

Bis[hexaamminecobalt(III)] penta-chloride nitrate

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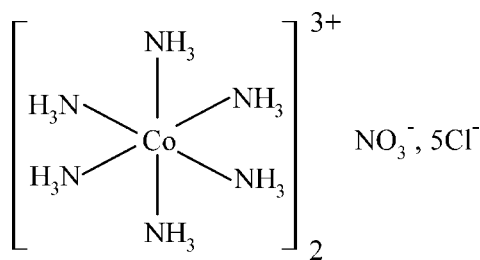
Received 26 April 2012; accepted 10 May 2012

Key indicators: single-crystal X-ray study; $T = 296$ K; mean $\sigma(\text{O}-\text{N}) = 0.005$ Å; R factor = 0.050; wR factor = 0.140; data-to-parameter ratio = 23.6.

The title compound, $[\text{Co}(\text{NH}_3)_6]_2\text{Cl}_5(\text{NO}_3)$, was obtained under hydrothermal conditions. The asymmetric unit contains three Co^{3+} ions, one lying on an inversion center and the other two located at $2/m$ positions. All Co^{3+} ions are six-coordinated by NH_3 molecules, forming $[\text{Co}(\text{NH}_3)_6]^{3+}$ octahedra, with $\text{Co}-\text{N}$ distances in the range 1.945 (4)–1.967 (3) Å. The nitrate N atom and one of the O atoms lie at a mirror plane. Among the Cl^- anions, one lies in a general position, one on a twofold axis and two on a mirror plane. $\text{N}-\text{H}\cdots\text{O}$ and $\text{N}-\text{H}\cdots\text{Cl}$ hydrogen bonds link the cations and anions into a three-dimensional network.

Related literature

For metal phosphates and germanates prepared using metal complexes as templates, see: Wang *et al.* (2003*a,b*); Pan *et al.* (2005, 2008). For our continued research interest focused on the synthesis of microporous open-framework metal-organic hybrid materials by introducing transition metal complexes as templates, see: Pan *et al.* (2010*a,b*, 2011); Tong & Pan (2011); Liang *et al.* (2011). For a structure containing a $[\text{Co}(\text{NH}_3)_6]^{3+}$ cation, see: Han *et al.* (2012).



Experimental

Crystal data

$[\text{Co}(\text{NH}_3)_6]_2\text{Cl}_5(\text{NO}_3)$	$V = 2165.8$ (6) Å ³
$M_r = 561.53$	$Z = 4$
Monoclinic, $C2/m$	Mo $K\alpha$ radiation
$a = 21.118$ (4) Å	$\mu = 2.18$ mm ⁻¹
$b = 14.985$ (3) Å	$T = 296$ K
$c = 6.8491$ (11) Å	$0.20 \times 0.12 \times 0.10$ mm
$\beta = 92.147$ (3)°	

Data collection

Bruker APEXII CCD area-detector diffractometer	7927 measured reflections
Absorption correction: multi-scan (<i>SADABS</i> ; Bruker, 2005)	2813 independent reflections
$T_{\min} = 0.738$, $T_{\max} = 0.770$	1870 reflections with $I > 2\sigma(I)$
	$R_{\text{int}} = 0.046$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.050$	119 parameters
$wR(F^2) = 0.140$	H-atom parameters constrained
$S = 1.02$	$\Delta\rho_{\max} = 0.65$ e Å ⁻³
2813 reflections	$\Delta\rho_{\min} = -0.71$ e Å ⁻³

Table 1

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
N1–H1A \cdots Cl1	0.89	2.89	3.427 (4)	120
N1–H1A \cdots Cl3 ⁱ	0.89	2.90	3.484 (4)	125
N1–H1B \cdots Cl1 ⁱⁱ	0.89	2.59	3.410 (4)	154
N1–H1C \cdots Cl3 ⁱⁱⁱ	0.89	2.63	3.431 (4)	150
N3–H3A \cdots O2 ^{iv}	0.89	2.53	3.155 (6)	128
N4–H4A \cdots Cl3 ^v	0.89	2.79	3.287 (4)	117
N4–H4B \cdots Cl4	0.89	2.62	3.448 (5)	155
N4–H4C \cdots Cl2 ^v	0.89	2.73	3.321 (4)	125
N5–H5A \cdots Cl1 ^{vi}	0.89	2.77	3.375 (4)	127
N5–H5A \cdots Cl4 ^{vii}	0.89	2.91	3.456 (4)	122
N5–H5B \cdots O2 ^{viii}	0.89	2.17	3.048 (5)	168
N5–H5C \cdots Cl3 ^{vi}	0.89	2.56	3.337 (4)	146
N6–H6A \cdots Cl4 ^{vii}	0.89	2.76	3.339 (4)	124
N6–H6C \cdots Cl3 ^{viii}	0.89	2.93	3.445 (4)	118
N7–H7A \cdots Cl4 ^{iv}	0.89	2.78	3.368 (4)	125
N7–H7B \cdots Cl3 ^{viii}	0.89	2.87	3.394 (4)	119

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

Data collection: *APEX2* (Bruker, 2005); cell refinement: *SAINTE* (Bruker, 2005); data reduction: *SAINTE*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL*.

This work was supported by the Program for New Century Excellent Talents in Universities (NCET-11-0929), the National Natural Science Foundation of China (No. 21101047), the Natural Science Foundation of Hainan Province (No. 211010) and the Priming Scientific Research Foundation of Hainan University (No. kyqd1051).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: YK2056).

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supporting information

Acta Cryst. (2012). E68, i45–i46 [doi:10.1107/S1600536812021332]

Bis[hexaamminecobalt(III)] pentachloride nitrate**Qihui Wu, Chunyu Du, Yang Lv, Guoliang Chen and Qinhe Pan****S1. Comment**

Recently, more attention has been paid to transition metal complexes, because they can be employed as templates in the synthesis of various open-framework materials, including metal phosphates (Wang *et al.*, 2003*a,b*) and germanates (Pan *et al.*, 2005,2008). Our continued interest has been focused on the synthesis of microporous open-framework metal-organic hybrid materials by introducing transition metal complexes as templates (Pan *et al.*, 2010*a,b*, 2011; Tong & Pan, 2011; Liang *et al.*, 2011). Unexpectedly, the title compound, $[\text{Co}(\text{NH}_3)_6]_2(\text{NO}_3)\text{Cl}_5$, was obtained.

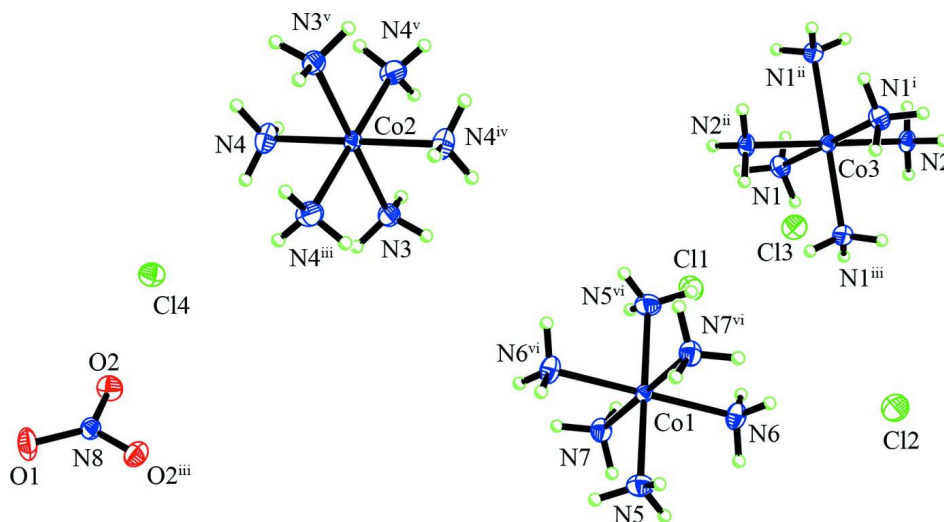
The title compound is composed of $[\text{Co}(\text{NH}_3)_6]^{3+}$ cations and the counterions Cl^- and NO_3^- , as shown in Fig. 1. The asymmetric part of this crystal structure contains three Co^{3+} ions; one is located on an inversion center, and the other two are positioned on the twofold rotation axis with center of symmetry (2/m). All Co(III) ions are six coordinated by NH_3 molecules to form $[\text{Co}(\text{NH}_3)_6]^{3+}$ cations, having a slightly distorted octahedral geometry, as in the structure of $[\text{Co}(\text{NH}_3)_6]_3[\text{Zn}_8(\text{HPO}_4)_8(\text{PO}_4)_2](\text{PO}_4)$ (Han *et al.*, 2012). The Co—N bond distances are in the range from 1.945 (4) to 1.967 (3) Å. For the counterions, the N8 atom of NO_3^- anion is located on mirror plane and displays a trigonal geometry by bonded to three O atoms with the N—O distances of 1.234 (6)–1.253 (4) Å. The Cl^- anions are located in different positions: inversion center for Cl2, mirror plane for Cl1 and Cl4, and general position for Cl3. The $[\text{Co}(\text{NH}_3)_6]^{3+}$ cations interact with the counterions Cl^- and NO_3^- via hydrogen bonds; the distances of N—H \cdots O hydrogen bonds are in the range 3.048 (5)–3.155 (6) Å, and the distances of N—H \cdots Cl hydrogen bonds lie in the range from 3.287 (4) to 3.484 (4) Å (Table 1), to form an extensive three-dimensional hydrogen-bonding network.

S2. Experimental

In a typical synthesis, a mixture of $\text{Cd}(\text{NO}_3)_2 \cdot 4\text{H}_2\text{O}$ (0.231 g), pyromellitic acid (0.0254 g), $[\text{Co}(\text{NH}_3)_6]\text{Cl}_3$ (0.03 g), NaOH (0.016 g) and H_2O (10 ml) were added in a 20 ml Teflon-lined reactor under autogenous pressure at 100°C for 3 days. Yellow rod-like crystals were obtained.

S3. Refinement

All H atoms were positioned geometrically (N—H = 0.89 Å) and allowed to ride on their parent atoms, with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{parent atom})$.

**Figure 1**

A view of the asymmetric unit of title compound showing the atom labelling scheme. Ellipsoids are drawn at the 30% probability level. [Symmetry codes: (i) $-x, 1 - y, -z$; (ii) $-x, y, -z$; (iii) $x, 1 - y, z$; (iv) $1 - x, 1 - y, -z$; (v) $1 - x, y, -z$; (vi) $1/2 - x, 1/2 - y, 1 - z$. (iv) $x, -y + 1, z$; (v) $-x, -y + 1, -z$; (vi) $-x, y, -z$.

Bis[hexaamminecobalt(III)] pentachloride nitrate

Crystal data

$[\text{Co}(\text{NH}_3)_6]_2\text{Cl}_5(\text{NO}_3)$

$M_r = 561.53$

Monoclinic, $C2/m$

Hall symbol: $-C 2y$

$a = 21.118 (4) \text{ \AA}$

$b = 14.985 (3) \text{ \AA}$

$c = 6.8491 (11) \text{ \AA}$

$\beta = 92.147 (3)^\circ$

$V = 2165.8 (6) \text{ \AA}^3$

$Z = 4$

$F(000) = 1160$

$D_x = 1.722 \text{ Mg m}^{-3}$

Mo $K\alpha$ radiation, $\lambda = 0.71073 \text{ \AA}$

Cell parameters from 7927 reflections

$\theta = 1.7\text{--}28.4^\circ$

$\mu = 2.18 \text{ mm}^{-1}$

$T = 296 \text{ K}$

Rod, yellow

$0.2 \times 0.12 \times 0.10 \text{ mm}$

Data collection

Bruker APEXII CCD area-detector
diffractometer

Radiation source: fine-focus sealed tube

Graphite monochromator

Detector resolution: $83.66 \text{ pixels mm}^{-1}$

φ and ω scans

Absorption correction: multi-scan

(*SADABS*; Bruker, 2005)

$T_{\min} = 0.738, T_{\max} = 0.770$

7927 measured reflections

2813 independent reflections

1870 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.046$

$\theta_{\max} = 28.4^\circ, \theta_{\min} = 1.7^\circ$

$h = -27 \rightarrow 28$

$k = -19 \rightarrow 20$

$l = -6 \rightarrow 9$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.050$

$wR(F^2) = 0.140$

$S = 1.02$

2813 reflections

119 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 constrained

$$w = 1/[\sigma^2(F_o^2) + (0.0641P)^2 + 4.8344P]$$

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

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

$$\Delta\rho_{\max} = 0.65 \text{ e } \text{\AA}^{-3}$$

$$\Delta\rho_{\min} = -0.71 \text{ e } \text{\AA}^{-3}$$

Special details

Geometry. All s.u.'s (except the s.u. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell s.u.'s are taken into account individually in the estimation of s.u.'s in distances, angles and torsion angles; correlations between s.u.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell s.u.'s is used for estimating s.u.'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>	$U_{\text{iso}}^*/U_{\text{eq}}$
Co1	0.2500	0.2500	0.5000	0.0193 (2)
N7	0.25395 (17)	0.3197 (3)	0.7422 (5)	0.0329 (9)
H7A	0.2923	0.3440	0.7585	0.040*
H7B	0.2465	0.2842	0.8429	0.040*
H7C	0.2249	0.3627	0.7353	0.040*
N6	0.16170 (16)	0.2158 (3)	0.5415 (5)	0.0342 (9)
H6A	0.1477	0.1812	0.4434	0.041*
H6B	0.1378	0.2646	0.5463	0.041*
H6C	0.1596	0.1861	0.6535	0.041*
N5	0.27844 (19)	0.1439 (3)	0.6414 (6)	0.0401 (10)
H5A	0.2811	0.0984	0.5585	0.048*
H5B	0.2509	0.1306	0.7323	0.048*
H5C	0.3164	0.1541	0.6982	0.048*
Co2	0.5000	0.5000	0.0000	0.0212 (3)
Cl4	0.66930 (8)	0.5000	0.4229 (2)	0.0350 (4)
N4	0.55640 (18)	0.5926 (3)	0.1076 (6)	0.0411 (10)
H4A	0.5852	0.6062	0.0208	0.049*
H4B	0.5758	0.5727	0.2168	0.049*
H4C	0.5339	0.6410	0.1341	0.049*
N3	0.4522 (2)	0.5000	0.2394 (7)	0.0329 (12)
H3A	0.4278	0.4517	0.2435	0.040*
H3B	0.4787	0.5000	0.3435	0.040*
Co3	0.0000	0.5000	0.0000	0.0208 (3)
N2	-0.0927 (2)	0.5000	-0.0085 (7)	0.0289 (11)
H2A	-0.1072	0.4517	-0.0712	0.035*
H2B	-0.1075	0.5000	0.1114	0.035*
N1	0.00050 (17)	0.5934 (3)	0.2019 (5)	0.0330 (9)
H1A	0.0403	0.6075	0.2360	0.040*
H1B	-0.0191	0.5734	0.3061	0.040*
H1C	-0.0195	0.6415	0.1551	0.040*

Cl3	0.12244 (5)	0.28432 (8)	0.00154 (16)	0.0351 (3)
Cl2	0.0000	0.19040 (14)	0.5000	0.0485 (5)
Cl1	0.11173 (8)	0.5000	0.5167 (2)	0.0459 (5)
O2	0.68054 (15)	0.5722 (2)	0.9173 (5)	0.0392 (8)
N8	0.7099 (2)	0.5000	0.9396 (7)	0.0291 (11)
O1	0.7671 (2)	0.5000	0.9832 (8)	0.0507 (14)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Co1	0.0190 (4)	0.0185 (4)	0.0206 (4)	0.0001 (3)	0.0021 (3)	0.0002 (3)
N7	0.032 (2)	0.039 (2)	0.028 (2)	-0.0044 (17)	0.0031 (15)	-0.0072 (15)
N6	0.0265 (19)	0.036 (2)	0.041 (2)	-0.0052 (17)	0.0084 (16)	-0.0079 (18)
N5	0.046 (2)	0.032 (2)	0.042 (2)	0.0034 (19)	-0.0037 (18)	0.0093 (17)
Co2	0.0179 (5)	0.0211 (6)	0.0247 (6)	0.000	0.0025 (4)	0.000
Cl4	0.0419 (9)	0.0284 (8)	0.0347 (9)	0.000	-0.0006 (7)	0.000
N4	0.033 (2)	0.044 (3)	0.047 (2)	-0.0102 (19)	0.0093 (18)	-0.0124 (19)
N3	0.027 (3)	0.043 (3)	0.028 (3)	0.000	0.005 (2)	0.000
Co3	0.0165 (5)	0.0220 (6)	0.0239 (6)	0.000	0.0019 (4)	0.000
N2	0.017 (2)	0.029 (3)	0.040 (3)	0.000	-0.001 (2)	0.000
N1	0.030 (2)	0.035 (2)	0.034 (2)	0.0027 (17)	-0.0011 (16)	-0.0044 (16)
Cl3	0.0334 (6)	0.0315 (6)	0.0405 (7)	0.0048 (5)	0.0037 (5)	0.0012 (5)
Cl2	0.0462 (10)	0.0521 (12)	0.0478 (11)	0.000	0.0079 (8)	0.000
Cl1	0.0361 (9)	0.0683 (13)	0.0337 (9)	0.000	0.0056 (7)	0.000
O2	0.0395 (19)	0.036 (2)	0.043 (2)	0.0092 (15)	0.0046 (15)	-0.0019 (14)
N8	0.024 (3)	0.037 (3)	0.027 (3)	0.000	0.004 (2)	0.000
O1	0.022 (2)	0.053 (4)	0.077 (4)	0.000	-0.005 (2)	0.000

Geometric parameters (Å, °)

Co1—N5 ⁱ	1.945 (4)	Co2—N3 ⁱⁱ	1.958 (5)
Co1—N5	1.945 (4)	N4—H4A	0.8900
Co1—N7	1.960 (3)	N4—H4B	0.8900
Co1—N7 ⁱ	1.960 (3)	N4—H4C	0.8900
Co1—N6	1.965 (3)	N3—H3A	0.8900
Co1—N6 ⁱ	1.965 (3)	N3—H3B	0.8900
N7—H7A	0.8900	Co3—N2	1.956 (5)
N7—H7B	0.8900	Co3—N2 ^v	1.956 (5)
N7—H7C	0.8900	Co3—N1	1.967 (3)
N6—H6A	0.8900	Co3—N1 ^{vi}	1.967 (3)
N6—H6B	0.8900	Co3—N1 ^v	1.967 (3)
N6—H6C	0.8900	Co3—N1 ^{iv}	1.967 (3)
N5—H5A	0.8900	N2—H2A	0.8900
N5—H5B	0.8900	N2—H2B	0.8900
N5—H5C	0.8900	N1—H1A	0.8900
Co2—N4	1.955 (4)	N1—H1B	0.8900
Co2—N4 ⁱⁱ	1.955 (4)	N1—H1C	0.8900
Co2—N4 ⁱⁱⁱ	1.955 (4)	O2—N8	1.253 (4)

Co2—N4 ^{iv}	1.955 (4)	N8—O1	1.234 (6)
Co2—N3	1.958 (5)	N8—O2 ^{iv}	1.253 (4)
N5 ⁱ —Co1—N5	180.000 (1)	N4 ^{iv} —Co2—N3	90.59 (16)
N5 ⁱ —Co1—N7	89.33 (16)	N4—Co2—N3 ⁱⁱ	89.41 (16)
N5—Co1—N7	90.67 (16)	N4 ⁱⁱ —Co2—N3 ⁱⁱ	90.59 (16)
N5 ⁱ —Co1—N7 ⁱ	90.67 (16)	N4 ⁱⁱⁱ —Co2—N3 ⁱⁱ	90.59 (16)
N5—Co1—N7 ⁱ	89.33 (16)	N4 ^{iv} —Co2—N3 ⁱⁱ	89.41 (16)
N7—Co1—N7 ⁱ	180.0	N3—Co2—N3 ⁱⁱ	180.000 (1)
N5 ⁱ —Co1—N6	90.47 (17)	Co2—N4—H4A	109.5
N5—Co1—N6	89.53 (17)	Co2—N4—H4B	109.5
N7—Co1—N6	91.56 (15)	H4A—N4—H4B	109.5
N7 ⁱ —Co1—N6	88.44 (15)	Co2—N4—H4C	109.5
N5 ⁱ —Co1—N6 ⁱ	89.53 (17)	H4A—N4—H4C	109.5
N5—Co1—N6 ⁱ	90.47 (17)	H4B—N4—H4C	109.5
N7—Co1—N6 ⁱ	88.44 (15)	Co2—N3—H3A	110.1
N7 ⁱ —Co1—N6 ⁱ	91.56 (15)	Co2—N3—H3B	110.0
N6—Co1—N6 ⁱ	180.00 (6)	H3A—N3—H3B	108.9
Co1—N7—H7A	109.5	N2—Co3—N2 ^v	180.0
Co1—N7—H7B	109.5	N2—Co3—N1	90.00 (15)
H7A—N7—H7B	109.5	N2 ^v —Co3—N1	90.00 (15)
Co1—N7—H7C	109.5	N2—Co3—N1 ^{vi}	90.00 (15)
H7A—N7—H7C	109.5	N2 ^v —Co3—N1 ^{vi}	90.00 (15)
H7B—N7—H7C	109.5	N1—Co3—N1 ^{vi}	89.3 (2)
Co1—N6—H6A	109.5	N2—Co3—N1 ^v	90.00 (15)
Co1—N6—H6B	109.5	N2 ^v —Co3—N1 ^v	90.00 (15)
H6A—N6—H6B	109.5	N1—Co3—N1 ^v	180.0 (2)
Co1—N6—H6C	109.5	N1 ^{vi} —Co3—N1 ^v	90.7 (2)
H6A—N6—H6C	109.5	N2—Co3—N1 ^{iv}	90.00 (15)
H6B—N6—H6C	109.5	N2 ^v —Co3—N1 ^{iv}	90.00 (15)
Co1—N5—H5A	109.5	N1—Co3—N1 ^{iv}	90.7 (2)
Co1—N5—H5B	109.5	N1 ^{vi} —Co3—N1 ^{iv}	180.00 (16)
H5A—N5—H5B	109.5	N1 ^v —Co3—N1 ^{iv}	89.3 (2)
Co1—N5—H5C	109.5	Co3—N2—H2A	109.9
H5A—N5—H5C	109.5	Co3—N2—H2B	111.0
H5B—N5—H5C	109.5	H2A—N2—H2B	108.6
N4—Co2—N4 ⁱⁱ	180.0	Co3—N1—H1A	109.5
N4—Co2—N4 ⁱⁱⁱ	89.6 (3)	Co3—N1—H1B	109.5
N4 ⁱⁱ —Co2—N4 ⁱⁱⁱ	90.4 (3)	H1A—N1—H1B	109.5
N4—Co2—N4 ^{iv}	90.4 (3)	Co3—N1—H1C	109.5
N4 ⁱⁱ —Co2—N4 ^{iv}	89.6 (3)	H1A—N1—H1C	109.5
N4 ⁱⁱⁱ —Co2—N4 ^{iv}	180.00 (17)	H1B—N1—H1C	109.5
N4—Co2—N3	90.59 (16)	O1—N8—O2 ^{iv}	120.3 (3)
N4 ⁱⁱ —Co2—N3	89.41 (16)	O1—N8—O2	120.3 (3)
N4 ⁱⁱⁱ —Co2—N3	89.41 (16)	O2 ^{iv} —N8—O2	119.4 (5)

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

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 C11	0.89	2.89	3.427 (4)	120
N1—H1A \cdots C13 ^{iv}	0.89	2.90	3.484 (4)	125
N1—H1B \cdots C11 ^{vii}	0.89	2.59	3.410 (4)	154
N1—H1C \cdots C13 ^v	0.89	2.63	3.431 (4)	150
N3—H3A \cdots O2 ^{viii}	0.89	2.53	3.155 (6)	128
N4—H4A \cdots C13 ^{ix}	0.89	2.79	3.287 (4)	117
N4—H4B \cdots C14	0.89	2.62	3.448 (5)	155
N4—H4C \cdots C12 ^{ix}	0.89	2.73	3.321 (4)	125
N5—H5A \cdots C11 ⁱ	0.89	2.77	3.375 (4)	127
N5—H5A \cdots C14 ^x	0.89	2.91	3.456 (4)	122
N5—H5B \cdots O2 ^x	0.89	2.17	3.048 (5)	168
N5—H5C \cdots C13 ⁱ	0.89	2.56	3.337 (4)	146
N6—H6A \cdots C14 ^x	0.89	2.76	3.339 (4)	124
N6—H6C \cdots C13 ^{xi}	0.89	2.93	3.445 (4)	118
N7—H7A \cdots C14 ^{viii}	0.89	2.78	3.368 (4)	125
N7—H7B \cdots C13 ^{xi}	0.89	2.87	3.394 (4)	119

Symmetry codes: (i) $-x+1/2, -y+1/2, -z+1$; (iv) $x, -y+1, z$; (v) $-x, -y+1, -z$; (vii) $-x, -y+1, -z+1$; (viii) $-x+1, -y+1, -z+1$; (ix) $x+1/2, y+1/2, z$; (x) $x-1/2, y-1/2, z$; (xi) $x, y, z+1$.