-carboxy-2-propyl-1*H*-imidazole-4-carboxylato-k^{2}N^3,*O*^{4}) manganese(II)]*N*,*N*-dimethylformamide(Yan *et al.*, 2010), [Diaquabis(5-carboxy-2-propyl-1*H*-imidazole-4-carboxylato-k^2 *N*^{3},*O*^{4})nickle(II)]*N*,*N*-dimethylformamide disolvate(Li *et al.*, 2010*a*), Diaquabis(4-carboxy-2-propyl-1*H*-imidazole-5-carboxylato- k^{2}N^3,*O*^{4})copper(II) *N*,*N*-dimethylformamide disolvate(He *et al.*, 2010), Diaquabis(5-carboxy-2-propyl-1*H*-imidazole- 4-carboxylato-k^{2}N^3,*O*^{4})nickle(II) tetrahedrate(Fan *et al.*, 2010), Diaquabis(5-carboxy-2-propyl-1*H*-imidazole-4-carboxylato- k^{2}N^3,*O*^{4})-manganese(II) 3.5-hydrate(Li *et al.* 2010*c*), Diaquabis (5-carboxy-2-propyl-1*H*-imidazole-4-carboxylato-K^{2}N^3,*O*^{4})zinc(II) 3.5-hydrate(Li *et al.* 2010*b*), Diaquabis(5-carboxy-2-propyl-1*H*- imidazole-4-carboxylato-k^{2}N^3,*O*^{4})cadmium(II) 3.5-hydrate (Li *et al.* 2010*d*), In this paper, we will report the synthesis and structure of a new Co^{II} complex based the same ligand.

As illustrated in figure 1, the title complex molecule is isomorphous with Ni(II), Mn(II) and Cu(II) analogs (Li *et al.*, 2010a,b,c,d; Yan *et al.*, 2010; He *et al.*, 2010), Similar structural description applies to the present isomorphous complex.the Co^{II} cation lying on the inversion center, is six-coordinated CoN_2O_4 in a slightly distorted octahedral geometry, constructed by the two pairs of N and O atoms from H_2pimda in the equatorial plane, and two coordinate water O atoms occipying the axial position. The Co—O bond lengths and Co—N bond lengths, all of which are within the range of those observed for other Co complexes based on the similar ligand (Lu *et al.*, 2008; Wang *et al.*, 2004). Each H_3pimda adopts bidentate coordination mode to chelate Co^{II} atom through imidazole N atom and O atom from the protonated carboxyl group, the complex molecules and dimethylformamide solvent molecules are linked by extensive O—H···O and N—H···O hydrogen bonds into a two-dimensional supramolecular network parallel to (001).

S2. Experimental

A mixture of $Co(NO3)_2$ (0.5 mmol, 0.06 g) and 2-propyl-1*H*-imidazole-4,5-dicarboxylic acid(0.5 mmol, 0.99 g) in 15 ml of DMF solution was sealed in an autoclave equipped with a Teflon liner (20 ml) and then heated at 413k for 3 days. Crystals of the title compound were obtained by slow evaporation of the solvent at room temperature.

S3. Refinement

Water H atoms were located in a difference Fourier map and were allowed to ride on the parent atom, with U_{iso}(H) = 1.5U_{eq}(O). Carboxyl H atoms were located in a difference map and refined with distance restraints, U_{iso}(H) = 1.5U_{eq}(O). Other H atoms were placed at calculated positions and were treated as riding on parent atoms with C—H = 0.96 (methyl), 0.97 (methylene) and N—H = 0.86 Å, U_{iso}(H) = 1.2 or 1.5U_{eq}(C,*N*).

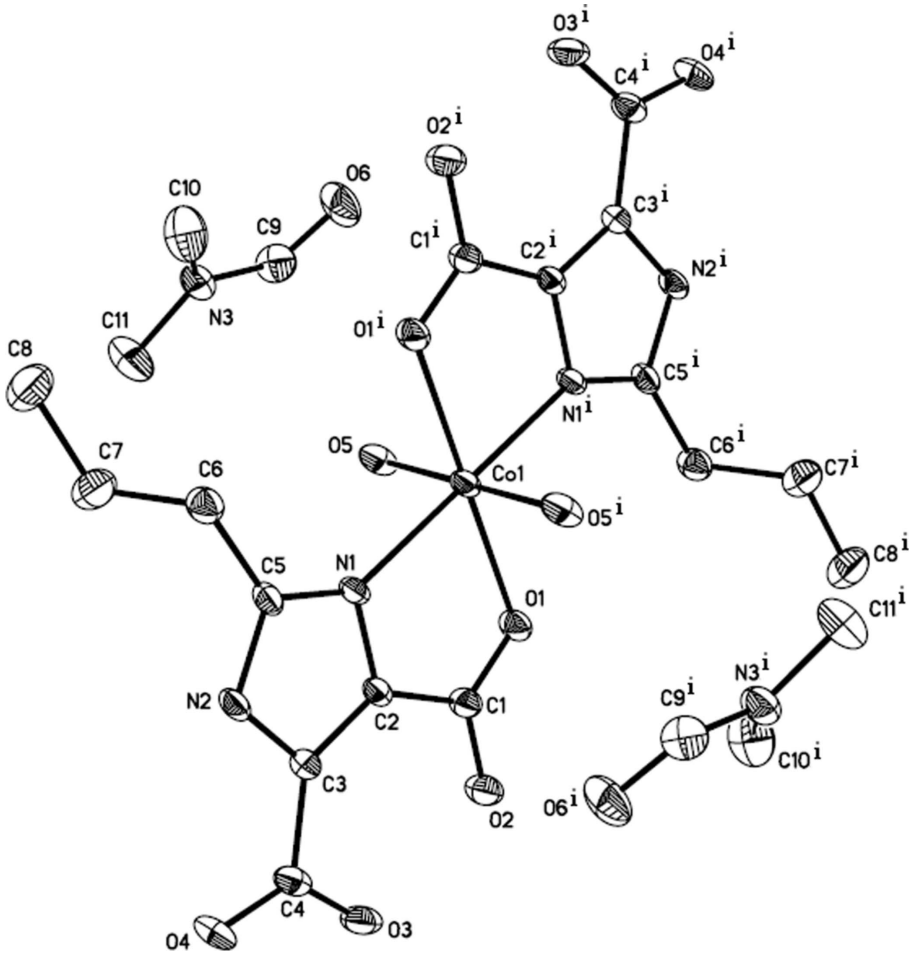

Figure 1

The structure of the title compound, showing the atomic numbering scheme. Non-H atoms are shown with 30% probability displacement ellipsoids. (Symmetry codes: (i)1 - *x*,1 - *y*,1 - *z*;)

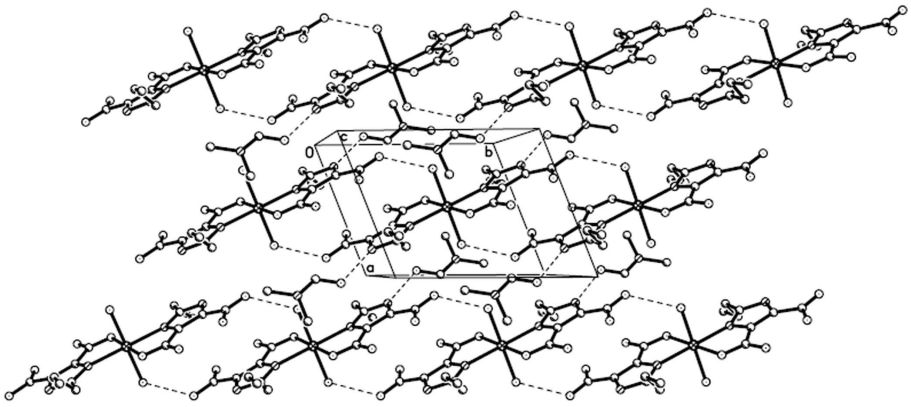

Figure 2

A view of the infinite two-dimensional structure. (H atoms are omitted for clarity)

Diaquabis(4-carboxy-2-propyl-1*H*-imidazole-5-carboxylato-κ^2N^3,O^4)cobalt(II) *N*,*N*-dimethylformamide disolvate

Crystal data

$[Co(C_8H_9N_2O_4)_2(H_2O)_2]\cdot 2C_3H_7NO$
$M_r = 635.50$
Triclinic, $P\overline{1}$
Hall symbol: -P 1
$a = 7.3325\ (7)$ Å
$b = 9.330\ (1)$ Å
$c = 11.2255\ (12)$ Å
$\alpha = 76.930\ (1)°$
$\beta = 87.564\ (2)°$
$\gamma = 68.857\ (1)°$
$V = 697.06\ (12)$ Å^3
$Z = 1$
$F(000) = 333$
$D_x = 1.514$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 1702 reflections
$\theta = 2.5–25.9°$
$\mu = 0.69$ mm^{-1}
$T = 298$ K
Cubic, purple
0.28 × 0.16 × 0.12 mm

Data collection

Bruker SMART 1000 CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2007)
$T_{min} = 0.831$, $T_{max} = 0.922$
3602 measured reflections
2393 independent reflections
1785 reflections with $I > 2\sigma(I)$
$R_{int} = 0.025$
$\theta_{max} = 25.0°$, $\theta_{min} = 1.9°$
$h = -8\rightarrow 8$
$k = -11\rightarrow 10$
$l = -13\rightarrow 12$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.046$
$wR(F^2) = 0.120$
$S = 1.06$
2393 reflections
191 parameters
0 restraints
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
$w = 1/[\sigma^2(F_o^2) + (0.0593P)^2 + 0.0702P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.37$ e Å^{-3}
$\Delta\rho_{min} = -0.52$ 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}
Co1	0.5000	0.5000	0.5000	0.0276 (2)
N1	0.6372 (4)	0.2538 (3)	0.5508 (2)	0.0262 (6)
N2	0.8031 (4)	−0.0015 (3)	0.6076 (2)	0.0299 (7)
H2	0.8735	−0.0911	0.6524	0.036*
N3	0.1217 (5)	0.4898 (4)	0.8633 (3)	0.0431 (8)
O1	0.4446 (3)	0.4305 (3)	0.3378 (2)	0.0342 (6)
O2	0.4995 (4)	0.2241 (3)	0.2558 (2)	0.0410 (6)
H2A	0.5618	0.1289	0.2735	0.061*
O3	0.6877 (4)	−0.0632 (3)	0.3176 (2)	0.0422 (6)
O4	0.8630 (4)	−0.2427 (3)	0.4793 (2)	0.0415 (6)
O5	0.2300 (3)	0.4898 (3)	0.5643 (2)	0.0393 (6)
H5C	0.2094	0.4117	0.5526	0.047*
H5D	0.1309	0.5698	0.5403	0.047*
O6	0.0385 (4)	0.7471 (3)	0.7696 (3)	0.0600 (8)
C1	0.5195 (5)	0.2858 (4)	0.3436 (3)	0.0300 (8)
C2	0.6307 (5)	0.1832 (4)	0.4565 (3)	0.0257 (7)
C3	0.7326 (5)	0.0238 (4)	0.4905 (3)	0.0274 (7)
C4	0.7665 (5)	−0.1054 (4)	0.4262 (3)	0.0325 (8)
C5	0.7426 (5)	0.1391 (4)	0.6406 (3)	0.0288 (8)
C6	0.7851 (6)	0.1544 (4)	0.7649 (3)	0.0380 (9)
H6A	0.7434	0.2655	0.7652	0.046*
H6B	0.9254	0.1081	0.7822	0.046*
C7	0.6851 (7)	0.0760 (5)	0.8653 (3)	0.0535 (11)
H7A	0.7339	−0.0364	0.8688	0.064*
H7B	0.5458	0.1168	0.8449	0.064*
C8	0.7158 (7)	0.1009 (6)	0.9906 (3)	0.0587 (12)
H8A	0.8492	0.0418	1.0192	0.088*
H8B	0.6301	0.0656	1.0467	0.088*
H8C	0.6876	0.2110	0.9853	0.088*
C9	0.0104 (6)	0.6217 (5)	0.7892 (4)	0.0482 (10)
H9	−0.0967	0.6196	0.7490	0.058*
C10	0.2965 (6)	0.4851 (5)	0.9218 (4)	0.0659 (13)
H10A	0.4092	0.4333	0.8796	0.099*
H10B	0.3077	0.4281	1.0055	0.099*
H10C	0.2887	0.5907	0.9190	0.099*

C11	0.0896 (9)	0.3443 (6)	0.8724 (5)	0.0855 (17)
H11A	−0.0306	0.3653	0.8290	0.128*
H11B	0.0817	0.2973	0.9570	0.128*
H11C	0.1962	0.2733	0.8375	0.128*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Co1	0.0338 (4)	0.0169 (4)	0.0301 (4)	−0.0063 (3)	−0.0011 (3)	−0.0059 (3)
N1	0.0333 (16)	0.0169 (15)	0.0287 (15)	−0.0088 (12)	−0.0018 (12)	−0.0059 (12)
N2	0.0349 (17)	0.0144 (14)	0.0346 (16)	−0.0038 (12)	−0.0030 (13)	−0.0019 (12)
N3	0.049 (2)	0.0271 (18)	0.0475 (19)	−0.0089 (16)	−0.0012 (16)	−0.0055 (15)
O1	0.0437 (15)	0.0207 (13)	0.0315 (13)	−0.0046 (11)	−0.0077 (11)	−0.0025 (10)
O2	0.0544 (18)	0.0285 (14)	0.0357 (14)	−0.0071 (13)	−0.0098 (12)	−0.0098 (12)
O3	0.0545 (17)	0.0317 (15)	0.0424 (16)	−0.0108 (13)	0.0002 (13)	−0.0197 (12)
O4	0.0462 (16)	0.0189 (14)	0.0572 (17)	−0.0063 (12)	−0.0018 (13)	−0.0125 (12)
O5	0.0390 (15)	0.0270 (14)	0.0549 (16)	−0.0118 (12)	0.0054 (12)	−0.0158 (12)
O6	0.066 (2)	0.0279 (16)	0.070 (2)	−0.0047 (14)	−0.0209 (16)	0.0049 (14)
C1	0.033 (2)	0.027 (2)	0.0322 (19)	−0.0115 (16)	0.0004 (15)	−0.0091 (16)
C2	0.0293 (18)	0.0177 (16)	0.0285 (17)	−0.0072 (14)	0.0001 (14)	−0.0043 (14)
C3	0.0319 (19)	0.0228 (18)	0.0295 (18)	−0.0119 (15)	0.0023 (15)	−0.0067 (14)
C4	0.030 (2)	0.025 (2)	0.045 (2)	−0.0092 (16)	0.0079 (17)	−0.0144 (17)
C5	0.034 (2)	0.0179 (18)	0.0322 (19)	−0.0084 (15)	−0.0024 (15)	−0.0016 (15)
C6	0.046 (2)	0.030 (2)	0.036 (2)	−0.0113 (17)	−0.0087 (17)	−0.0054 (16)
C7	0.068 (3)	0.061 (3)	0.040 (2)	−0.029 (2)	0.009 (2)	−0.019 (2)
C8	0.065 (3)	0.068 (3)	0.039 (2)	−0.019 (3)	0.006 (2)	−0.014 (2)
C9	0.043 (2)	0.050 (3)	0.048 (2)	−0.011 (2)	−0.0044 (19)	−0.012 (2)
C10	0.049 (3)	0.055 (3)	0.071 (3)	−0.004 (2)	−0.017 (2)	0.009 (2)
C11	0.126 (5)	0.045 (3)	0.094 (4)	−0.043 (3)	0.017 (4)	−0.016 (3)

Geometric parameters (Å, º)

Co1—N1^{i}	2.098 (3)	O6—C9	1.230 (5)
Co1—N1	2.098 (3)	C1—C2	1.471 (5)
Co1—O5^{i}	2.105 (2)	C2—C3	1.372 (4)
Co1—O5	2.105 (2)	C3—C4	1.482 (4)
Co1—O1^{i}	2.165 (2)	C5—C6	1.491 (4)
Co1—O1	2.165 (2)	C6—C7	1.513 (5)
N1—C5	1.319 (4)	C6—H6A	0.9700
N1—C2	1.377 (4)	C6—H6B	0.9700
N2—C5	1.357 (4)	C7—C8	1.515 (5)
N2—C3	1.371 (4)	C7—H7A	0.9700
N2—H2	0.8600	C7—H7B	0.9700
N3—C9	1.320 (5)	C8—H8A	0.9600
N3—C11	1.440 (5)	C8—H8B	0.9600
N3—C10	1.447 (5)	C8—H8C	0.9600
O1—C1	1.248 (4)	C9—H9	0.9300
O2—C1	1.286 (4)	C10—H10A	0.9600

O2—H2A	0.8200	C10—H10B	0.9600
O3—C4	1.286 (4)	C10—H10C	0.9600
O4—C4	1.238 (4)	C11—H11A	0.9600
O5—H5C	0.8333	C11—H11B	0.9600
O5—H5D	0.8318	C11—H11C	0.9600

N1^{i}—Co1—N1	180.0	O4—C4—C3	119.3 (3)
N1^{i}—Co1—O5^{i}	92.07 (10)	O3—C4—C3	115.5 (3)
N1—Co1—O5^{i}	87.93 (10)	N1—C5—N2	110.7 (3)
N1^{i}—Co1—O5	87.93 (10)	N1—C5—C6	126.4 (3)
N1—Co1—O5	92.07 (10)	N2—C5—C6	122.8 (3)
O5^{i}—Co1—O5	180.0	C5—C6—C7	113.5 (3)
N1^{i}—Co1—O1^{i}	78.33 (9)	C5—C6—H6A	108.9
N1—Co1—O1^{i}	101.67 (9)	C7—C6—H6A	108.9
O5^{i}—Co1—O1^{i}	88.69 (9)	C5—C6—H6B	108.9
O5—Co1—O1^{i}	91.31 (9)	C7—C6—H6B	108.9
N1^{i}—Co1—O1	101.67 (9)	H6A—C6—H6B	107.7
N1—Co1—O1	78.33 (9)	C6—C7—C8	113.8 (3)
O5^{i}—Co1—O1	91.31 (9)	C6—C7—H7A	108.8
O5—Co1—O1	88.69 (9)	C8—C7—H7A	108.8
O1^{i}—Co1—O1	180.0	C6—C7—H7B	108.8
C5—N1—C2	105.8 (3)	C8—C7—H7B	108.8
C5—N1—Co1	142.0 (2)	H7A—C7—H7B	107.7
C2—N1—Co1	111.9 (2)	C7—C8—H8A	109.5
C5—N2—C3	108.3 (3)	C7—C8—H8B	109.5
C5—N2—H2	125.8	H8A—C8—H8B	109.5
C3—N2—H2	125.8	C7—C8—H8C	109.5
C9—N3—C11	121.0 (4)	H8A—C8—H8C	109.5
C9—N3—C10	119.5 (3)	H8B—C8—H8C	109.5
C11—N3—C10	118.7 (4)	O6—C9—N3	124.5 (4)
C1—O1—Co1	114.2 (2)	O6—C9—H9	117.7
C1—O2—H2A	109.5	N3—C9—H9	117.7
Co1—O5—H5C	113.1	N3—C10—H10A	109.5
Co1—O5—H5D	116.9	N3—C10—H10B	109.5
H5C—O5—H5D	108.6	H10A—C10—H10B	109.5
O1—C1—O2	122.4 (3)	N3—C10—H10C	109.5
O1—C1—C2	118.2 (3)	H10A—C10—H10C	109.5
O2—C1—C2	119.5 (3)	H10B—C10—H10C	109.5
C3—C2—N1	110.3 (3)	N3—C11—H11A	109.5
C3—C2—C1	132.5 (3)	N3—C11—H11B	109.5
N1—C2—C1	117.2 (3)	H11A—C11—H11B	109.5
N2—C3—C2	104.9 (3)	N3—C11—H11C	109.5
N2—C3—C4	122.9 (3)	H11A—C11—H11C	109.5
C2—C3—C4	132.2 (3)	H11B—C11—H11C	109.5
O4—C4—O3	125.2 (3)		

N1^{i}—Co1—N1—C5	156 (25)	O1—C1—C2—N1	2.7 (5)
O5^{i}—Co1—N1—C5	85.2 (4)	O2—C1—C2—N1	−175.9 (3)

O5—Co1—N1—C5	−94.8 (4)	C5—N2—C3—C2	0.4 (3)
O1^{i}—Co1—N1—C5	−3.0 (4)	C5—N2—C3—C4	−178.4 (3)
O1—Co1—N1—C5	177.0 (4)	N1—C2—C3—N2	−0.5 (3)
N1^{i}—Co1—N1—C2	−17 (25)	C1—C2—C3—N2	−179.6 (3)
O5^{i}—Co1—N1—C2	−88.1 (2)	N1—C2—C3—C4	178.1 (3)
O5—Co1—N1—C2	91.9 (2)	C1—C2—C3—C4	−1.0 (6)
O1^{i}—Co1—N1—C2	−176.3 (2)	N2—C3—C4—O4	−0.3 (5)
O1—Co1—N1—C2	3.7 (2)	C2—C3—C4—O4	−178.6 (3)
N1^{i}—Co1—O1—C1	177.5 (2)	N2—C3—C4—O3	178.7 (3)
N1—Co1—O1—C1	−2.5 (2)	C2—C3—C4—O3	0.4 (5)
O5^{i}—Co1—O1—C1	85.2 (2)	C2—N1—C5—N2	−0.1 (4)
O5—Co1—O1—C1	−94.8 (2)	Co1—N1—C5—N2	−173.7 (2)
O1^{i}—Co1—O1—C1	26 (45)	C2—N1—C5—C6	−177.2 (3)
Co1—O1—C1—O2	179.3 (2)	Co1—N1—C5—C6	9.3 (6)
Co1—O1—C1—C2	0.7 (4)	C3—N2—C5—N1	−0.2 (4)
C5—N1—C2—C3	0.4 (4)	C3—N2—C5—C6	177.1 (3)
Co1—N1—C2—C3	176.1 (2)	N1—C5—C6—C7	110.9 (4)
C5—N1—C2—C1	179.6 (3)	N2—C5—C6—C7	−65.8 (5)
Co1—N1—C2—C1	−4.7 (3)	C5—C6—C7—C8	−175.9 (3)
O1—C1—C2—C3	−178.2 (3)	C11—N3—C9—O6	−174.1 (4)
O2—C1—C2—C3	3.2 (6)	C10—N3—C9—O6	−3.8 (6)

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

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O5—H5*D*···O4^{ii}	0.83	2.12	2.946 (3)	174
O5—H5*C*···O4^{iii}	0.83	1.94	2.773 (3)	175
O2—H2*A*···O3	0.82	1.66	2.478 (3)	177
N2—H2···O6^{iv}	0.86	1.84	2.685 (4)	166

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