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Bis[N^5,N^7-bis(pyridin-2-yl)-6,7-dihydro-5*H*-pyrrolo[3,4-*b*]pyrazine-5,7-diimine]cobalt(III) perchlorate acetonitrile disolvate

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Keywords: crystal structure; pyrrolopyrazine; pincer ligand; isoindoline analogue; cobalt(III); hydrogen bonding; supramolecular framework.

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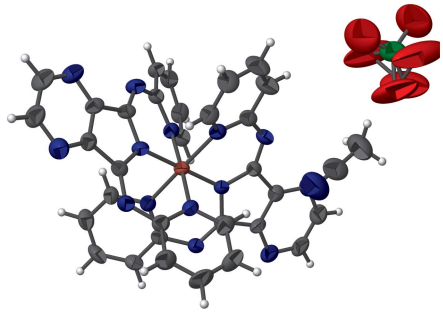
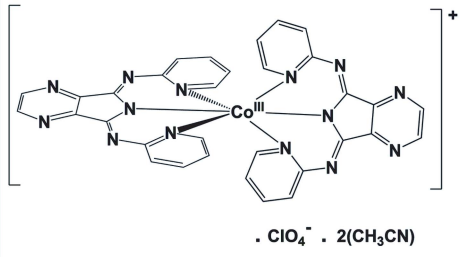
Structural data: full structural data are available from iucrdata.iucr.org

In the title complex, $[Co(C_{16}H_{10}N_7)_2]ClO_4\cdot 2CH_3CN$, the cation possesses twofold rotational symmetry. The Co^{III} ion is located on a twofold rotation axis and is octahedrally coordinated to two tridentate 'pincer' ligands. The Cl atom of the perchlorate anion is located on a fourfold rotoinversion axis. In the crystal, the cations are linked *via* C—H···O and C—H···N hydrogen bonds involving the perchlorate anion and the solvate acetonitrile molecules. These interactions lead to the formation of a supramolecular three-dimensional framework.

3D view



Chemical scheme



Structure description

Symmetrically substituted isoindolines, such as 1,3-bis(2-pyridylinimo)isoindoline (Schilf, 2004), are ideal tridentate 'pincer' ligands. For example, two isotypic cobalt(II) complexes of deprotonated 1,3-bis(2-pyridylinimo)isoindoline have been synthesized and their interaction with calf-thymus DNA studied (Selvi *et al.*, 2005). The same ligand has been used to form a neutral square-planar platinum(II) complex that has a bright-orange to red room temperature luminescence in fluid dichloromethane solutions (Wen *et al.*, 2010).

The pyrazine analogue of 1,3-bis(2-pyridylinimo)isoindoline, *viz*. (5*Z*,7*Z*)-N^5,N^7-di(pyridin-2-yl)-5*H*-pyrrolo[3,4-*b*]pyrazine-5,7(6*H*)-diimine (**L**) (Posel & Stoeckli-Evans, 2018), was synthesized in order to study its coordination behaviour with transition metals (Posel, 1998). Herein, we describe one such complex synthesized by the reaction of **L** with cobalt perchlorate.

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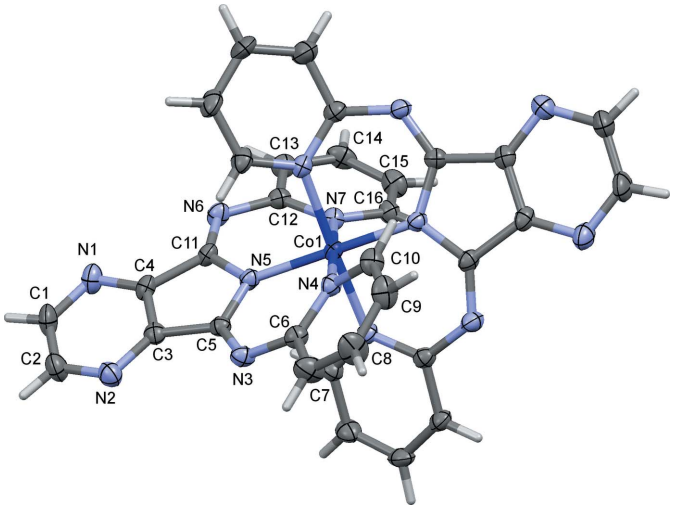

Figure 1
The molecular structure of the cation of the title complex, with atom labelling and displacement ellipsoids drawn at the 50% probability level. Unlabelled atoms are related to labelled atoms by the twofold rotation symmetry operation $-x+\frac{1}{2}, y, -z+\frac{3}{4}$.

The molecular structure of the title complex cation is illustrated in Fig. 1. It possesses twofold rotational symmetry with the cobalt atom located on a twofold rotation axis. It is ligated by six N atoms from two deprotonated tridentate **L** ligands, hence it has an almost perfect octahedral coordination sphere. The Co—N_{imine} bond length (Co1—N5) is 1.885 (5) Å, shorter than the Co—$N_{pyridine}$ bond lengths (Co1—N4 and Co1—N7) of 1.983 (6) and 1.979 (5) Å. These bond lengths are very similar to those observed in the two isotypic bis(1,3-bis(2-pyridylimino)isoindoline)cobalt(III) perchlorate methanol solvate complexes mentioned above (space groups $C2$ and $P2_1/c$), where the Co—N_{imine} bond lengths vary from *ca* 1.885 to 1.890 Å, and the Co—$N_{pyridine}$ bond lengths vary from *ca* 1.971 to 1.986 Å.

On coordination, the ligand molecules are extremely twisted compared to the situation in the free ligand, which is relatively planar with an r.m.s. deviation of 0.061 Å for all 23 non-H atoms (Posel & Stoeckli-Evans, 2018). In the complex cation, the pyridine rings (N4/C6–C10) and (N7/C12–C16) are inclined to the mean plane of the pyrrolopyrazine unit (N1/N2/N5/C1–C5/C11) by 28.3 (3) and 30.9 (3)°, respectively, and by 53.6 (3)° to each other. This arrangement is similar to that observed for the isotypic bis(1,3-bis(2-pyridylimino)-isoindoline)cobalt(III) perchlorate methanol solvate complexes mentioned above.

In the crystal, the cations are linked *via* C—H···$O_{perchlorate}$ and C—H···$N_{acetonitrile}$ hydrogen bonds, forming a supramolecular three-dimensional framework (Table 1 and Fig. 2).

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

D—H···A	D—H	H···A	D···A	D—H···A
C10—H10···N8	0.93	2.61	3.372 (12)	139
C14—H14···O1^{i}	0.93	2.55	3.256 (13)	133
C16—H16···O3^{ii}	0.93	2.51	3.213 (19)	133
C18—H18C···O2	0.96	2.42	3.31 (3)	154

Symmetry codes: (i) $x, -y+\frac{1}{2}, -z+\frac{1}{4}$; (ii) $y, x+\frac{1}{2}, z+\frac{1}{4}$.

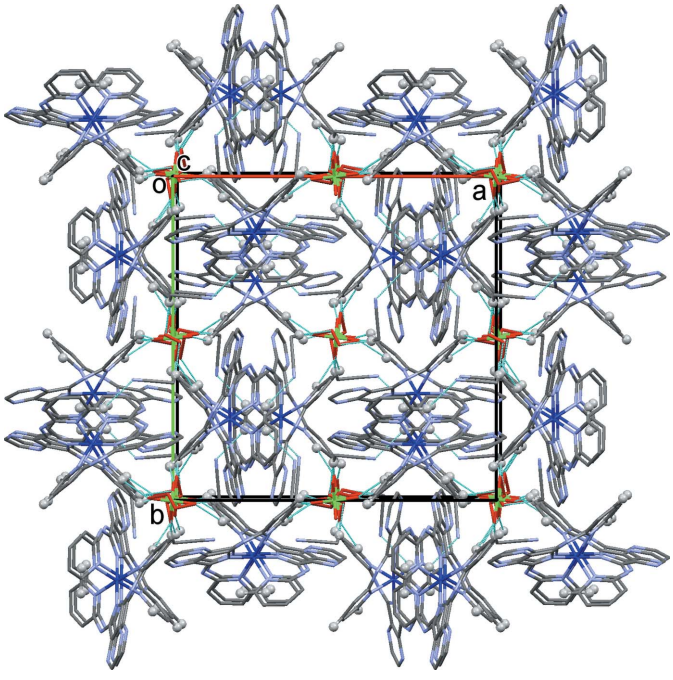

Figure 2
A view along the *c* axis of the crystal packing of the title compound. The hydrogen bonds are shown as dashed lines [see Table 1; only the H atoms (grey balls) involved in hydrogen bonding have been included].

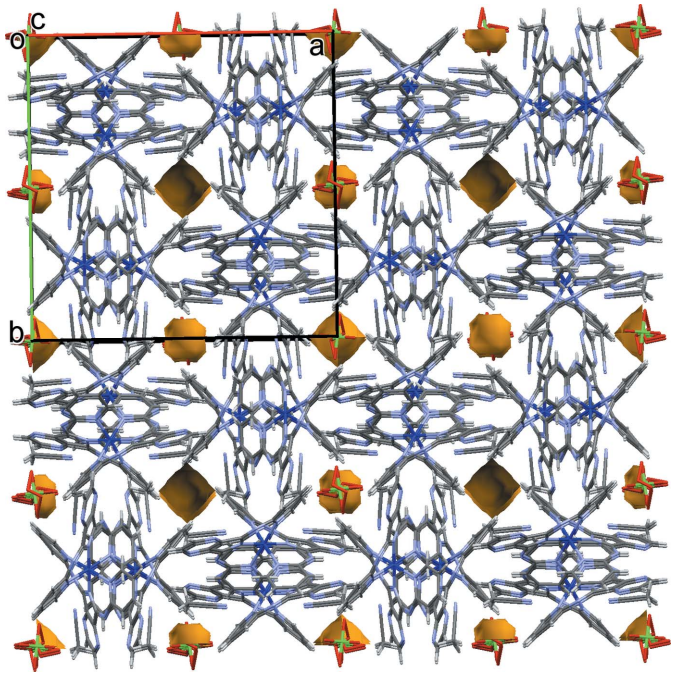

Figure 3
A view along the *c* axis of the crystal packing of the title compound. The small cavities in the crystal structure are represented in yellow–brown (*Mercury*; Macrae *et al.*, 2008).

Table 2
Experimental details.

Crystal data	
Chemical formula	$[Co(C_{16}H_{10}N_7)_2]ClO_4{\cdot}2C_2H_3N$
M_r	841.11
Crystal system, space group	Tetragonal, $I\overline{4}2d$
Temperature (K)	293
a, c (Å)	19.9756 (17), 18.3409 (18)
V (Å^3)	7318.5 (14)
Z	8
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.61
Crystal size (mm)	0.61 × 0.57 × 0.51
Data collection	
Diffractometer	Stoe–Siemens AED2 4-circle
Absorption correction	–
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	3245, 3148, 2352
R_{int}	0.046
$(\sin\theta/\lambda)_{max}$ (Å^{-1})	0.594
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.048, 0.113, 0.98
No. of reflections	3148
No. of parameters	273
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.28, −0.30
Absolute structure	Flack x determined using 815 quotients $[(I^+)-(I^-)]/[(I^+)+(I^-)]$ (Parsons *et al.*, 2013)
Absolute structure parameter	0.05 (3)

Computer programs: *STADI4* and *X-RED* (Stoe & Cie, 1997), *SHELXS97* (Sheldrick, 2008), *SHELXL2018* (Sheldrick, 2015), *Mercury* (Macrae *et al.*, 2008), *PLATON* (Spek, 2009) and *publCIF* (Westrip, 2010).

There are small cavities in the crystal structure, with a total potential solvent area volume of *ca* 72 Å^3 (*ca* 1% of the unit-cell volume). They are represented in brown–yellow in Fig. 3. There is no evidence of any residual electron density being present in these cavities on examination of the final difference-Fourier map (see Table 2).

Synthesis and crystallization

The title compound was synthesized by the reaction of (5*Z*,7*Z*)-N^5,N^7-di(pyridin-2-yl)-5*H*-pyrrolo[3,4-*b*]pyrazine-5,7(6*H*)-diimine (**L**) (Posel & Stoeckli-Evans, 2018) with $Co(ClO_4)_2$.

In a round-bottomed flask were mixed 0.0646 g (0.00021 mol) of ligand **L** in 7 ml of dry methanol and 0.1 ml of triethylamine. Then a solution of 0.0366 g (0.0001 mol) of $Co(ClO_4)_2{\cdot}6H_2O$ in 3 ml of dry methanol was added. The mixture was stirred at room temperature for 48 h. The main product, a brown–black powder, was filtered off and dried in a vacuum desiccator over silica (yield ∼0.03 g, 36%; m.p. >623 K). This solid was then used for recrystallization from a mixture of acetonitrile/methanol (1/1, *v*/*v*), which gave a small amount of brown–black block-like crystals. Analysis for $[(C_{16}H_{10}N_7)_2Co]{\cdot}ClO_4{\cdot}2(CH_3CN)$ (840.0931 g mol^{-1}): calculated C 51.47, H 3.12, N 26.65%; found C 50.68, H 3.11, N 26.18%. IR (KBr pellet. cm^{-1}): 2244, 1611, 1579, 1537, 1450, 1359, 1221, 1144, 1089, 782, 748, 650, 548, 437.

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. The Cl atom of the perchlorate anion is located on a fourfold rotoinversion axis, and two O atoms (O2 and O3) are partially disordered (occupancies of 0.5 each). The intensity data were measured at room temperature using a four-circle diffractometer. No absorption correction was applied as there were no suitable reflections for ψ scans.

Funding information

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full crystallographic data

IUCrData (2018). **3**, x180754 [https://doi.org/10.1107/S241431461800754X]

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Crystal data

$[Co(C_{16}H_{10}N_7)_2]ClO_4·2C_2H_3N$
M_r = 841.11
Tetragonal, $I\bar{4}2d$
a = 19.9756 (17) Å
c = 18.3409 (18) Å
V = 7318.5 (14) Å^3
Z = 8
$F(000)$ = 3440
D_x = 1.527 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 18 reflections
θ = 14.0–17.5°
μ = 0.61 mm^{-1}
T = 293 K
Block, brown–black
0.61 × 0.57 × 0.51 mm

Data collection

Stoe–Siemens AED2 4-circle diffractometer
Radiation source: fine-focus sealed tube
Plane graphite monochromator
$\omega/2\theta$ scans
3245 measured reflections
3148 independent reflections
2352 reflections with $I > 2\sigma(I)$
R_{int} = 0.046
θ_{max} = 25.0°, θ_{min} = 2.0°
h = −16→16
k = 0→23
l = 0→21
2 standard reflections every 60 min
intensity decay: 2%

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.048
$wR(F^2)$ = 0.113
S = 0.98
3148 reflections
273 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
$w = 1/[\sigma^2(F_o^2) + (0.0532P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.28 e Å^{-3}
$\Delta\rho_{min}$ = −0.30 e Å^{-3}
Absolute structure: Flack x determined using 815 quotients $[(I^+)-(I^-)]/[(I^+)+(I^-)]$ (Parsons *et al.*, 2013)
Absolute structure parameter: 0.05 (3)

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
Co1	0.250000	0.32578 (6)	0.375000	0.0317 (3)	
N1	0.4124 (3)	0.3449 (3)	0.1426 (3)	0.0523 (16)	
N2	0.4962 (3)	0.2988 (3)	0.2590 (3)	0.0496 (16)	
N3	0.4069 (3)	0.2768 (3)	0.3910 (3)	0.0383 (13)	
N4	0.2948 (3)	0.2569 (3)	0.4357 (3)	0.0356 (12)	
N5	0.3249 (3)	0.3256 (3)	0.3125 (2)	0.0333 (12)	
N6	0.2759 (3)	0.3747 (3)	0.2050 (3)	0.0410 (14)	
N7	0.2088 (3)	0.3960 (3)	0.3135 (3)	0.0355 (13)	
C1	0.4774 (4)	0.3335 (4)	0.1360 (4)	0.059 (2)	
H1	0.496793	0.340028	0.090421	0.071*	
C2	0.5184 (4)	0.3124 (4)	0.1922 (4)	0.056 (2)	
H2	0.563872	0.307431	0.182886	0.067*	
C3	0.4310 (3)	0.3115 (3)	0.2660 (4)	0.0373 (16)	
C4	0.3912 (3)	0.3331 (3)	0.2099 (3)	0.0375 (16)	
C5	0.3881 (3)	0.3036 (3)	0.3308 (3)	0.0338 (16)	
C6	0.3625 (3)	0.2532 (4)	0.4425 (3)	0.0388 (15)	
C7	0.3912 (4)	0.2167 (4)	0.5000 (4)	0.061 (2)	
H7	0.437456	0.216834	0.505894	0.074*	
C8	0.3531 (4)	0.1815 (5)	0.5469 (4)	0.068 (3)	
H8	0.372497	0.158673	0.585743	0.082*	
C9	0.2845 (4)	0.1798 (4)	0.5360 (4)	0.059 (2)	
H9	0.257089	0.154050	0.565874	0.071*	
C10	0.2578 (4)	0.2170 (3)	0.4802 (4)	0.0450 (17)	
H10	0.211885	0.214784	0.472461	0.054*	
C11	0.3235 (4)	0.3455 (3)	0.2405 (3)	0.0355 (15)	
C12	0.2207 (3)	0.4021 (3)	0.2399 (4)	0.0361 (16)	
C13	0.1813 (4)	0.4438 (3)	0.1971 (4)	0.0410 (17)	
H13	0.187905	0.445373	0.146947	0.049*	
C14	0.1324 (4)	0.4828 (4)	0.2286 (4)	0.0503 (19)	
H14	0.104580	0.509249	0.199938	0.060*	
C15	0.1255 (4)	0.4820 (4)	0.3025 (4)	0.0489 (19)	
H15	0.096083	0.511310	0.325368	0.059*	
C16	0.1623 (3)	0.4377 (3)	0.3429 (4)	0.0406 (17)	
H16	0.155166	0.436012	0.392920	0.049*	
N8	0.1199 (5)	0.1258 (4)	0.4430 (5)	0.097 (3)	
C17	0.0661 (6)	0.1296 (5)	0.4271 (5)	0.072 (3)	
C18	−0.0026 (5)	0.1357 (6)	0.4052 (6)	0.092 (3)	
H18A	−0.013282	0.182072	0.398060	0.138*	
H18B	−0.030970	0.117374	0.442438	0.138*	
H18C	−0.009440	0.111691	0.360476	0.138*	
Cl1	0.000000	0.000000	0.21977 (17)	0.0721 (9)	
O1	0.0549 (4)	0.0048 (9)	0.1770 (6)	0.185 (5)	
O2	−0.0216 (13)	0.011 (2)	0.2881 (8)	0.175 (12)	0.5
O3	−0.0089 (16)	0.0710 (8)	0.2249 (8)	0.179 (11)	0.5

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Co1	0.0355 (7)	0.0326 (7)	0.0270 (6)	0.000	−0.0011 (6)	0.000
N1	0.061 (4)	0.058 (4)	0.038 (4)	0.008 (3)	0.012 (3)	0.003 (3)
N2	0.040 (3)	0.056 (4)	0.053 (4)	0.004 (3)	0.003 (3)	0.000 (3)
N3	0.037 (3)	0.041 (3)	0.037 (3)	−0.001 (2)	−0.007 (3)	0.007 (3)
N4	0.041 (3)	0.035 (3)	0.031 (3)	−0.002 (3)	0.002 (2)	0.002 (3)
N5	0.036 (3)	0.037 (3)	0.027 (3)	0.004 (3)	−0.002 (3)	0.000 (2)
N6	0.047 (3)	0.044 (3)	0.032 (3)	0.010 (3)	−0.003 (3)	0.002 (3)
N7	0.038 (3)	0.033 (3)	0.035 (3)	0.001 (3)	0.001 (3)	0.002 (3)
C1	0.060 (5)	0.073 (5)	0.044 (5)	0.008 (4)	0.025 (4)	0.000 (4)
C2	0.045 (5)	0.069 (6)	0.054 (5)	0.002 (4)	0.016 (4)	0.005 (4)
C3	0.040 (4)	0.032 (4)	0.041 (4)	−0.003 (3)	0.003 (3)	−0.002 (3)
C4	0.051 (4)	0.033 (4)	0.029 (4)	0.004 (3)	0.005 (3)	−0.003 (3)
C5	0.035 (4)	0.031 (4)	0.035 (4)	0.001 (3)	−0.003 (3)	−0.003 (3)
C6	0.043 (4)	0.036 (4)	0.037 (4)	0.000 (4)	−0.003 (3)	0.004 (3)
C7	0.055 (5)	0.073 (5)	0.056 (5)	−0.004 (4)	−0.010 (4)	0.022 (5)
C8	0.067 (6)	0.089 (7)	0.049 (5)	0.009 (5)	−0.004 (4)	0.039 (5)
C9	0.073 (6)	0.049 (5)	0.054 (5)	0.006 (4)	0.014 (4)	0.023 (4)
C10	0.056 (5)	0.033 (3)	0.045 (4)	0.000 (4)	0.008 (4)	0.008 (3)
C11	0.044 (4)	0.036 (4)	0.026 (3)	0.003 (3)	0.000 (3)	−0.004 (3)
C12	0.038 (4)	0.035 (4)	0.035 (4)	−0.003 (3)	−0.004 (3)	0.001 (3)
C13	0.047 (4)	0.040 (4)	0.036 (4)	−0.002 (3)	−0.004 (3)	0.011 (3)
C14	0.040 (4)	0.050 (5)	0.061 (5)	0.005 (4)	−0.013 (4)	0.019 (4)
C15	0.047 (5)	0.036 (4)	0.063 (5)	0.008 (3)	0.004 (4)	0.008 (4)
C16	0.037 (4)	0.040 (4)	0.045 (4)	0.005 (3)	0.003 (3)	0.000 (3)
N8	0.091 (6)	0.081 (6)	0.118 (8)	−0.002 (6)	−0.028 (6)	−0.002 (6)
C17	0.087 (8)	0.063 (6)	0.067 (6)	−0.002 (6)	−0.009 (6)	−0.015 (5)
C18	0.070 (7)	0.111 (8)	0.096 (8)	−0.010 (6)	−0.009 (6)	−0.027 (7)
Cl1	0.059 (2)	0.108 (3)	0.0493 (18)	0.010 (2)	0.000	0.000
O1	0.067 (5)	0.343 (17)	0.146 (8)	−0.008 (8)	0.010 (6)	0.002 (10)
O2	0.19 (3)	0.26 (3)	0.075 (10)	0.08 (2)	0.008 (12)	−0.076 (19)
O3	0.40 (4)	0.071 (11)	0.066 (10)	0.060 (16)	0.005 (17)	0.004 (9)

Geometric parameters (Å, º)

Co1—N5^{i}	1.885 (5)	C7—H7	0.9300
Co1—N5	1.885 (5)	C8—C9	1.386 (11)
Co1—N7	1.979 (5)	C8—H8	0.9300
Co1—N7^{i}	1.979 (5)	C9—C10	1.372 (10)
Co1—N4	1.983 (6)	C9—H9	0.9300
Co1—N4^{i}	1.983 (6)	C10—H10	0.9300
N1—C1	1.325 (9)	C12—C13	1.389 (9)
N1—C4	1.326 (8)	C13—C14	1.375 (10)
N2—C2	1.331 (9)	C13—H13	0.9300
N2—C3	1.332 (8)	C14—C15	1.363 (11)
N3—C5	1.284 (8)	C14—H14	0.9300

N3—C6	1.378 (8)	C15—C16	1.368 (9)
N4—C10	1.359 (8)	C15—H15	0.9300
N4—C6	1.361 (8)	C16—H16	0.9300
N5—C5	1.378 (8)	N8—C17	1.116 (11)
N5—C11	1.381 (7)	C17—C18	1.436 (14)
N6—C11	1.291 (8)	C18—H18A	0.9600
N6—C12	1.387 (8)	C18—H18B	0.9600
N7—C16	1.357 (8)	C18—H18C	0.9600
N7—C12	1.377 (8)	Cl1—O2^{ii}	1.343 (15)
C1—C2	1.383 (11)	Cl1—O2	1.343 (15)
C1—H1	0.9300	Cl1—O1	1.352 (9)
C2—H2	0.9300	Cl1—O1^{ii}	1.352 (9)
C3—C4	1.371 (9)	Cl1—O3	1.433 (16)
C3—C5	1.473 (9)	Cl1—O3^{ii}	1.433 (16)
C4—C11	1.485 (9)	O2—O2^{ii}	0.96 (4)
C6—C7	1.406 (10)	O2—O3	1.69 (4)
C7—C8	1.346 (11)		

N5^{i}—Co1—N5	179.7 (3)	C9—C8—H8	120.7
N5^{i}—Co1—N7	91.0 (2)	C10—C9—C8	118.6 (8)
N5—Co1—N7	89.2 (2)	C10—C9—H9	120.7
N5^{i}—Co1—N7^{i}	89.2 (2)	C8—C9—H9	120.7
N5—Co1—N7^{i}	91.0 (2)	N4—C10—C9	123.7 (7)
N7—Co1—N7^{i}	89.7 (3)	N4—C10—H10	118.1
N5^{i}—Co1—N4	90.9 (2)	C9—C10—H10	118.1
N5—Co1—N4	88.9 (2)	N6—C11—N5	128.9 (6)
N7—Co1—N4	177.8 (2)	N6—C11—C4	123.8 (6)
N7^{i}—Co1—N4	89.1 (2)	N5—C11—C4	107.1 (6)
N5^{i}—Co1—N4^{i}	88.9 (2)	N7—C12—N6	123.7 (6)
N5—Co1—N4^{i}	90.9 (2)	N7—C12—C13	120.6 (6)
N7—Co1—N4^{i}	89.1 (2)	N6—C12—C13	115.3 (6)
N7^{i}—Co1—N4^{i}	177.8 (2)	C14—C13—C12	120.3 (7)
N4—Co1—N4^{i}	92.1 (3)	C14—C13—H13	119.8
C1—N1—C4	111.6 (7)	C12—C13—H13	119.8
C2—N2—C3	112.0 (6)	C15—C14—C13	118.9 (7)
C5—N3—C6	122.9 (6)	C15—C14—H14	120.6
C10—N4—C6	116.9 (6)	C13—C14—H14	120.6
C10—N4—Co1	120.0 (5)	C14—C15—C16	119.4 (7)
C6—N4—Co1	122.5 (5)	C14—C15—H15	120.3
C5—N5—C11	110.1 (5)	C16—C15—H15	120.3
C5—N5—Co1	125.5 (4)	N7—C16—C15	123.4 (7)
C11—N5—Co1	124.4 (4)	N7—C16—H16	118.3
C11—N6—C12	122.1 (5)	C15—C16—H16	118.3
C16—N7—C12	116.9 (6)	N8—C17—C18	178.5 (14)
C16—N7—Co1	119.6 (4)	C17—C18—H18A	109.5
C12—N7—Co1	123.3 (5)	C17—C18—H18B	109.5
N1—C1—C2	124.4 (7)	H18A—C18—H18B	109.5
N1—C1—H1	117.8	C17—C18—H18C	109.5

C2—C1—H1	117.8	H18A—C18—H18C	109.5
N2—C2—C1	123.5 (7)	H18B—C18—H18C	109.5
N2—C2—H2	118.2	O2^{ii}—Cl1—O2	42.0 (16)
C1—C2—H2	118.2	O2^{ii}—Cl1—O1	107.0 (12)
N2—C3—C4	123.7 (6)	O2—Cl1—O1	142.4 (15)
N2—C3—C5	128.7 (6)	O2^{ii}—Cl1—O1^{ii}	142.4 (15)
C4—C3—C5	107.5 (6)	O2—Cl1—O1^{ii}	107.0 (12)
N1—C4—C3	124.7 (6)	O1—Cl1—O1^{ii}	109.0 (9)
N1—C4—C11	127.8 (6)	O2^{ii}—Cl1—O3	97.7 (19)
C3—C4—C11	107.3 (5)	O2—Cl1—O3	75.1 (18)
N3—C5—N5	127.5 (6)	O1—Cl1—O3	94.0 (14)
N3—C5—C3	124.7 (6)	O1^{ii}—Cl1—O3	90.4 (13)
N5—C5—C3	107.7 (5)	O2^{ii}—Cl1—O3^{ii}	75.1 (18)
N4—C6—N3	124.0 (6)	O2—Cl1—O3^{ii}	97.7 (19)
N4—C6—C7	120.1 (6)	O1—Cl1—O3^{ii}	90.4 (13)
N3—C6—C7	115.4 (6)	O1^{ii}—Cl1—O3^{ii}	94.0 (14)
C8—C7—C6	121.4 (8)	O3—Cl1—O3^{ii}	172.5 (13)
C8—C7—H7	119.3	O2^{ii}—O2—Cl1	69.0 (8)
C6—C7—H7	119.3	O2^{ii}—O2—O3	100 (4)
C7—C8—C9	118.7 (8)	Cl1—O2—O3	54.9 (13)
C7—C8—H8	120.7	Cl1—O3—O2	50.0 (10)

N7—Co1—N5—C5	157.8 (5)	C6—N4—C10—C9	7.6 (10)
N7^{i}—Co1—N5—C5	68.1 (5)	Co1—N4—C10—C9	−163.8 (5)
N4—Co1—N5—C5	−21.0 (5)	C8—C9—C10—N4	−1.6 (12)
N4^{i}—Co1—N5—C5	−113.1 (5)	C12—N6—C11—N5	12.3 (10)
N7—Co1—N5—C11	−24.6 (5)	C12—N6—C11—C4	−161.7 (6)
N7^{i}—Co1—N5—C11	−114.3 (5)	C5—N5—C11—N6	−172.9 (6)
N4—Co1—N5—C11	156.6 (5)	Co1—N5—C11—N6	9.2 (9)
N4^{i}—Co1—N5—C11	64.5 (5)	C5—N5—C11—C4	1.9 (7)
C4—N1—C1—C2	−0.6 (11)	Co1—N5—C11—C4	−176.0 (4)
C3—N2—C2—C1	−3.5 (11)	N1—C4—C11—N6	−4.7 (11)
N1—C1—C2—N2	2.7 (13)	C3—C4—C11—N6	170.5 (6)
C2—N2—C3—C4	2.8 (10)	N1—C4—C11—N5	−179.9 (6)
C2—N2—C3—C5	−179.5 (7)	C3—C4—C11—N5	−4.6 (7)
C1—N1—C4—C3	−0.2 (10)	C16—N7—C12—N6	165.1 (6)
C1—N1—C4—C11	174.3 (7)	Co1—N7—C12—N6	−20.1 (9)
N2—C3—C4—N1	−1.1 (11)	C16—N7—C12—C13	−7.1 (9)
C5—C3—C4—N1	−179.2 (6)	Co1—N7—C12—C13	167.8 (5)
N2—C3—C4—C11	−176.5 (6)	C11—N6—C12—N7	−5.7 (10)
C5—C3—C4—C11	5.4 (7)	C11—N6—C12—C13	166.8 (6)
C6—N3—C5—N5	13.9 (11)	N7—C12—C13—C14	4.1 (10)
C6—N3—C5—C3	−161.2 (6)	N6—C12—C13—C14	−168.6 (6)
C11—N5—C5—N3	−174.4 (6)	C12—C13—C14—C15	2.9 (11)
Co1—N5—C5—N3	3.4 (10)	C13—C14—C15—C16	−6.7 (12)
C11—N5—C5—C3	1.4 (7)	C12—N7—C16—C15	3.3 (10)
Co1—N5—C5—C3	179.3 (4)	Co1—N7—C16—C15	−171.8 (6)
N2—C3—C5—N3	−6.4 (11)	C14—C15—C16—N7	3.6 (11)

C4—C3—C5—N3	171.6 (6)	O1—Cl1—O2—O2^{ii}	−43 (7)
N2—C3—C5—N5	177.6 (6)	O1^{ii}—Cl1—O2—O2^{ii}	154 (5)
C4—C3—C5—N5	−4.4 (7)	O3—Cl1—O2—O2^{ii}	−120 (6)
C10—N4—C6—N3	163.4 (6)	O3^{ii}—Cl1—O2—O2^{ii}	57 (5)
Co1—N4—C6—N3	−25.4 (10)	O2^{ii}—Cl1—O2—O3	120 (6)
C10—N4—C6—C7	−8.6 (10)	O1—Cl1—O2—O3	77 (2)
Co1—N4—C6—C7	162.6 (6)	O1^{ii}—Cl1—O2—O3	−85.8 (18)
C5—N3—C6—N4	−1.4 (11)	O3^{ii}—Cl1—O2—O3	177.6 (4)
C5—N3—C6—C7	170.9 (7)	O2^{ii}—Cl1—O3—O2	−36 (3)
N4—C6—C7—C8	4.0 (13)	O1—Cl1—O3—O2	−143.4 (14)
N3—C6—C7—C8	−168.7 (8)	O1^{ii}—Cl1—O3—O2	107.5 (13)
C6—C7—C8—C9	2.2 (14)	O2^{ii}—O2—O3—Cl1	55 (4)
C7—C8—C9—C10	−3.4 (14)		

Symmetry codes: (i) −*x*+1/2, *y*, −*z*+3/4; (ii) −*x*, −*y*, *z*.

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C10—H10···N8	0.93	2.61	3.372 (12)	139
C14—H14···O1^{iii}	0.93	2.55	3.256 (13)	133
C16—H16···O3^{iv}	0.93	2.51	3.213 (19)	133
C18—H18*C*···O2	0.96	2.42	3.31 (3)	154

Symmetry codes: (iii) *x*, −*y*+1/2, −*z*+1/4; (iv) *y*, *x*+1/2, *z*+1/4.