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[2,6-Dioxo-1,2,3,6-tetrahydropyrimidine-4-carboxylato(2−)]bis(pyrazino-[2,3-*f*][1,10]phenanthroline)cobalt(II) dihydrate

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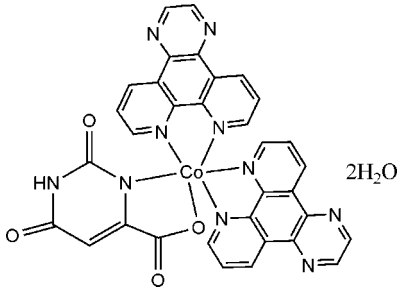
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.003 Å; R factor = 0.030; wR factor = 0.105; data-to-parameter ratio = 11.5.

The title complex, $[Co(C_5H_2N_2O_4)(C_{14}H_8N_4)_2]\cdot 2H_2O$, features a slightly distorted octahedral geometry for Co due to the sterical requirements of the orotic acid and pyrazino[2,3-*f*]-[1,10]phenanthroline ligands. Intermolecular hydrogen bonding between the uncoordinated water molecules and the ligand stablizes the structure of the complex.

Related literature

For related literature, see: Darensbourg *et al.* (1998); Lieberman *et al.* (1955); Lalioti *et al.* (1998).



Experimental

Crystal data

$[Co(C_5H_2N_2O_4)(C_{14}H_8N_4)_2]\cdot 2H_2O$
M_r = 713.54
Monoclinic, $P2_1/c$
a = 15.9468 (7) Å
b = 13.3765 (6) Å
c = 15.5661 (7) Å
β = 117.5610 (10)°
V = 2943.6 (2) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.65 mm^{-1}
T = 293 (2) K
0.16 × 0.12 × 0.10 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.903, T_{max} = 0.938
32977 measured reflections
5185 independent reflections
4601 reflections with $I > 2\sigma(I)$
R_{int} = 0.026

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.030
$wR(F^2)$ = 0.105
S = 1.00
5185 reflections
451 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.30 e Å^{-3}
$\Delta\rho_{min}$ = −0.44 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Co1—O1	2.0622 (13)	Co1—N1	2.1299 (14)
Co1—N3	2.1223 (15)	Co1—N4	2.1542 (15)
Co1—N7	2.1280 (15)	Co1—N8	2.1827 (15)
O1—Co1—N3	96.18 (5)	N7—Co1—N4	97.38 (6)
O1—Co1—N7	96.39 (5)	N1—Co1—N4	158.47 (5)
N3—Co1—N7	165.47 (5)	O1—Co1—N8	169.75 (6)
O1—Co1—N1	78.09 (5)	N3—Co1—N8	90.07 (5)
N3—Co1—N1	99.75 (5)	N7—Co1—N8	76.48 (5)
N7—Co1—N1	89.95 (6)	N1—Co1—N8	108.90 (6)
O1—Co1—N4	80.99 (5)	N4—Co1—N8	92.51 (6)
N3—Co1—N4	77.45 (5)		

Table 2
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
O5—H33···O4^{i}	0.85	2.22	3.007 (3)	155
O5—H34···O6^{ii}	0.85	2.16	2.903 (3)	146
O6—H35···O4^{iii}	0.85	2.02	2.822 (2)	156
O6—H36···O3^{i}	0.85	2.16	2.990 (2)	166
N2—H2···O3^{iv}	0.83	2.03	2.850 (2)	169

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

Data collection: *SMART* (Siemens, 1996); cell refinement: *SAINT* (Siemens, 1996); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997*a*); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997*a*); molecular graphics: *SHELXTL* (Sheldrick, 1997*b*); 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: FI2050).

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supporting information

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[2,6-Dioxo-1,2,3,6-tetrahydropyrimidine-4-carboxylato(2−)]bis(pyrazino[2,3-*f*][1,10]phenanthroline)cobalt(II) dihydrate

Rentao Wu, Jikun Li, Zebao Zheng and Wenzeng Duan

S1. Comment

Orotic acid is an important pyrimidine derivative as the effective precursor in the biosythesis of the pyrimidine base of nucleic acids in living organisms and plays a unique role in bioinorganic and pharmaceutical chemistry (Lieberman *et al.*, 1955). Aside from the biological interest, orotic acid is also interesting in coordination chemistry (Lalioti *et al.*, 1998). In this contribution, the title compound (I) was synthesized and its crystal structure determined (Fig. 1 and Table 1). The central Co is coordinated by five nitrogen atoms (four from pyrazino[2,3-*f*][1,10]phenanthroline ligand and one from orotic acid ligand) and one carboxylate oxygen from the orotic acid ligand,yielding a slightly distorted octahedral coordination geometry. The geometric parameters are in good agreement with those found in literature (Darensbourg *et al.*, 1998). The intermolecular hydrogen bonding between the uncoordinated water molecules and the ligand stablizes the structure of the complex (Fig. 2).

S2. Experimental

The orotic acid (Lancaster, 98%) and solvents were commercially available, and they were used without further purification. The orotic acid (0.035 g, 0.2 mmol) $CoCl_2$ $6H_2O$ (0.047 g, 0.2 mmol) and pyrazino[2,3-*f*][1,10]phenanthroline were added to 40 ml EtOH-water(1:2 V:V) and heated to 353 K and stirred for 20 min.A few drops of ammonia were added to adjust the pH value to about 6 and then the resulting mixture was filtered. Orange single crystals were obtained after a few days. Yield, 0.096 g, 75%. m.p. 450–452 K.

Analysis found: C 55.50, H 3.14, N 19.58, O 13.42%; $C_{33}H_{22}N_{10}O_6Co$ requires: C 55.55, H 3.11, N 19.63, O 13.45%.

S3. Refinement

All H atoms were initially located in diffrence Fourier map. The C, O and N bound H atoms were then constrained to an ideal geometry, with C—H = 0.93 Å and refined as riding with U_{iso}(H) = 1.2U_{eq}(C-aromatic) and with the O—H = 0.8494 - 0.8512 Å, N—H = 0.8321 Å and refined as riding with U_{iso}(H) = 1.2U_{eq}(O, N).

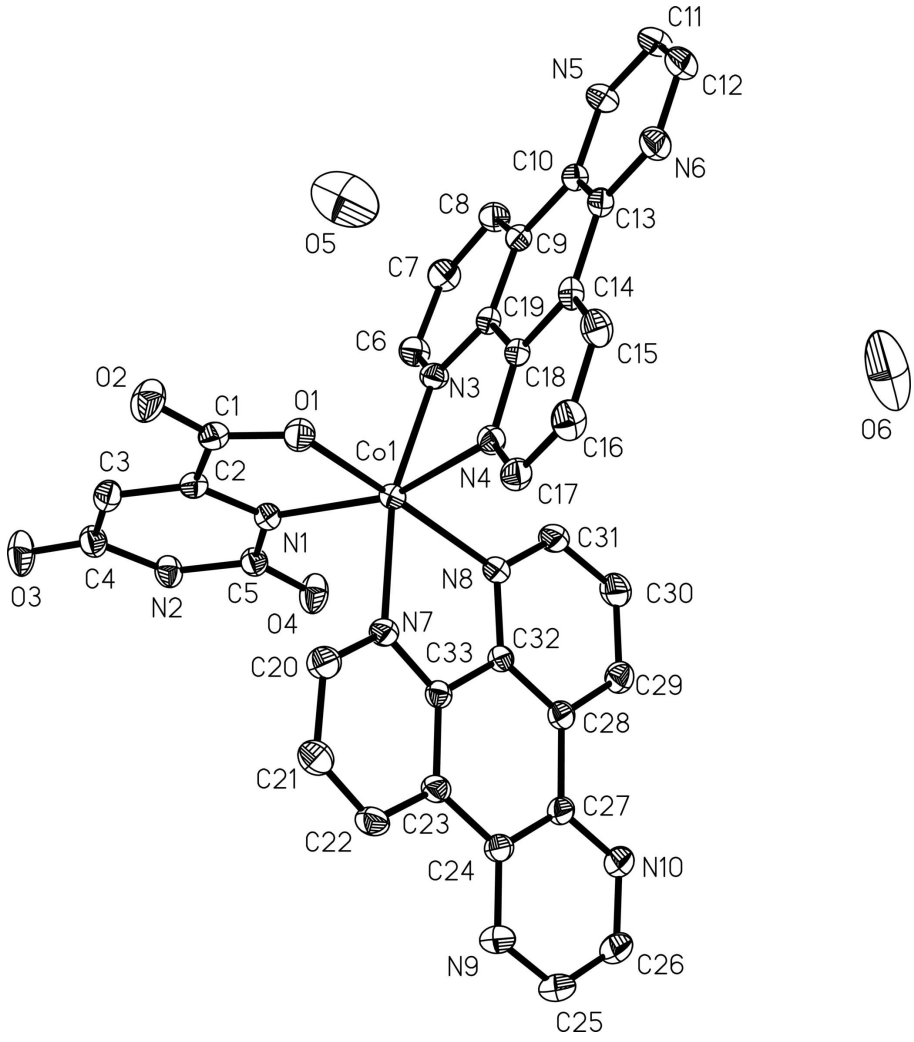

Figure 1

The structure of (I) showing 30% probability displacement ellipsoids and the atom-numbering scheme. The H atoms are omitted for clarity.

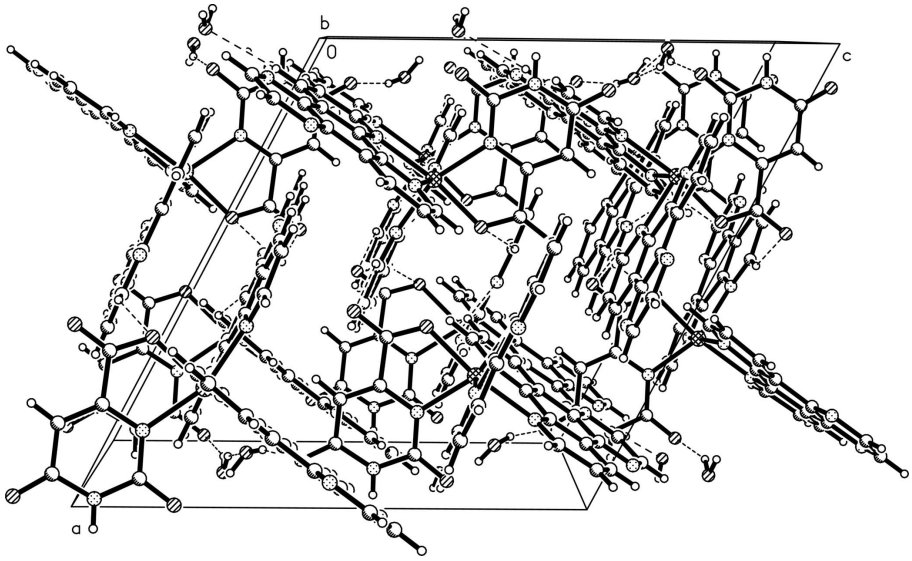

Figure 2

The intermolecular hydrogen bonding in the complex.

[2,6-Dioxo-1,2,3,6-tetrahydropyrimidine-4- carboxylato(2-)](dipyrazino[2,3-*f*][1,10]phenanthroline)cobalt(II) dihydrate

Crystal data

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Hall symbol: -P 2ybc
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$b = 13.3765\ (6)$ Å
$c = 15.5661\ (7)$ Å
$\beta = 117.561\ (1)°$
$V = 2943.6\ (2)$ Å^3
$Z = 4$
$F(000) = 1460$
$D_x = 1.610$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 14858 reflections
$\theta = 2.6–28.1°$
$\mu = 0.65$ mm^{-1}
$T = 293$ K
Block, orange
0.16 × 0.12 × 0.10 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Radiation source: sealed tube
Graphite monochromator
φ & ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.903$, $T_{max} = 0.938$
32977 measured reflections
5185 independent reflections
4601 reflections with $I > 2\sigma(I)$
$R_{int} = 0.026$
$\theta_{max} = 25.0°$, $\theta_{min} = 1.4°$
$h = -18\rightarrow18$
$k = -15\rightarrow15$
$l = -18\rightarrow18$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.030$
$wR(F^2) = 0.105$
$S = 1.00$
5185 reflections
451 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
$w = 1/[\sigma^2(F_o^2) + (0.0839P)^2 + 0.3838P]$
where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.30$ e Å^{-3}
$\Delta\rho_{min} = -0.44$ 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 (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
Co1	0.302202 (16)	0.138211 (16)	0.366964 (15)	0.02739 (11)
O1	0.40452 (10)	0.12832 (10)	0.50951 (9)	0.0376 (3)
O2	0.43227 (10)	0.09578 (13)	0.66013 (10)	0.0538 (4)
O3	0.10352 (10)	−0.00194 (13)	0.60522 (10)	0.0557 (4)
O4	0.07356 (9)	0.08288 (12)	0.31027 (9)	0.0472 (4)
O5	0.98177 (15)	0.12594 (16)	0.76679 (18)	0.0891 (7)
H33	0.9531	0.0701	0.7512	0.107*
H34	0.9388	0.1683	0.7580	0.107*
O6	0.90804 (17)	0.18193 (17)	0.28686 (18)	0.1009 (8)
H35	0.9491	0.1518	0.2759	0.121*
H36	0.8946	0.1343	0.3145	0.121*
N1	0.22079 (10)	0.09749 (11)	0.43806 (10)	0.0287 (3)
N2	0.09212 (11)	0.04177 (12)	0.45940 (11)	0.0354 (4)
H2	0.0343	0.0305	0.4329	0.042*
N3	0.28705 (10)	0.29594 (11)	0.36494 (10)	0.0299 (3)
N4	0.42213 (10)	0.18951 (11)	0.35070 (10)	0.0299 (3)
N5	0.45316 (12)	0.60117 (12)	0.37989 (12)	0.0406 (4)
N6	0.60438 (11)	0.48810 (13)	0.38628 (11)	0.0398 (4)
N7	0.30777 (10)	−0.01439 (11)	0.33132 (10)	0.0311 (3)
N8	0.21162 (11)	0.13331 (10)	0.21056 (11)	0.0303 (3)
N9	0.17387 (14)	−0.25488 (13)	0.07249 (12)	0.0474 (4)
N10	0.08181 (13)	−0.09711 (13)	−0.05752 (12)	0.0460 (4)
C1	0.37945 (13)	0.10401 (14)	0.57318 (12)	0.0337 (4)
C2	0.27470 (12)	0.08264 (12)	0.53502 (12)	0.0295 (4)
C3	0.24123 (13)	0.04902 (14)	0.59542 (13)	0.0360 (4)
H3A	0.2820	0.0402	0.6610	0.043*
C4	0.14344 (13)	0.02734 (15)	0.55768 (13)	0.0370 (4)
C5	0.12786 (13)	0.07517 (13)	0.39814 (12)	0.0317 (4)
C6	0.21428 (14)	0.34805 (14)	0.36155 (14)	0.0353 (4)
H6	0.1630	0.3133	0.3599	0.042*
C7	0.21152 (14)	0.45158 (15)	0.36044 (14)	0.0395 (4)
H7	0.1584	0.4851	0.3556	0.047*

C8	0.28830 (14)	0.50429 (15)	0.36655 (13)	0.0363 (4)
H8	0.2888	0.5738	0.3685	0.044*
C9	0.36554 (13)	0.45180 (13)	0.36978 (12)	0.0289 (4)
C10	0.45001 (12)	0.50074 (13)	0.37630 (12)	0.0309 (4)
C11	0.53149 (17)	0.64312 (15)	0.38635 (16)	0.0468 (5)
H11	0.5365	0.7124	0.3883	0.056*
C12	0.60592 (15)	0.58649 (16)	0.39021 (15)	0.0456 (5)
H12	0.6595	0.6195	0.3959	0.055*
C13	0.52507 (13)	0.44397 (14)	0.37875 (12)	0.0310 (4)
C14	0.51799 (13)	0.33593 (14)	0.37159 (12)	0.0305 (4)
C15	0.58863 (13)	0.27483 (16)	0.37097 (14)	0.0390 (4)
H15	0.6449	0.3029	0.3782	0.047*
C16	0.57528 (14)	0.17395 (16)	0.35985 (15)	0.0419 (5)
H16	0.6222	0.1327	0.3597	0.050*
C17	0.49038 (14)	0.13382 (14)	0.34878 (14)	0.0351 (4)
H17	0.4809	0.0652	0.3397	0.042*
C18	0.43614 (12)	0.28890 (13)	0.36294 (11)	0.0266 (4)
C19	0.36096 (12)	0.34745 (13)	0.36641 (12)	0.0270 (4)
C20	0.35704 (15)	−0.08618 (14)	0.39335 (14)	0.0406 (5)
H20	0.3975	−0.0688	0.4572	0.049*
C21	0.35049 (16)	−0.18542 (15)	0.36665 (15)	0.0453 (5)
H21	0.3856	−0.2336	0.4122	0.054*
C22	0.29230 (14)	−0.21251 (14)	0.27315 (14)	0.0382 (4)
H22	0.2871	−0.2792	0.2546	0.046*
C23	0.24054 (13)	−0.13879 (12)	0.20537 (13)	0.0320 (4)
C24	0.18141 (14)	−0.15951 (14)	0.10363 (15)	0.0345 (4)
C25	0.11973 (18)	−0.26838 (17)	−0.02203 (16)	0.0560 (6)
H25	0.1120	−0.3330	−0.0466	0.067*
C26	0.07401 (19)	−0.19040 (18)	−0.08593 (16)	0.0558 (6)
H26	0.0366	−0.2050	−0.1512	0.067*
C27	0.13568 (13)	−0.08080 (14)	0.03829 (13)	0.0343 (4)
C28	0.14542 (12)	0.02137 (14)	0.07340 (12)	0.0323 (4)
C29	0.10276 (14)	0.10256 (15)	0.01198 (14)	0.0393 (4)
H29	0.0660	0.0928	−0.0543	0.047*
C30	0.11575 (15)	0.19611 (16)	0.05054 (14)	0.0441 (5)
H30	0.0887	0.2511	0.0106	0.053*
C31	0.16973 (14)	0.20886 (14)	0.15002 (13)	0.0391 (4)
H31	0.1769	0.2731	0.1754	0.047*
C32	0.20028 (12)	0.04064 (13)	0.17205 (12)	0.0276 (4)
C33	0.25063 (12)	−0.04016 (13)	0.23834 (12)	0.0276 (4)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Co1	0.03091 (17)	0.02377 (17)	0.02886 (16)	−0.00288 (9)	0.01500 (12)	−0.00119 (8)
O1	0.0316 (7)	0.0471 (8)	0.0316 (7)	−0.0091 (6)	0.0124 (6)	−0.0019 (5)
O2	0.0407 (8)	0.0803 (12)	0.0311 (7)	−0.0083 (8)	0.0088 (6)	0.0007 (7)
O3	0.0465 (9)	0.0841 (12)	0.0447 (8)	−0.0048 (8)	0.0280 (7)	0.0161 (8)

O4	0.0330 (7)	0.0733 (11)	0.0317 (7)	−0.0048 (7)	0.0118 (6)	0.0063 (7)
O5	0.0666 (13)	0.0695 (13)	0.1107 (18)	−0.0005 (10)	0.0236 (12)	0.0099 (11)
O6	0.1180 (18)	0.0916 (15)	0.145 (2)	0.0530 (14)	0.1050 (17)	0.0658 (15)
N1	0.0301 (8)	0.0286 (7)	0.0285 (7)	−0.0021 (6)	0.0143 (6)	−0.0001 (6)
N2	0.0299 (8)	0.0425 (9)	0.0360 (8)	−0.0033 (7)	0.0172 (7)	0.0031 (7)
N3	0.0305 (8)	0.0281 (8)	0.0338 (8)	−0.0039 (6)	0.0173 (6)	−0.0042 (6)
N4	0.0339 (8)	0.0277 (8)	0.0309 (7)	0.0013 (6)	0.0173 (6)	0.0013 (6)
N5	0.0516 (10)	0.0265 (8)	0.0447 (9)	−0.0061 (7)	0.0233 (8)	−0.0001 (7)
N6	0.0373 (9)	0.0448 (10)	0.0393 (9)	−0.0107 (7)	0.0193 (7)	−0.0002 (7)
N7	0.0358 (8)	0.0259 (7)	0.0305 (8)	0.0013 (6)	0.0145 (6)	0.0006 (6)
N8	0.0349 (9)	0.0254 (8)	0.0308 (8)	−0.0022 (6)	0.0155 (7)	0.0006 (6)
N9	0.0634 (11)	0.0342 (9)	0.0505 (10)	−0.0090 (8)	0.0314 (9)	−0.0114 (8)
N10	0.0582 (11)	0.0467 (10)	0.0352 (9)	−0.0150 (9)	0.0233 (8)	−0.0078 (7)
C1	0.0361 (10)	0.0321 (9)	0.0296 (9)	−0.0044 (8)	0.0123 (8)	−0.0037 (7)
C2	0.0339 (9)	0.0258 (9)	0.0289 (8)	−0.0007 (7)	0.0146 (7)	−0.0022 (7)
C3	0.0391 (11)	0.0397 (10)	0.0288 (9)	−0.0008 (8)	0.0155 (8)	0.0013 (8)
C4	0.0420 (11)	0.0369 (10)	0.0380 (10)	−0.0006 (8)	0.0235 (9)	0.0038 (8)
C5	0.0336 (10)	0.0312 (9)	0.0328 (9)	−0.0005 (8)	0.0173 (8)	0.0013 (7)
C6	0.0322 (10)	0.0357 (10)	0.0440 (11)	−0.0016 (8)	0.0226 (9)	−0.0033 (8)
C7	0.0389 (11)	0.0366 (10)	0.0487 (11)	0.0072 (8)	0.0251 (9)	−0.0003 (8)
C8	0.0435 (11)	0.0275 (10)	0.0411 (11)	0.0043 (8)	0.0222 (9)	−0.0002 (7)
C9	0.0351 (10)	0.0264 (9)	0.0265 (8)	−0.0009 (7)	0.0154 (7)	−0.0009 (7)
C10	0.0387 (10)	0.0279 (9)	0.0255 (8)	−0.0049 (7)	0.0143 (7)	−0.0003 (7)
C11	0.0582 (14)	0.0322 (11)	0.0499 (12)	−0.0155 (9)	0.0251 (11)	−0.0023 (8)
C12	0.0473 (12)	0.0467 (13)	0.0448 (11)	−0.0188 (10)	0.0228 (9)	−0.0017 (9)
C13	0.0345 (10)	0.0338 (10)	0.0250 (8)	−0.0063 (7)	0.0141 (7)	−0.0001 (7)
C14	0.0313 (9)	0.0361 (10)	0.0266 (8)	0.0006 (8)	0.0154 (7)	0.0048 (7)
C15	0.0339 (10)	0.0451 (12)	0.0455 (11)	0.0006 (8)	0.0246 (9)	0.0044 (9)
C16	0.0404 (11)	0.0441 (12)	0.0510 (11)	0.0115 (9)	0.0294 (9)	0.0059 (9)
C17	0.0426 (11)	0.0308 (10)	0.0372 (10)	0.0060 (8)	0.0229 (9)	0.0009 (7)
C18	0.0307 (9)	0.0268 (9)	0.0244 (8)	−0.0003 (7)	0.0144 (7)	0.0007 (6)
C19	0.0306 (9)	0.0281 (9)	0.0228 (8)	−0.0005 (7)	0.0129 (7)	0.0008 (6)
C20	0.0464 (12)	0.0337 (10)	0.0348 (10)	0.0060 (9)	0.0129 (8)	0.0030 (8)
C21	0.0561 (13)	0.0311 (10)	0.0461 (12)	0.0106 (9)	0.0214 (10)	0.0091 (9)
C22	0.0466 (11)	0.0245 (9)	0.0466 (11)	0.0021 (8)	0.0242 (9)	−0.0001 (8)
C23	0.0353 (10)	0.0283 (10)	0.0387 (10)	−0.0041 (7)	0.0224 (9)	−0.0034 (7)
C24	0.0389 (10)	0.0335 (10)	0.0393 (10)	−0.0085 (8)	0.0250 (8)	−0.0079 (8)
C25	0.0813 (17)	0.0403 (12)	0.0524 (13)	−0.0186 (12)	0.0361 (12)	−0.0187 (10)
C26	0.0767 (16)	0.0548 (14)	0.0397 (11)	−0.0248 (12)	0.0301 (11)	−0.0182 (10)
C27	0.0387 (10)	0.0370 (10)	0.0328 (9)	−0.0106 (8)	0.0212 (8)	−0.0068 (8)
C28	0.0325 (10)	0.0343 (10)	0.0335 (9)	−0.0047 (7)	0.0182 (8)	−0.0010 (7)
C29	0.0408 (11)	0.0436 (11)	0.0301 (9)	−0.0028 (9)	0.0135 (8)	0.0015 (8)
C30	0.0506 (12)	0.0379 (11)	0.0379 (10)	0.0045 (9)	0.0155 (9)	0.0104 (8)
C31	0.0507 (12)	0.0277 (9)	0.0364 (10)	0.0000 (8)	0.0180 (9)	0.0015 (8)
C32	0.0292 (9)	0.0272 (9)	0.0296 (8)	−0.0035 (7)	0.0164 (7)	−0.0015 (7)
C33	0.0287 (9)	0.0271 (9)	0.0326 (9)	−0.0012 (7)	0.0188 (7)	−0.0004 (7)

Geometric parameters (Å, º)

Co1—O1	2.0622 (13)	C7—C8	1.378 (3)
Co1—N3	2.1223 (15)	C7—H7	0.9300
Co1—N7	2.1280 (15)	C8—C9	1.398 (3)
Co1—N1	2.1299 (14)	C8—H8	0.9300
Co1—N4	2.1542 (15)	C9—C19	1.397 (2)
Co1—N8	2.1827 (15)	C9—C10	1.459 (2)
O1—C1	1.271 (2)	C10—C13	1.403 (3)
O2—C1	1.224 (2)	C11—C12	1.386 (3)
O3—C4	1.242 (2)	C11—H11	0.9300
O4—C5	1.239 (2)	C12—H12	0.9300
O5—H33	0.8499	C13—C14	1.450 (3)
O5—H34	0.8500	C14—C15	1.395 (3)
O6—H35	0.8512	C14—C18	1.398 (2)
O6—H36	0.8494	C15—C16	1.365 (3)
N1—C5	1.349 (2)	C15—H15	0.9300
N1—C2	1.362 (2)	C16—C17	1.391 (3)
N2—C4	1.374 (2)	C16—H16	0.9300
N2—C5	1.392 (2)	C17—H17	0.9300
N2—H2	0.8321	C18—C19	1.454 (2)
N3—C6	1.334 (2)	C20—C21	1.380 (3)
N3—C19	1.356 (2)	C20—H20	0.9300
N4—C17	1.331 (2)	C21—C22	1.364 (3)
N4—C18	1.347 (2)	C21—H21	0.9300
N5—C11	1.330 (3)	C22—C23	1.400 (3)
N5—C10	1.345 (2)	C22—H22	0.9300
N6—C12	1.317 (3)	C23—C33	1.398 (2)
N6—C13	1.351 (2)	C23—C24	1.446 (3)
N7—C20	1.330 (2)	C24—C27	1.410 (3)
N7—C33	1.350 (2)	C25—C26	1.392 (3)
N8—C31	1.332 (2)	C25—H25	0.9300
N8—C32	1.352 (2)	C26—H26	0.9300
N9—C25	1.329 (3)	C27—C28	1.453 (3)
N9—C24	1.350 (2)	C28—C32	1.395 (2)
N10—C26	1.310 (3)	C28—C29	1.398 (3)
N10—C27	1.351 (2)	C29—C30	1.362 (3)
C1—C2	1.519 (3)	C29—H29	0.9300
C2—C3	1.355 (2)	C30—C31	1.391 (3)
C3—C4	1.419 (3)	C30—H30	0.9300
C3—H3A	0.9300	C31—H31	0.9300
C6—C7	1.385 (3)	C32—C33	1.453 (2)
C6—H6	0.9300		
O1—Co1—N3	96.18 (5)	N5—C11—C12	121.89 (18)
O1—Co1—N7	96.39 (5)	N5—C11—H11	119.1
N3—Co1—N7	165.47 (5)	C12—C11—H11	119.1
O1—Co1—N1	78.09 (5)	N6—C12—C11	123.17 (19)

N3—Co1—N1	99.75 (5)	N6—C12—H12	118.4
N7—Co1—N1	89.95 (6)	C11—C12—H12	118.4
O1—Co1—N4	80.99 (5)	N6—C13—C10	121.24 (17)
N3—Co1—N4	77.45 (5)	N6—C13—C14	118.61 (16)
N7—Co1—N4	97.38 (6)	C10—C13—C14	120.15 (15)
N1—Co1—N4	158.47 (5)	C15—C14—C18	117.16 (17)
O1—Co1—N8	169.75 (6)	C15—C14—C13	123.36 (16)
N3—Co1—N8	90.07 (5)	C18—C14—C13	119.47 (16)
N7—Co1—N8	76.48 (5)	C16—C15—C14	120.07 (18)
N1—Co1—N8	108.90 (6)	C16—C15—H15	120.0
N4—Co1—N8	92.51 (6)	C14—C15—H15	120.0
C1—O1—Co1	118.54 (12)	C15—C16—C17	118.88 (18)
H33—O5—H34	104.6	C15—C16—H16	120.6
H35—O6—H36	98.3	C17—C16—H16	120.6
C5—N1—C2	118.28 (14)	N4—C17—C16	122.72 (17)
C5—N1—Co1	128.40 (11)	N4—C17—H17	118.6
C2—N1—Co1	112.90 (11)	C16—C17—H17	118.6
C4—N2—C5	125.88 (16)	N4—C18—C14	122.96 (16)
C4—N2—H2	118.6	N4—C18—C19	116.83 (15)
C5—N2—H2	115.5	C14—C18—C19	120.21 (16)
C6—N3—C19	117.94 (15)	N3—C19—C9	122.54 (16)
C6—N3—Co1	127.68 (12)	N3—C19—C18	116.80 (15)
C19—N3—Co1	114.38 (11)	C9—C19—C18	120.65 (16)
C17—N4—C18	118.16 (16)	N7—C20—C21	122.59 (18)
C17—N4—Co1	127.17 (12)	N7—C20—H20	118.7
C18—N4—Co1	113.32 (11)	C21—C20—H20	118.7
C11—N5—C10	116.12 (17)	C22—C21—C20	119.74 (18)
C12—N6—C13	115.93 (18)	C22—C21—H21	120.1
C20—N7—C33	118.21 (15)	C20—C21—H21	120.1
C20—N7—Co1	125.81 (12)	C21—C22—C23	119.32 (17)
C33—N7—Co1	115.82 (11)	C21—C22—H22	120.3
C31—N8—C32	117.49 (15)	C23—C22—H22	120.3
C31—N8—Co1	128.53 (12)	C33—C23—C22	117.41 (17)
C32—N8—Co1	113.94 (11)	C33—C23—C24	119.27 (16)
C25—N9—C24	115.47 (19)	C22—C23—C24	123.26 (16)
C26—N10—C27	116.04 (19)	N9—C24—C27	121.07 (18)
O2—C1—O1	125.55 (18)	N9—C24—C23	118.61 (18)
O2—C1—C2	119.03 (17)	C27—C24—C23	120.28 (17)
O1—C1—C2	115.41 (15)	N9—C25—C26	123.1 (2)
C3—C2—N1	124.61 (16)	N9—C25—H25	118.4
C3—C2—C1	120.41 (16)	C26—C25—H25	118.4
N1—C2—C1	114.96 (15)	N10—C26—C25	122.4 (2)
C2—C3—C4	119.40 (16)	N10—C26—H26	118.8
C2—C3—H3A	120.3	C25—C26—H26	118.8
C4—C3—H3A	120.3	N10—C27—C24	121.89 (18)
O3—C4—N2	120.15 (17)	N10—C27—C28	118.03 (17)
O3—C4—C3	125.87 (18)	C24—C27—C28	120.08 (16)
N2—C4—C3	113.98 (15)	C32—C28—C29	117.91 (17)

O4—C5—N1	123.22 (16)	C32—C28—C27	119.42 (16)
O4—C5—N2	118.98 (16)	C29—C28—C27	122.67 (16)
N1—C5—N2	117.80 (15)	C30—C29—C28	119.07 (17)
N3—C6—C7	123.02 (17)	C30—C29—H29	120.5
N3—C6—H6	118.5	C28—C29—H29	120.5
C7—C6—H6	118.5	C29—C30—C31	119.54 (18)
C8—C7—C6	119.25 (18)	C29—C30—H30	120.2
C8—C7—H7	120.4	C31—C30—H30	120.2
C6—C7—H7	120.4	N8—C31—C30	122.98 (18)
C7—C8—C9	119.05 (18)	N8—C31—H31	118.5
C7—C8—H8	120.5	C30—C31—H31	118.5
C9—C8—H8	120.5	N8—C32—C28	122.98 (16)
C19—C9—C8	118.06 (17)	N8—C32—C33	116.77 (15)
C19—C9—C10	118.78 (16)	C28—C32—C33	120.22 (16)
C8—C9—C10	123.16 (17)	N7—C33—C23	122.72 (16)
N5—C10—C13	121.65 (16)	N7—C33—C32	116.64 (15)
N5—C10—C9	117.83 (16)	C23—C33—C32	120.63 (16)
C13—C10—C9	120.52 (16)		

N3—Co1—O1—C1	99.21 (14)	C13—N6—C12—C11	−0.4 (3)
N7—Co1—O1—C1	−88.09 (14)	N5—C11—C12—N6	1.1 (3)
N1—Co1—O1—C1	0.51 (13)	C12—N6—C13—C10	−0.6 (2)
N4—Co1—O1—C1	175.42 (14)	C12—N6—C13—C14	178.44 (16)
N8—Co1—O1—C1	−133.4 (3)	N5—C10—C13—N6	1.0 (3)
O1—Co1—N1—C5	−174.59 (16)	C9—C10—C13—N6	−178.97 (15)
N3—Co1—N1—C5	91.09 (15)	N5—C10—C13—C14	−178.01 (16)
N7—Co1—N1—C5	−78.04 (15)	C9—C10—C13—C14	2.0 (2)
N4—Co1—N1—C5	171.59 (15)	N6—C13—C14—C15	−0.7 (3)
N8—Co1—N1—C5	−2.37 (16)	C10—C13—C14—C15	178.29 (16)
O1—Co1—N1—C2	−2.29 (11)	N6—C13—C14—C18	−179.48 (15)
N3—Co1—N1—C2	−96.62 (12)	C10—C13—C14—C18	−0.4 (2)
N7—Co1—N1—C2	94.25 (12)	C18—C14—C15—C16	1.6 (3)
N4—Co1—N1—C2	−16.1 (2)	C13—C14—C15—C16	−177.18 (17)
N8—Co1—N1—C2	169.93 (11)	C14—C15—C16—C17	0.3 (3)
O1—Co1—N3—C6	−108.60 (15)	C18—N4—C17—C16	0.7 (3)
N7—Co1—N3—C6	101.6 (2)	Co1—N4—C17—C16	−165.11 (14)
N1—Co1—N3—C6	−29.67 (15)	C15—C16—C17—N4	−1.5 (3)
N4—Co1—N3—C6	172.09 (15)	C17—N4—C18—C14	1.4 (2)
N8—Co1—N3—C6	79.53 (15)	Co1—N4—C18—C14	169.10 (12)
O1—Co1—N3—C19	72.07 (12)	C17—N4—C18—C19	−178.96 (14)
N7—Co1—N3—C19	−77.7 (3)	Co1—N4—C18—C19	−11.25 (18)
N1—Co1—N3—C19	150.99 (11)	C15—C14—C18—N4	−2.5 (2)
N4—Co1—N3—C19	−7.25 (11)	C13—C14—C18—N4	176.31 (15)
N8—Co1—N3—C19	−99.80 (12)	C15—C14—C18—C19	177.85 (15)
O1—Co1—N4—C17	77.88 (15)	C13—C14—C18—C19	−3.3 (2)
N3—Co1—N4—C17	176.33 (15)	C6—N3—C19—C9	3.5 (2)
N7—Co1—N4—C17	−17.47 (15)	Co1—N3—C19—C9	−177.07 (12)
N1—Co1—N4—C17	91.6 (2)	C6—N3—C19—C18	−175.63 (15)

N8—Co1—N4—C17	−94.15 (15)	Co1—N3—C19—C18	3.77 (18)
O1—Co1—N4—C18	−88.50 (12)	C8—C9—C19—N3	−3.3 (2)
N3—Co1—N4—C18	9.96 (11)	C10—C9—C19—N3	176.82 (15)
N7—Co1—N4—C18	176.16 (11)	C8—C9—C19—C18	175.84 (15)
N1—Co1—N4—C18	−74.8 (2)	C10—C9—C19—C18	−4.1 (2)
N8—Co1—N4—C18	99.47 (12)	N4—C18—C19—N3	5.2 (2)
O1—Co1—N7—C20	7.01 (17)	C14—C18—C19—N3	−175.14 (14)
N3—Co1—N7—C20	156.8 (2)	N4—C18—C19—C9	−173.98 (15)
N1—Co1—N7—C20	−71.00 (16)	C14—C18—C19—C9	5.7 (2)
N4—Co1—N7—C20	88.70 (16)	C33—N7—C20—C21	−1.2 (3)
N8—Co1—N7—C20	179.53 (17)	Co1—N7—C20—C21	173.85 (15)
O1—Co1—N7—C33	−177.80 (12)	N7—C20—C21—C22	0.6 (3)
N3—Co1—N7—C33	−28.0 (3)	C20—C21—C22—C23	0.5 (3)
N1—Co1—N7—C33	104.20 (12)	C21—C22—C23—C33	−0.9 (3)
N4—Co1—N7—C33	−96.10 (12)	C21—C22—C23—C24	176.28 (19)
N8—Co1—N7—C33	−5.28 (12)	C25—N9—C24—C27	−1.2 (3)
O1—Co1—N8—C31	−127.7 (3)	C25—N9—C24—C23	−178.90 (18)
N3—Co1—N8—C31	0.04 (17)	C33—C23—C24—N9	178.66 (17)
N7—Co1—N8—C31	−174.40 (18)	C22—C23—C24—N9	1.5 (3)
N1—Co1—N8—C31	100.38 (17)	C33—C23—C24—C27	1.0 (3)
N4—Co1—N8—C31	−77.41 (17)	C22—C23—C24—C27	−176.18 (18)
O1—Co1—N8—C32	50.1 (3)	C24—N9—C25—C26	0.6 (3)
N3—Co1—N8—C32	177.92 (12)	C27—N10—C26—C25	−1.2 (3)
N7—Co1—N8—C32	3.48 (12)	N9—C25—C26—N10	0.7 (4)
N1—Co1—N8—C32	−81.74 (13)	C26—N10—C27—C24	0.5 (3)
N4—Co1—N8—C32	100.47 (12)	C26—N10—C27—C28	−179.22 (18)
Co1—O1—C1—O2	−179.64 (16)	N9—C24—C27—N10	0.7 (3)
Co1—O1—C1—C2	1.2 (2)	C23—C24—C27—N10	178.37 (17)
C5—N1—C2—C3	−1.7 (3)	N9—C24—C27—C28	−179.52 (17)
Co1—N1—C2—C3	−174.80 (15)	C23—C24—C27—C28	−1.9 (3)
C5—N1—C2—C1	176.70 (15)	N10—C27—C28—C32	179.74 (16)
Co1—N1—C2—C1	3.55 (18)	C24—C27—C28—C32	0.0 (3)
O2—C1—C2—C3	−4.0 (3)	N10—C27—C28—C29	−1.1 (3)
O1—C1—C2—C3	175.16 (17)	C24—C27—C28—C29	179.19 (18)
O2—C1—C2—N1	177.54 (17)	C32—C28—C29—C30	−0.4 (3)
O1—C1—C2—N1	−3.3 (2)	C27—C28—C29—C30	−179.66 (18)
N1—C2—C3—C4	−0.3 (3)	C28—C29—C30—C31	−1.0 (3)
C1—C2—C3—C4	−178.53 (17)	C32—N8—C31—C30	0.0 (3)
C5—N2—C4—O3	179.30 (19)	Co1—N8—C31—C30	177.86 (15)
C5—N2—C4—C3	−0.5 (3)	C29—C30—C31—N8	1.3 (3)
C2—C3—C4—O3	−178.5 (2)	C31—N8—C32—C28	−1.6 (3)
C2—C3—C4—N2	1.3 (3)	Co1—N8—C32—C28	−179.74 (13)
C2—N1—C5—O4	−177.54 (17)	C31—N8—C32—C33	176.74 (16)
Co1—N1—C5—O4	−5.6 (3)	Co1—N8—C32—C33	−1.39 (19)
C2—N1—C5—N2	2.3 (2)	C29—C28—C32—N8	1.8 (3)
Co1—N1—C5—N2	174.28 (12)	C27—C28—C32—N8	−178.94 (16)
C4—N2—C5—O4	178.55 (18)	C29—C28—C32—C33	−176.47 (16)
C4—N2—C5—N1	−1.3 (3)	C27—C28—C32—C33	2.8 (2)

C19—N3—C6—C7	−0.6 (3)	C20—N7—C33—C23	0.8 (3)
Co1—N3—C6—C7	−179.95 (14)	Co1—N7—C33—C23	−174.80 (13)
N3—C6—C7—C8	−2.4 (3)	C20—N7—C33—C32	−178.09 (16)
C6—C7—C8—C9	2.5 (3)	Co1—N7—C33—C32	6.33 (19)
C7—C8—C9—C19	0.1 (2)	C22—C23—C33—N7	0.3 (3)
C7—C8—C9—C10	−179.97 (16)	C24—C23—C33—N7	−177.03 (16)
C11—N5—C10—C13	−0.3 (3)	C22—C23—C33—C32	179.12 (16)
C11—N5—C10—C9	179.64 (16)	C24—C23—C33—C32	1.8 (3)
C19—C9—C10—N5	−179.72 (15)	N8—C32—C33—N7	−3.2 (2)
C8—C9—C10—N5	0.4 (2)	C28—C32—C33—N7	175.18 (15)
C19—C9—C10—C13	0.3 (2)	N8—C32—C33—C23	177.88 (15)
C8—C9—C10—C13	−179.64 (16)	C28—C32—C33—C23	−3.7 (2)
C10—N5—C11—C12	−0.7 (3)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O5—H33···O4^{i}	0.85	2.22	3.007 (3)	155
O5—H34···O6^{ii}	0.85	2.16	2.903 (3)	146
O6—H35···O4^{iii}	0.85	2.02	2.822 (2)	156
O6—H36···O3^{i}	0.85	2.16	2.990 (2)	166
N2—H2···O3^{iv}	0.83	2.03	2.850 (2)	169

Symmetry codes: (i) −*x*+1, −*y*, −*z*+1; (ii) *x*, −*y*+1/2, *z*+1/2; (iii) *x*+1, *y*, *z*; (iv) −*x*, −*y*, −*z*+1.