

Crystal structure of bis(2-amino-5-chloropyridinium) tetrachloridocobaltate(II)

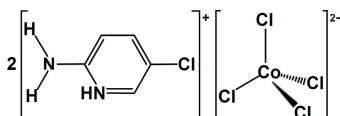
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The title salt, $(C_5H_6ClN_2)_2[CoCl_4]$, was synthesized by slow evaporation of an aqueous solution at room temperature. The asymmetric unit consists of two essentially planar $(C_5H_6ClN_2)^+$ cations [maximum deviations = 0.010 (3) and 0.014 (3) Å] that are nearly perpendicular to each other [dihedral angle = 84.12 (7)°]. They are bonded through N—H...Cl hydrogen bonds to distorted $[CoCl_4]^{2-}$ tetrahedra, leading to the formation of undulating layers parallel to (100). The structure is isotypic with the Zn analogue [Kefi *et al.* (2011). *Acta Cryst. E* **67**, m355–m356.]

1. Chemical context

Organic–inorganic hybrid compounds frequently exhibit self-organized structures and can combine organic and inorganic characteristics (Parent *et al.*, 2007; Zheng *et al.*, 2010; Chang *et al.*, 2011). In particular, anionic cobalt halides associated with organic counter-cations have some interesting physical properties, such as luminescence, in which we are interested. In this communication, we report the synthesis and crystal structure of the new organic–inorganic hybrid compound bis(2-amino-5-chloropyridinium) tetrachloridocobaltate(II), $(C_5H_6ClN_2)_2[CoCl_4]$.



2. Structural commentary

The asymmetric unit of the title compound consists of two 2-amino-5-chloropyridinium cations (cat1 consists of ring C1–

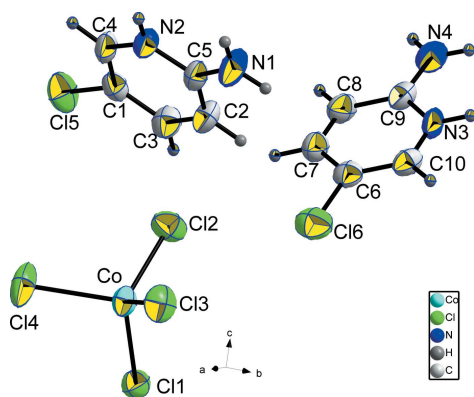
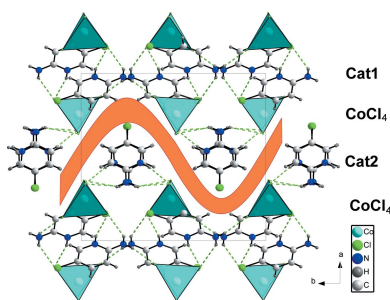


Figure 1

The molecular entities of $(C_5H_6ClN_2)_2[CoCl_4]$, showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level.

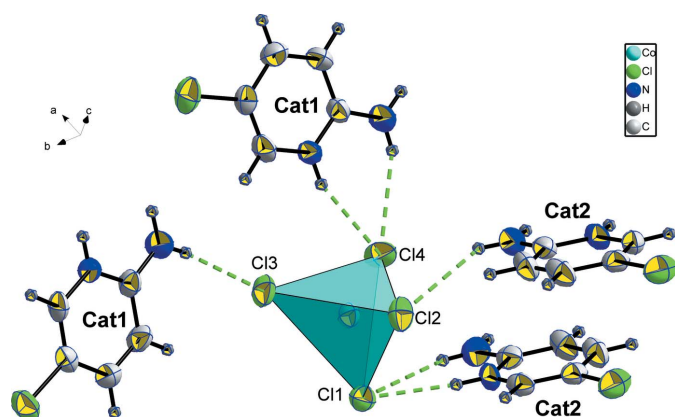


Figure 2
The environment of the CoCl_4 tetrahedron.

C5/N2 and cat2 consists of ring C9-C10/N3 and one isolated $[\text{CoCl}_4]^{2-}$ anion (Fig. 1).

The organic cations are nearly planar exhibiting small maximum deviations of 0.010 (3) and 0.014 (3) Å for atoms N2 and C6, respectively. The two least-squares planes of the two cations are nearly perpendicular to each other [84.12 (7)°]. The bond angles C4-N2-C5 [123.6 (3)°] and C9-N3-C10 [123.3 (3)°] in the rings of cat1 and cat2 , respectively, confirm the presence of pyridinium cations. Previous studies (Jin *et al.*, 2001) showed that a pyridinium cation possesses an expanded C-N(H)-C angle in comparison with the parent pyridine (117°). This geometrical characteristic is in agreement with an imine-enamine resonance (Jin *et al.*, 2005) and contributes to the structural stability.

In the $[\text{CoCl}_4]^{2-}$ anion, the Co-Cl bond lengths range from 2.2645 (12) to 2.2934 (12) Å and the Cl-Co-Cl angles range from 104.84 (5) to 118.58 (5)°, revealing considerable distortions from the ideal tetrahedral geometry. These values are in agreement with those observed in similar compounds (Dhieb *et al.*, 2014; Mghandef & Boughzala, 2014; Oh *et al.*, 2011). The different Co-Cl bond lengths in the $[\text{CoCl}_4]^{2-}$ anion are related to the number of hydrogen bonds accepted by the Cl atoms. The Co-Cl1 and Co-Cl4 bonds are longer than the Co-Cl2 and Co-Cl3 bonds because atoms Cl1 and Cl4 are

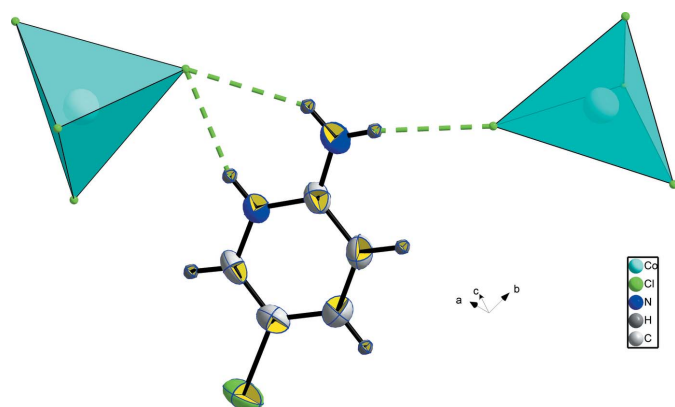


Figure 3
The environment around the cations (cat1 or cat2).

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

| $D-H\cdots A$ | $D-H$ | $H\cdots A$ | $D\cdots A$ | $D-H\cdots A$ |
|---------------------------------------|-------|-------------|-------------|---------------|
| $\text{N1-H1A}\cdots\text{Cl4}^i$ | 0.86 | 2.64 | 3.400 (4) | 148 |
| $\text{N1-H1B}\cdots\text{Cl3}^{ii}$ | 0.86 | 2.47 | 3.317 (3) | 169 |
| $\text{N2-HN2}\cdots\text{Cl4}^i$ | 0.86 | 2.42 | 3.238 (3) | 160 |
| $\text{N3-HN3}\cdots\text{Cl1}^{iii}$ | 0.86 | 2.42 | 3.251 (3) | 164 |
| $\text{N4-H4A}\cdots\text{Cl1}^{iii}$ | 0.86 | 2.77 | 3.519 (4) | 147 |
| $\text{N4-H4B}\cdots\text{Cl2}^{iv}$ | 0.86 | 2.80 | 3.541 (4) | 145 |

Symmetry codes: (i) $-x+2, -y+1, -z+1$; (ii) $x, -y+\frac{3}{2}, z+\frac{1}{2}$; (iii) $-x+1, y+\frac{1}{2}, -z+\frac{1}{2}$; (iv) $-x+1, -y+1, -z+1$.

each acceptors of two hydrogen bonds from cat2 and cat1 , respectively.

3. Supramolecular features

Each CoCl_4 tetrahedron is linked to four cations (two cat1 and two cat2) by hydrogen bonds (Fig. 2 and Table 1). Atom Cl1 is doubly linked to one cat2 cation by $\text{N3-HN3}\cdots\text{Cl1}$ and $\text{N4-H4A}\cdots\text{Cl1}$, and atom Cl2 establishes one hydrogen bond with a symmetry-related cat2 cation *via* $\text{N4-H4B}\cdots\text{Cl2}$. Atom Cl3 is linked to cation cat1 by $\text{N1-H1B}\cdots\text{Cl3}$ and atom Cl4 again shares two hydrogen bonds ($\text{N1-H1A}\cdots\text{Cl4}$ and $\text{N2-HN2}\cdots\text{Cl4}$) with a second symmetry-related cat1 cation. The hydrogen-bonding environments of the two cations are similar. Both are linked to two CoCl_4 tetrahedra by three hydrogen bonds (Fig. 3)

The crystal packing can be described by an alternate stacking of cations and anions with a $-\text{cat1}-[\text{CoCl}_4]-\text{cat2}-[\text{CoCl}_4]-$ sequence along [100], as shown in Fig. 4. Between antiparallel aligned cat2 cations, $\pi-\pi$ interactions are also present [centroid-to-centroid separation = 3.900 (2) Å]. The

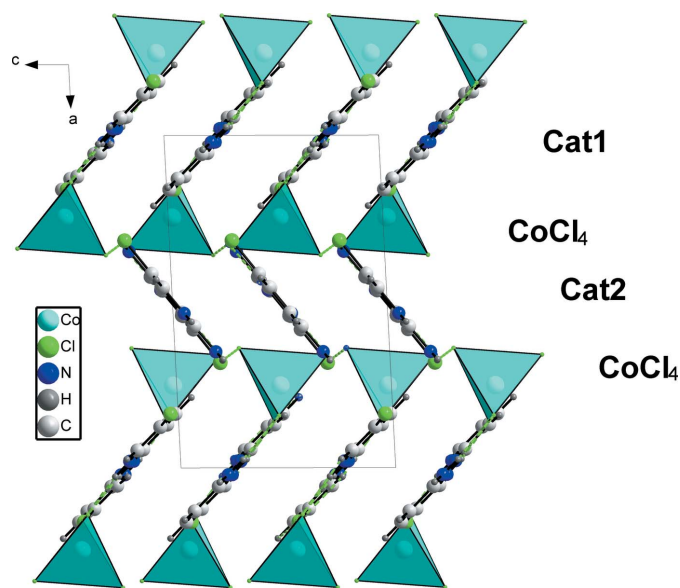


Figure 4
Projection of the crystal structure along [010] showing the $-\text{cat1}-[\text{CoCl}_4]-\text{cat2}-[\text{CoCl}_4]-$ sequence stacked along [100].

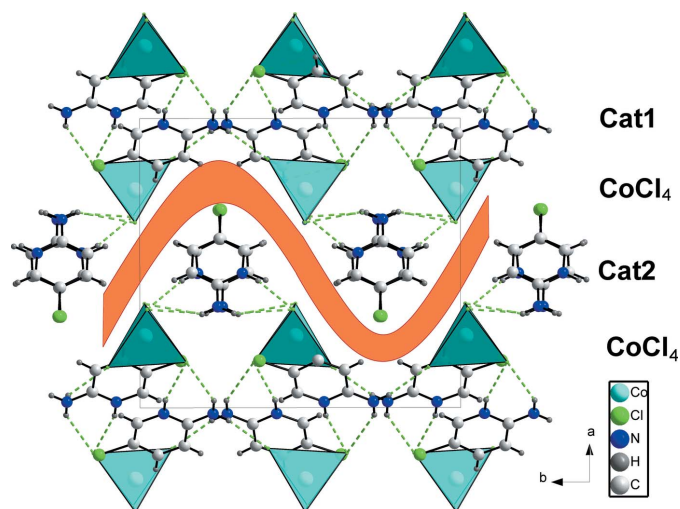


Figure 5
Projection of the crystal structure along [001] showing the layered character of the hydrogen-bonded components.

stacked cations and anions are linked through N—H...Cl hydrogen bonds into zigzag layers parallel to (100) (Fig. 5).

4. Database survey

A systematic search procedure in the Cambridge Structural Database (Groom & Allen, 2014) indicates a total of 32 hits for the 2-amino-5-chloropyridinium cation with various counter-anions. For tetrahalogenidometalate anions, the following structures have been reported: $(C_5H_6ClN_2)_2 \cdot [ZnCl_4] \cdot H_2O$ (Coomer *et al.*, 2007); $(C_5H_6ClN_2)_2 [ZnCl_4]$ (Kefi *et al.*, 2011a); $(C_5H_6ClN_2)_2 [CdCl_4] \cdot H_2O$ (Kefi *et al.*, 2011b); $(C_5H_6ClN_2)_2 [CuCl_4]$ (Parsons *et al.*, 2006); $(C_5H_6ClN_2)_2 [CuBr_4]$ (Woodward *et al.*, 2002). The title compound is isotopic with the Zn analogue $(C_5H_6ClN_2)_2 [ZnCl_4]$ (Kefi *et al.*, 2011a).

5. Synthesis and crystallization

A mixture of cobalt(II) chloride and 2-amino-5-chloropyridine (molar ratio 1:1) was dissolved in an aqueous solution of hydrochloric acid with 5 ml of ethanol. The mixture was stirred and then kept at room temperature. Blue crystals of the title compound were obtained after two weeks.

6. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. H atoms were placed geometrically and included as riding contributions, with N—H = 0.86 Å and C—H = 0.93 Å and with $U_{iso}(H) = 1.2U_{eq}(N,C)$.

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Table 2
Experimental details.

| | |
|--|--|
| Crystal data | |
| Chemical formula | $(C_5H_6ClN_2)_2 [CoCl_4]$ |
| M_r | 459.87 |
| Crystal system, space group | Monoclinic, $P2_1/c$ |
| Temperature (K) | 298 |
| a, b, c (Å) | 13.519 (2), 14.945 (3), 8.725 (2) |
| β (°) | 92.858 (3) |
| V (Å ³) | 1760.6 (6) |
| Z | 4 |
| Radiation type | Mo $K\alpha$ |
| μ (mm ⁻¹) | 1.88 |
| Crystal size (mm) | 0.5 × 0.3 × 0.2 |
| Data collection | |
| Diffractometer | Enraf–Nonius CAD-4 |
| Absorption correction | ψ scan (North <i>et al.</i> , 1968) |
| T_{min}, T_{max} | 0.423, 0.649 |
| No. of measured, independent and observed [$I > 2\sigma(I)$] reflections | 6241, 3707, 2121 |
| R_{int} | 0.039 |
| $(\sin \theta/\lambda)_{max}$ (Å ⁻¹) | 0.638 |
| Refinement | |
| $R[F^2 > 2\sigma(F^2)], wR(F^2), S$ | 0.041, 0.109, 0.99 |
| No. of reflections | 3707 |
| No. of parameters | 190 |
| H-atom treatment | H-atom parameters not refined |
| $\Delta\rho_{max}, \Delta\rho_{min}$ (e Å ⁻³) | 0.52, -0.34 |

Computer programs: *CAD-4 EXPRESS* (Enraf–Nonius, 1994), *XCAD4* (Harms & Wocadlo, 1995), *SHELXS97* and *SHELXL97* (Sheldrick, 2008), *DIAMOND* (Brandenburg, 2008) and *publCIF* (Westrip, 2010).

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supporting information

Acta Cryst. (2015). E71, 555-557 [https://doi.org/10.1107/S2056989015007707]

Crystal structure of bis(2-amino-5-chloropyridinium) tetrachloridocobaltate(II)

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Computing details

Data collection: *CAD-4 EXPRESS* (Enraf–Nonius, 1994); cell refinement: *CAD-4 EXPRESS* (Enraf–Nonius, 1994); data reduction: *XCAD4* (Harms & Wocadlo, 1995); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *DIAMOND* (Brandenburg, 2008); software used to prepare material for publication: *publCIF* (Westrip, 2010).

Bis(2-amino-5-chloropyridinium) tetrachloridocobaltate(II)

Crystal data

$(C_5H_6ClN_2)_2[CoCl_4]$

$M_r = 459.87$

Monoclinic, $P2_1/c$

Hall symbol: -P 2ybc

$a = 13.519$ (2) Å

$b = 14.945$ (3) Å

$c = 8.725$ (2) Å

$\beta = 92.858$ (3)°

$V = 1760.6$ (6) Å³

$Z = 4$

$F(000) = 916$

$D_x = 1.735$ Mg m⁻³

Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å

Cell parameters from 25 reflections

$\theta = 10\text{--}15^\circ$

$\mu = 1.88$ mm⁻¹

$T = 298$ K

Prism, blue

$0.5 \times 0.3 \times 0.2$ mm

Data collection

Enraf–Nonius CAD-4
diffractometer

Radiation source: fine-focus sealed tube

Graphite monochromator

non-profiled $\omega/2\theta$ scans

Absorption correction: ψ scan
(North *et al.*, 1968)

$T_{\min} = 0.423$, $T_{\max} = 0.649$

6241 measured reflections

3707 independent reflections

2121 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.039$

$\theta_{\max} = 27.0^\circ$, $\theta_{\min} = 2.0^\circ$

$h = -17 \rightarrow 17$

$k = -19 \rightarrow 1$

$l = -11 \rightarrow 5$

2 standard reflections every 120 min

intensity decay: 6%

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.041$

$wR(F^2) = 0.109$

$S = 0.99$

3707 reflections

190 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 not refined

$w = 1/[\sigma^2(F_o^2) + (0.0443P)^2]$

where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{\max} < 0.001$

$\Delta\rho_{\max} = 0.52$ e Å⁻³

$\Delta\rho_{\min} = -0.34$ 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 (\AA^2)

| | <i>x</i> | <i>y</i> | <i>z</i> | $U_{\text{iso}}^*/U_{\text{eq}}$ |
|-----|-------------|-------------|---------------|----------------------------------|
| Co | 0.75262 (3) | 0.48488 (3) | 0.01742 (6) | 0.03927 (16) |
| Cl1 | 0.66040 (7) | 0.47789 (7) | -0.20888 (12) | 0.0475 (3) |
| Cl2 | 0.64020 (8) | 0.48540 (8) | 0.20135 (13) | 0.0580 (3) |
| Cl3 | 0.85951 (8) | 0.60044 (7) | 0.05556 (14) | 0.0580 (3) |
| Cl4 | 0.84305 (8) | 0.35504 (7) | 0.03059 (15) | 0.0690 (4) |
| Cl5 | 0.83772 (8) | 0.37281 (8) | 0.53616 (14) | 0.0646 (3) |
| Cl6 | 0.68358 (8) | 0.75291 (9) | 0.29194 (14) | 0.0672 (4) |
| N1 | 0.9792 (2) | 0.7278 (2) | 0.7188 (4) | 0.0616 (11) |
| H1A | 1.0247 | 0.7306 | 0.7912 | 0.074* |
| H1B | 0.9565 | 0.7762 | 0.6768 | 0.074* |
| N2 | 0.9798 (2) | 0.5740 (2) | 0.7372 (4) | 0.0430 (8) |
| HN2 | 1.0261 | 0.5790 | 0.8078 | 0.052* |
| N3 | 0.4647 (2) | 0.8197 (2) | 0.5514 (4) | 0.0444 (8) |
| HN3 | 0.4394 | 0.8686 | 0.5834 | 0.053* |
| N4 | 0.3491 (2) | 0.7428 (2) | 0.6902 (4) | 0.0557 (9) |
| H4A | 0.3264 | 0.7931 | 0.7210 | 0.067* |
| H4B | 0.3233 | 0.6935 | 0.7195 | 0.067* |
| C1 | 0.8770 (3) | 0.4802 (3) | 0.5868 (5) | 0.0427 (9) |
| C2 | 0.8694 (3) | 0.6385 (3) | 0.5537 (5) | 0.0498 (11) |
| H2 | 0.8425 | 0.6887 | 0.5045 | 0.060* |
| C3 | 0.8370 (3) | 0.5557 (3) | 0.5125 (5) | 0.0503 (11) |
| H3 | 0.7880 | 0.5492 | 0.4346 | 0.060* |
| C4 | 0.9472 (3) | 0.4907 (2) | 0.6989 (5) | 0.0458 (10) |
| H4 | 0.9736 | 0.4411 | 0.7504 | 0.055* |
| C5 | 0.9440 (3) | 0.6484 (2) | 0.6714 (5) | 0.0418 (9) |
| C6 | 0.5837 (3) | 0.7483 (3) | 0.4092 (4) | 0.0451 (10) |
| C7 | 0.5437 (3) | 0.6658 (3) | 0.4521 (5) | 0.0550 (11) |
| H7 | 0.5707 | 0.6129 | 0.4168 | 0.066* |
| C8 | 0.4669 (3) | 0.6625 (3) | 0.5436 (5) | 0.0536 (11) |
| H8 | 0.4413 | 0.6075 | 0.5720 | 0.064* |
| C9 | 0.4253 (3) | 0.7413 (3) | 0.5959 (4) | 0.0444 (10) |
| C10 | 0.5418 (3) | 0.8250 (3) | 0.4591 (4) | 0.0433 (9) |
| H10 | 0.5659 | 0.8804 | 0.4301 | 0.052* |

Atomic displacement parameters (\AA^2)

| | U^{11} | U^{22} | U^{33} | U^{12} | U^{13} | U^{23} |
|-----|-------------|-------------|-------------|--------------|--------------|--------------|
| Co | 0.0394 (3) | 0.0288 (3) | 0.0492 (4) | -0.0023 (2) | -0.0018 (2) | -0.0013 (3) |
| C11 | 0.0502 (5) | 0.0460 (6) | 0.0459 (6) | 0.0005 (5) | -0.0002 (4) | 0.0005 (5) |
| C12 | 0.0679 (6) | 0.0542 (7) | 0.0534 (7) | -0.0144 (5) | 0.0158 (5) | -0.0045 (6) |
| C13 | 0.0587 (6) | 0.0409 (6) | 0.0740 (8) | -0.0159 (5) | -0.0008 (5) | -0.0049 (6) |
| C14 | 0.0673 (7) | 0.0336 (6) | 0.1025 (10) | 0.0110 (5) | -0.0328 (7) | -0.0098 (6) |
| C15 | 0.0688 (7) | 0.0414 (6) | 0.0842 (9) | -0.0114 (5) | 0.0087 (6) | -0.0175 (6) |
| C16 | 0.0545 (6) | 0.0911 (10) | 0.0556 (7) | 0.0035 (6) | -0.0007 (5) | 0.0019 (7) |
| N1 | 0.072 (2) | 0.031 (2) | 0.079 (3) | -0.0005 (17) | -0.020 (2) | 0.0032 (19) |
| N2 | 0.0468 (17) | 0.0315 (18) | 0.050 (2) | 0.0029 (14) | -0.0070 (15) | 0.0019 (16) |
| N3 | 0.058 (2) | 0.0224 (16) | 0.052 (2) | 0.0068 (15) | -0.0028 (17) | -0.0015 (16) |
| N4 | 0.060 (2) | 0.048 (2) | 0.058 (2) | -0.0021 (17) | -0.0021 (19) | 0.0081 (19) |
| C1 | 0.046 (2) | 0.035 (2) | 0.048 (2) | -0.0022 (18) | 0.0102 (18) | -0.008 (2) |
| C2 | 0.049 (2) | 0.041 (2) | 0.058 (3) | 0.0069 (19) | -0.009 (2) | 0.010 (2) |
| C3 | 0.044 (2) | 0.050 (3) | 0.055 (3) | 0.0022 (19) | -0.0083 (19) | -0.002 (2) |
| C4 | 0.054 (2) | 0.025 (2) | 0.058 (3) | 0.0077 (17) | 0.005 (2) | 0.003 (2) |
| C5 | 0.044 (2) | 0.031 (2) | 0.051 (3) | 0.0023 (17) | 0.0027 (18) | 0.006 (2) |
| C6 | 0.049 (2) | 0.048 (3) | 0.038 (2) | 0.0016 (19) | -0.0102 (18) | -0.001 (2) |
| C7 | 0.082 (3) | 0.035 (2) | 0.048 (3) | 0.007 (2) | -0.002 (2) | -0.001 (2) |
| C8 | 0.080 (3) | 0.032 (2) | 0.049 (3) | -0.006 (2) | 0.003 (2) | 0.005 (2) |
| C9 | 0.050 (2) | 0.037 (2) | 0.045 (2) | -0.0010 (18) | -0.0099 (19) | 0.006 (2) |
| C10 | 0.049 (2) | 0.037 (2) | 0.043 (2) | -0.0078 (18) | -0.0065 (19) | 0.0046 (19) |

Geometric parameters (\AA , $^\circ$)

| | | | |
|------------|-------------|----------|-----------|
| Co—C12 | 2.2645 (12) | N4—H4A | 0.8600 |
| Co—C13 | 2.2657 (11) | N4—H4B | 0.8600 |
| Co—C11 | 2.2843 (12) | C1—C4 | 1.337 (5) |
| Co—C14 | 2.2934 (12) | C1—C3 | 1.397 (6) |
| C15—C1 | 1.741 (4) | C2—C3 | 1.355 (6) |
| C16—C6 | 1.735 (4) | C2—C5 | 1.410 (5) |
| N1—C5 | 1.337 (5) | C2—H2 | 0.9300 |
| N1—H1A | 0.8600 | C3—H3 | 0.9300 |
| N1—H1B | 0.8600 | C4—H4 | 0.9300 |
| N2—C5 | 1.331 (4) | C6—C10 | 1.360 (5) |
| N2—C4 | 1.357 (5) | C6—C7 | 1.405 (6) |
| N2—HN2 | 0.8600 | C7—C8 | 1.342 (6) |
| N3—C10 | 1.351 (5) | C7—H7 | 0.9300 |
| N3—C9 | 1.352 (5) | C8—C9 | 1.392 (6) |
| N3—HN3 | 0.8600 | C8—H8 | 0.9300 |
| N4—C9 | 1.351 (5) | C10—H10 | 0.9300 |
| C12—Co—C13 | 109.81 (5) | C2—C3—C1 | 120.1 (4) |
| C12—Co—C11 | 104.84 (5) | C2—C3—H3 | 119.9 |
| C13—Co—C11 | 118.58 (5) | C1—C3—H3 | 119.9 |
| C12—Co—C14 | 110.02 (5) | C1—C4—N2 | 119.9 (4) |

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| C13—Co—C14 | 107.65 (5) | C1—C4—H4 | 120.1 |
| C11—Co—C14 | 105.73 (4) | N2—C4—H4 | 120.1 |
| C5—N1—H1A | 120.0 | N2—C5—N1 | 119.5 (3) |
| C5—N1—H1B | 120.0 | N2—C5—C2 | 117.2 (3) |
| H1A—N1—H1B | 120.0 | N1—C5—C2 | 123.3 (3) |
| C5—N2—C4 | 123.6 (3) | C10—C6—C7 | 118.8 (4) |
| C5—N2—HN2 | 118.2 | C10—C6—Cl6 | 120.2 (3) |
| C4—N2—HN2 | 118.2 | C7—C6—Cl6 | 120.9 (3) |
| C10—N3—C9 | 123.3 (3) | C8—C7—C6 | 120.7 (4) |
| C10—N3—HN3 | 118.4 | C8—C7—H7 | 119.7 |
| C9—N3—HN3 | 118.4 | C6—C7—H7 | 119.7 |
| C9—N4—H4A | 120.0 | C7—C8—C9 | 120.1 (4) |
| C9—N4—H4B | 120.0 | C7—C8—H8 | 120.0 |
| H4A—N4—H4B | 120.0 | C9—C8—H8 | 120.0 |
| C4—C1—C3 | 119.2 (4) | N4—C9—N3 | 118.9 (4) |
| C4—C1—Cl5 | 119.4 (3) | N4—C9—C8 | 123.1 (4) |
| C3—C1—Cl5 | 121.4 (3) | N3—C9—C8 | 117.9 (4) |
| C3—C2—C5 | 119.9 (4) | N3—C10—C6 | 119.2 (4) |
| C3—C2—H2 | 120.0 | N3—C10—H10 | 120.4 |
| C5—C2—H2 | 120.0 | C6—C10—H10 | 120.4 |

Hydrogen-bond geometry (Å, °)

| <i>D</i> —H... <i>A</i> | <i>D</i> —H | H... <i>A</i> | <i>D</i> ... <i>A</i> | <i>D</i> —H... <i>A</i> |
|-----------------------------|-------------|---------------|-----------------------|-------------------------|
| N1—H1A...Cl4 ⁱ | 0.86 | 2.64 | 3.400 (4) | 148 |
| N1—H1B...Cl3 ⁱⁱ | 0.86 | 2.47 | 3.317 (3) | 169 |
| N2—HN2...Cl4 ⁱ | 0.86 | 2.42 | 3.238 (3) | 160 |
| N3—HN3...Cl1 ⁱⁱⁱ | 0.86 | 2.42 | 3.251 (3) | 164 |
| N4—H4A...Cl1 ⁱⁱⁱ | 0.86 | 2.77 | 3.519 (4) | 147 |
| N4—H4B...Cl2 ^{iv} | 0.86 | 2.80 | 3.541 (4) | 145 |

Symmetry codes: (i) $-x+2, -y+1, -z+1$; (ii) $x, -y+3/2, z+1/2$; (iii) $-x+1, y+1/2, -z+1/2$; (iv) $-x+1, -y+1, -z+1$.