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# Bis(2-phenylethylammonium) tetrachloridocobaltate(II)

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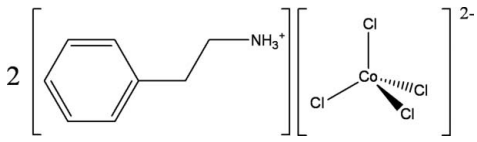
Key indicators: single-crystal X-ray study; $T$ = 296 K; mean $\sigma$(C–C) = 0.011 Å; $R$ factor = 0.055; $wR$ factor = 0.161; data-to-parameter ratio = 17.0.

Crystals of the title compound, $(C_6H_5CH_2CH_2NH_3)_2[CoCl_4]$, 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* N—H···Cl hydrogen bonds. The $CoCl_4$ tetrahedra connect to the cations through N—H···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

$(C_8H_{12}N)_2[CoCl_4]$
$M_r$ = 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) Å$^3$
$Z$ = 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)
$T_{min}$ = 0.237, $T_{max}$ = 0.265
4692 measured reflections
3595 independent reflections
1566 reflections with $I > 2\sigma(I)$
$R_{int}$ = 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
$\Delta\rho_{max}$ = 0.43 e Å$^{-3}$
$\Delta\rho_{min}$ = −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, °).

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| N2—H2$C$···Cl1$^{i}$ | 0.89 | 2.62 | 3.445 (6) | 156 |
| N2—H2$A$···Cl4$^{ii}$ | 0.89 | 2.51 | 3.321 (6) | 152 |
| N1—H1$C$···Cl3$^{iii}$ | 0.89 | 2.42 | 3.291 (8) | 167 |
| N1—H1$B$···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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# supplementary materials

*Acta Cryst.* (2011). E**67**, m522-m523 [ **doi:10.1107/S1600536811011603** ]

# Bis(2-phenylethylammonium) tetrachloridocobaltate(II)

**I.-H. Oh, D. Kim, Y.-D. Huh, Y. Park, J. M. S. Park and S.-H. Park**

## Comment

The title compound, $(C_6H_5CH_2CH_2NH_3)_2CoCl_4$, 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 $(C_6H_5CH_2CH_2NH_3)_2CoCl_4$. Among the phenethylammonium-based compounds, several examples with tetrahedral anions are known to literature, for example, $(C_6H_5C_2H_4NH_3)_2ZnBr_4$ (Huh *et al.*, 2006), $(C_6H_5(CH_2)_2NH_3)_2Cd_{0.75}Hg_{0.25}Br_4$ (Zouari & Ben Salah, 2004), $(C_8H_{12}N)TlBr_4$ (Abdi *et al.*, 2005). Except for $(C_8H_{12}N)TlBr_4$, 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 $(C_6H_5CH_2CH_2NH_3)_2CoCl_4$. 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 N—H···Cl hydrogen bonds *via* the $NH_3$-groups. Tab. 2 and Fig. 2 display also the N—H···Cl hydrogen bonds of $(C_6H_5CH_2CH_2NH_3)_2CoCl_4$. Between the $CoCl_4$ layers, —$CNH_3^+$ ions are located in the space between $CoCl_4$ tetrahedra, which is formed by Cl atoms. N—H···Cl hydrogen bonds connect the two groups. The $CoCl_4$ tetrahedra connect the $C_6H_5CH_2CH_2NH_3^+$ ions through hydrogen bonds to build a two-dimensional hydrogen-bonded $NH_3$—$CoCl_4$ 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 N—H···Cl hydrogen bonds in the structure can be classified as weak (Steiner, 1998; Steiner, 2002).

## Experimental

$CoCl_2{\cdot}6H_2O$ (99%, Aldrich), phenethylamine ($C_6H_5CH_2CH_2NH_2$, 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 $(C_6H_5CH_2CH_2NH_3)_2CoCl_4$, 10 ml of a 0.25*M* $CoCl_2{\cdot}6H_2O$ methanol solution were mixed with 10 ml of a 0.5*M* phenethylamine methanol solution. 1 mL of an HCl solution was added to the mixed solution. Blue crystals of $(C_6H_5CH_2CH_2NH_3)_2CoCl_4$ 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%.

### Refinement

H atoms bonded to C were positioned geometrically and refined based on a riding model (C—H = 0.95Å in aromatic ring and 0.99 Å 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 Å, and with $U_{iso}$(H) = 1.2$U_{eq}$(N). C7—C8 and C15—C16 bond lengths were refined with restrained distances 1.545 (2) Å.

### Figures

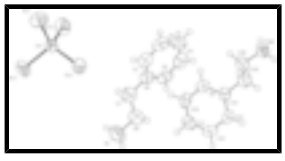

Fig. 1. Molecular structure of $(C_6H_5CH_2CH_2NH_3)_2CoCl_4$, showing the atomic labeling and 50% probability displacement elllisoids for non-H atoms.

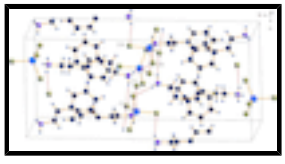

Fig. 2. Crystal structure of $(C_6H_5CH_2CH_2NH_3)_2CoCl_4$ viewed along the *a* axis, showing the N—H···Cl hydrogen bonds as dashed lines.

### Bis(2-phenylethylammonium) tetrachloridocobaltate(II)

*Crystal data*

| | |
|---|---|
| $(C_8H_{12}N)_2[CoCl_4]$ | $F(000) = 916$ |
| $M_r = 445.10$ | $D_x = 1.435$ Mg m$^{-3}$ |
| Monoclinic, $P2_1/c$ | Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å |
| Hall symbol: -P 2ybc | Cell parameters from 38 reflections |
| $a = 7.4623$ (13) Å | $\theta = 3.3$–$12.3°$ |
| $b = 24.664$ (3) Å | $\mu = 1.35$ mm$^{-1}$ |
| $c = 11.1997$ (16) Å | $T = 296$ K |
| $\beta = 91.769$ (13)° | Rectangle, blue |
| $V = 2060.3$ (5) Å$^3$ | 0.5 × 0.4 × 0.35 mm |
| $Z = 4$ | |

*Data collection*

| | |
|---|---|
| Bruker P4 diffractometer | 1566 reflections with $I > 2\sigma(I)$ |
| Radiation source: fine-focus sealed tube | $R_{int} = 0.041$ |
| graphite | $\theta_{max} = 25.0°$, $\theta_{min} = 2.0°$ |
| 2θ/ω scans | $h = -1 \rightarrow 8$ |
| Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996) | $k = -1 \rightarrow 29$ |

| | |
|---|---|
| $T_{min}$ = 0.237, $T_{max}$ = 0.265 | $l = -13 \rightarrow 13$ |
| 4692 measured reflections | 3 standard reflections every 97 reflections |
| 3595 independent reflections | intensity decay: none |

*Refinement*

| | |
|---|---|
| Refinement on $F^2$ | Secondary atom site location: difference Fourier map |
| Least-squares matrix: full | Hydrogen site location: inferred from neighbouring sites |
| $R[F^2 > 2\sigma(F^2)] = 0.055$ | H-atom parameters constrained |
| $wR(F^2) = 0.161$ | $w = 1/[\sigma^2(F_o^2) + (0.0502P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$ |
| $S = 1.03$ | $(\Delta/\sigma)_{max} = 0.001$ |
| 3595 reflections | $\Delta\rho_{max} = 0.43$ e Å$^{-3}$ |
| 211 parameters | $\Delta\rho_{min} = -0.30$ e Å$^{-3}$ |
| 2 restraints | Extinction correction: *SHELXL*, $Fc^* = kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$ |
| Primary atom site location: structure-invariant direct methods | Extinction coefficient: 0.0018 (7) |

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

| | *x* | *y* | *z* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| 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 (Å$^2$)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| 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—Cl4 | 2.229 (2) | C15—C16 | 1.451 (9) |
| Co1—Cl2 | 2.251 (2) | C16—N2 | 1.485 (8) |
| Co1—Cl1 | 2.272 (2) | C1—H1 | 0.931 |
| Co1—Cl3 | 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 |
| Cl4—Co1—Cl2 | 108.41 (8) | C16—C15—C14 | 114.6 (6) |
| Cl4—Co1—Cl1 | 107.67 (11) | C15—C16—N2 | 112.8 (7) |
| Cl2—Co1—Cl1 | 111.10 (9) | H5—C5—C4 | 119.6 |
| Cl4—Co1—Cl3 | 110.19 (10) | H2A—N2—H2C | 109.5 |
| Cl2—Co1—Cl3 | 111.65 (9) | H2C—N2—H2B | 109.4 |
| Cl1—Co1—Cl3 | 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 (Å, °)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| N2—H2C···Cl1$^{i}$ | 0.89 | 2.62 | 3.445 (6) | 156. |
| N2—H2A···Cl4$^{ii}$ | 0.89 | 2.51 | 3.321 (6) | 152. |
| N1—H1C···Cl3$^{iii}$ | 0.89 | 2.42 | 3.291 (8) | 167. |
| N1—H1B···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.

**Fig. 1**

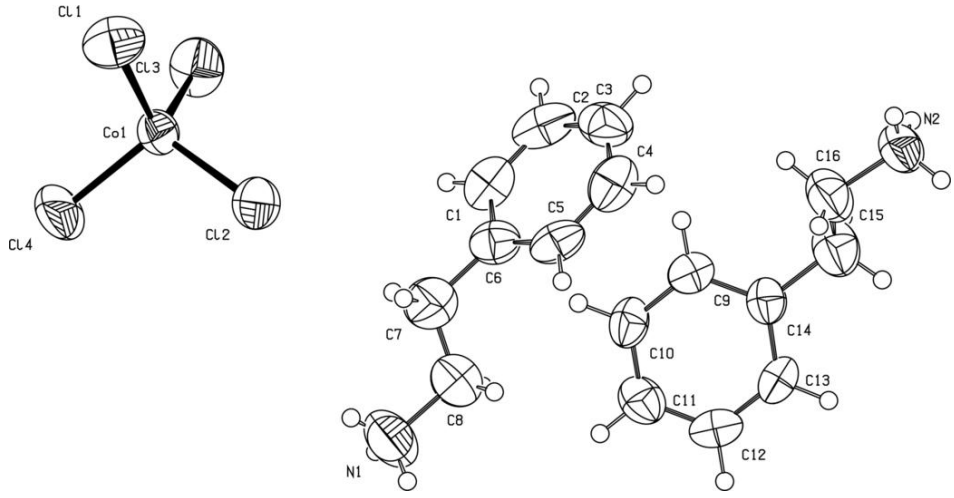
Cl1
Cl3
Co1
Cl4
Cl2
C2
C3
C4
C1
C5
C6
C7
C8
N1
C9
C10
C11
C12
C13
C14
C15
C16
N2

**Fig. 2**