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Bis(2-phenylethylammonium) tetrachloridocobaltate(II)

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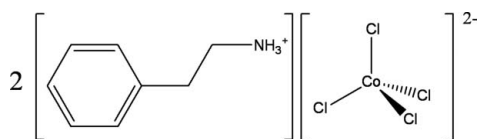
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Key indicators: single-crystal X-ray study; $T = 296$ K; mean $\sigma(\text{C}-\text{C}) = 0.011$ Å; R factor = 0.055; wR factor = 0.161; data-to-parameter ratio = 17.0.

Crystals of the title compound, $(\text{C}_6\text{H}_5\text{CH}_2\text{CH}_2\text{NH}_3)_2[\text{CoCl}_4]$, were grown by the solvent-evaporation method. This inorganic–organic hybrid compound exhibits a layered structure in which isolated CoCl_4 inorganic layers alternate with bilayers of phenylethylammonium cations. Although the inorganic anion is zero-dimensional, the layered structure is stabilized via $\text{N}-\text{H}\cdots\text{Cl}$ hydrogen bonds. The CoCl_4 tetrahedra connect to the cations through $\text{N}-\text{H}\cdots\text{Cl}$ hydrogen bonds, building a two-dimensional network extending parallel to (010).

Related literature

For inorganic–organic hybrids containing tetrahedral anions, see: Abdi *et al.* (2005); Huh *et al.* (2006); Zouari & Ben Salah, (2004). For low-dimensional magnetism in inorganic–organic perovskite systems, see: de Jongh (1986); Park & Lee (2005, 2006); Depmeier (2009); Mitzi (1999). For classification of hydrogen bonds depending on bond lengths, see: Steiner (1998, 2002).



Experimental

Crystal data

$(\text{C}_8\text{H}_{12}\text{N})_2[\text{CoCl}_4]$
 $M_r = 445.10$
 Monoclinic, $P2_1/c$
 $a = 7.4623$ (13) Å
 $b = 24.664$ (3) Å

$c = 11.1997$ (16) Å
 $\beta = 91.769$ (13)°
 $V = 2060.3$ (5) Å³
 $Z = 4$
 Mo $K\alpha$ radiation

$\mu = 1.35$ mm⁻¹
 $T = 296$ K

0.50 × 0.40 × 0.35 mm

Data collection

Bruker P4 diffractometer
 Absorption correction: multi-scan
 (*SADABS*; Sheldrick, 1996)
 $T_{\text{min}} = 0.237$, $T_{\text{max}} = 0.265$
 4692 measured reflections
 3595 independent reflections

1566 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.041$
 3 standard reflections every 97 reflections
 intensity decay: none

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.055$
 $wR(F^2) = 0.161$
 $S = 1.03$
 3595 reflections
 211 parameters

2 restraints
 H-atom parameters constrained
 $\Delta\rho_{\text{max}} = 0.43$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.30$ e Å⁻³

Table 1

Selected bond lengths (Å).

Co1—Cl4	2.229 (2)	Co1—Cl1	2.272 (2)
Co1—Cl2	2.251 (2)	Co1—Cl3	2.276 (2)

Table 2

Hydrogen-bond geometry (Å, °).

$D-\text{H}\cdots A$	$D-\text{H}$	$\text{H}\cdots A$	$D\cdots A$	$D-\text{H}\cdots A$
N2—H2C \cdots Cl1 ⁱ	0.89	2.62	3.445 (6)	156
N2—H2A \cdots Cl4 ⁱⁱ	0.89	2.51	3.321 (6)	152
N1—H1C \cdots Cl3 ⁱⁱⁱ	0.89	2.42	3.291 (8)	167
N1—H1B \cdots Cl1	0.89	2.55	3.382 (7)	156

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

Data collection: *XSCANS* (Bruker, 1996); cell refinement: *XSCANS*; data reduction: *XSCANS*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *PLATON* (Spek, 2009) and *DIAMOND* (Brandenburg, 1999); software used to prepare material for publication: *SHELXL97*.

IHO thanks Professor G. Heger for discussion of the results and for suggestions.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: SI2347).

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supporting information

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Bis(2-phenylethylammonium) tetrachloridocobaltate(II)

In-Hwan Oh, Dahye Kim, Young-Duk Huh, Younbong Park, J. M. Sungil Park and Seong-Hun Park

S1. Comment

The title compound, $(\text{C}_6\text{H}_5\text{CH}_2\text{CH}_2\text{NH}_3)_2\text{CoCl}_4$, belongs to the layered inorganic-organic hybrid systems of general formula A_2MX_4 (where A = organic cation, M = divalent metal, X = halides). These systems are of special interest because of typical low-dimensional magnetic systems (de Jongh, 1986; Mitzi, 1999). To investigate the role of interlayer spacing on the magnetic properties, a variety of hybrid systems using long-chain alkylamine have been developed. However, their crystallographic studies are limited because their insolubility make it difficult to obtain a good single-crystal. As a part of our research interest in the low-dimensional magnetism (Park & Lee 2005, 2006), we synthesized a series of the layered inorganic-organic perovskite materials using phenethylamine and present the crystal structure of $(\text{C}_6\text{H}_5\text{CH}_2\text{CH}_2\text{NH}_3)_2\text{CoCl}_4$. Among the phenethylammonium-based compounds, several examples with tetrahedral anions are known to literature, for example, $(\text{C}_6\text{H}_5\text{C}_2\text{H}_4\text{NH}_3)_2\text{ZnBr}_4$ (Huh *et al.*, 2006), $(\text{C}_6\text{H}_5(\text{CH}_2)_2\text{NH}_3)_2\text{Cd}_{0.75}\text{Hg}_{0.25}\text{Br}_4$ (Zouari & Ben Salah, 2004), $(\text{C}_8\text{H}_{12}\text{N})\text{TlBr}_4$ (Abdi *et al.*, 2005). Except for $(\text{C}_8\text{H}_{12}\text{N})\text{TlBr}_4$, in which the heavy atom has trivalent, the other bivalent compounds have tetrahedral MBr_4 anions with non-magnetic ions in common. The present paper is the first report of the tetrahedral MCl_4 with magnetic ion using phenethylamine.

Fig. 1 shows the molecular structure of $(\text{C}_6\text{H}_5\text{CH}_2\text{CH}_2\text{NH}_3)_2\text{CoCl}_4$. The asymmetric unit of the title compound consists of two phenethylammonium cations and one isolated CoCl_4 anion; the latter is arranged as an distorted tetrahedron, whose bond lengths ranging from 2.229 (2) to 2.276 (2) Å (Table 1). Interestingly, the crystal structure exhibits a layered inorganic-organic structure although the dimension of inorganic backbone is 0-dimensional or isolated CoCl_4 tetrahedra, as shown in Fig. 2. The CoCl_4 tetrahedral groups are isolated and are connected to the organic cations by $\text{N—H}\cdots\text{Cl}$ hydrogen bonds *via* the NH_3 -groups. Tab. 2 and Fig. 2 display also the $\text{N—H}\cdots\text{Cl}$ hydrogen bonds of $(\text{C}_6\text{H}_5\text{CH}_2\text{CH}_2\text{NH}_3)_2\text{CoCl}_4$. Between the CoCl_4 layers, $-\text{CNH}_3^+$ ions are located in the space between CoCl_4 tetrahedra, which is formed by Cl atoms. $\text{N—H}\cdots\text{Cl}$ hydrogen bonds connect the two groups. The CoCl_4 tetrahedra connect the $\text{C}_6\text{H}_5\text{CH}_2\text{CH}_2\text{NH}_3^+$ ions through hydrogen bonds to build a two-dimensional hydrogen-bonded $\text{NH}_3-\text{CoCl}_4$ network. Due to the hydrogen bonds, the Co—Cl bond lengths increase, resulting in slightly deformed CoCl_4 tetrahedra. The obtained bond lengths suggest that the strength of the $\text{N—H}\cdots\text{Cl}$ hydrogen bonds in the structure can be classified as weak (Steiner, 1998; Steiner, 2002).

S2. Experimental

$\text{CoCl}_2\cdot 6\text{H}_2\text{O}$ (99%, Aldrich), phenethylamine ($\text{C}_6\text{H}_5\text{CH}_2\text{CH}_2\text{NH}_2$, 99.5%, Aldrich), HCl (37 wt % in water, Aldrich), and methanol (anhydrous, 99.8%, Aldrich) are used as received. For the preparation of single-crystal $(\text{C}_6\text{H}_5\text{CH}_2\text{CH}_2\text{NH}_3)_2\text{CoCl}_4$, 10 ml of a 0.25M $\text{CoCl}_2\cdot 6\text{H}_2\text{O}$ methanol solution were mixed with 10 ml of a 0.5M phenethylamine methanol solution. 1 mL of an HCl solution was added to the mixed solution. Blue crystals of $(\text{C}_6\text{H}_5\text{CH}_2\text{CH}_2\text{NH}_3)_2\text{CoCl}_4$ were obtained after 7 days at room temperature. Elemental analysis of C, H, and N was carried

out by CHNS analysis (CE Instrument EA 1112 series). The expected formula of $C_{16}H_{24}N_2Cl_4Co$ was confirmed. The relative weights calculated for $C_{16}H_{24}N_2Cl_4Co$ were: C, 43.17%, H, 5.43%, N, 6.29%; found: C, 43.14%, H, 5.44%, N, 6.23%.

S3. Refinement

H atoms bonded to C were positioned geometrically and refined based on a riding model ($C-H = 0.95 \text{ \AA}$ in aromatic ring and 0.99 \AA for CH_2) with $U_{iso}(H) = 1.2$ of their parent atoms. H atoms at N atoms were located in a difference map and refined with distance constrained of $N-H = 0.89 \text{ \AA}$, and with $U_{iso}(H) = 1.2U_{eq}(N)$. $C7-C8$ and $C15-C16$ bond lengths were refined with restrained distances $1.545(2) \text{ \AA}$.

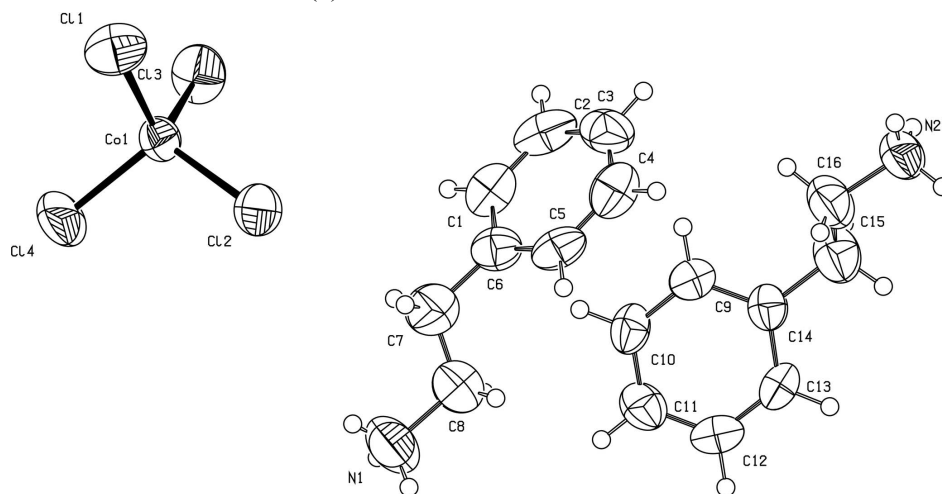


Figure 1

Molecular structure of $(C_6H_5CH_2CH_2NH_3)_2CoCl_4$, showing the atomic labeling and 50% probability displacement ellipsoids for non-H atoms.

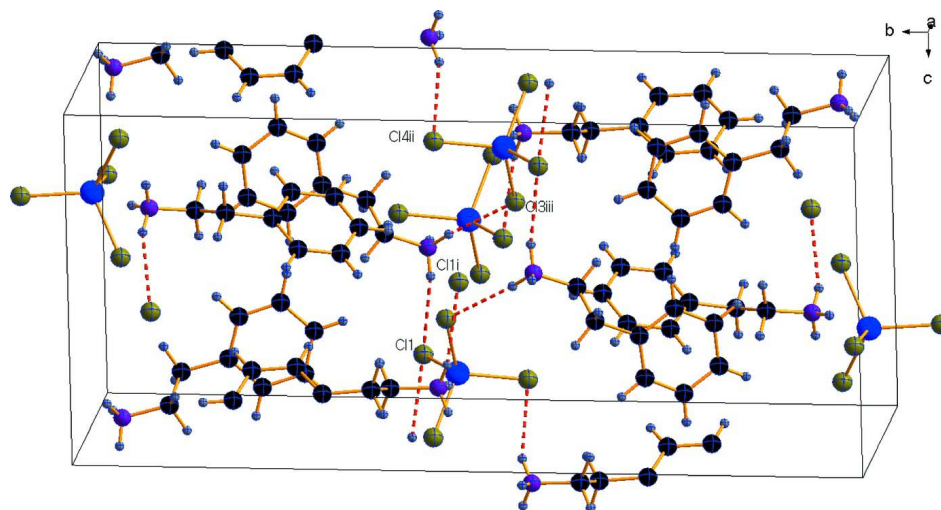


Figure 2

Crystal structure of $(C_6H_5CH_2CH_2NH_3)_2CoCl_4$ viewed along the a axis, showing the $N-H \cdots Cl$ hydrogen bonds as dashed lines.

Bis(2-phenylethylammonium) tetrachloridocobaltate(II)

Crystal data

(C₈H₁₂N)₂[CoCl₄]
M_r = 445.10
 Monoclinic, *P*2₁/*c*
 Hall symbol: -*P* 2ybc
a = 7.4623 (13) Å
b = 24.664 (3) Å
c = 11.1997 (16) Å
 β = 91.769 (13)°
V = 2060.3 (5) Å³
Z = 4

F(000) = 916
D_x = 1.435 Mg m⁻³
 Mo *K*α radiation, λ = 0.71073 Å
 Cell parameters from 38 reflections
 θ = 3.3–12.3°
 μ = 1.35 mm⁻¹
T = 296 K
 Rectangle, blue
 0.5 × 0.4 × 0.35 mm

Data collection

Bruker P4
 diffractometer
 Radiation source: fine-focus sealed tube
 Graphite monochromator
 2 θ / ω scans
 Absorption correction: multi-scan
 (*SADABS*; Sheldrick, 1996)
T_{min} = 0.237, *T_{max}* = 0.265
 4692 measured reflections

3595 independent reflections
 1566 reflections with *I* > 2σ(*I*)
R_{int} = 0.041
 θ_{\max} = 25.0°, θ_{\min} = 2.0°
h = -1→8
k = -1→29
l = -13→13
 3 standard reflections every 97 reflections
 intensity decay: none

Refinement

Refinement on *F*²
 Least-squares matrix: full
R[*F*² > 2σ(*F*²)] = 0.055
wR(*F*²) = 0.161
S = 1.03
 3595 reflections
 211 parameters
 2 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/[σ²(*F_o*²) + (0.0502*P*)²]
 where *P* = (*F_o*² + 2*F_c*²)/3
 (Δ/σ)_{max} = 0.001
 Δρ_{max} = 0.43 e Å⁻³
 Δρ_{min} = -0.30 e Å⁻³
 Extinction correction: *SHELXL*,
 $F_c^* = kF_c [1 + 0.001x F_c^2 \lambda^3 / \sin(2\theta)]^{-1/4}$
 Extinction coefficient: 0.0018 (7)

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

	<i>x</i>	<i>y</i>	<i>z</i>	<i>U_{iso}</i> [*] / <i>U_{eq}</i>
Co1	0.25951 (13)	0.52176 (4)	0.77334 (8)	0.0581 (3)
Cl1	0.0134 (3)	0.55281 (9)	0.67021 (18)	0.0911 (7)
Cl2	0.2717 (3)	0.55493 (8)	0.96063 (16)	0.0901 (7)
Cl3	0.5051 (3)	0.54580 (9)	0.67008 (18)	0.0895 (7)
Cl4	0.2382 (4)	0.43175 (8)	0.78339 (19)	0.1218 (11)
C1	0.3714 (10)	0.6982 (4)	0.1447 (7)	0.075 (2)
H1	0.3974	0.6694	0.0946	0.090*
C2	0.4215 (10)	0.7492 (4)	0.1131 (6)	0.081 (3)
H31	0.4849	0.7546	0.0439	0.097*
C3	0.3783 (11)	0.7927 (3)	0.1835 (8)	0.083 (2)
H3	0.4077	0.8278	0.1608	0.099*

C4	0.2910 (10)	0.7836 (4)	0.2879 (7)	0.081 (2)
H4	0.2642	0.8125	0.3376	0.097*
C5	0.2433 (9)	0.7316 (4)	0.3188 (6)	0.068 (2)
H5	0.1823	0.7258	0.3888	0.082*
C6	0.2847 (10)	0.6882 (3)	0.2473 (6)	0.066 (2)
C7	0.2286 (12)	0.6304 (4)	0.2746 (7)	0.099 (3)
H7A	0.0987	0.6285	0.2720	0.118*
H7B	0.2717	0.6067	0.2126	0.118*
C8	0.2921 (13)	0.6110 (3)	0.3860 (7)	0.106 (3)
H8A	0.2501	0.6346	0.4484	0.127*
H8B	0.4221	0.6121	0.3886	0.127*
C9	0.2308 (9)	0.2503 (3)	0.1306 (5)	0.0560 (17)
H9	0.2728	0.2687	0.1983	0.067*
C10	0.2513 (9)	0.1950 (3)	0.1235 (6)	0.0627 (19)
H10	0.3066	0.1762	0.1866	0.075*
C11	0.1908 (10)	0.1675 (3)	0.0243 (7)	0.069 (2)
H11	0.2044	0.1301	0.0198	0.083*
C12	0.1107 (10)	0.1951 (3)	-0.0676 (6)	0.067 (2)
H12	0.0702	0.1763	-0.1353	0.080*
C13	0.0887 (9)	0.2501 (3)	-0.0622 (5)	0.0608 (18)
H13	0.0334	0.2684	-0.1260	0.073*
C14	0.1485 (9)	0.2788 (3)	0.0380 (6)	0.0562 (17)
C15	0.1166 (11)	0.3392 (3)	0.0449 (7)	0.086 (2)
H15A	0.0752	0.3519	-0.0331	0.103*
H15B	0.0215	0.3458	0.1002	0.103*
C16	0.2724 (11)	0.3707 (3)	0.0826 (7)	0.085 (2)
H16A	0.3704	0.3625	0.0307	0.102*
H16B	0.3088	0.3602	0.1632	0.102*
N1	0.2316 (11)	0.5540 (3)	0.4099 (6)	0.115 (3)
H1A	0.1329	0.5469	0.3661	0.172*
H1B	0.2083	0.5505	0.4870	0.172*
H1C	0.3177	0.5309	0.3909	0.172*
N2	0.2383 (8)	0.4300 (2)	0.0799 (5)	0.0758 (18)
H2A	0.2107	0.4403	0.0053	0.114*
H2B	0.3362	0.4475	0.1059	0.114*
H2C	0.1476	0.4378	0.1267	0.114*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Co1	0.0607 (6)	0.0511 (5)	0.0628 (6)	0.0000 (5)	0.0052 (4)	-0.0041 (5)
Cl1	0.0673 (13)	0.1124 (17)	0.0931 (14)	0.0206 (13)	-0.0035 (11)	0.0131 (12)
Cl2	0.135 (2)	0.0655 (12)	0.0702 (12)	0.0041 (13)	0.0055 (13)	-0.0163 (10)
Cl3	0.0707 (13)	0.1058 (16)	0.0931 (14)	-0.0135 (13)	0.0222 (11)	-0.0084 (12)
Cl4	0.225 (3)	0.0497 (11)	0.0914 (15)	-0.0165 (16)	0.0130 (18)	-0.0131 (10)
C1	0.060 (5)	0.098 (6)	0.066 (5)	0.007 (5)	0.001 (4)	-0.013 (4)
C2	0.048 (5)	0.140 (8)	0.055 (4)	0.009 (6)	0.004 (4)	0.020 (5)
C3	0.068 (6)	0.082 (6)	0.097 (6)	-0.007 (5)	-0.017 (5)	0.030 (5)

C4	0.068 (6)	0.099 (7)	0.076 (5)	0.006 (5)	-0.005 (4)	-0.017 (5)
C5	0.059 (5)	0.104 (6)	0.043 (4)	0.009 (5)	0.007 (3)	0.006 (4)
C6	0.057 (5)	0.077 (5)	0.065 (5)	0.006 (4)	0.000 (4)	0.009 (4)
C7	0.101 (7)	0.099 (7)	0.095 (6)	-0.012 (6)	-0.019 (6)	0.013 (5)
C8	0.130 (9)	0.090 (7)	0.097 (6)	-0.034 (6)	-0.008 (6)	0.013 (5)
C9	0.056 (4)	0.063 (4)	0.049 (4)	-0.012 (4)	0.003 (3)	0.000 (3)
C10	0.062 (5)	0.060 (5)	0.065 (4)	-0.007 (4)	-0.007 (4)	0.019 (4)
C11	0.071 (5)	0.052 (4)	0.085 (5)	-0.007 (4)	0.002 (4)	-0.002 (4)
C12	0.066 (5)	0.083 (6)	0.050 (4)	-0.009 (4)	0.001 (4)	-0.016 (4)
C13	0.061 (5)	0.072 (5)	0.049 (4)	0.000 (4)	-0.009 (3)	0.014 (4)
C14	0.053 (4)	0.051 (4)	0.064 (4)	0.000 (4)	0.001 (4)	0.008 (3)
C15	0.077 (6)	0.066 (5)	0.115 (6)	-0.001 (5)	-0.010 (5)	0.007 (5)
C16	0.089 (6)	0.054 (5)	0.112 (6)	0.003 (5)	-0.011 (5)	-0.003 (4)
N1	0.177 (8)	0.066 (4)	0.103 (5)	-0.025 (5)	0.033 (5)	-0.003 (4)
N2	0.099 (5)	0.050 (4)	0.079 (4)	0.002 (3)	0.005 (4)	0.003 (3)

Geometric parameters (Å, °)

Co1—C14	2.229 (2)	C15—C16	1.451 (9)
Co1—C12	2.251 (2)	C16—N2	1.485 (8)
Co1—C11	2.272 (2)	C1—H1	0.931
Co1—C13	2.276 (2)	C2—H31	0.931
C1—C6	1.358 (9)	C3—H3	0.931
C1—C2	1.363 (10)	C4—H4	0.929
C2—C3	1.376 (10)	C5—H5	0.929
C3—C4	1.374 (10)	C7—H7A	0.970
C4—C5	1.377 (10)	C7—H7B	0.970
C5—C6	1.379 (10)	C8—H8A	0.968
C6—C7	1.519 (10)	C8—H8B	0.969
C7—C8	1.405 (9)	C9—H9	0.930
C8—N1	1.502 (9)	C10—H10	0.930
C9—C10	1.376 (8)	C11—H11	0.929
C9—C14	1.380 (8)	C12—H12	0.929
C10—C11	1.367 (9)	C13—H13	0.930
C11—C12	1.358 (9)	C15—H15A	0.970
C12—C13	1.368 (9)	C15—H15B	0.970
C13—C14	1.389 (8)	C16—H16A	0.970
C14—C15	1.510 (9)	C16—H16B	0.970
C14—Co1—C12	108.41 (8)	C16—C15—C14	114.6 (6)
C14—Co1—C11	107.67 (11)	C15—C16—N2	112.8 (7)
C12—Co1—C11	111.10 (9)	H5—C5—C4	119.6
C14—Co1—C13	110.19 (10)	H2A—N2—H2C	109.5
C12—Co1—C13	111.65 (9)	H2C—N2—H2B	109.4
C11—Co1—C13	107.75 (9)	H2A—N2—H2B	109.4
C6—C1—C2	122.0 (7)	C16—N2—H2A	109.4
C1—C2—C3	120.0 (7)	C16—N2—H2A	109.4
C4—C3—C2	119.1 (8)	C16—N2—H2B	109.5

C3—C4—C5	119.9 (8)	H1A—N1—C8	109.3
C4—C5—C6	120.9 (7)	H1B—N1—C8	109.4
C1—C6—C5	118.1 (7)	H1C—N1—C8	109.4
C1—C6—C7	118.9 (7)	H1A—N1—H1B	109.5
C5—C6—C7	123.0 (7)	H1B—N1—H1C	109.5
C8—C7—C6	114.3 (7)	H1A—N1—H1C	109.6
C7—C8—N1	112.5 (7)	C3—C4—H4	119.9
C10—C9—C14	120.6 (6)	C2—C3—H3	120.5
C11—C10—C9	120.3 (6)	C2—C1—H1	119.0
C12—C11—C10	119.6 (7)	H1—C1—C6	118.8
C11—C12—C13	121.0 (6)	C6—C7—H7B	108.5
C12—C13—C14	120.3 (6)	C6—C7—H7A	108.4
C9—C14—C13	118.2 (6)	C7—C8—H8B	108.9
C9—C14—C15	122.0 (6)	C7—C8—H8A	109.0
C13—C14—C15	119.7 (6)		
C6—C1—C2—C3	-2.5 (12)	C14—C9—C10—C11	0.2 (11)
C1—C2—C3—C4	2.6 (12)	C9—C10—C11—C12	0.2 (11)
C2—C3—C4—C5	-2.0 (11)	C10—C11—C12—C13	-0.4 (11)
C3—C4—C5—C6	1.1 (11)	C11—C12—C13—C14	0.1 (11)
C2—C1—C6—C5	1.7 (11)	C10—C9—C14—C13	-0.5 (10)
C2—C1—C6—C7	178.3 (7)	C10—C9—C14—C15	177.3 (6)
C4—C5—C6—C1	-0.9 (11)	C12—C13—C14—C9	0.4 (10)
C4—C5—C6—C7	-177.4 (7)	C12—C13—C14—C15	-177.5 (7)
C1—C6—C7—C8	125.0 (9)	C9—C14—C15—C16	49.4 (10)
C5—C6—C7—C8	-58.6 (11)	C13—C14—C15—C16	-132.8 (8)
C6—C7—C8—N1	179.3 (7)	C14—C15—C16—N2	176.0 (6)

Hydrogen-bond geometry (\AA , $^\circ$)

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
N2—H2C \cdots C11 ⁱ	0.89	2.62	3.445 (6)	156
N2—H2A \cdots C14 ⁱⁱ	0.89	2.51	3.321 (6)	152
N1—H1C \cdots C13 ⁱⁱⁱ	0.89	2.42	3.291 (8)	167
N1—H1B \cdots C11	0.89	2.55	3.382 (7)	156

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