

Bis[2-(2-aminoethyl)-1*H*-benzimidazole- κ^2N^2,N^3](nitrate- κ^2O,O')cobalt(II) chloride trihydrate

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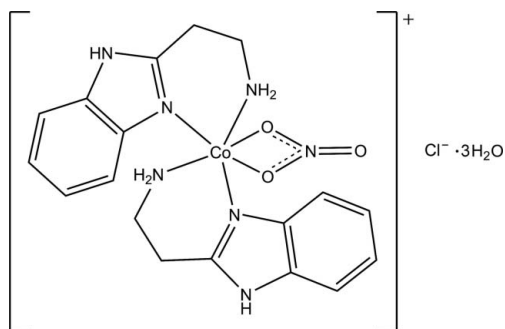
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Key indicators: single-crystal X-ray study; $T = 296$ K; mean $\sigma(C-C) = 0.007$ Å; R factor = 0.050; wR factor = 0.131; data-to-parameter ratio = 13.2.

In the title compound, $[Co(NO_3)(C_9H_{11}N_3)_2]Cl \cdot 3H_2O$, the Co^{II} atom is coordinated by four N atoms from two chelating 2-(2-aminoethyl)-1*H*-benzimidazole ligands and two O atoms from one nitrate anion in a distorted octahedral coordination environment. In the crystal, $N-H \cdots Cl$, $N-H \cdots O$, $O-H \cdots Cl$ and $O-H \cdots O$ hydrogen bonds link the complex cations, chloride anions and solvent water molecules into a three-dimensional network. $\pi-\pi$ interactions between the imidazole and benzene rings and between the benzene rings are observed [centroid-centroid distances = 3.903 (3), 3.720 (3), 3.774 (3) and 3.926 (3) Å].

Related literature

For background to the coordination chemistry of benzimidazole and 2-substituted benzimidazole derivatives towards transition metal ions, see: Téllez *et al.* (2008). For the structures and properties of transition metal complexes with 2-(2-aminoethyl)benzimidazole, see: Dash *et al.* (1995); Zhang *et al.* (2008). For the synthesis of the 2-(2-aminoethyl)benzimidazole ligand, see: Cescon & Day (1962).



Experimental

Crystal data

$[Co(NO_3)(C_9H_{11}N_3)_2]Cl \cdot 3H_2O$
 $M_r = 532.85$
 Triclinic, $P\bar{1}$
 $a = 7.408$ (2) Å
 $b = 9.808$ (3) Å
 $c = 17.280$ (6) Å
 $\alpha = 76.238$ (7)°
 $\beta = 89.203$ (7)°

$\gamma = 67.867$ (5)°
 $V = 1125.6$ (6) Å³
 $Z = 2$
 Mo $K\alpha$ radiation
 $\mu = 0.93$ mm⁻¹
 $T = 296$ K
 $0.28 \times 0.27 \times 0.26$ mm

Data collection

Bruker APEXII CCD diffractometer
 Absorption correction: multi-scan (SADABS; Sheldrick, 1996)
 $T_{min} = 0.780$, $T_{max} = 0.794$

5677 measured reflections
 3936 independent reflections
 2895 reflections with $I > 2\sigma(I)$
 $R_{int} = 0.029$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.050$
 $wR(F^2) = 0.131$
 $S = 0.99$
 3936 reflections
 298 parameters

3 restraints
 H-atom parameters constrained
 $\Delta\rho_{max} = 0.35$ e Å⁻³
 $\Delta\rho_{min} = -0.86$ e Å⁻³

Table 1

Hydrogen-bond geometry (Å, °).

$D-H \cdots A$	$D-H$	$H \cdots A$	$D \cdots A$	$D-H \cdots A$
$N2-H2 \cdots O4$	0.86	1.91	2.757 (5)	168
$N3-H3B \cdots Cl1^i$	0.90	2.56	3.322 (3)	143
$N3-H3C \cdots O3^{ii}$	0.90	2.08	2.897 (4)	150
$N5-H5 \cdots Cl1^{iii}$	0.86	2.29	3.148 (4)	174
$N6-H6A \cdots O4^i$	0.90	2.54	3.299 (5)	142
$N6-H6B \cdots O3^{ii}$	0.90	2.12	2.897 (4)	145
$O4-H1O4 \cdots O5$	0.85	1.92	2.766 (4)	179
$O4-H2O4 \cdots O6^{iv}$	0.85	1.93	2.781 (5)	179
$O5-H1O5 \cdots Cl1^v$	0.85	2.41	3.189 (3)	153
$O5-H2O5 \cdots O1^{vi}$	0.85	2.03	2.872 (4)	174
$O6-H1O6 \cdots O2$	0.85	2.01	2.828 (4)	162
$O6-H2O6 \cdots Cl1^{vi}$	0.85	2.34	3.192 (4)	176

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

Data collection: APEX2 (Bruker, 2007); cell refinement: SAINT (Bruker, 2007); data reduction: SAINT; 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.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HY2542).

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supporting information

Acta Cryst. (2012). E68, m711–m712 [doi:10.1107/S1600536812018612]

Bis[2-(2-aminoethyl)-1*H*-benzimidazole- κ^2 N²,N³](nitrate- κ^2 O,O')cobalt(II) chloride trihydrate

Jing Zhao, Heng Zhang and Guoyi Zhu

S1. Comment

Benzimidazole and 2-substituted benzimidazole derivatives are important heteroaromatic compounds acting as multidentate ligands towards transition metal ions in coordination chemistry (Télliez *et al.*, 2008). 2-(2-Aminoethyl)-benzimidazole is a bidentate ligand possessing two aromatic rings and can chelate a 3d transition-metal ion through two N atoms of the pendant aminoethyl group and the imidazole ring (Zhang *et al.*, 2008). Furthermore, this ligand has a larger conjugated π -system than imidazole, which is expected to display a stability-enhancement due to the hydrophobic interaction with the substituted group of the amino acids or to be involved in aromatic ring π - π stacking effects with purine and pyrimidine bases. Based on the inherent characters of the benzimidazole group, a large number of studies have been reported on metal complexes of benzimidazole-based ligands (Dash *et al.*, 1995). To our knowledge, Co^{II} complexes with 2-(2-aminoethyl)benzimidazole ligand have not been reported. In this paper, we report the crystal structure of one such complex.

The title compound consists of a [Co(NO₃)(C₉H₁₁N₃)₂]⁺ complex cation, a chloride anion and three hydrate solvent molecules. As shown in Fig. 1, two bidentate 2-(2-aminoethyl)benzimidazole ligands are coordinated to the Co^{II} atom solely *via* two N atoms. A bidentate nitrate is coordinated to the Co^{II} atom *via* two O atoms. The coordination geometry around the Co^{II} atom is distorted octahedral, with bite angles of 68.37 (12)° for the nitrate anion and 89.44 (13) and 89.37 (14)° for the two bidentate ligands. The other *cis* bond angles at the Co^{II} atom fall in the range of 89.37 (14)–98.11 (13)° and the *trans* bond angles are 166.29 (13), 166.39 (13) and 178.40 (14)°, suggesting a significant deviation from a perfect octahedral coordination. The Co—N bond lengths range from 1.948 (3) to 1.957 (3) Å, with an average of 1.952 (3) Å. The Co—O bond lengths are 1.928 (3) and 1.930 (3) Å. Extensive hydrogen bonds in the crystal, as shown in Fig. 2 and Table 1, link the complex cations, chloride anions and hydrate solvent molecules into a three-dimensional network.

S2. Experimental

The title compound was prepared by adding a methanol solution (5 ml) of Co(NO₃)₂·6H₂O (0.1 mmol) to a methanol solution (5 ml) of 2-(2-aminoethyl)benzimidazole dihydrochloride (0.2 mmol) neutralized by sodium hydroxide (Cescon & Day, 1962). The mixture was stirred at room temperature for 15 h and then filtered. Purple crystals suitable for X-ray diffraction were obtained by slow evaporation of the solvent after several days. Analysis, calculated for C₁₈H₂₈ClCoN₇O₆: C 40.57, H 5.30, N 18.40%; found: C 40.42, H 5.48, N 18.36%.

S3. Refinement

H atoms bonded to C and N atoms were positioned geometrically and refined as riding atoms, with C—H = 0.93 (aromatic), 0.97 (CH₂) and N—H = 0.86 (NH), 0.90 (NH₂) Å and with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C},\text{N})$. H atoms of water

molecules were found from a difference Fourier map and refined as riding atoms, with O—H = 0.85 Å and with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{O})$.

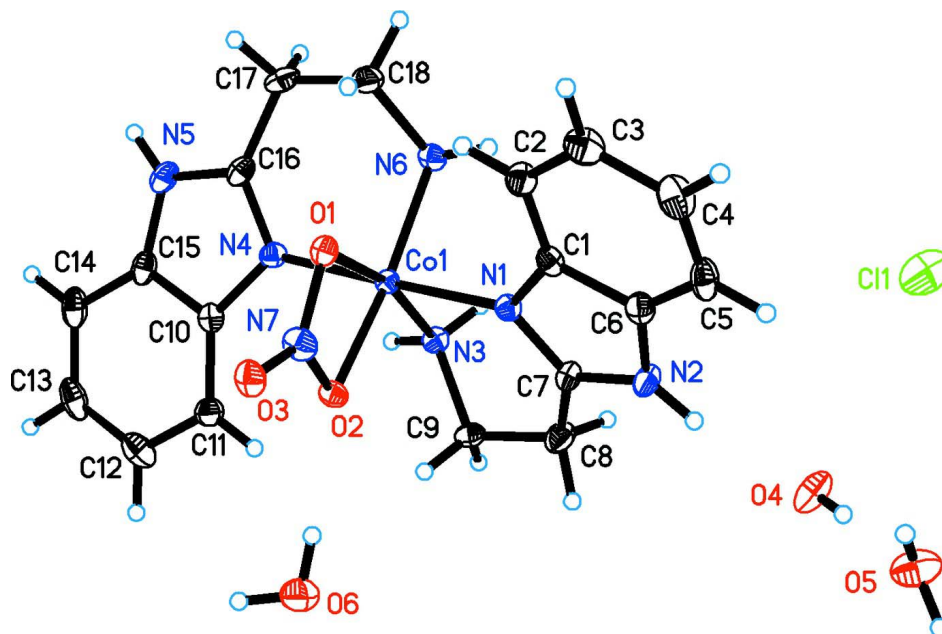


Figure 1

Molecular structure of the title complex, with displacement ellipsoids drawn at the 30% probability level.

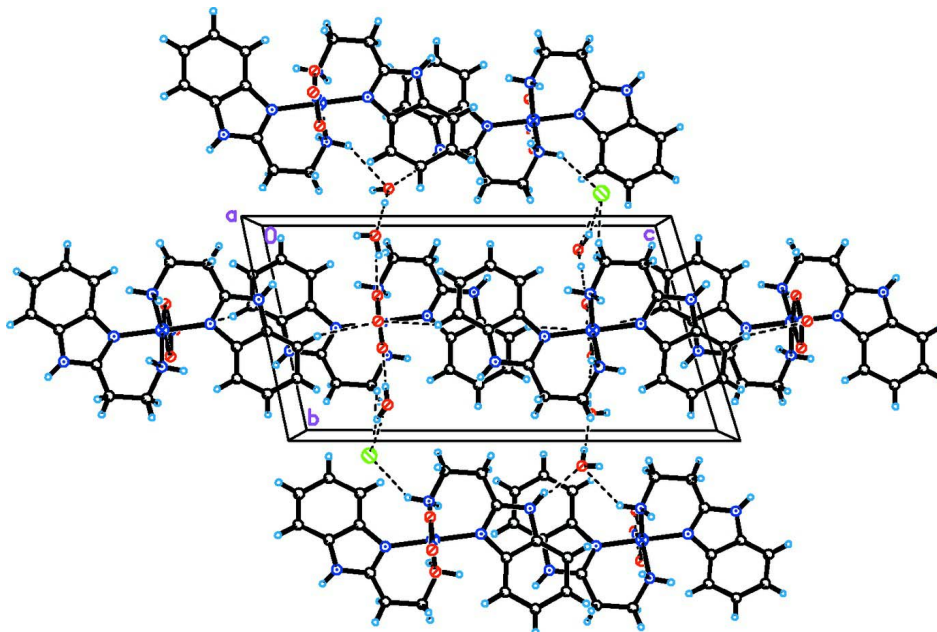


Figure 2

The packing diagram viewed along the *a* axis. Dashed lines denote hydrogen bonds.

Bis[2-(2-aminoethyl)-1H-benzimidazole- κ^2N^2,N^3](nitrate- κ^2O,O')cobalt(II) chloride trihydrate*Crystal data*[Co(NO₃)(C₉H₁₁N₃)₂]Cl·3H₂O $M_r = 532.85$ Triclinic, $P\bar{1}$

Hall symbol: -P 1

 $a = 7.408$ (2) Å $b = 9.808$ (3) Å $c = 17.280$ (6) Å $\alpha = 76.238$ (7)° $\beta = 89.203$ (7)° $\gamma = 67.867$ (5)° $V = 1125.6$ (6) Å³ $Z = 2$ $F(000) = 554$ $D_x = 1.572$ Mg m⁻³Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å

Cell parameters from 1285 reflections

 $\theta = 2.9$ – 23.7 ° $\mu = 0.93$ mm⁻¹ $T = 296$ K

Cube, purple

 $0.28 \times 0.27 \times 0.26$ mm*Data collection*

Bruker APEXII CCD

diffractometer

Radiation source: fine-focus sealed tube

Graphite monochromator

 φ and ω scans

Absorption correction: multi-scan

(SADABS; Sheldrick, 1996)

 $T_{\min} = 0.780$, $T_{\max} = 0.794$

5677 measured reflections

3936 independent reflections

2895 reflections with $I > 2\sigma(I)$ $R_{\text{int}} = 0.029$ $\theta_{\text{max}} = 25.0$ °, $\theta_{\text{min}} = 2.3$ ° $h = -8 \rightarrow 8$ $k = -9 \rightarrow 11$ $l = -20 \rightarrow 20$ *Refinement*Refinement on F^2

Least-squares matrix: full

 $R[F^2 > 2\sigma(F^2)] = 0.050$ $wR(F^2) = 0.131$ $S = 0.99$

3936 reflections

298 parameters

3 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

 $w = 1/[\sigma^2(F_o^2) + (0.0713P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$ $(\Delta/\sigma)_{\text{max}} = 0.001$ $\Delta\rho_{\text{max}} = 0.35$ e Å⁻³ $\Delta\rho_{\text{min}} = -0.86$ 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 (Å²)

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
Co1	0.76176 (7)	0.51980 (6)	0.74870 (3)	0.01888 (18)
Cl1	1.08278 (18)	0.11248 (13)	0.14279 (7)	0.0416 (3)
C1	0.7611 (6)	0.4443 (5)	0.5882 (2)	0.0240 (9)

C2	0.7801 (6)	0.2936 (5)	0.6108 (3)	0.0324 (10)
H2A	0.7928	0.2425	0.6644	0.039*
C3	0.7796 (7)	0.2221 (6)	0.5509 (3)	0.0413 (12)
H3	0.7923	0.1211	0.5646	0.050*
C4	0.7604 (7)	0.2986 (6)	0.4698 (3)	0.0430 (12)
H4	0.7585	0.2476	0.4310	0.052*
C5	0.7445 (6)	0.4455 (6)	0.4467 (3)	0.0371 (11)
H5A	0.7321	0.4959	0.3929	0.045*
C6	0.7475 (6)	0.5175 (5)	0.5072 (2)	0.0291 (10)
C7	0.7441 (6)	0.6755 (5)	0.5797 (2)	0.0248 (9)
C8	0.7469 (7)	0.8163 (5)	0.5963 (3)	0.0361 (11)
H8A	0.6403	0.9022	0.5633	0.043*
H8B	0.8678	0.8260	0.5794	0.043*
C9	0.7298 (6)	0.8281 (5)	0.6815 (2)	0.0285 (10)
H9A	0.7666	0.9102	0.6877	0.034*
H9B	0.5949	0.8524	0.6939	0.034*
C10	0.6666 (6)	0.5948 (5)	0.9090 (2)	0.0239 (9)
C11	0.5304 (6)	0.7426 (5)	0.8863 (2)	0.0317 (10)
H11	0.4912	0.7924	0.8328	0.038*
C12	0.4541 (7)	0.8140 (6)	0.9470 (3)	0.0439 (13)
H12	0.3620	0.9134	0.9332	0.053*
C13	0.5108 (7)	0.7422 (6)	1.0267 (3)	0.0447 (13)
H13	0.4561	0.7941	1.0652	0.054*
C14	0.6464 (7)	0.5955 (6)	1.0504 (3)	0.0399 (12)
H14	0.6846	0.5462	1.1040	0.048*
C15	0.7235 (6)	0.5244 (5)	0.9898 (2)	0.0294 (10)
C16	0.8857 (6)	0.3640 (5)	0.9178 (2)	0.0265 (9)
C17	1.0300 (7)	0.2219 (5)	0.9025 (3)	0.0362 (11)
H17A	1.0044	0.1368	0.9349	0.043*
H17B	1.1595	0.2109	0.9203	0.043*
C18	1.0314 (7)	0.2116 (5)	0.8160 (3)	0.0336 (10)
H18A	1.1505	0.1298	0.8095	0.040*
H18B	0.9214	0.1882	0.8028	0.040*
N1	0.7582 (5)	0.5483 (4)	0.63286 (18)	0.0229 (7)
N2	0.7352 (5)	0.6619 (4)	0.50395 (19)	0.0317 (8)
H2	0.7239	0.7317	0.4612	0.038*
N3	0.8577 (5)	0.6833 (4)	0.73877 (18)	0.0249 (8)
H3B	0.8654	0.7008	0.7872	0.030*
H3C	0.9790	0.6530	0.7222	0.030*
N4	0.7730 (5)	0.4905 (4)	0.86430 (18)	0.0233 (8)
N5	0.8614 (5)	0.3800 (4)	0.9931 (2)	0.0346 (9)
H5	0.9212	0.3121	1.0359	0.042*
N6	1.0196 (4)	0.3571 (4)	0.76028 (19)	0.0247 (8)
H6A	1.0511	0.3406	0.7119	0.030*
H6B	1.1082	0.3872	0.7783	0.030*
N7	0.4435 (5)	0.5208 (4)	0.7462 (2)	0.0332 (8)
O1	0.6072 (4)	0.3975 (3)	0.75714 (15)	0.0238 (6)
O2	0.4853 (4)	0.6428 (3)	0.73689 (15)	0.0248 (6)

O3	0.2770 (4)	0.5211 (3)	0.74554 (16)	0.0325 (7)
O4	0.7163 (5)	0.8522 (4)	0.35574 (18)	0.0491 (9)
H1O4	0.6480	0.8549	0.3158	0.059*
H2O4	0.7584	0.9225	0.3391	0.059*
O5	0.4947 (5)	0.8627 (4)	0.2253 (2)	0.0512 (9)
H1O5	0.4095	0.9325	0.1902	0.061*
H2O5	0.4738	0.7817	0.2302	0.061*
O6	0.1492 (5)	0.9162 (4)	0.7010 (2)	0.0515 (9)
H1O6	0.2360	0.8278	0.7051	0.062*
H2O6	0.0865	0.9132	0.7425	0.062*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Co1	0.0188 (3)	0.0192 (3)	0.0200 (3)	-0.0091 (2)	0.0009 (2)	-0.0046 (2)
Cl1	0.0477 (7)	0.0351 (7)	0.0390 (7)	-0.0174 (6)	-0.0086 (5)	-0.0009 (5)
C1	0.022 (2)	0.030 (2)	0.022 (2)	-0.0093 (19)	0.0009 (17)	-0.0119 (18)
C2	0.039 (3)	0.032 (2)	0.031 (2)	-0.017 (2)	0.005 (2)	-0.011 (2)
C3	0.050 (3)	0.036 (3)	0.048 (3)	-0.020 (2)	0.004 (2)	-0.022 (2)
C4	0.049 (3)	0.054 (3)	0.040 (3)	-0.027 (3)	0.005 (2)	-0.028 (3)
C5	0.037 (3)	0.059 (3)	0.023 (2)	-0.022 (2)	0.0043 (19)	-0.017 (2)
C6	0.021 (2)	0.037 (3)	0.027 (2)	-0.010 (2)	0.0001 (18)	-0.007 (2)
C7	0.028 (2)	0.028 (2)	0.020 (2)	-0.0139 (19)	0.0017 (17)	-0.0045 (18)
C8	0.048 (3)	0.028 (2)	0.032 (2)	-0.017 (2)	0.005 (2)	-0.001 (2)
C9	0.032 (2)	0.018 (2)	0.033 (2)	-0.0085 (19)	-0.0006 (19)	-0.0039 (18)
C10	0.024 (2)	0.029 (2)	0.025 (2)	-0.0147 (19)	0.0019 (17)	-0.0097 (18)
C11	0.036 (3)	0.030 (2)	0.026 (2)	-0.009 (2)	0.0018 (19)	-0.0075 (19)
C12	0.036 (3)	0.049 (3)	0.050 (3)	-0.012 (3)	0.011 (2)	-0.028 (3)
C13	0.046 (3)	0.069 (4)	0.037 (3)	-0.028 (3)	0.019 (2)	-0.036 (3)
C14	0.046 (3)	0.064 (4)	0.020 (2)	-0.030 (3)	0.007 (2)	-0.016 (2)
C15	0.036 (3)	0.039 (3)	0.021 (2)	-0.023 (2)	0.0021 (18)	-0.0062 (19)
C16	0.031 (2)	0.028 (2)	0.024 (2)	-0.018 (2)	-0.0026 (18)	-0.0012 (18)
C17	0.037 (3)	0.025 (2)	0.035 (3)	-0.006 (2)	-0.009 (2)	0.006 (2)
C18	0.032 (2)	0.023 (2)	0.041 (3)	-0.009 (2)	0.005 (2)	-0.003 (2)
N1	0.0239 (18)	0.0219 (18)	0.0241 (18)	-0.0094 (15)	0.0024 (14)	-0.0071 (15)
N2	0.041 (2)	0.032 (2)	0.0208 (18)	-0.0159 (18)	0.0025 (16)	-0.0005 (16)
N3	0.0266 (19)	0.0244 (19)	0.0246 (18)	-0.0107 (16)	0.0009 (14)	-0.0064 (15)
N4	0.0250 (19)	0.0222 (18)	0.0219 (17)	-0.0082 (16)	-0.0014 (14)	-0.0055 (15)
N5	0.041 (2)	0.037 (2)	0.0193 (18)	-0.0133 (19)	-0.0047 (16)	0.0021 (16)
N6	0.0179 (17)	0.0263 (19)	0.0310 (19)	-0.0096 (15)	0.0020 (14)	-0.0075 (15)
N7	0.0252 (12)	0.0359 (15)	0.043 (2)	-0.0149 (11)	0.0013 (16)	-0.0121 (18)
O1	0.0239 (13)	0.0269 (14)	0.0258 (14)	-0.0155 (10)	0.0026 (12)	-0.0062 (12)
O2	0.0180 (14)	0.0258 (15)	0.0295 (15)	-0.0068 (12)	0.0002 (12)	-0.0075 (13)
O3	0.0229 (14)	0.0463 (19)	0.0324 (16)	-0.0175 (14)	0.0022 (13)	-0.0103 (14)
O4	0.064 (2)	0.050 (2)	0.0339 (18)	-0.0329 (19)	-0.0067 (16)	0.0074 (16)
O5	0.050 (2)	0.037 (2)	0.064 (2)	-0.0182 (18)	-0.0146 (18)	-0.0055 (17)
O6	0.047 (2)	0.037 (2)	0.059 (2)	-0.0079 (17)	0.0078 (17)	-0.0037 (17)

Geometric parameters (Å, °)

Co1—O1	1.928 (3)	C12—C13	1.379 (7)
Co1—O2	1.930 (3)	C12—H12	0.9300
Co1—N4	1.948 (3)	C13—C14	1.375 (7)
Co1—N6	1.949 (3)	C13—H13	0.9300
Co1—N1	1.953 (3)	C14—C15	1.392 (6)
Co1—N3	1.957 (3)	C14—H14	0.9300
C1—C2	1.388 (6)	C15—N5	1.388 (6)
C1—C6	1.400 (6)	C16—N4	1.337 (5)
C1—N1	1.412 (5)	C16—N5	1.349 (5)
C2—C3	1.383 (6)	C16—C17	1.483 (6)
C2—H2A	0.9300	C17—C18	1.521 (6)
C3—C4	1.404 (7)	C17—H17A	0.9700
C3—H3	0.9300	C17—H17B	0.9700
C4—C5	1.360 (7)	C18—N6	1.491 (5)
C4—H4	0.9300	C18—H18A	0.9700
C5—C6	1.399 (6)	C18—H18B	0.9700
C5—H5A	0.9300	N2—H2	0.8600
C6—N2	1.372 (5)	N3—H3B	0.9000
C7—N1	1.331 (5)	N3—H3C	0.9000
C7—N2	1.351 (5)	N5—H5	0.8600
C7—C8	1.484 (6)	N6—H6A	0.9000
C8—C9	1.504 (5)	N6—H6B	0.9000
C8—H8A	0.9700	N7—O3	1.233 (4)
C8—H8B	0.9700	N7—O2	1.319 (4)
C9—N3	1.496 (5)	N7—O1	1.327 (4)
C9—H9A	0.9700	O4—H1O4	0.8500
C9—H9B	0.9700	O4—H2O4	0.8496
C10—C11	1.383 (6)	O5—H1O5	0.8501
C10—C15	1.394 (5)	O5—H2O5	0.8500
C10—N4	1.419 (5)	O6—H1O6	0.8500
C11—C12	1.394 (6)	O6—H2O6	0.8499
C11—H11	0.9300		
O1—Co1—O2	68.37 (12)	C14—C13—C12	121.3 (4)
O1—Co1—N4	89.76 (12)	C14—C13—H13	119.3
O2—Co1—N4	92.05 (12)	C12—C13—H13	119.3
O1—Co1—N6	98.11 (13)	C13—C14—C15	116.5 (4)
O2—Co1—N6	166.39 (13)	C13—C14—H14	121.7
N4—Co1—N6	89.37 (14)	C15—C14—H14	121.7
O1—Co1—N1	91.42 (12)	N5—C15—C14	131.0 (4)
O2—Co1—N1	89.38 (12)	N5—C15—C10	106.1 (3)
N4—Co1—N1	178.40 (14)	C14—C15—C10	122.9 (4)
N6—Co1—N1	89.40 (13)	N4—C16—N5	111.3 (4)
O1—Co1—N3	166.29 (13)	N4—C16—C17	128.0 (4)
O2—Co1—N3	97.97 (13)	N5—C16—C17	120.6 (4)
N4—Co1—N3	89.66 (13)	C16—C17—C18	115.8 (3)

N6—Co1—N3	95.58 (14)	C16—C17—H17A	108.3
N1—Co1—N3	89.44 (13)	C18—C17—H17A	108.3
C2—C1—C6	120.0 (4)	C16—C17—H17B	108.3
C2—C1—N1	132.3 (4)	C18—C17—H17B	108.3
C6—C1—N1	107.7 (4)	H17A—C17—H17B	107.4
C3—C2—C1	117.8 (4)	N6—C18—C17	111.2 (3)
C3—C2—H2A	121.1	N6—C18—H18A	109.4
C1—C2—H2A	121.1	C17—C18—H18A	109.4
C2—C3—C4	121.4 (5)	N6—C18—H18B	109.4
C2—C3—H3	119.3	C17—C18—H18B	109.4
C4—C3—H3	119.3	H18A—C18—H18B	108.0
C5—C4—C3	121.5 (4)	C7—N1—C1	106.1 (3)
C5—C4—H4	119.2	C7—N1—Co1	125.7 (3)
C3—C4—H4	119.2	C1—N1—Co1	128.2 (3)
C4—C5—C6	117.2 (4)	C7—N2—C6	108.1 (3)
C4—C5—H5A	121.4	C7—N2—H2	125.9
C6—C5—H5A	121.4	C6—N2—H2	125.9
N2—C6—C5	131.4 (4)	C9—N3—Co1	112.9 (2)
N2—C6—C1	106.5 (3)	C9—N3—H3B	109.0
C5—C6—C1	122.0 (4)	Co1—N3—H3B	109.0
N1—C7—N2	111.6 (4)	C9—N3—H3C	109.0
N1—C7—C8	127.2 (3)	Co1—N3—H3C	109.0
N2—C7—C8	121.1 (4)	H3B—N3—H3C	107.8
C7—C8—C9	116.8 (4)	C16—N4—C10	106.1 (3)
C7—C8—H8A	108.1	C16—N4—Co1	125.6 (3)
C9—C8—H8A	108.1	C10—N4—Co1	128.3 (3)
C7—C8—H8B	108.1	C16—N5—C15	108.5 (3)
C9—C8—H8B	108.1	C16—N5—H5	125.8
H8A—C8—H8B	107.3	C15—N5—H5	125.8
N3—C9—C8	111.6 (3)	C18—N6—Co1	113.3 (2)
N3—C9—H9A	109.3	C18—N6—H6A	108.9
C8—C9—H9A	109.3	Co1—N6—H6A	108.9
N3—C9—H9B	109.3	C18—N6—H6B	108.9
C8—C9—H9B	109.3	Co1—N6—H6B	108.9
H9A—C9—H9B	108.0	H6A—N6—H6B	107.7
C11—C10—C15	119.7 (4)	O3—N7—O2	125.0 (4)
C11—C10—N4	132.3 (4)	O3—N7—O1	125.0 (4)
C15—C10—N4	108.0 (4)	O2—N7—O1	110.0 (3)
C10—C11—C12	117.4 (4)	N7—O1—Co1	90.7 (2)
C10—C11—H11	121.3	N7—O2—Co1	90.9 (2)
C12—C11—H11	121.3	H104—O4—H2O4	104.9
C13—C12—C11	122.1 (5)	H105—O5—H2O5	107.7
C13—C12—H12	118.9	H106—O6—H2O6	107.7
C11—C12—H12	118.9		

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>
N2—H2 \cdots O4	0.86	1.91	2.757 (5)	168
N3—H3 <i>B</i> \cdots C11 ⁱ	0.90	2.56	3.322 (3)	143
N3—H3 <i>C</i> \cdots O3 ⁱⁱ	0.90	2.08	2.897 (4)	150
N5—H5 \cdots C11 ⁱⁱⁱ	0.86	2.29	3.148 (4)	174
N6—H6 <i>A</i> \cdots O4 ⁱ	0.90	2.54	3.299 (5)	142
N6—H6 <i>B</i> \cdots O3 ⁱⁱ	0.90	2.12	2.897 (4)	145
O4—H1 <i>O</i> 4 \cdots O5	0.85	1.92	2.766 (4)	179
O4—H2 <i>O</i> 4 \cdots O6 ^{iv}	0.85	1.93	2.781 (5)	179
O5—H1 <i>O</i> 5 \cdots C11 ^v	0.85	2.41	3.189 (3)	153
O5—H2 <i>O</i> 5 \cdots O1 ^{vi}	0.85	2.03	2.872 (4)	174
O6—H1 <i>O</i> 6 \cdots O2	0.85	2.01	2.828 (4)	162
O6—H2 <i>O</i> 6 \cdots C11 ^{vi}	0.85	2.34	3.192 (4)	176

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