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1*H*-Benzotriazol-3-ium (1*H*-benzotriazole-κN^3)trichloridocobaltate(II) monohydrate: a reformulation

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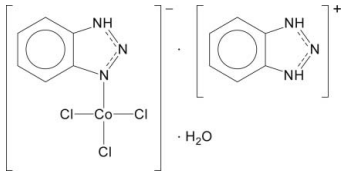
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.006 Å; R factor = 0.029; wR factor = 0.078; data-to-parameter ratio = 11.6.

The asymmetric unit of the title compound, $(C_6H_6N_3)[CoCl_3(C_6H_5N_3)]\cdot H_2O$, contains two crystallographically independent cations, two anions and two water molecules. The structure has been reported previously [Zhang, Li, Wang, Xie, Wang & Shen (2004). *Acta Cryst* E**60**, m498–m500] as a neutral cobalt(III) complex accompanied by unprotonated benzotriazole molecules and here has been redetermined as an anionic cobalt(II) complex accompanied by protonated benzotriazole cations. For both complex anions, a tetrahedral $CoNCl_3$ geometry arises. A network of N—H···O, N—H···Cl, O—H···O and O—H···Cl hydrogen bonds helps to establish the packing.

Related literature

For the previous stucture, see: Zhang *et al.* (2004). For related Co(II)-containing structures, see: Hahn *et al.* (1997); Krawczyk & Gdaniec (2005); Pan & Xu (2004); Zhang *et al.* (2006);



Experimental

Crystal data

$(C_6H_6N_3)[CoCl_3(C_6H_5N_3)]\cdot H_2O$
M_r = 422.56
Triclinic, $P\overline{1}$
a = 6.8760 (8) Å
b = 7.8033 (12) Å
c = 16.657 (3) Å
α = 95.450 (13)°
β = 95.962 (8)°
γ = 103.989 (9)°
V = 855.8 (2) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 1.48 mm^{-1}
T = 293 (2) K
0.40 × 0.40 × 0.20 mm

Data collection

Bruker P4 diffractometer
Absorption correction: ψ scan (North *et al.*, 1968)
T_{min} = 0.611, T_{max} = 0.744
4906 measured reflections
4846 independent reflections
4526 reflections with $I > 2\sigma(I)$
R_{int} = 0.078
3 standard reflections
every 100 reflections
intensity decay: none

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.029
$wR(F^2)$ = 0.078
S = 1.08
4846 reflections
417 parameters
3 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.34 e Å^{-3}
$\Delta\rho_{min}$ = −0.26 e Å^{-3}
Absolute structure: Flack (1983), 920 Friedel pairs
Flack parameter: −0.008 (13)

Table 1
Selected bond lengths (Å).

Co1—Cl1	2.2649 (13)	Co2—Cl4	2.2441 (13)
Co1—Cl2	2.2616 (13)	Co2—Cl5	2.2450 (15)
Co1—Cl3	2.2195 (16)	Co2—Cl6	2.2584 (16)
Co1—N1	2.027 (3)	Co2—N11	2.022 (3)

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

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1*B*···Cl6	0.82	2.79	3.279 (5)	120
O2—H2*A*···O1^{i}	0.82	2.41	3.142 (7)	148
O2—H2*B*···Cl6	0.82	2.52	3.295 (5)	159
N3—H3···O2^{ii}	0.86	1.87	2.721 (4)	173
N13—H13···Cl2^{iii}	0.86	2.28	3.127 (3)	169
N21—H21···Cl4	0.86	2.80	3.458 (4)	134
N21—H21···Cl6^{iv}	0.86	2.75	3.316 (4)	125
N23—H23···Cl1^{v}	0.86	2.30	3.123 (3)	160
N31—H31···Cl3^{vi}	0.86	2.61	3.214 (4)	128
N33—H33···O1^{i}	0.86	1.79	2.646 (5)	170

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

Data collection: *XSCANS* (Bruker, 1997); cell refinement: *XSCANS*; data reduction: *XSCANS*; program(s) used to solve structure: *SHELXTL* (Bruker, 2003); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *PLATON* (Spek, 2003).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB2664).

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supplementary materials

Acta Cryst. (2008). E**64**, m58 [**doi:10.1107/S1600536807063131**]

1*H*-Benzotriazol-3-ium (1*H*-benzotriazole-κN^3)trichloridocobaltate(II) monohydrate: a reformulation

L. Sieron

Comment

The crystal structure of the salt-like title compound, (I), $C_6H_6N_3^+.[CoCl_3(C_6H_5N_3)]^-.H_2O$, was originally modelled as a $[CoCl_3(C_6H_5N_3)].C_6H_5N_3.H_2O$ complex (Zhang *et al.*, 2004). A few facts point that the structure was incorrectly described as Co^{III} instead of Co^{II} complex. The blue colour of the crystal and a tetrahedral coordination geometry around the central metal atom is typical for the $Co^{II}Cl_3N$ chromophore, *e.g.* in pyridinium trichloro-pyridine-cobalt(II) (Hahn *et al.*, 1997), quinolinium trichloro-quinoline-cobalt(II) (Pan & Xu, 2004) and 2-aminopyridinium (2-aminopyridine)-trichloro-cobalt(II) (Zhang *et al.*, 2006).

A decrease of the metal oxidation number in (I) from III to II requires the presence of an additional proton for charge balance. In fact, an analysis of difference Fourier maps has shown two peaks in the positions expected for missing benzotriazole H atoms (N–Q = 0.85 and 0.89 Å). Both of these are involved in short, strong N–H···O_{water} hydrogen bonds which confirms the supposition (Fig. 1). The N–N bond lengths in the benzimidazolium cations are practically equalized and range from 1.309 (4) to 1.316 (5) Å, indicating full delocalization of their π electrons, which is not observed in neutral benzotriazole molecules (Krawczyk & Gdaniec, 2005). The metal bond distances and hydrogen bonds are listed in Tables 1 and 2, respectively.

Experimental

Due to the unsuccesful attempts at the synthesis of (I), the deposited structure factors and other data have been taken from the original paper of Zhang *et al.* (2004).

Refinement

All H atoms were located in difference Fourier syntheses but were repositioned with ideal geometry (C–H = 0.93, N–H = 0.86 and O–H = 0.82 Å) and refined as riding with $U_{iso}(H) = 1.2U_{eq}(C, N)$ or $1.5U_{eq}(O)$.

Figures

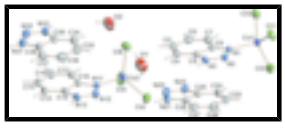


Fig. 1. A view of (I), showing displacement ellipsoids for the non-H atoms drawn at the 30% probability level.

1*H*-Benzotriazol-3-ium (1*H*-benzotriazole-κN^3)trichloridocobalt(II) monohydrate

Crystal data

$(C_6H_6N_3)[CoCl_3(C_6H_5N_3)]\cdot H_2O$	$Z = 2$
$M_r = 422.56$	$F_{000} = 426$
Triclinic, $P\overline{1}$	$D_x = 1.640$ Mg m^{-3}
Hall symbol: P -1	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
$a = 6.8760$ (8) Å	Cell parameters from 28 reflections
$b = 7.8033$ (12) Å	$\theta = 5.3$–12.6º
$c = 16.657$ (3) Å	$\mu = 1.48$ mm^{-1}
$\alpha = 95.450$ (13)º	$T = 293$ (2) K
$\beta = 95.962$ (8)º	Prism, blue
$\gamma = 103.989$ (9)º	0.40 × 0.40 × 0.20 mm
$V = 855.8$ (2) Å^3	

Data collection

Bruker P4 diffractometer	$R_{int} = 0.078$
Radiation source: fine-focus sealed tube	$\theta_{max} = 27.5$º
Monochromator: graphite	$\theta_{min} = 2.5$º
$T = 293$(2) K	$h = -8\rightarrow1$
ω scans	$k = -9\rightarrow10$
Absorption correction: ψ scan (North *et al.*, 1968)	$l = -21\rightarrow21$
$T_{min} = 0.611$, $T_{max} = 0.744$	3 standard reflections
4906 measured reflections	every 100 reflections
4846 independent reflections	intensity decay: none
4526 reflections with $I > 2\sigma(I)$	

Refinement

Refinement on F^2	Hydrogen site location: difference Fourier map
Least-squares matrix: full	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)] = 0.029$	$w = 1/[\sigma^2(F_o^2) + (0.0331P)^2 + 0.2297P]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.078$	$(\Delta/\sigma)_{max} < 0.001$
$S = 1.08$	$\Delta\rho_{max} = 0.34$ e Å^{-3}
4846 reflections	$\Delta\rho_{min} = -0.26$ e Å^{-3}
417 parameters	Extinction correction: none
3 restraints	Absolute structure: Flack (1983), 920 Friedel pairs
Primary atom site location: structure-invariant direct methods	Flack parameter: −0.008 (13)

Secondary atom site location: structure-invariant direct methods

Special details

Geometry. Bond distances, angles *etc*. have been calculated using the rounded fractional coordinates. All su's are estimated from the variances of the (full) variance-covariance matrix. The cell e.s.d.'s are taken into account in the estimation of distances, angles and torsion angles

Refinement. Refinement on F^2 for ALL reflections except those flagged by the user for potential systematic errors. Weighted *R*-factors *wR* and all goodnesses 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 observed criterion of $F^2 > \sigma(F^2)$ is used only for calculating -*R*-factor-obs *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	0.44420 (6)	0.01369 (5)	0.90042 (3)	0.0462 (1)
Cl1	0.1994 (2)	−0.24333 (13)	0.89041 (6)	0.0706 (3)
Cl2	0.3415 (2)	0.22168 (14)	0.97717 (6)	0.0707 (4)
Cl3	0.7529 (2)	−0.0156 (3)	0.93735 (8)	0.0969 (6)
N1	0.4450 (5)	0.0908 (4)	0.78758 (16)	0.0436 (8)
N2	0.3859 (5)	−0.0327 (4)	0.72406 (17)	0.0491 (9)
N3	0.3929 (5)	0.0501 (4)	0.65771 (17)	0.0487 (9)
C4	0.4831 (7)	0.3714 (6)	0.6303 (3)	0.0585 (12)
C5	0.5466 (8)	0.5379 (6)	0.6726 (3)	0.0669 (16)
C6	0.5824 (8)	0.5658 (5)	0.7580 (3)	0.0674 (15)
C7	0.5560 (6)	0.4277 (5)	0.8042 (2)	0.0560 (11)
C8	0.4911 (5)	0.2557 (4)	0.7616 (2)	0.0441 (9)
C9	0.4567 (5)	0.2298 (5)	0.6770 (2)	0.0446 (9)
Co2	0.55479 (7)	0.48473 (5)	0.39999 (3)	0.0484 (1)
Cl4	0.6620 (2)	0.24123 (14)	0.42163 (7)	0.0745 (4)
Cl5	0.7823 (3)	0.72314 (15)	0.46890 (8)	0.0979 (6)
Cl6	0.2402 (2)	0.4745 (2)	0.43067 (8)	0.0891 (5)
N11	0.5282 (5)	0.5107 (4)	0.27999 (16)	0.0445 (8)
N12	0.4780 (6)	0.3689 (4)	0.22487 (17)	0.0514 (9)
N13	0.4662 (6)	0.4279 (4)	0.15251 (17)	0.0542 (9)
C14	0.5165 (7)	0.7309 (6)	0.1018 (2)	0.0570 (11)
C15	0.5618 (8)	0.9044 (6)	0.1336 (3)	0.0630 (16)
C16	0.5992 (7)	0.9600 (5)	0.2186 (3)	0.0606 (13)
C17	0.5933 (6)	0.8414 (5)	0.2737 (2)	0.0512 (10)
C18	0.5479 (5)	0.6616 (4)	0.24206 (18)	0.0409 (9)
C19	0.5082 (6)	0.6077 (5)	0.1583 (2)	0.0453 (10)
N21	0.9897 (6)	0.4698 (4)	0.59051 (19)	0.0554 (10)
N22	1.0593 (6)	0.6201 (4)	0.6387 (2)	0.0608 (11)
N23	1.0793 (5)	0.5710 (4)	0.71148 (18)	0.0531 (9)
C24	1.0184 (7)	0.2821 (6)	0.7735 (2)	0.0581 (11)
C25	0.9546 (7)	0.1017 (6)	0.7485 (3)	0.0670 (16)

C26	0.8995 (7)	0.0348 (6)	0.6655 (3)	0.0695 (16)
C27	0.9026 (7)	0.1394 (5)	0.6052 (3)	0.0605 (14)
C28	0.9658 (6)	0.3237 (5)	0.6305 (2)	0.0462 (10)
C29	1.0242 (5)	0.3911 (5)	0.7118 (2)	0.0439 (10)
N31	0.0523 (6)	0.8803 (5)	0.0749 (2)	0.0609 (13)
N32	0.0951 (7)	1.0044 (5)	0.1374 (2)	0.0673 (14)
N33	0.0884 (6)	0.9186 (5)	0.2018 (2)	0.0581 (11)
C34	0.0247 (7)	0.5974 (7)	0.2283 (3)	0.0671 (16)
C35	−0.0210 (9)	0.4337 (7)	0.1856 (4)	0.0788 (19)
C36	−0.0493 (8)	0.4068 (6)	0.1003 (4)	0.0805 (18)
C37	−0.0293 (8)	0.5435 (6)	0.0545 (3)	0.0688 (14)
C38	0.0182 (7)	0.7128 (5)	0.0974 (2)	0.0531 (11)
C39	0.0438 (6)	0.7406 (5)	0.1818 (2)	0.0514 (11)
O1	0.1150 (10)	0.0529 (7)	0.3557 (2)	0.127 (2)
O2	0.3201 (10)	0.8988 (6)	0.4999 (2)	0.124 (2)
H3	0.36100	−0.00330	0.60880	0.0580*
H4	0.45880	0.35330	0.57380	0.0710*
H5	0.56690	0.63600	0.64400	0.0810*
H6	0.62540	0.68190	0.78410	0.0810*
H7	0.57990	0.44690	0.86070	0.0670*
H13	0.43520	0.35920	0.10710	0.0650*
H14	0.49230	0.69560	0.04600	0.0680*
H15	0.56870	0.99050	0.09830	0.0760*
H16	0.62860	1.08080	0.23720	0.0730*
H17	0.61810	0.87790	0.32940	0.0620*
H21	0.96190	0.46410	0.53860	0.074 (15)*
H23	1.12300	0.64520	0.75490	0.0640*
H24	1.05520	0.32800	0.82800	0.0700*
H25	0.94790	0.02270	0.78710	0.0800*
H26	0.85880	−0.08790	0.65150	0.0840*
H27	0.86550	0.09280	0.55080	0.0730*
H31	0.04630	0.90190	0.02520	0.0730*
H33	0.11010	0.97010	0.25110	0.10 (2)*
H34	0.04250	0.61440	0.28480	0.0810*
H35	−0.03420	0.33520	0.21380	0.0940*
H36	−0.08290	0.29080	0.07420	0.0970*
H37	−0.04650	0.52480	−0.00210	0.0820*
H1A	0.23890	0.07600	0.36260	0.1910*
H1B	0.04880	0.12670	0.36090	0.1910*
H2A	0.30780	0.97330	0.46940	0.1850*
H2B	0.27160	0.79140	0.48810	0.1850*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Co1	0.0523 (3)	0.0539 (2)	0.0332 (2)	0.0160 (2)	0.0026 (2)	0.0071 (2)
Cl1	0.0959 (8)	0.0581 (5)	0.0467 (4)	−0.0033 (5)	0.0175 (5)	0.0019 (4)
Cl2	0.1015 (9)	0.0690 (6)	0.0423 (4)	0.0284 (6)	0.0096 (5)	−0.0074 (4)

Cl3	0.0682 (7)	0.1819 (15)	0.0594 (6)	0.0585 (9)	0.0058 (5)	0.0423 (7)
N1	0.0503 (16)	0.0458 (13)	0.0372 (12)	0.0171 (13)	0.0039 (12)	0.0076 (10)
N2	0.0596 (18)	0.0496 (14)	0.0389 (13)	0.0173 (14)	0.0029 (13)	0.0050 (11)
N3	0.0563 (18)	0.0541 (15)	0.0365 (12)	0.0166 (15)	0.0054 (13)	0.0034 (11)
C4	0.060 (2)	0.072 (2)	0.055 (2)	0.026 (2)	0.0196 (19)	0.0287 (19)
C5	0.066 (3)	0.061 (2)	0.088 (3)	0.024 (2)	0.030 (2)	0.038 (2)
C6	0.065 (3)	0.0468 (19)	0.093 (3)	0.0146 (19)	0.019 (2)	0.0109 (19)
C7	0.057 (2)	0.0533 (18)	0.0544 (19)	0.0098 (18)	0.0087 (18)	−0.0001 (15)
C8	0.0424 (17)	0.0504 (16)	0.0423 (15)	0.0161 (14)	0.0055 (14)	0.0084 (13)
C9	0.0431 (18)	0.0526 (16)	0.0426 (15)	0.0169 (15)	0.0089 (14)	0.0118 (13)
Co2	0.0625 (3)	0.0495 (2)	0.0336 (2)	0.0159 (2)	0.0033 (2)	0.0060 (2)
Cl4	0.1100 (10)	0.0605 (5)	0.0572 (5)	0.0355 (6)	−0.0038 (6)	0.0083 (4)
Cl5	0.1390 (14)	0.0598 (6)	0.0697 (7)	0.0027 (8)	−0.0386 (8)	−0.0015 (5)
Cl6	0.0837 (9)	0.1346 (11)	0.0667 (6)	0.0474 (9)	0.0314 (6)	0.0256 (7)
N11	0.0564 (17)	0.0426 (13)	0.0350 (11)	0.0145 (13)	0.0044 (12)	0.0038 (10)
N12	0.069 (2)	0.0467 (14)	0.0382 (13)	0.0191 (15)	0.0004 (14)	0.0000 (11)
N13	0.069 (2)	0.0590 (16)	0.0355 (12)	0.0233 (16)	0.0014 (14)	−0.0013 (11)
C14	0.061 (2)	0.077 (2)	0.0418 (17)	0.027 (2)	0.0099 (17)	0.0230 (17)
C15	0.067 (3)	0.073 (3)	0.062 (2)	0.029 (2)	0.017 (2)	0.035 (2)
C16	0.068 (3)	0.0489 (18)	0.069 (2)	0.0182 (19)	0.010 (2)	0.0174 (17)
C17	0.061 (2)	0.0456 (16)	0.0485 (18)	0.0161 (17)	0.0085 (17)	0.0057 (14)
C18	0.0440 (17)	0.0461 (15)	0.0353 (14)	0.0155 (14)	0.0053 (13)	0.0083 (11)
C19	0.048 (2)	0.0568 (18)	0.0362 (14)	0.0211 (16)	0.0094 (14)	0.0070 (13)
N21	0.065 (2)	0.0601 (17)	0.0392 (14)	0.0147 (16)	−0.0007 (15)	0.0087 (12)
N22	0.069 (2)	0.0514 (16)	0.0605 (19)	0.0148 (16)	−0.0018 (18)	0.0115 (14)
N23	0.0579 (19)	0.0524 (15)	0.0470 (15)	0.0168 (15)	−0.0020 (14)	−0.0018 (12)
C24	0.058 (2)	0.078 (2)	0.0472 (18)	0.028 (2)	0.0105 (18)	0.0202 (17)
C25	0.056 (2)	0.073 (3)	0.084 (3)	0.024 (2)	0.019 (2)	0.040 (2)
C26	0.055 (2)	0.0473 (19)	0.105 (4)	0.0122 (19)	0.005 (2)	0.011 (2)
C27	0.057 (2)	0.0491 (19)	0.071 (3)	0.0143 (18)	−0.003 (2)	−0.0047 (17)
C28	0.0429 (18)	0.0501 (17)	0.0452 (16)	0.0122 (15)	0.0032 (14)	0.0064 (13)
C29	0.0408 (18)	0.0527 (17)	0.0400 (15)	0.0162 (15)	0.0043 (14)	0.0044 (13)
N31	0.072 (3)	0.0657 (19)	0.0476 (16)	0.0224 (19)	0.0014 (17)	0.0150 (14)
N32	0.079 (3)	0.063 (2)	0.063 (2)	0.0251 (19)	0.0019 (19)	0.0135 (16)
N33	0.060 (2)	0.0635 (19)	0.0504 (17)	0.0182 (17)	0.0014 (15)	0.0054 (14)
C34	0.053 (2)	0.088 (3)	0.069 (3)	0.023 (2)	0.013 (2)	0.034 (2)
C35	0.069 (3)	0.066 (3)	0.109 (4)	0.019 (2)	0.019 (3)	0.036 (3)
C36	0.068 (3)	0.056 (2)	0.116 (4)	0.013 (2)	0.017 (3)	0.005 (2)
C37	0.069 (3)	0.070 (2)	0.065 (2)	0.016 (2)	0.011 (2)	−0.0019 (19)
C38	0.052 (2)	0.063 (2)	0.0476 (17)	0.0197 (18)	0.0068 (16)	0.0093 (15)
C39	0.045 (2)	0.0578 (18)	0.0526 (19)	0.0151 (17)	0.0035 (16)	0.0111 (15)
O1	0.161 (5)	0.126 (4)	0.074 (2)	0.015 (4)	0.002 (3)	−0.019 (2)
O2	0.187 (6)	0.111 (3)	0.065 (2)	0.033 (4)	0.016 (3)	−0.014 (2)

Geometric parameters (Å, °)

Co1—Cl1	2.2649 (13)	C6—C7	1.371 (6)
Co1—Cl2	2.2616 (13)	C7—C8	1.403 (5)
Co1—Cl3	2.2195 (16)	C8—C9	1.392 (5)

Co1—N1	2.027 (3)	C4—H4	0.93
Co2—Cl4	2.2441 (13)	C5—H5	0.93
Co2—Cl5	2.2450 (15)	C6—H6	0.93
Co2—Cl6	2.2584 (16)	C7—H7	0.93
Co2—N11	2.022 (3)	C14—C15	1.355 (6)
O1—H1B	0.82	C14—C19	1.404 (5)
O1—H1A	0.82	C15—C16	1.419 (7)
N1—C8	1.371 (4)	C16—C17	1.361 (6)
N1—N2	1.320 (4)	C17—C18	1.399 (5)
N2—N3	1.332 (4)	C18—C19	1.397 (4)
N3—C9	1.360 (5)	C14—H14	0.93
O2—H2B	0.82	C15—H15	0.93
O2—H2A	0.82	C16—H16	0.93
N3—H3	0.86	C17—H17	0.93
N11—N12	1.320 (4)	C24—C25	1.378 (6)
N11—C18	1.373 (4)	C24—C29	1.393 (5)
N12—N13	1.332 (4)	C25—C26	1.409 (7)
N13—C19	1.354 (5)	C26—C27	1.352 (7)
N13—H13	0.86	C27—C28	1.407 (5)
N21—C28	1.359 (5)	C28—C29	1.386 (5)
N21—N22	1.311 (4)	C24—H24	0.93
N22—N23	1.309 (4)	C25—H25	0.93
N23—C29	1.363 (5)	C26—H26	0.93
N21—H21	0.86	C27—H27	0.93
N23—H23	0.86	C34—C39	1.407 (6)
N31—C38	1.366 (5)	C34—C35	1.350 (8)
N31—N32	1.310 (5)	C35—C36	1.403 (9)
N32—N33	1.316 (5)	C36—C37	1.358 (7)
N33—C39	1.349 (5)	C37—C38	1.388 (6)
N31—H31	0.86	C38—C39	1.388 (5)
N33—H33	0.86	C34—H34	0.93
C4—C5	1.365 (7)	C35—H35	0.93
C4—C9	1.398 (6)	C36—H36	0.93
C5—C6	1.405 (7)	C37—H37	0.93
Cl1—Co1—Cl2	106.81 (5)	C5—C6—H6	119
Cl1—Co1—Cl3	113.73 (7)	C8—C7—H7	122
Cl1—Co1—N1	106.87 (10)	C6—C7—H7	122
Cl2—Co1—Cl3	116.75 (6)	C15—C14—C19	115.9 (3)
Cl2—Co1—N1	105.84 (10)	C14—C15—C16	122.6 (4)
Cl3—Co1—N1	106.16 (11)	C15—C16—C17	121.8 (4)
Cl6—Co2—N11	102.70 (11)	C16—C17—C18	116.4 (3)
Cl4—Co2—Cl6	114.49 (6)	C17—C18—C19	121.4 (3)
Cl4—Co2—N11	110.22 (10)	N11—C18—C19	107.4 (3)
Cl4—Co2—Cl5	108.33 (6)	N11—C18—C17	131.2 (3)
Cl5—Co2—N11	109.56 (10)	N13—C19—C14	134.5 (3)
Cl5—Co2—Cl6	111.40 (7)	C14—C19—C18	121.8 (3)
H1A—O1—H1B	125	N13—C19—C18	103.7 (3)
N2—N1—C8	109.5 (3)	C15—C14—H14	122
Co1—N1—N2	118.5 (2)	C19—C14—H14	122

Co1—N1—C8	131.9 (2)	C16—C15—H15	119
N1—N2—N3	107.4 (3)	C14—C15—H15	119
N2—N3—C9	111.5 (3)	C15—C16—H16	119
H2A—O2—H2B	124	C17—C16—H16	119
C9—N3—H3	124	C18—C17—H17	122
N2—N3—H3	124	C16—C17—H17	122
N12—N11—C18	109.6 (3)	C25—C24—C29	115.7 (3)
Co2—N11—N12	120.6 (2)	C24—C25—C26	121.3 (4)
Co2—N11—C18	129.7 (2)	C25—C26—C27	123.6 (4)
N11—N12—N13	106.7 (3)	C26—C27—C28	115.4 (4)
N12—N13—C19	112.7 (3)	N21—C28—C29	104.7 (3)
N12—N13—H13	124	N21—C28—C27	133.7 (3)
C19—N13—H13	124	C27—C28—C29	121.6 (4)
N22—N21—C28	113.5 (3)	C24—C29—C28	122.5 (4)
N21—N22—N23	104.1 (3)	N23—C29—C24	133.3 (3)
N22—N23—C29	113.6 (3)	N23—C29—C28	104.3 (3)
C28—N21—H21	123	C29—C24—H24	122
N22—N21—H21	123	C25—C24—H24	122
N22—N23—H23	123	C24—C25—H25	119
C29—N23—H23	123	C26—C25—H25	119
N32—N31—C38	112.6 (3)	C25—C26—H26	118
N31—N32—N33	105.2 (3)	C27—C26—H26	118
N32—N33—C39	112.3 (3)	C28—C27—H27	122
C38—N31—H31	124	C26—C27—H27	122
N32—N31—H31	124	C35—C34—C39	115.8 (5)
C39—N33—H33	124	C34—C35—C36	122.5 (5)
N32—N33—H33	124	C35—C36—C37	122.5 (5)
C5—C4—C9	116.0 (4)	C36—C37—C38	115.8 (5)
C4—C5—C6	122.1 (4)	N31—C38—C39	104.2 (3)
C5—C6—C7	122.2 (4)	N31—C38—C37	133.7 (4)
C6—C7—C8	116.4 (3)	C37—C38—C39	122.1 (4)
N1—C8—C9	107.2 (3)	C34—C39—C38	121.3 (4)
N1—C8—C7	131.9 (3)	N33—C39—C34	133.0 (4)
C7—C8—C9	120.9 (3)	N33—C39—C38	105.7 (3)
N3—C9—C8	104.5 (3)	C35—C34—H34	122
N3—C9—C4	133.1 (3)	C39—C34—H34	122
C4—C9—C8	122.4 (4)	C36—C35—H35	119
C5—C4—H4	122	C34—C35—H35	119
C9—C4—H4	122	C35—C36—H36	119
C6—C5—H5	119	C37—C36—H36	119
C4—C5—H5	119	C38—C37—H37	122
C7—C6—H6	119	C36—C37—H37	122

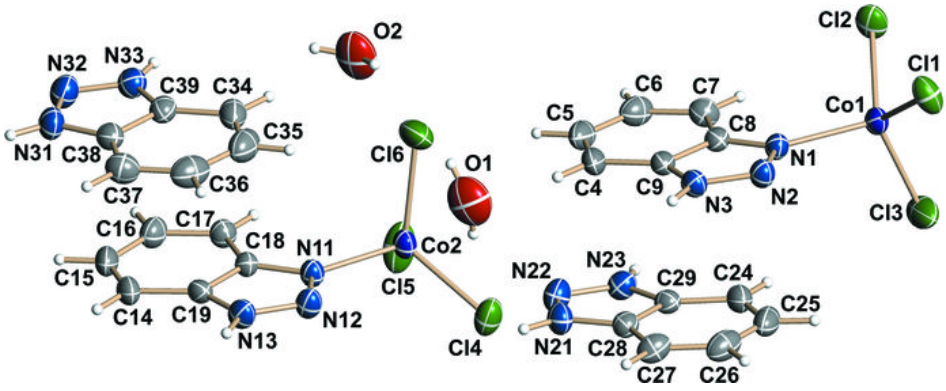
Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1B···Cl6	0.82	2.79	3.279 (5)	120
O2—H2A···O1^{i}	0.82	2.41	3.142 (7)	148
O2—H2B···Cl6	0.82	2.52	3.295 (5)	159

N3—H3···O2^{ii}	0.86	1.87	2.721 (4)	173
N13—H13···Cl2^{iii}	0.86	2.28	3.127 (3)	169
N21—H21···Cl4	0.86	2.80	3.458 (4)	134
N21—H21···Cl6^{iv}	0.86	2.75	3.316 (4)	125
N23—H23···Cl1^{v}	0.86	2.30	3.123 (3)	160
N31—H31···Cl3^{vi}	0.86	2.61	3.214 (4)	128
N33—H33···O1^{i}	0.86	1.79	2.646 (5)	170

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

Fig. 1


O2
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C39
C34
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N31
C38
C37
C36
Cl6
O1
C16
C17
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Co2
C15
Cl5
C14
C19
N12
N13
Cl4
Cl2
Cl1
C6
C7
C5
C8
Co1
N1
C4
C9
N3
N2
Cl3
N22
N23
C29
C24
C25
N21
C28
C27
C26