

Acta Crystallographica Section E

Structure Reports

Online

ISSN 1600-5368

1-Phenylpiperazine-1,4-dium tetrachloridocobalt(II)

Abdelhamid Chiheb Dhib, ^a Daron E. Janzen, ^b Mohamed Rzaigui^a and Wajda Smirani Sta^{a*}^aLaboratoire de Chimie des Matériaux, Faculté des Sciences de Bizerte, 7021 Zarzouna Bizerte, Tunisia, and ^bDepartment of Chemistry and Biochemistry, St Catherine University, 2004 Randolph Avenue, #4282, St Paul, MN 55105, USA
Correspondence e-mail: wajda_sta@yahoo.fr

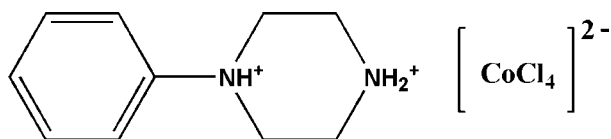
Received 12 March 2014; accepted 14 March 2014

Key indicators: single-crystal X-ray study; $T = 173$ K; mean $\sigma(\text{C}-\text{C}) = 0.003$ Å; R factor = 0.023; wR factor = 0.054; data-to-parameter ratio = 20.1.

In the title molecular salt, $(\text{C}_{10}\text{H}_{16}\text{N}_2)[\text{CoCl}_4]$, the piperazine ring of the phenylpiperazine dication adopts a chair conformation and the phenyl ring occupies an equatorial orientation. In the tetrachloridocobaltate(II) dianion, the Co—Cl bond lengths for the chloride ions not accepting hydrogen bonds are significantly shorter than those for the chloride ions accepting such bonds. In the crystal, the components are linked by $\text{N}-\text{H}\cdots\text{Cl}$ hydrogen bonds, generating [001] chains.

Related literature

For background to organic-inorganic hybrid materials, see: Bringley & Rajeswaran (2006); Brammer *et al.* (2002). For phenylpiperazinium cations, see: Ben Garbia *et al.* (2005). For related structures, see: Mghandef & Boughzala (2014); Wang *et al.* (2012).



Experimental

Crystal data

 $(\text{C}_{10}\text{H}_{16}\text{N}_2)[\text{CoCl}_4]$
 $M_r = 365.00$
Monoclinic, $P2_1/c$
 $a = 7.7400$ (9) Å
 $b = 20.278$ (3) Å
 $c = 9.6257$ (12) Å
 $\beta = 105.121$ (8)° $V = 1458.5$ (3) Å³
 $Z = 4$
Mo $K\alpha$ radiation
 $\mu = 1.89$ mm⁻¹
 $T = 173$ K
 $0.46 \times 0.32 \times 0.28$ mm

Data collection

Rigaku XtaLAB mini diffractometer
Absorption correction: multi-scan (*REQAB*; Rigaku, 1998)
 $T_{\min} = 0.465$, $T_{\max} = 0.589$ 15030 measured reflections
3335 independent reflections
3034 reflections with $F^2 > 2\sigma(F^2)$
 $R_{\text{int}} = 0.023$

Refinement

 $R[F^2 > 2\sigma(F^2)] = 0.023$
 $wR(F^2) = 0.054$
 $S = 1.14$
3335 reflections
166 parametersH atoms treated by a mixture of independent and constrained refinement
 $\Delta\rho_{\max} = 0.26$ e Å⁻³
 $\Delta\rho_{\min} = -0.36$ e Å⁻³**Table 1**
Selected bond lengths (Å).

Co1—Cl1	2.3182 (5)	Co1—Cl3	2.2738 (5)
Co1—Cl2	2.2431 (5)	Co1—Cl4	2.2811 (6)

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

$D-\text{H}\cdots A$	$D-\text{H}$	$\text{H}\cdots A$	$D\cdots A$	$D-\text{H}\cdots A$
$\text{N1}-\text{H1A}\cdots\text{Cl4}$	0.90 (3)	2.21 (3)	3.1043 (14)	173 (3)
$\text{N1}-\text{H1B}\cdots\text{Cl1}^i$	0.85 (2)	2.66 (3)	3.2963 (14)	132.2 (18)
$\text{N2}-\text{H2}\cdots\text{Cl1}^{ii}$	0.89 (3)	2.36 (2)	3.2262 (13)	164.6 (17)

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

Data collection: *CrystalClear-SM Expert* (Rigaku, 2011); cell refinement: *CrystalClear-SM Expert*; data reduction: *CrystalClear-SM Expert*; program(s) used to solve structure: *SIR2004* (Burla *et al.*, 2005); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 2012); software used to prepare material for publication: *CrystalStructure* (Rigaku, 2010).

We acknowledge the NSF-MRI grant No. 1125975 "MRI Consortium Acquisition of a Single Crystal X-ray Diffractometer for a Regional PUI Molecular Structure Facility".

Supporting information for this paper is available from the IUCr electronic archives (Reference: HB7210).

References

- Ben Garbia, I., Kefi, R., Rayes, A. & Ben Nasr, C. (2005). *Z. Kristallogr. New Cryst. Struct.* **220**, 333–334.
- Brammer, L., Swearingen, J. K., Bruton, E. A. & Sherwood, P. (2002). *Proc Natl Acad Sci USA*, **99**, 4956–4961.
- Bringley, J. F. & Rajeswaran, M. (2006). *Acta Cryst.* **E62**, m1304–m1305.
- Burla, M. C., Caliandro, R., Camalli, M., Carrozzini, B., Cascarano, G. L., De Caro, L., Giacovazzo, C., Polidori, G. & Spagna, R. (2005). *J. Appl. Cryst.* **38**, 381–388.
- Farrugia, L. J. (2012). *J. Appl. Cryst.* **45**, 849–854.
- Mghandef, M. & Boughzala, H. (2014). *Acta Cryst.* **E70**, m75.
- Rigaku (1998). *REQAB*. Rigaku Corporation, Tokyo, Japan.
- Rigaku (2010). *CrystalStructure*. Rigaku Corporation, Tokyo, Japan.
- Rigaku (2011). *CrystalClear-SM Expert*. Rigaku Corporation, Tokyo, Japan.
- Sheldrick, G. M. (2008). *Acta Cryst.* **A64**, 112–122.
- Wang, W.-Z., Ismayilov, R. H., Lee, G.-H., Wen, Y.-S. & Peng, S.-M. (2012). *Acta Cryst.* **E68**, m51.

supporting information

Acta Cryst. (2014). E70, m139 [doi:10.1107/S1600536814005790]

1-Phenylpiperazine-1,4-dium tetrachloridocobalt(II)

Abdelhamid Chiheb Dhieb, Daron E. Janzen, Mohamed Rzaigui and Wajda Smirani Sta

S1. Comment

Organic-inorganic hybrid materials have received extensive attention in recent years owing to their great fundamental and practical interest such as second-order nonlinear optical (NLO) responses, magnetism, luminescence, photography and drug delivery (Bringley & Rajeswaran, 2006). However, the energetics of $\text{NH}\cdots\text{Cl}-M$ ($M = \text{metal}$) hydrogen bonds and their possible roles in supramolecular chemistry have only been recently described in detail (Brammer *et al.*, 2002). It is therefore vital to design and synthesize new organic inorganic hybrid compound to explore their various properties.

The title inorganic-organic hybrid compound contains two basic components, the one $[\text{CoCl}_4]^{2-}$ anion and one $(\text{C}_{10}\text{H}_{16}\text{N}_2)^{2+}$ organic dication (Fig.1). The structure can be described by tetrachloridocobalt(II) units which form a hydrogen-bonded one-dimensional network with the phenylpiperazinium ($\text{N}-\text{H}\cdots\text{Cl}$: 3.1043 (14) Å, 3.2963 (14) Å, 3.2262 (13) Å of infinite ribbons located at $y = 0$ and $y = 1/2$ that translate along the c direction (Fig. 2). The vander Waals contacts between these ribbons give rise to a three-dimensional network in the structure and add stability to this structure. In the $[\text{CoCl}_4]$ tetrahedra, the $\text{Co}-\text{Cl}$ bond lengths and $\text{Cl}-\text{Co}-\text{Cl}$ angles, ranging from 2.2431 (5) to 2.3182 (5) Å and from 103.983 (1) to 116.304 (19)° respectively, are in agreement with those found in 1-(4-hydroxyphenyl)-piperazine-1,4-dium tetrachloridocobalt(II) monohydrate (Mghandef & Boughzala, 2014). The nearest $\text{Co}\cdots\text{Co}$ intra-chain distance is 6.044 Å, while that between adjacent chains is 7.441 Å. The organic cation, $(\text{C}_{10}\text{H}_{16}\text{N}_2)^{2+}$, contains a piperazindium ring in a chair conformation and a planar aromatic ring (atoms C5—C10 r.m.s. deviation = 0.003 Å). In this dication, the bond lengths of C5—C6, C5—C10, C6—C7, C7—C8, C8—C9 and C9—C10 are between single bonds and double bonds and are similar to those of benzene (Ben Garbia *et al.*, 2005). Furthermore, the distances N1—C4, N1—C1, N2—C5, N2—C2, N2—C3, C1—C2 and C3—C4 indicate single bonds.

In this compound, H1A and H2A attached to the N1 nitrogen atom and H2 attached to N2 nitrogen atom play an important role in forming the molecular association through hydrogen bonding. Here two chlorine atoms, Cl1 and Cl4, act as acceptors of $\text{N}-\text{H}\cdots\text{Cl}$ H-bonds. The chlorine atoms Cl2 and Cl3 do not participate in the hydrogen bonding network. The deviation from the perfect tetrahedral arrangement around Co(II) in the title compound can be explained by involvement of the chlorine ions in hydrogen bonding. Three different $[\text{CoCl}_4]^{2-}$ anions are act as hydrogen-bonding acceptors to each phenylpiperazinium dication forming two different hydrogen-bonding ring motifs, $R_2^4(14)$ and $R_4^4(12)$ (Fig.3). As Cl2 and Cl3 do not act as hydrogen-bond acceptors, the bond angles $\text{Cl2}-\text{Co}-\text{Cl3}$ and $\text{Cl2}-\text{Co}-\text{Cl4}$ (116.304 (19)° and 112.971 (19)°, respectively) display comparatively large deviations from the expected tetrahedral arrangement around Co(II). Similar features have been also observed in the structure of dimorpholinium tetrachloridocobaltate(II) (Wang *et al.*, 2012), where three chlorine atoms are engaged in the hydrogen-bonding network and distortions from tetrahedral predictions are present in the $\text{Cl}-\text{Co}-\text{Cl}$ angles. The structure of dimorpholinium tetrachloridocobaltate(II) also displays a $R_4^4(12)$ hydrogen bonding motif, but does not possess a second unique $R_2^4(14)$ motif that the title compound does exhibit.

S2. Experimental

A mixture of $\text{CoCl}_2 \cdot \text{H}_2\text{O}$ and phenylpiperazine was dissolved in an aqueous solution of hydrochloric acid (molar ratio 1:1:1). The obtained solution was stirred for 2 h and then kept at room temperature. Blue prisms of the title compound were obtained two weeks later.

S3. Refinement

Many hydrogen atoms were treated in calculated positions and refined in the model as riding with distances of $\text{C}-\text{H} = 0.95$ and 0.99 \AA for the phenyl and methylene groups, respectively, and with $U_{\text{iso}}(\text{H}) = k \times U_{\text{eq}}(\text{C})$, $k = 1.2$. Hydrogen atoms H1A, H1B, and H2 were located in the electron density map, and their positions were refined with $U_{\text{iso}}(\text{H}) = k \times U_{\text{eq}}(\text{C})$, $k = 1.2$.

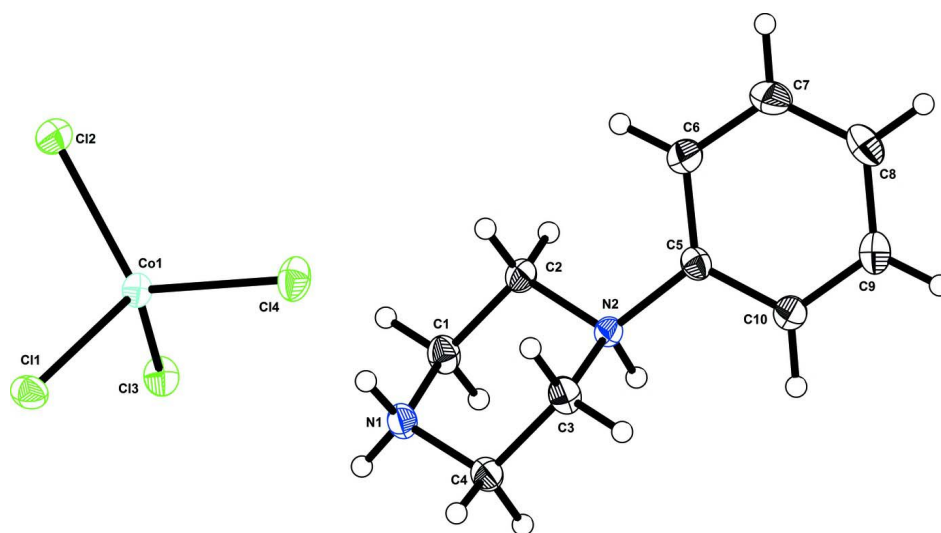


Figure 1

ORTEP-3 view of the title compound with displacement ellipsoids drawn at the 30% probability level.

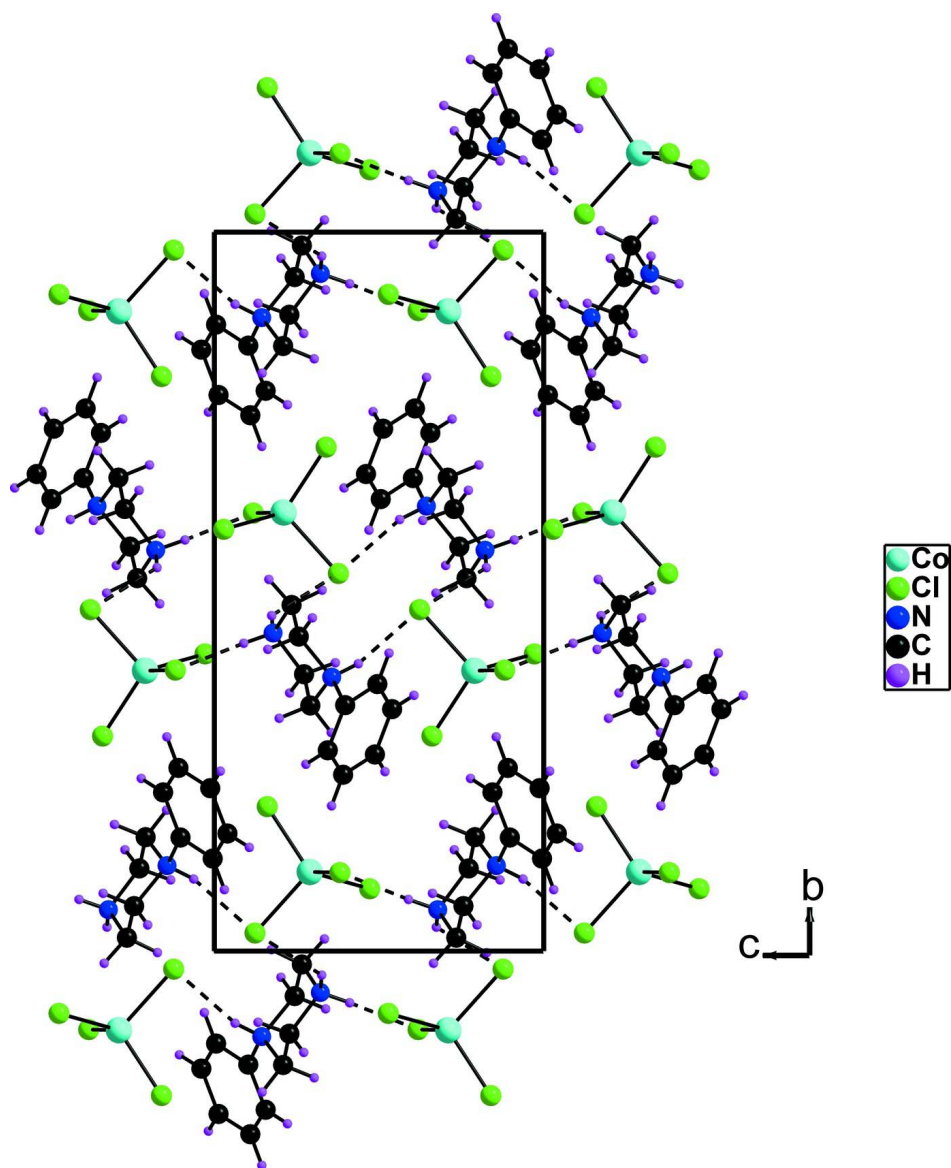


Figure 2

View of the atomic arrangement of the title compound along the a axis. Hydrogen bonds are shown as dashed lines.

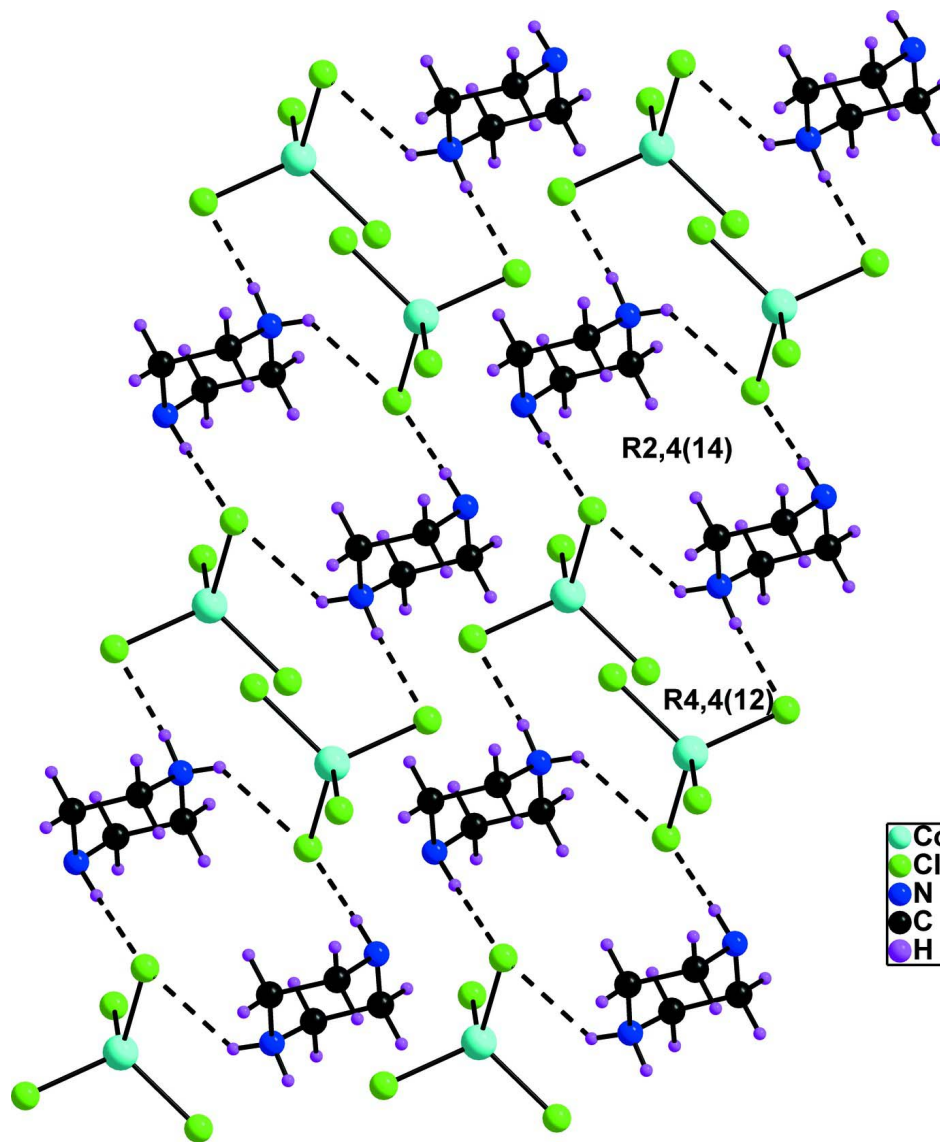


Figure 3

Graph-set description of ring types hydrogen bonding. Hydrogen bonds are shown as dashed lines.

1-Phenylpiperazine-1,4-dium tetrachloridocobalt(II)

Crystal data

(C₁₀H₁₆N₂)[CoCl₄]

$M_r = 365.00$

Monoclinic, $P2_1/c$

Hall symbol: -P 2ybc

$a = 7.7400$ (9) Å

$b = 20.278$ (3) Å

$c = 9.6257$ (12) Å

$\beta = 105.121$ (8)°

$V = 1458.5$ (3) Å³

$Z = 4$

$F(000) = 740.00$

$D_x = 1.662$ Mg m⁻³

Mo $K\alpha$ radiation, $\lambda = 0.71075$ Å

Cell parameters from 14000 reflections

$\theta = 3.0$ – 27.6 °

$\mu = 1.89$ mm⁻¹

$T = 173$ K

Prism, blue

$0.46 \times 0.32 \times 0.28$ mm

Data collection

Rigaku XtaLAB mini
diffractometer
Detector resolution: 6.849 pixels mm⁻¹
 ω scans
Absorption correction: multi-scan
(*REQAB*; Rigaku, 1998)
 $T_{\min} = 0.465$, $T_{\max} = 0.589$
15030 measured reflections

3335 independent reflections
3034 reflections with $F^2 > 2\sigma(F^2)$
 $R_{\text{int}} = 0.023$
 $\theta_{\text{max}} = 27.5^\circ$
 $h = -10 \rightarrow 10$
 $k = -26 \rightarrow 26$
 $l = -12 \rightarrow 12$

Refinement

Refinement on F^2
 $R[F^2 > 2\sigma(F^2)] = 0.023$
 $wR(F^2) = 0.054$
 $S = 1.14$
3335 reflections
166 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 atoms treated by a mixture of independent
and constrained refinement
 $w = 1/[\sigma^2(F_o^2) + (0.0197P)^2 + 0.6924P]$
where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\text{max}} = 0.001$
 $\Delta\rho_{\text{max}} = 0.26 \text{ e } \text{Å}^{-3}$
 $\Delta\rho_{\text{min}} = -0.36 \text{ e } \text{Å}^{-3}$

Special details

Geometry. ENTER SPECIAL DETAILS OF THE MOLECULAR GEOMETRY

Refinement. Refinement was performed using all reflections. The weighted R -factor (wR) and goodness of fit (S) are based on F^2 . R -factor (gt) are based on F . The threshold expression of $F^2 > 2.0 \sigma(F^2)$ is used only for calculating R -factor (gt).

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

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
Co1	0.14256 (3)	0.110059 (11)	0.71031 (2)	0.01829 (7)
Cl1	0.17830 (5)	0.025120 (19)	0.87659 (4)	0.02225 (9)
Cl2	0.12699 (6)	0.20091 (2)	0.83944 (4)	0.02466 (10)
Cl3	-0.10305 (5)	0.08669 (2)	0.52831 (4)	0.02264 (9)
Cl4	0.38614 (5)	0.10918 (2)	0.61855 (4)	0.02585 (10)
N1	0.16483 (19)	0.05757 (7)	0.32178 (15)	0.0196 (3)
N2	0.36753 (17)	0.11889 (6)	0.14374 (14)	0.0156 (3)
C1	0.0927 (3)	0.11496 (8)	0.22774 (18)	0.0212 (4)
C2	0.2443 (2)	0.15844 (8)	0.20870 (18)	0.0195 (4)
C3	0.4446 (2)	0.06256 (8)	0.24379 (18)	0.0207 (4)
C4	0.2953 (3)	0.01865 (8)	0.26558 (18)	0.0213 (4)
C5	0.5097 (2)	0.15791 (8)	0.10288 (16)	0.0171 (3)
C6	0.5541 (3)	0.22071 (9)	0.15569 (19)	0.0255 (4)
C7	0.6844 (3)	0.25474 (9)	0.1091 (2)	0.0291 (4)
C8	0.7669 (3)	0.22656 (9)	0.01261 (19)	0.0261 (4)
C9	0.7195 (3)	0.16350 (9)	-0.03960 (18)	0.0234 (4)
C10	0.5899 (3)	0.12865 (8)	0.00517 (18)	0.0204 (4)
H1C	0.0121	0.1409	0.2714	0.0255*
H1D	0.0222	0.0990	0.1326	0.0255*

H1A	0.221 (3)	0.0719 (12)	0.411 (3)	0.040 (7)*
H1B	0.076 (3)	0.0334 (11)	0.326 (3)	0.027 (6)*
H2A	0.1951	0.1961	0.1451	0.0234*
H2B	0.3115	0.1762	0.3032	0.0234*
H2	0.305 (3)	0.1003 (10)	0.063 (3)	0.025 (5)*
H3A	0.5136	0.0803	0.3377	0.0248*
H3B	0.5271	0.0364	0.2024	0.0248*
H4A	0.2329	-0.0020	0.1729	0.0256*
H4B	0.3465	-0.0169	0.3344	0.0256*
H6	0.4972	0.2401	0.2220	0.0306*
H7	0.7172	0.2980	0.1441	0.0349*
H8	0.8561	0.2503	-0.0181	0.0313*
H9	0.7761	0.1442	-0.1062	0.0281*
H10	0.5565	0.0855	-0.0303	0.0245*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Co1	0.01922 (12)	0.02023 (12)	0.01622 (11)	0.00007 (8)	0.00605 (9)	0.00011 (8)
Cl1	0.0271 (2)	0.01947 (19)	0.01833 (18)	-0.00352 (15)	0.00258 (15)	0.00167 (15)
Cl2	0.0297 (3)	0.0210 (2)	0.0247 (2)	0.00116 (16)	0.00976 (17)	-0.00198 (16)
Cl3	0.01909 (19)	0.0276 (2)	0.02077 (19)	-0.00029 (15)	0.00430 (15)	0.00099 (16)
Cl4	0.0190 (2)	0.0383 (3)	0.0214 (2)	-0.00280 (16)	0.00730 (16)	-0.00424 (17)
N1	0.0193 (7)	0.0222 (8)	0.0189 (7)	-0.0024 (6)	0.0078 (6)	0.0004 (6)
N2	0.0167 (7)	0.0167 (7)	0.0139 (7)	-0.0018 (5)	0.0048 (5)	-0.0016 (5)
C1	0.0188 (8)	0.0235 (9)	0.0228 (9)	0.0029 (7)	0.0079 (7)	0.0035 (7)
C2	0.0208 (8)	0.0184 (8)	0.0217 (8)	0.0023 (6)	0.0095 (7)	-0.0008 (7)
C3	0.0192 (8)	0.0211 (9)	0.0232 (8)	0.0038 (7)	0.0080 (7)	0.0050 (7)
C4	0.0243 (9)	0.0180 (8)	0.0243 (8)	0.0009 (7)	0.0111 (7)	0.0019 (7)
C5	0.0160 (8)	0.0194 (8)	0.0155 (8)	-0.0018 (6)	0.0033 (6)	0.0018 (6)
C6	0.0285 (9)	0.0239 (9)	0.0267 (9)	-0.0053 (7)	0.0118 (8)	-0.0064 (8)
C7	0.0293 (10)	0.0231 (9)	0.0360 (10)	-0.0087 (7)	0.0106 (8)	-0.0050 (8)
C8	0.0204 (9)	0.0296 (10)	0.0285 (9)	-0.0056 (7)	0.0066 (7)	0.0064 (8)
C9	0.0208 (8)	0.0307 (10)	0.0204 (8)	0.0016 (7)	0.0082 (7)	0.0019 (7)
C10	0.0209 (8)	0.0208 (8)	0.0201 (8)	-0.0007 (7)	0.0062 (7)	-0.0011 (7)

Geometric parameters (Å, °)

Co1—Cl1	2.3182 (5)	N1—H1A	0.90 (3)
Co1—Cl2	2.2431 (5)	N1—H1B	0.86 (3)
Co1—Cl3	2.2738 (5)	N2—H2	0.89 (2)
Co1—Cl4	2.2811 (6)	C1—H1C	0.990
N1—C1	1.491 (2)	C1—H1D	0.990
N1—C4	1.490 (3)	C2—H2A	0.990
N2—C2	1.502 (3)	C2—H2B	0.990
N2—C3	1.513 (2)	C3—H3A	0.990
N2—C5	1.489 (3)	C3—H3B	0.990
C1—C2	1.517 (3)	C4—H4A	0.990

C3—C4	1.516 (3)	C4—H4B	0.990
C5—C6	1.381 (3)	C6—H6	0.950
C5—C10	1.388 (3)	C7—H7	0.950
C6—C7	1.389 (3)	C8—H8	0.950
C7—C8	1.381 (3)	C9—H9	0.950
C8—C9	1.388 (3)	C10—H10	0.950
C9—C10	1.385 (3)		
C11—Co1—C12	103.983 (19)	N1—C1—H1C	109.580
C11—Co1—C13	107.597 (18)	N1—C1—H1D	109.572
C11—Co1—C14	107.440 (18)	C2—C1—H1C	109.578
C12—Co1—C13	116.304 (19)	C2—C1—H1D	109.582
C12—Co1—C14	112.971 (19)	H1C—C1—H1D	108.117
C13—Co1—C14	108.021 (19)	N2—C2—H2A	109.754
C1—N1—C4	112.03 (14)	N2—C2—H2B	109.749
C2—N2—C3	109.03 (13)	C1—C2—H2A	109.748
C2—N2—C5	114.81 (12)	C1—C2—H2B	109.747
C3—N2—C5	111.93 (12)	H2A—C2—H2B	108.227
N1—C1—C2	110.37 (13)	N2—C3—H3A	109.634
N2—C2—C1	109.60 (13)	N2—C3—H3B	109.651
N2—C3—C4	110.07 (12)	C4—C3—H3A	109.646
N1—C4—C3	110.63 (14)	C4—C3—H3B	109.646
N2—C5—C6	121.53 (16)	H3A—C3—H3B	108.161
N2—C5—C10	116.34 (14)	N1—C4—H4A	109.525
C6—C5—C10	122.09 (17)	N1—C4—H4B	109.519
C5—C6—C7	118.12 (18)	C3—C4—H4A	109.521
C6—C7—C8	120.89 (17)	C3—C4—H4B	109.518
C7—C8—C9	120.01 (18)	H4A—C4—H4B	108.083
C8—C9—C10	120.14 (18)	C5—C6—H6	120.943
C5—C10—C9	118.76 (16)	C7—C6—H6	120.939
C1—N1—H1A	109.7 (15)	C6—C7—H7	119.555
C1—N1—H1B	107.3 (13)	C8—C7—H7	119.550
C4—N1—H1A	108.0 (16)	C7—C8—H8	119.998
C4—N1—H1B	110.1 (15)	C9—C8—H8	119.996
H1A—N1—H1B	110 (3)	C8—C9—H9	119.930
C2—N2—H2	109.3 (15)	C10—C9—H9	119.935
C3—N2—H2	105.8 (13)	C5—C10—H10	120.626
C5—N2—H2	105.5 (15)	C9—C10—H10	120.617
C1—N1—C4—C3	55.10 (15)	N1—C1—C2—N2	58.69 (16)
C4—N1—C1—C2	-56.04 (16)	N2—C3—C4—N1	-56.76 (16)
C2—N2—C3—C4	59.86 (14)	N2—C5—C6—C7	-178.07 (11)
C3—N2—C2—C1	-60.67 (13)	N2—C5—C10—C9	178.25 (11)
C2—N2—C5—C6	16.73 (17)	C6—C5—C10—C9	0.5 (3)
C2—N2—C5—C10	-161.00 (11)	C10—C5—C6—C7	-0.5 (3)
C5—N2—C2—C1	172.84 (10)	C5—C6—C7—C8	0.1 (3)
C3—N2—C5—C6	-108.25 (14)	C6—C7—C8—C9	0.2 (3)
C3—N2—C5—C10	74.02 (15)	C7—C8—C9—C10	-0.2 (3)

C5—N2—C3—C4 -172.01 (11) C8—C9—C10—C5 -0.2 (3)

Hydrogen-bond geometry (Å, °)

<i>D</i> —H \cdots <i>A</i>	<i>D</i> —H	H \cdots <i>A</i>	<i>D</i> \cdots <i>A</i>	<i>D</i> —H \cdots <i>A</i>
N1—H1A \cdots C14	0.90 (3)	2.21 (3)	3.1043 (14)	173 (3)
N1—H1B \cdots C11 ⁱ	0.85 (2)	2.66 (3)	3.2963 (14)	132.2 (18)
N2—H2 \cdots C11 ⁱⁱ	0.89 (3)	2.36 (2)	3.2262 (13)	164.6 (17)

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