research communications

Investigation of nitro–nitrito photoisomerization: crystal structure of *trans*-chloridonitro(1,4,8,11-tetraazacyclotetradecane-κ^4N,N',N'',N''')-cobalt(III) chloride

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The reaction cavity of the nitro group in the crystal of the title compound, [CoCl(NO$_2$)(C$_{10}$H$_{24}$N$_4$)]Cl, (I), was investigated to confirm that it offers sufficient free space for linkage isomerization to occur in accordance with the observed photochemical reactivity. The complex cation has crystallographic $2/m$ symmetry and the nitro and chloro ligands at the *trans* positions are statistically disordered. The complete cyclam ligand is generated by symmetry from a quarter of the molecule. In the crystal of (I), the complex cations and Cl$^-$ ions are linked into a three-dimensional network by N—H$\cdots$Cl(counter-ion) hydrogen bonds.

1. Chemical context

The photochemical reactions of metal complexes in the solid state attract much attention from crystallographers and chemists (Coppens *et al.*, 2002; Vittal & Quah, 2017). The present authors have investigated photochemical linkage isomerization of a series of the nitrocobalt(III) complexes, *trans*-[Co(en)$_2$(NO$_2$)(NCS)]Cl·H$_2$O and other salts, (Ohba, Tsuchimoto & Kurachi, 2018), *trans*-[Co(acac)$_2$(NO$_2$)(pyridine derivative)] (Ohba, Tsuchimoto & Miyazaki, 2018), and *trans*-[Co(salen)(NO$_2$)(pyridine derivative)] (Ohba, Tsuchimoto & Yamada, 2018). In the present study, we describe our investigations of another type of nitrocobalt complex, *trans*-[Co(cyclam)(NO$_2$)Cl]Cl, (I), where cyclam stands for 1,4,8,11-tetraazacyclotetradecane. It is known that the stability of the nitrito–Co^{III} complexes greatly depends on the electronic effects of the co-existing ligands, and cyclam is expected to bring a small rate constant of the nitrito-to-nitro thermal reaction (Miyoshi *et al.*, 1983). The crystal structure of *trans*-[Co(cyclam)(NO$_2$)$_2$]ClO$_4$, (II), has already been reported by Ohba *et al.* (2001). For (II) and the related PF$_6$ salt, thermal conversion steps from the dinitrito to dinitro form were investigated by differential scanning calorimetry and DFT calculations (Eslami *et al.*, 2014).

When a KBr disk of (I) was irradiated for 30 min with a Xe lamp, the IR spectrum showed an apparent change involving an increase in intensity of the absorption peak of *ca* 1000 cm^{-1} (see the Figure in the supporting information), which corresponds to the symmetric N—O stretching mode of the nitrito form (Eslami *et al.*, 2014). The IR spectrum of the irradiated complex was almost unchanged on standing at room
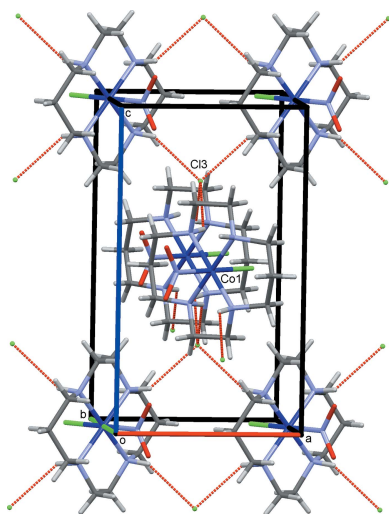
temperature for 2 h, indicating the long life-time of the nitrito form as in (II), and reverted to that before irradiation by heating at 55°C for 45 min. The crystal structure of (I) was determined to establish the dimensions of the reaction cavity and steric circumstance of the nitro group, and to compare them with those in (II).

(I)

(II)
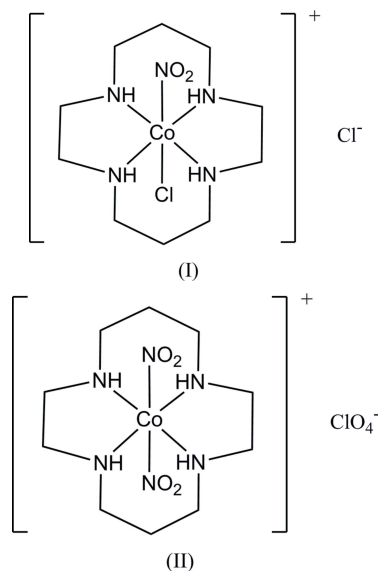
2. Structural commentary

The molecular structure of (I) is shown in Fig. 1. The coordination geometry around the Co atom is a distorted octahedron with the N5 (nitro) and Cl2 atoms at the *trans* positions. The macrocyclic ligand cyclam adopts the *trans*-III
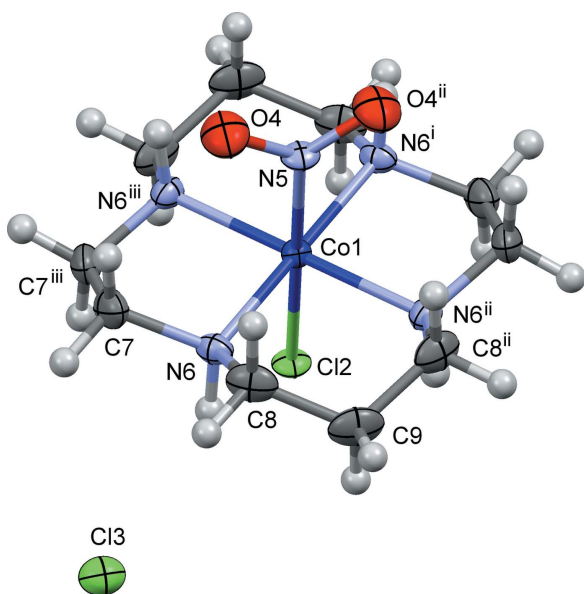

Figure 1
The molecular structure of (I), showing displacement ellipsoids at the 30% probability level. A crystallographic twofold axis runs through atom Co1 and the midpoint of the C7—C7^{iii} bond. Only one of two possible orientations of the nitro and chloride ions is shown for clarity. Symmetry codes: (i) $-x + 1$, $-y$, $-z + 1$; (ii) x, y, $-z + 1$; (iii) $-x + 1$, $-y$, z.

conformation of Tobe's classification (Bosnich *et al.*, 1965). The metal atom lies at site symmetry 2/*m*, and the atoms N5, Cl2 and C9 (the central C atom in the six-membered chelate ring) also lie on the mirror plane. There is a twofold axis running through the Co1 atom and midpoint of the C7—C7^{iii} bond in the five-membered chelate ring of cyclam, indicating that the positions of the Cl2 and nitro N5 atoms are exchanged. Similar orientational disorder of the chlorido-nitrocobalt complexes is observed for *trans*-[Co(en)$_2$Cl-(NO$_2$)]ClO$_4$ (Ohba & Eishima, 2000*a*) and the NO$_3$ salt (Ohba & Eishima, 2000*b*).

The Co—N(nitro) bond length is 1.9601 (10) Å, which is the result of restraint in the refinement of disorder, the length being similar to those in (II), 1.962 (5) and 1.968 (5) Å (Ohba, *et al.*, 2001). On the other hand, the Co—Cl bond distance is 2.2513 (12) Å, which is similar to that observed in *trans*-[Co(cyclam)Cl$_2$]Cl, 2.2533 (4) Å (Ivaniková *et al.*, 2006). There are intramolecular C—H···O/Cl hydrogen bonds (Table 1).

3. Supramolecular features

The crystal structure of (I) is shown in Fig. 2. The complex cations and chloride ions are connected by N—
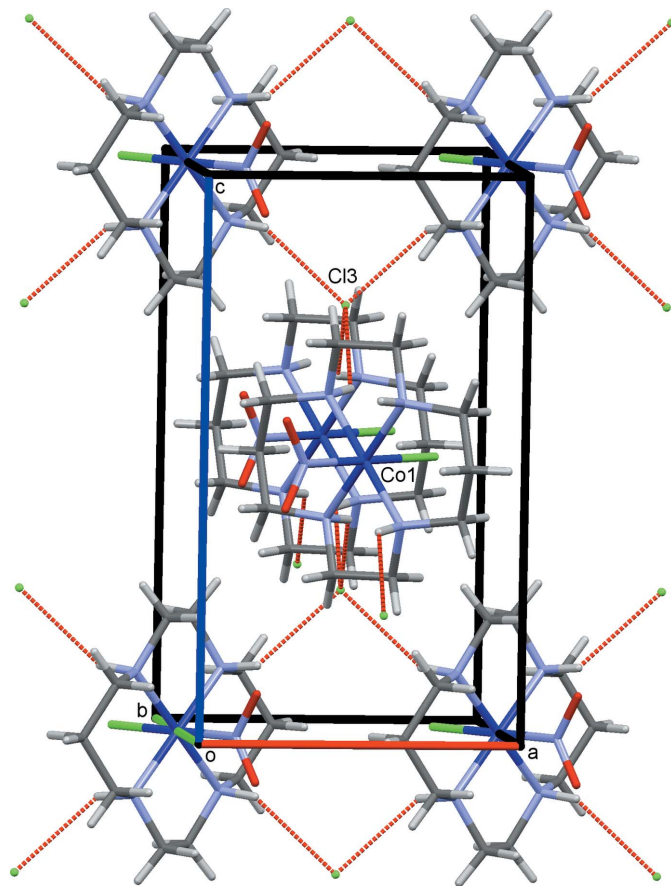

Figure 2
The crystal structure of (I), projected along *b*. The N—H···Cl hydrogen bonds are shown as red dashed lines. Only one of two possible orientations of the complex cation is shown for clarity.

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

D—H$\cdots A$	D—H	H$\cdots A$	$D\cdots A$	D—H$\cdots A$
N6—H6$\cdots$Cl3	0.98	2.64	3.3671 (16)	131
C7—H7$A\cdots$O4	0.97	2.28	2.929 (5)	124
C8—H8$B\cdots$Cl2^i	0.97	2.80	3.302 (4)	113

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

H$\cdots$Cl(counter-ion) hydrogen bonds, forming a three-dimensional network. In (II), there are two independent nitro ligands at the *trans* positions, and the O atoms of each nitro group show two possible positions (occupation factors 65 and 35%; Ohba, *et al.*, 2001). In the following discussion, the minor O(nitro) atoms will be neglected in (II). Slices of the reaction cavities around the NO_2^- group near its plane in (I) and (II) are compared in Fig. 3, where the radii of neighboring atoms are assumed to be 1.0 Å greater than the corresponding van der Waals radii (Bondi, 1964), except for Co, its radius being set to 1.90 Å. The shape of the cavity in the nitro plane is mainly defined by the N/C—H$\cdots$O(nitro) contacts which are shown in Figs. 4 and 5. Since the radius of the neighboring H atoms is assumed to be 2.20 Å, the cavity around the nitro O atoms is narrow in the intra- and intermolecular hydrogen-bond directions. In (I), the cavity has sufficient free space to both side of the nitro O atoms for rotation to become the nitrito form, as suggested by the observed photoreactivity. In (II), the cavities of the nitro groups have space at one of the O atoms for conversion to the mono- and di-nitrito forms. The bifurcated N—H$\cdots$O,O hydrogen bonds form an $R_2^2(4)$ ring (Fig. 5), which is also observed in the salts of *trans*-[Co(en)$_2$-

Figure 4
The steric circumstances of the nitro group in (I). Only parts of the complex are shown for clarity. The nitro group may be replaced with the Cl ligand due to the orientational disorder. There is a crystallographic twofold axis running vertical through the Co1^{xii} and Co1^{xv} atoms, another C8/C9 equivalent moiety which lies below the planes of the nitro groups being omitted for clarity. The N/C—H$\cdots$O hydrogen bonds are shown as blue dashed lines. The other O$\cdots$H contacts shorter than 2.9 Å (O4$\cdots$H7B^x = 2.78 Å and O4$\cdots$H8B^{iv} = 2.85 Å) are indicated as green dashed lines, and those of rather long distances (O4$\cdots$H9B^{iv} = 3.11 Å and O4$^{vi}\cdots$H9A^{iv} = 3.09 Å) are indicated as orange dashed lines. Symmetry codes: (i) $-x + 1, -y, -z + 1$; (ii) $x, y, -z + 1$; (iii) $-x + 1, -y, z$; (iv) $-x, -y, z$; (v) $-x, -y, -z + 1$; (vi) $-x, -y - 1, z$; (vii) $-x, -y - 1, -z + 1$; (viii) $x - 1, y - 1, z$; (ix) $x - 1, y - 1, -z + 1$; (x) $y, -x, -z + \frac{3}{2}$; (xi) $-y, x - 1, -z + \frac{3}{2}$; (xii) $-y, x - 1, z + \frac{1}{2}$; (xiii) $y, -x, z - \frac{1}{2}$; (xiv) $-y, x - 1, z - \frac{1}{2}$.
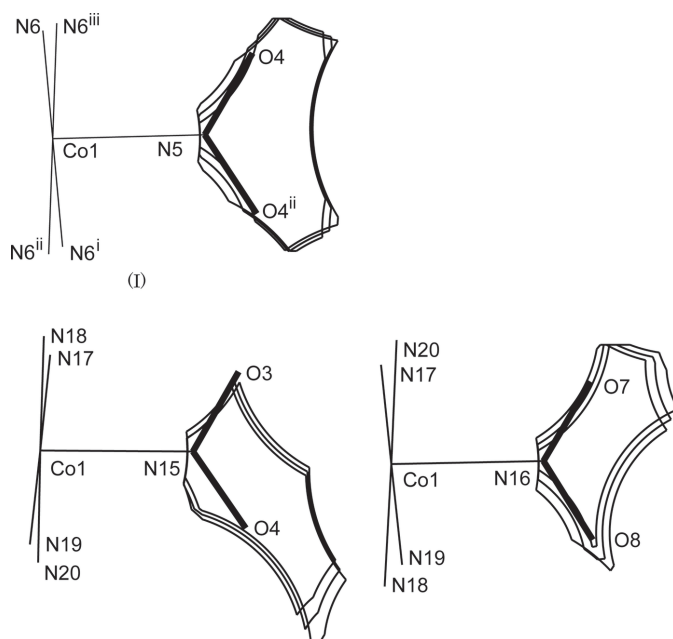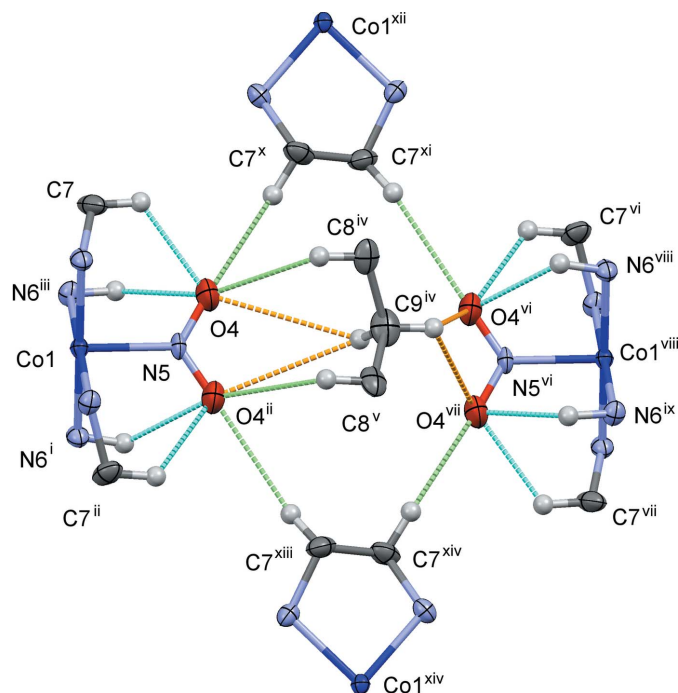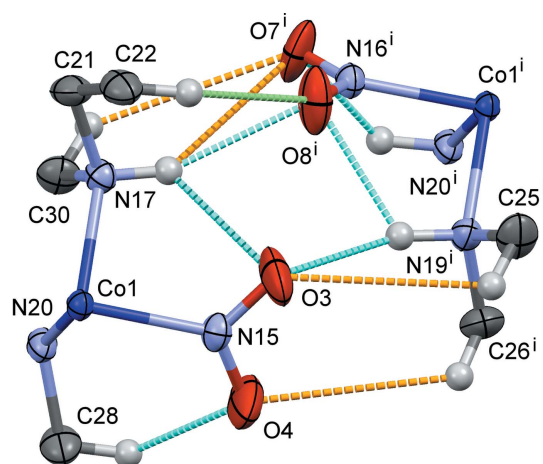

Figure 3
Comparison of the slices of the cavity around the nitro group within 0.1 Å from the plane in (I) and (II), where the minor O atoms (occupancy 35%) of each nitro ligand are omitted for clarity in (II). Symmetry codes for (I): (i) $-x + 1, -y, -z + 1$; (ii) $x, y, -z + 1$; (iii) $-x + 1, -y, z$.

Figure 5
The steric circumstance of the nitro groups in (II). The minor O atoms (occupancy 35%) of each nitro ligand are omitted, and only parts of the complex are shown for clarity. The N/C—H$\cdots$O hydrogen bonds are shown as blue dashed lines (H$\cdots$O distances 2.13–2.29 Å). A green dashed line indicates the O8$^i\cdots$H22B contact of 2.63 Å. Other O$\cdots$H contacts of rather long distances (3.03–3.09 Å) are indicated as orange dashed lines. Symmetry code: (i) $x, y, z + 1$.

Table 2
Experimental details.

Crystal data	
Chemical formula	$[CoCl(NO_2)(C_{10}H_{24}N_4)]Cl$
M_r	376.17
Crystal system, space group	Tetragonal, $P4_2/m$
Temperature (K)	301
a, c (Å)	7.6052 (3), 13.3873 (7)
V (Å^3)	774.31 (7)
Z	2
Radiation type	Mo $K\alpha$
μ (mm^{-1})	1.46
Crystal size (mm)	$0.25 \times 0.25 \times 0.10$
Data collection	
Diffractometer	Bruker D8 VENTURE
Absorption correction	Integration (*SADABS*; Bruker, 2016)
T_{min}, T_{max}	0.704, 0.876
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	7967, 953, 922
R_{int}	0.028
$(\sin \theta/\lambda)_{max}$ (Å^{-1})	0.659
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.033, 0.079, 1.19
No. of reflections	953
No. of parameters	58
No. of restraints	1
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}, \Delta\rho_{min}$ (e Å^{-3})	0.44, −0.26

Computer programs: *APEX3* and *SAINT* (Bruker, 2016), *SHELXT* (Sheldrick, 2015*a*), *SHELXL2014* (Sheldrick, 2015*b*), *Mercury* (Macrae *et al.*, 2008), *CAVITY* (Ohashi *et al.*, 1981) and *publCIF* (Westrip, 2010).

$(NO_2)(NCS)]^+$ complexes (Ohba, Tsuchimoto & Kurachi, 2018)

4. Database survey

There is no entry for a (cyclam)nitrocobalt(III) complex in the Cambridge Structural Database (CSD Version 5.39; Groom *et al.*, 2016), except for *trans*-[Co(cyclam)(NO$_2$)$_2$]ClO$_4$ (Ohba *et al.*, 2001). The nitrito coordination was reported for certain Co^{III} complexes with cyclam derivatives, for example *trans*-[Co(Me$_8$[14]ane)(ONO)$_2$]ClO$_4$ (Horn *et al.*, 2001), where Me$_8$[14]ane stands for 3,10-*C-meso*-3,5,7,7,10,12,14,14-octamethyl-1,4,8,11-tetraazacyclotetradecane, and *trans*-[Co(*L*)(NO$_2$)(ONO)]ClO$_4$ and *cis*-[Co(*L*)(NO$_2$)(ONO)]ClO$_4$ (Boyd *et al.*, 2007), where *L* stands for 1-(anthracen-9-ylmethyl)-1,4,8,11-tetraazacyclotetradecane.

The structures of *trans*-dichloro complexes have been published for several salts, *i.e. trans*-[Co(cyclam)Cl$_2$](Cl$^-$)$_{1.47}$(H$_3$O$^+$)$_{0.47}$(H$_2$O)$_{3.53}$ (Sosa-Torres *et al.*, 1997), *trans*-[Co(cyclam)Cl$_2$]Cl (Ivaniková *et al.*, 2006), *trans*-[Co(cyclam)Cl$_2$]PF$_6$ and *trans*-[Co(cyclam)Cl$_2$]Tf$_2$N, where Tf$_2$N$^-$ is bis(trifluoromethanesulfonyl)amide anion (Oba & Mochida, 2015), the conformation of cyclam in these crystals being *trans*-III according to Tobe's classification (Bosnich *et al.*, 1965). The (cyclam)chlorocobalt(III) alkynyl complexes such as *trans*-[Co(cyclam)Cl(1-ethynylnaphthalene)]CF$_3$SO$_3$·OEt$_2$ (Judkins *et al.*, 2018) have been studied for their structural and spectroscopic properties.

5. Synthesis and crystallization

trans-[Co(cyclam)Cl$_2$]Cl was prepared by a literature method (Nakahara & Shibata, 1977) from cobalt(II) chloride hexahydrate and cyclam, and converted to *trans*-[Co(cyclam)Cl(NH$_3$)]Cl$_2$·H$_2$O according to the method of Lee & Poon (1973). Then, *trans*-[Co(cyclam)Cl(NH$_3$)]Cl$_2$·H$_2$O (1.0 mmol) was dissolved in 11 ml of 1% NH$_3$ aqueous solution and neutralized with diluted HCl. To the solution sodium nitrite (8.0 mmol) and 1 ml of 1 *M* HCl were added, and the reaction mixture was stirred for 3 h at room temperature, and concentrated to precipitate the title compound, (I). Orange-red plate-like crystals of (I) were grown from a dimethyl sulfoxide solution by diffusion of diethyl ether vapour.

6. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. The electron densities of the nitro N5 and Cl2 atoms overlap with each other because of the orientational disorder of the complex cation. An EADP command was used for atoms N5 and Cl2, and the Co1—N5 bond distance was restrained to be 1.960 Å (s.u. = 0.001 Å) to obtain a reasonable geometry for the nitro group. The H atoms bound to C and N were positioned geometrically. They were refined as riding, with C—H/N—H = 0.97–0.98 Å, and U_{iso}(H) = 1.2U_{eq}(C/N). One reflection showing poor agreement was omitted from the final refinement.

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Investigation of nitro–nitrito photoisomerization: crystal structure of *trans*-chloridonitro(1,4,8,11-tetraazacyclotetradecane-κ^4N,N',N'',N''')cobalt(III) chloride

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Computing details

Data collection: *APEX3* (Bruker, 2016); cell refinement: *SAINT* (Bruker, 2016); data reduction: *SAINT* (Bruker, 2016); program(s) used to solve structure: SHELXT (Sheldrick, 2015a); program(s) used to refine structure: *SHELXL2014* (Sheldrick, 2015b); molecular graphics: *Mercury* (Macrae *et al.*, 2008) and *CAVITY* (Ohashi *et al.*, 1981); software used to prepare material for publication: *SHELXL2014* (Sheldrick, 2015b) and *publCIF* (Westrip, 2010).

trans-Chloridonitro(1,4,8,11-tetraazacyclotetradecane-\ κ^4N,N',N'',N''')cobalt(III) chloride

Crystal data

[CoCl(NO$_2$)(C$_{10}$H$_{24}$N$_4$)]Cl	D_x = 1.613 Mg m^{-3}
M_r = 376.17	Mo $K\alpha$ radiation, λ = 0.71073 Å
Tetragonal, $P4_2/m$	Cell parameters from 6699 reflections
a = 7.6052 (3) Å	θ = 2.7–27.9°
c = 13.3873 (7) Å	μ = 1.46 mm^{-1}
V = 774.31 (7) Å^3	T = 301 K
Z = 2	Plate, orange
$F(000)$ = 392	0.25 × 0.25 × 0.10 mm

Data collection

Bruker D8 VENTURE diffractometer	953 independent reflections
	922 reflections with $I > 2\sigma(I)$
φ and ω scans	R_{int} = 0.028
Absorption correction: integration (SADABS; Bruker, 2016)	θ_{max} = 27.9°, θ_{min} = 2.7°
	$h = -9 \rightarrow 10$
T_{min} = 0.704, T_{max} = 0.876	$k = -10 \rightarrow 9$
7967 measured reflections	$l = -15 \rightarrow 17$

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	
$R[F^2 > 2\sigma(F^2)]$ = 0.033	H-atom parameters constrained
$wR(F^2)$ = 0.079	$w = 1/[\sigma^2(F_o^2) + (0.0224P)^2 + 0.627P]$
S = 1.19	where $P = (F_o^2 + 2F_c^2)/3$
953 reflections	$(\Delta/\sigma)_{max} < 0.001$
58 parameters	$\Delta\rho_{max}$ = 0.44 e Å^{-3}
1 restraint	$\Delta\rho_{min}$ = −0.26 e Å^{-3}
Primary atom site location: structure-invariant direct methods	

Extinction correction: SHELXL2014
(Sheldrick, 2015b),
$Fc^* = kFc[1 + 0.001 x Fc^2 \lambda^3 / \sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.056 (7)

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.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	*y*	*z*	$U_{iso}*/U_{eq}$	Occ. (<1)
Co1	0.5000	0.0000	0.5000	0.02498 (19)	
Cl2	0.7410 (3)	0.1720 (4)	0.5000	0.0336 (3)	0.5
Cl3	0.5000	0.5000	0.7500	0.0529 (3)	
O4	0.2278 (5)	−0.2075 (6)	0.5775 (3)	0.0664 (11)	0.5
N5	0.2929 (11)	−0.1534 (15)	0.5000	0.0336 (3)	0.5
N6	0.4033 (2)	0.1478 (2)	0.60785 (13)	0.0352 (4)	
H6	0.4853	0.2464	0.6151	0.042*	
C7	0.4146 (4)	0.0476 (3)	0.70245 (16)	0.0519 (6)	
H7A	0.3180	−0.0353	0.7071	0.062*	
H7B	0.4085	0.1269	0.7591	0.062*	
C8	0.2278 (3)	0.2279 (3)	0.5944 (2)	0.0535 (6)	
H8A	0.2023	0.3034	0.6510	0.064*	
H8B	0.1396	0.1358	0.5927	0.064*	
C9	0.2167 (5)	0.3338 (5)	0.5000	0.0618 (11)	
H9A	0.3113	0.4194	0.5000	0.074*	
H9B	0.1066	0.3981	0.5000	0.074*	

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Co1	0.0221 (3)	0.0253 (3)	0.0275 (3)	0.00039 (16)	0.000	0.000
Cl2	0.0237 (10)	0.0297 (8)	0.0476 (6)	−0.0111 (5)	0.000	0.000
Cl3	0.0454 (4)	0.0454 (4)	0.0678 (8)	0.000	0.000	0.000
O4	0.054 (2)	0.075 (3)	0.071 (2)	−0.0275 (19)	0.0046 (19)	0.004 (2)
N5	0.0237 (10)	0.0297 (8)	0.0476 (6)	−0.0111 (5)	0.000	0.000
N6	0.0349 (8)	0.0325 (8)	0.0383 (9)	−0.0020 (6)	0.0069 (7)	−0.0065 (7)
C7	0.0729 (17)	0.0515 (14)	0.0313 (10)	−0.0072 (11)	0.0128 (10)	−0.0039 (9)
C8	0.0368 (11)	0.0490 (13)	0.0746 (17)	0.0073 (9)	0.0170 (11)	−0.0152 (12)
C9	0.0433 (19)	0.0421 (18)	0.100 (3)	0.0182 (15)	0.000	0.000

Geometric parameters (Å, º)

Co1—N5^i	1.9601 (10)	N6—C7	1.481 (3)
Co1—N5	1.9601 (10)	N6—H6	0.9800
Co1—N6	1.9720 (16)	C7—C7^{iii}	1.486 (6)

Co1—N6[i]	1.9720 (16)	C7—H7A	0.9700
Co1—N6[ii]	1.9720 (16)	C7—H7B	0.9700
Co1—N6[iii]	1.9720 (16)	C8—C9	1.501 (4)
Co1—Cl2	2.2513 (12)	C8—H8A	0.9700
Co1—Cl2[i]	2.2513 (12)	C8—H8B	0.9700
O4—N5	1.221 (4)	C9—C8[ii]	1.501 (4)
N5—O4[ii]	1.221 (4)	C9—H9A	0.9700
N6—C8	1.478 (3)	C9—H9B	0.9700
N5[i]—Co1—N5	180.0	O4[ii]—N5—Co1	121.76 (19)
N5[i]—Co1—N6	87.7 (3)	O4—N5—Co1	121.76 (19)
N5—Co1—N6	92.3 (3)	C8—N6—C7	111.64 (19)
N5[i]—Co1—N6[i]	92.3 (3)	C8—N6—Co1	118.86 (15)
N5—Co1—N6[i]	87.7 (3)	C7—N6—Co1	108.13 (13)
N6—Co1—N6[i]	180.0	C8—N6—H6	105.8
N5[i]—Co1—N6[ii]	87.7 (3)	C7—N6—H6	105.8
N5—Co1—N6[ii]	92.3 (3)	Co1—N6—H6	105.8
N6—Co1—N6[ii]	94.14 (10)	N6—C7—C7[iii]	107.55 (16)
N6[i]—Co1—N6[ii]	85.86 (10)	N6—C7—H7A	110.2
N5[i]—Co1—N6[iii]	92.3 (3)	C7[iii]—C7—H7A	110.2
N5—Co1—N6[iii]	87.7 (3)	N6—C7—H7B	110.2
N6—Co1—N6[iii]	85.86 (10)	C7[iii]—C7—H7B	110.2
N6[i]—Co1—N6[iii]	94.14 (10)	H7A—C7—H7B	108.5
N6[ii]—Co1—N6[iii]	180.0	N6—C8—C9	112.0 (2)
N5—Co1—Cl2	179.0 (5)	N6—C8—H8A	109.2
N6—Co1—Cl2	88.42 (7)	C9—C8—H8A	109.2
N6[i]—Co1—Cl2	91.58 (7)	N6—C8—H8B	109.2
N6[ii]—Co1—Cl2	88.42 (7)	C9—C8—H8B	109.2
N6[iii]—Co1—Cl2	91.58 (7)	H8A—C8—H8B	107.9
N5[i]—Co1—Cl2[i]	179.0 (5)	C8—C9—C8[ii]	114.7 (3)
N6—Co1—Cl2[i]	91.58 (7)	C8—C9—H9A	108.6
N6[i]—Co1—Cl2[i]	88.42 (7)	C8[ii]—C9—H9A	108.6
N6[ii]—Co1—Cl2[i]	91.58 (7)	C8—C9—H9B	108.6
N6[iii]—Co1—Cl2[i]	88.42 (7)	C8[ii]—C9—H9B	108.6
O4[ii]—N5—O4	116.4 (4)	H9A—C9—H9B	107.6
C8—N6—C7—C7[iii]	172.3 (2)	Co1—N6—C8—C9	−54.6 (3)
Co1—N6—C7—C7[iii]	39.7 (3)	N6—C8—C9—C8[ii]	67.3 (4)
C7—N6—C8—C9	178.5 (2)		

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

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N6—H6···Cl3	0.98	2.64	3.3671 (16)	131

C7—H7A···O4	0.97	2.28	2.929 (5)	124
C8—H8B···Cl2^i	0.97	2.80	3.302 (4)	113

Symmetry code: (i) −x+1, −y, −z+1.