Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

Piperazine-1,4-diium bis(hexahydroxido-heptaoxidohexaborato-κ^3O,O',O'')-cobaltate(II) hexahydrate

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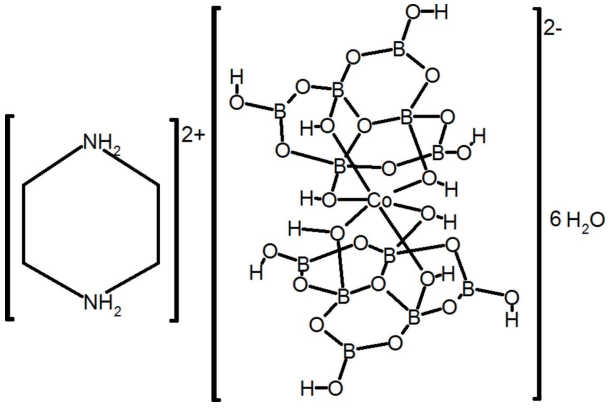
Received 3 March 2014; accepted 30 March 2014

Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.004 Å; R factor = 0.049; wR factor = 0.153; data-to-parameter ratio = 30.1.

In the title hydrate, $(C_4H_{12}N_2)[Co\{B_6O_7(OH)_6\}_2]\cdot 6H_2O$, both the dication and dianion are generated by crystallographic inversion symmetry. The Co^{2+} ion in the dianion adopts a fairly regular CoO_6 octahedral coordination geometry arising from the two O,O',O''-tridentate ligands. In the crystal, the dianions and water molecules are linked by O—H···O hydrogen bonds, generating a framework with large [100] channels, which are occupied by the organic dications. N—H···O and C—H···O hydrogen bonds consolidate the structure.

Related literature

For related structures, see: Natarajan *et al.* (2003); Negro *et al.* (1971); Zhihong *et al.* (2005); Yue *et al.* (2003).



Experimental

Crystal data

$(C_4H_{12}N_2)[Co(H_6B_6O_{13})_2]\cdot 6H_2O$
M_r = 813.00
Triclinic, $P\overline{1}$
a = 8.226 (3) Å
b = 10.157 (2) Å
c = 11.298 (4) Å
α = 65.98 (2)°
β = 74.20 (3)°
γ = 69.03 (5)°
V = 796.2 (4) Å^3
Z = 1
Ag $K\alpha$ radiation
λ = 0.56087 Å
μ = 0.35 mm^{-1}
T = 298 K
0.23 × 0.15 × 0.11 mm

Data collection

Enraf–Nonius CAD-4 diffractometer
9895 measured reflections
7785 independent reflections
6118 reflections with $I > 2\sigma(I)$
R_{int} = 0.014
2 standard reflections every 120 min
intensity decay: 2%

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.049
$wR(F^2)$ = 0.153
S = 1.06
7785 reflections
259 parameters
12 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 2.42 e Å^{-3}
$\Delta\rho_{min}$ = −0.99 e Å^{-3}

Table 1
Selected bond lengths (Å).

Co1—O2	2.0539 (17)	Co1—O4	2.1926 (12)
Co1—O1	2.0648 (14)		

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

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1···O2W	0.82 (1)	2.00 (2)	2.7525 (19)	153 (3)
O2—H2···O6^{i}	0.81 (1)	2.11 (1)	2.876 (2)	157 (3)
O3—H3···O23^{ii}	0.82	1.93	2.745 (2)	172
O4—H4···O2W	0.81 (1)	2.08 (1)	2.864 (2)	164 (3)
O5—H5···O45^{iii}	0.82	1.91	2.7159 (18)	169
O6—H6···O4^{i}	0.82	1.95	2.734 (2)	160
O1W—H1W1···O5	0.86 (1)	1.96 (2)	2.771 (2)	158 (4)
O1W—H2W1···O26^{iv}	0.86 (1)	2.27 (1)	3.108 (3)	167 (3)
O1W—H2W1···O23^{iv}	0.86 (1)	2.51 (3)	3.158 (3)	133 (3)
O2W—H1W2···O3^{v}	0.85 (1)	2.05 (2)	2.861 (2)	159 (3)
O2W—H2W2···O1W^{vi}	0.85 (1)	2.01 (1)	2.838 (3)	164 (3)
O3W—H2W3···O1W^{vii}	0.85 (1)	2.05 (2)	2.842 (3)	155 (3)
O3W—H1W3···O1W^{viii}	0.85 (1)	2.24 (1)	3.088 (3)	179 (1)
N1—H1A···O16	0.90	1.78	2.654 (2)	165
N1—H1A···O6	0.90	2.46	2.986 (3)	117
N1—H1B···O3W	0.90	1.98	2.836 (3)	157
C1—H1C···O34^{v}	0.97	2.56	3.321 (3)	136

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

Data collection: *CAD-4 EXPRESS* (Enraf–Nonius, 1994); cell refinement: *CAD-4 EXPRESS*; data reduction: *XCAD4* (Harms & Wocadlo, 1996); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 2012) and *DIAMOND* (Brandenburg & Putz, 2005); software used to prepare material for publication: *WinGX* (Farrugia, 2012).

Supporting information for this paper is available from the IUCr electronic archives (Reference: HB7207).

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supporting information

Acta Cryst. (2014). E**70**, m167–m168 [doi:10.1107/S1600536814007090]

Piperazine-1,4-diium bis(hexahydroxidoheptaoxidohexaborato-κ^3O,O',O'')cobaltate(II) hexahydrate

Nabil Jamai, Mohamed Rzaigui and Samah Akriche Toumi

S1. Comment

The mode of condensation of trigonal planar $B(OH)_3$ and tetrahedral $[B(OH)_4]^-$ primary structural units, leads to a variety of hydrated polyborate structures such as rings, cages, chains, sheets or extended networks. In particular, the polymerization of three tetrahedral $BO_3(OH)$ (3Δ) and three trigonal BO2(OH)(3 T) moieties form tricyclic $[B_6O_7(OH)_6]^{2-}$ anions featuring an unusual three-coordinate oxygen atom (μ_3–O). To date, various hydrated hexaborate structures including inorganic metals have been extensively studied. In contrast, those with organic and inorganic cations are less explored. On the best of our knowledge only one hydrated hexaborate with transition metal and organic cations, is earlier cited; $[(Me)_2NH(CH_2)_2NH(Me)_2]\{Zn[B_6O_7(OH)_6]2\}\cdot 2H_2O$ (with Me = methyl)(Natarajan *et al.*, 2003). In this work, we report the synthesis and structure of a new organic-inorganic hydrated hexaborate, $[C_4N_2H_{12}]\{Co[B_6O_7(OH)_6]_2\}\cdot 6H_2O$ (I).

The asymmetric unit of the title complex consists of a half $[C_4H_{12}N_2]^{2+}$ diprotonated cation, a half of $\{Co[B_6O_7(OH)_6]_2\}^{2-}$ complex hexaborate anions and three lattice water molecules as shown in Figure 1. As the Co^{2+} ion is located on centre of inversion so is bonded to six O atoms of two chelating $[B_6O_7(OH)_6]^{2-}$ anions forming thus a distorted octahedron. The Co—O distances range from 2.0539 (17) to 2.1926 (12) Å and the O—Co—O angles are between 87.03 (5)–180.00 (7)° (Table 1). The $[B_6O_7(OH)_6]^{2-}$ unit is formed by three tetrahedral B and three trigonal B atoms (3Δ + 3 T), linked through six double bridged (μ_2–O) and one triple bridged (μ_3–O) oxygen atoms in which each B atom possesses one terminal OH group, resulting in the formation of a tricyclic honeycomb-like structure anion (Fig. 2). Similar hexaborate anions have been encountered in the mineral aksaite (Negro *et al.*, 1971).

The B—O and O—B—O bond lengths range from 1.434 (2) to 1.5123 (18) Å and from 105.58 (12) to 112.53 (12) ° respectively for the tetrahedral B atoms and those for trigonal ones are in the range 1.355 (2)–1.371 (2) Å and from 114.61 (14) to 122.88 (14) °. The longer B—O distances are observed for the tetrahedral B atoms associated with the μ_3 oxygen atom. These structural parameters are in good agreement with those observed for other hydrated hexaborate associated with some alkali and transition metals, such as $K_2Mg[B_6O_7(OH)_6]_2\cdot 4H_2O$ (Zhihong *et al.*, 2005) and $Rb_2Co[B_6O_7(OH)_6]_2\cdot 4H_2O$ (Yue *et al.*, 2003).

The $[B_6O_7(OH)_6]^{2-}$ anions are further interconnected through O—H···O hydrogen-bonding interactions of the hydroxyl groups (Table 2) yelding to a three-dimensional framework with channels along the *a* axis. The negative excess charges of the anionic framework is compensated by $[C_4H_{12}N_2]^{2+}$ cations, which occupy the voids along with water molecules (Fig. 3). It'to be noted that the diprotonated piperazine ring adopts a chair conformation, with puckering parameters Q = 1.7803 Å, θ = 171.58° and φ = 90°.

S2. Experimental

Piperazine (0.086 g), $CoCl_2·6H_2O$ (0.8 g) and H_3BO_3 (2 g) in a molar ratio: piperazine/Co/ B = 1/4/32 were dissolved in a mixture of 30 ml of distilled water and 20 ml of ethanol and then stirred for 1 h. The pH was adjusted to 9 by addition of 5 ml of pyridine. Within two weeks, pink prisms of the title compound were obtained. The existence of hexaborate anion in the prepared compound is evidenced by characteristic IR absorption band at 685 cm^{-1}. IR (KBr, cm^{-1}): 1358 $\nu_{as}(BO_3)$, 908–850 $\nu_s(BO_3)$, 1028$\nu_{as}(BO_4)$,807 $\nu_s(BO_4)$,1095 ν(BOH) and 685$\delta(BO_3)$+$\delta(BO_4)$.

S3. Refinement

All H atoms attached to C and N atoms were fixed geometrically and treated as riding, with C—H = 0.97 Å and N—H = 0.90 Å with U_{iso}(H) = 1.2Ueq(C, N) for piperazine ring. The H atoms of OH groups are fixed using restraint O—H = 0.82 Å and those of water molecules are located using restraints [O—H = 0.85 (1) Å, H···H = 1.44 (2) Å and U_{iso}(H) = 1.5Ueq(O). Four bad reflections with (Iobs-Icalc)/SigmaW > 10 are omitted on the final refinement.

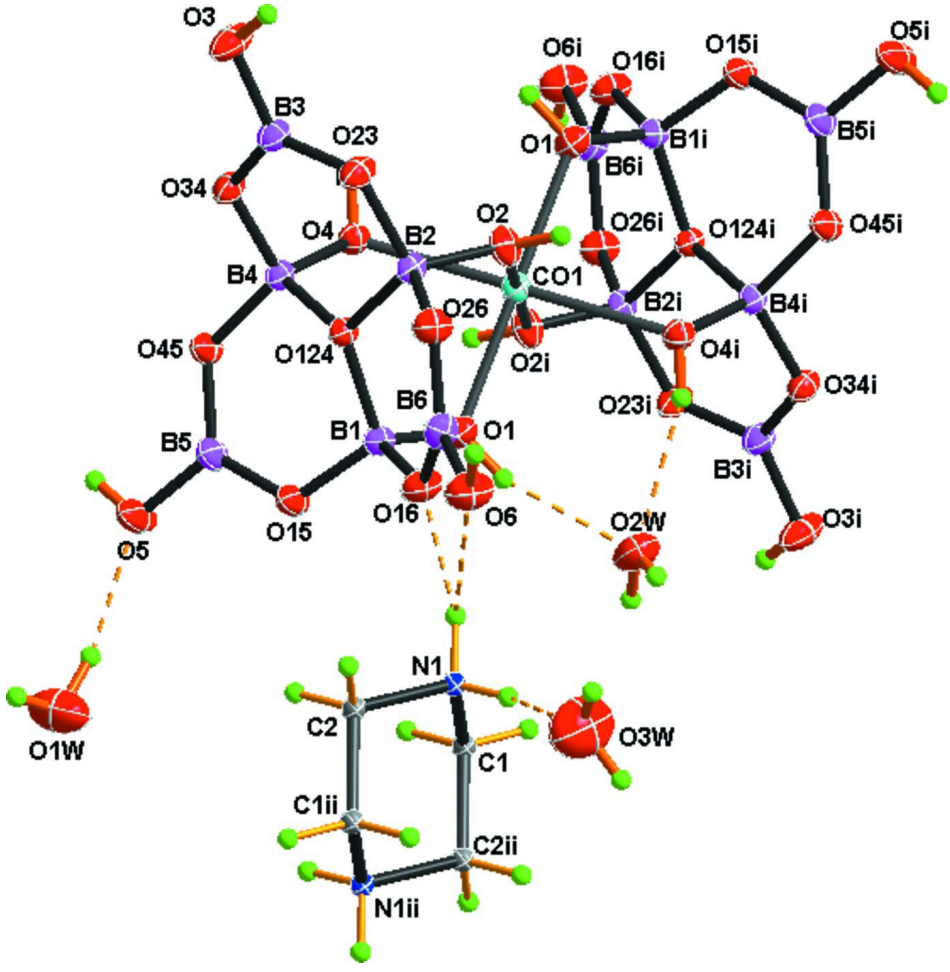

Figure 1

An *ORTEP* view of (I) with displacement ellipsoids drawn at the 30% probability level. Hydrogen bonds are represented as dashed lines. [Symmetry code: (i) 1 - *x*, 1 - *y*, 1 - *z*]

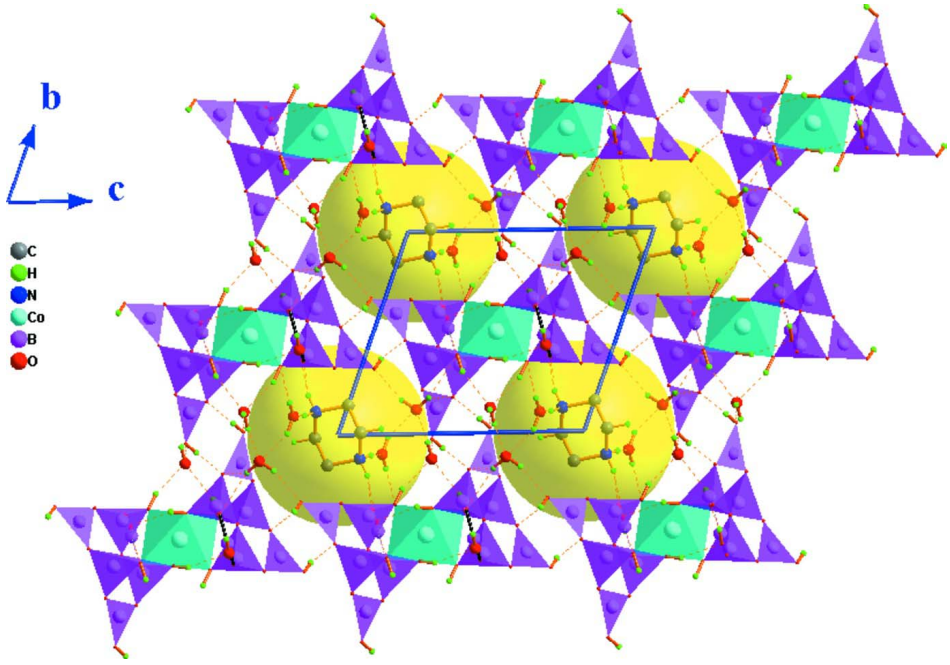

Figure 2

Crystal structure of I viewed along *a* axis showing a three-dimensional-supramolecular structure featuring the voids represented as large yellow ball. The H-atoms not included in H-bond scheme are omitted.

Piperazine-1,4-diium bis(hexahydroxidoheptaoxidohexaborato-κ^3O,O',O'')cobaltate(II) hexahydrate

Crystal data

$(C_4H_{12}N_2)[Co(H_6B_6O_{13})_2]\cdot 6H_2O$
$M_r = 813.00$
Triclinic, $P\overline{1}$
Hall symbol: -P 1
$a = 8.226$ (3) Å
$b = 10.157$ (2) Å
$c = 11.298$ (4) Å
$\alpha = 65.98$ (2)°
$\beta = 74.20$ (3)°
$\gamma = 69.03$ (5)°
$V = 796.2$ (4) Å^3
$Z = 1$
$F(000) = 417$
$D_x = 1.696$ Mg m^{-3}
Ag $K\alpha$ radiation, $\lambda = 0.56087$ Å
Cell parameters from 25 reflections
$\theta = 9$–11°
$\mu = 0.35$ mm^{-1}
$T = 298$ K
Prism, pink
0.23 × 0.15 × 0.11 mm

Data collection

Enraf–Nonius CAD-4 diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
non–profiled ω scans
9895 measured reflections
7785 independent reflections
6118 reflections with $I > 2\sigma(I)$
$R_{int} = 0.014$
$\theta_{max} = 28.0°$, $\theta_{min} = 2.1°$
$h = -13\rightarrow13$
$k = -16\rightarrow16$
$l = -3\rightarrow18$
2 standard reflections every 120 min
intensity decay: 2%

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.049$
$wR(F^2) = 0.153$
$S = 1.06$
7785 reflections
259 parameters
12 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
$w = 1/[\sigma^2(F_o^2) + (0.0924P)^2 + 0.2147P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 2.42$ e Å^{-3}
$\Delta\rho_{min} = -0.99$ 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_{iso}*/U_{eq}
Co1	0.5000	0.5000	0.5000	0.01614 (7)
B1	0.7384 (2)	0.59885 (17)	0.23924 (15)	0.0163 (2)
B2	0.8734 (2)	0.33738 (17)	0.39832 (16)	0.0167 (2)
B3	0.8346 (2)	0.12594 (18)	0.36263 (17)	0.0200 (3)
B4	0.6375 (2)	0.37212 (16)	0.26842 (15)	0.0161 (2)
B5	0.6174 (2)	0.59847 (19)	0.06603 (16)	0.0210 (3)
B6	1.0368 (2)	0.5217 (2)	0.29973 (17)	0.0203 (3)
O124	0.77220 (13)	0.43050 (11)	0.28482 (10)	0.01562 (17)
O45	0.58438 (15)	0.46319 (12)	0.14086 (11)	0.02026 (19)
O34	0.71305 (15)	0.21657 (12)	0.28139 (12)	0.02037 (19)
O16	0.89561 (14)	0.62883 (13)	0.24323 (12)	0.0225 (2)
O15	0.69605 (17)	0.66434 (13)	0.10864 (11)	0.0232 (2)
O23	0.91602 (16)	0.17965 (12)	0.41590 (12)	0.0229 (2)
O1	0.58976 (15)	0.65398 (12)	0.33104 (12)	0.02076 (19)
H1	0.595 (4)	0.7336 (18)	0.330 (3)	0.031*
O2	0.75590 (15)	0.36962 (14)	0.51227 (11)	0.0222 (2)
H2	0.793 (4)	0.361 (3)	0.5750 (18)	0.033*
O3	0.8757 (2)	−0.02567 (13)	0.38981 (16)	0.0321 (3)
H3	0.9463	−0.0701	0.4421	0.048*
O4	0.51422 (14)	0.61177 (12)	0.62547 (11)	0.01811 (18)
H4	0.528 (4)	0.6931 (17)	0.578 (2)	0.027*
O5	0.5670 (2)	0.67326 (16)	−0.05561 (13)	0.0352 (3)
H5	0.5205	0.6238	−0.0708	0.053*
O6	1.17955 (16)	0.57172 (15)	0.27863 (15)	0.0286 (3)

H6	1.2628	0.5003	0.3070	0.043*
O26	1.03454 (14)	0.37793 (13)	0.37106 (12)	0.0223 (2)
O1W	0.6861 (3)	0.8794 (2)	−0.2835 (2)	0.0489 (4)
H1W1	0.622 (4)	0.833 (4)	−0.216 (3)	0.073*
H2W1	0.773 (3)	0.818 (3)	−0.314 (3)	0.073*
O2W	0.5784 (2)	0.87545 (16)	0.41668 (16)	0.0349 (3)
H1W2	0.676 (2)	0.882 (3)	0.423 (3)	0.052*
H2W2	0.511 (3)	0.959 (2)	0.375 (3)	0.052*
O3W	1.2705 (3)	0.9010 (3)	0.2089 (3)	0.0675 (7)
H2W3	1.253 (5)	0.981 (2)	0.223 (5)	0.101*
H1W3	1.3578	0.8334	0.2430	0.101*
N1	0.9898 (3)	0.8815 (2)	0.1223 (2)	0.0443 (4)
H1A	0.9538	0.8001	0.1763	0.053*
H1B	1.0545	0.8982	0.1646	0.053*
C1	0.8360 (3)	1.0119 (2)	0.0893 (2)	0.0355 (4)
H1C	0.7653	1.0290	0.1686	0.043*
H1D	0.7638	0.9935	0.0458	0.043*
C2	1.1021 (4)	0.8520 (2)	−0.0001 (3)	0.0441 (5)
H2A	1.2028	0.7651	0.0235	0.053*
H2B	1.0339	0.8314	−0.0450	0.053*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Co1	0.01484 (11)	0.01703 (12)	0.01733 (12)	−0.00406 (8)	−0.00425 (8)	−0.00587 (9)
B1	0.0158 (5)	0.0161 (5)	0.0180 (6)	−0.0053 (4)	−0.0062 (5)	−0.0038 (5)
B2	0.0157 (5)	0.0159 (5)	0.0194 (6)	−0.0025 (4)	−0.0083 (5)	−0.0050 (5)
B3	0.0214 (6)	0.0157 (6)	0.0240 (7)	−0.0030 (5)	−0.0078 (5)	−0.0070 (5)
B4	0.0168 (5)	0.0154 (5)	0.0179 (6)	−0.0039 (4)	−0.0071 (5)	−0.0053 (5)
B5	0.0255 (7)	0.0211 (6)	0.0173 (6)	−0.0073 (5)	−0.0086 (5)	−0.0034 (5)
B6	0.0160 (6)	0.0245 (7)	0.0241 (7)	−0.0074 (5)	−0.0055 (5)	−0.0090 (6)
O124	0.0151 (4)	0.0150 (4)	0.0180 (4)	−0.0037 (3)	−0.0070 (3)	−0.0046 (3)
O45	0.0244 (5)	0.0208 (4)	0.0182 (4)	−0.0091 (4)	−0.0102 (4)	−0.0025 (4)
O34	0.0233 (5)	0.0158 (4)	0.0252 (5)	−0.0029 (3)	−0.0108 (4)	−0.0078 (4)
O16	0.0176 (4)	0.0203 (4)	0.0316 (6)	−0.0072 (4)	−0.0091 (4)	−0.0058 (4)
O15	0.0321 (6)	0.0206 (5)	0.0194 (5)	−0.0107 (4)	−0.0116 (4)	−0.0014 (4)
O23	0.0262 (5)	0.0148 (4)	0.0294 (5)	−0.0011 (4)	−0.0159 (4)	−0.0058 (4)
O1	0.0199 (4)	0.0178 (4)	0.0254 (5)	−0.0055 (3)	−0.0020 (4)	−0.0088 (4)
O2	0.0187 (4)	0.0287 (5)	0.0192 (5)	−0.0025 (4)	−0.0074 (4)	−0.0091 (4)
O3	0.0400 (7)	0.0156 (5)	0.0460 (8)	−0.0014 (4)	−0.0265 (6)	−0.0085 (5)
O4	0.0174 (4)	0.0182 (4)	0.0203 (4)	−0.0065 (3)	−0.0039 (3)	−0.0061 (3)
O5	0.0583 (9)	0.0321 (6)	0.0227 (6)	−0.0253 (6)	−0.0218 (6)	0.0042 (5)
O6	0.0177 (5)	0.0287 (6)	0.0403 (7)	−0.0093 (4)	−0.0100 (5)	−0.0069 (5)
O26	0.0156 (4)	0.0235 (5)	0.0282 (5)	−0.0055 (4)	−0.0087 (4)	−0.0059 (4)
O1W	0.0409 (9)	0.0369 (8)	0.0484 (10)	−0.0071 (7)	0.0027 (7)	−0.0038 (7)
O2W	0.0407 (7)	0.0262 (6)	0.0426 (8)	−0.0149 (5)	−0.0062 (6)	−0.0116 (6)
O3W	0.0612 (14)	0.0639 (14)	0.0861 (17)	−0.0129 (11)	−0.0395 (13)	−0.0203 (13)
N1	0.0550 (12)	0.0363 (9)	0.0406 (10)	−0.0197 (8)	−0.0131 (9)	−0.0026 (8)

C1	0.0392 (10)	0.0318 (8)	0.0291 (8)	−0.0099 (7)	0.0008 (7)	−0.0081 (7)
C2	0.0509 (13)	0.0232 (8)	0.0485 (12)	−0.0079 (8)	0.0024 (10)	−0.0111 (8)

Geometric parameters (Å, º)

Co1—O2	2.0539 (17)	B6—O6	1.368 (2)
Co1—O2^{i}	2.0539 (17)	B6—O16	1.369 (2)
Co1—O1	2.0648 (14)	O1—H1	0.820 (10)
Co1—O1^{i}	2.0648 (14)	O2—H2	0.811 (10)
Co1—O4^{i}	2.1926 (12)	O3—H3	0.8200
Co1—O4	2.1926 (12)	O4—B4^{i}	1.490 (2)
B1—O15	1.434 (2)	O4—H4	0.810 (10)
B1—O16	1.4462 (19)	O5—H5	0.8200
B1—O1	1.475 (2)	O6—H6	0.8200
B1—O124	1.5123 (18)	O1W—H1W1	0.861 (10)
B2—O26	1.4447 (19)	O1W—H2W1	0.856 (10)
B2—O23	1.4510 (19)	O2W—H1W2	0.852 (10)
B2—O2	1.462 (2)	O2W—H2W2	0.854 (10)
B2—O124	1.5041 (19)	O3W—H2W3	0.846 (10)
B3—O34	1.357 (2)	O3W—H1W3	0.847 (2)
B3—O23	1.363 (2)	N1—C1	1.466 (3)
B3—O3	1.371 (2)	N1—C2	1.517 (4)
B4—O34	1.4360 (19)	N1—H1A	0.9000
B4—O45	1.4463 (19)	N1—H1B	0.9000
B4—O4^{i}	1.490 (2)	C1—C2^{ii}	1.508 (3)
B4—O124	1.5117 (18)	C1—H1C	0.9700
B5—O15	1.356 (2)	C1—H1D	0.9700
B5—O5	1.368 (2)	C2—C1^{ii}	1.508 (3)
B5—O45	1.368 (2)	C2—H2A	0.9700
B6—O26	1.355 (2)	C2—H2B	0.9700
O2—Co1—O2^{i}	180.0	B2—O124—B4	118.01 (11)
O2—Co1—O1	88.68 (6)	B2—O124—B1	116.87 (11)
O2^{i}—Co1—O1	91.32 (6)	B4—O124—B1	117.76 (11)
O2—Co1—O1^{i}	91.32 (6)	B5—O45—B4	124.30 (12)
O2^{i}—Co1—O1^{i}	88.68 (6)	B3—O34—B4	120.52 (12)
O1—Co1—O1^{i}	180.0	B6—O16—B1	124.47 (12)
O2—Co1—O4^{i}	88.17 (5)	B5—O15—B1	120.85 (12)
O2^{i}—Co1—O4^{i}	91.83 (5)	B3—O23—B2	123.44 (12)
O1—Co1—O4^{i}	87.03 (5)	B1—O1—Co1	118.94 (9)
O1^{i}—Co1—O4^{i}	92.97 (5)	B1—O1—H1	109.3 (19)
O2—Co1—O4	91.83 (5)	Co1—O1—H1	121.9 (19)
O2^{i}—Co1—O4	88.17 (5)	B2—O2—Co1	121.28 (9)
O1—Co1—O4	92.97 (5)	B2—O2—H2	122 (2)
O1^{i}—Co1—O4	87.03 (5)	Co1—O2—H2	114 (2)
O4^{i}—Co1—O4	180.0	B3—O3—H3	109.5
O15—B1—O16	110.89 (12)	B4^{i}—O4—Co1	116.22 (9)
O15—B1—O1	110.91 (13)	B4^{i}—O4—H4	110.6 (19)

O16—B1—O1	110.56 (12)	Co1—O4—H4	107.3 (19)
O15—B1—O124	109.07 (12)	B5—O5—H5	109.5
O16—B1—O124	108.17 (12)	B6—O6—H6	109.5
O1—B1—O124	107.12 (12)	B6—O26—B2	119.33 (13)
O26—B2—O23	109.16 (13)	H1W1—O1W—H2W1	112 (2)
O26—B2—O2	112.53 (12)	H1W2—O2W—H2W2	113 (2)
O23—B2—O2	110.85 (13)	H2W3—O3W—H1W3	111 (2)
O26—B2—O124	109.35 (12)	C1—N1—C2	110.90 (19)
O23—B2—O124	109.28 (12)	C1—N1—H1A	109.5
O2—B2—O124	105.58 (12)	C2—N1—H1A	109.5
O34—B3—O23	122.88 (14)	C1—N1—H1B	109.5
O34—B3—O3	117.27 (14)	C2—N1—H1B	109.5
O23—B3—O3	119.85 (14)	H1A—N1—H1B	108.0
O34—B4—O45	111.78 (12)	N1—C1—C2^{ii}	109.0 (2)
O34—B4—O4^{i}	109.79 (12)	N1—C1—H1C	109.9
O45—B4—O4^{i}	110.85 (12)	C2^{ii}—C1—H1C	109.9
O34—B4—O124	109.48 (12)	N1—C1—H1D	109.9
O45—B4—O124	107.67 (11)	C2^{ii}—C1—H1D	109.9
O4^{i}—B4—O124	107.13 (11)	H1C—C1—H1D	108.3
O15—B5—O5	117.83 (14)	C1^{ii}—C2—N1	109.18 (18)
O15—B5—O45	122.48 (14)	C1^{ii}—C2—H2A	109.8
O5—B5—O45	119.68 (14)	N1—C2—H2A	109.8
O26—B6—O6	122.85 (15)	C1^{ii}—C2—H2B	109.8
O26—B6—O16	122.54 (14)	N1—C2—H2B	109.8
O6—B6—O16	114.61 (14)	H2A—C2—H2B	108.3

O26—B2—O124—B4	158.42 (12)	O1—B1—O15—B5	−88.84 (17)
O23—B2—O124—B4	38.99 (17)	O124—B1—O15—B5	28.90 (19)
O2—B2—O124—B4	−80.28 (14)	O34—B3—O23—B2	4.1 (3)
O26—B2—O124—B1	−52.13 (16)	O3—B3—O23—B2	−176.41 (15)
O23—B2—O124—B1	−171.56 (11)	O26—B2—O23—B3	−136.34 (15)
O2—B2—O124—B1	69.17 (15)	O2—B2—O23—B3	99.17 (17)
O34—B4—O124—B2	−47.01 (16)	O124—B2—O23—B3	−16.8 (2)
O45—B4—O124—B2	−168.73 (11)	O15—B1—O1—Co1	128.21 (10)
O4^{i}—B4—O124—B2	71.99 (15)	O16—B1—O1—Co1	−108.36 (12)
O34—B4—O124—B1	163.82 (12)	O124—B1—O1—Co1	9.28 (14)
O45—B4—O124—B1	42.10 (16)	O2—Co1—O1—B1	37.04 (10)
O4^{i}—B4—O124—B1	−77.18 (14)	O2^{i}—Co1—O1—B1	−142.96 (10)
O15—B1—O124—B2	160.84 (12)	O1^{i}—Co1—O1—B1	3 (100)
O16—B1—O124—B2	40.14 (16)	O4^{i}—Co1—O1—B1	−51.19 (10)
O1—B1—O124—B2	−79.05 (14)	O4—Co1—O1—B1	128.81 (10)
O15—B1—O124—B4	−49.63 (16)	O26—B2—O2—Co1	125.40 (11)
O16—B1—O124—B4	−170.33 (12)	O23—B2—O2—Co1	−112.03 (12)
O1—B1—O124—B4	70.47 (15)	O124—B2—O2—Co1	6.19 (15)
O15—B5—O45—B4	−3.7 (3)	O2^{i}—Co1—O2—B2	−124 (100)
O5—B5—O45—B4	177.61 (16)	O1—Co1—O2—B2	−47.25 (11)
O34—B4—O45—B5	−135.19 (15)	O1^{i}—Co1—O2—B2	132.75 (11)
O4^{i}—B4—O45—B5	101.96 (17)	O4^{i}—Co1—O2—B2	39.82 (11)

O124—B4—O45—B5	−14.9 (2)	O4—Co1—O2—B2	−140.18 (11)
O23—B3—O34—B4	−12.8 (2)	O2—Co1—O4—B4^{i}	−134.31 (9)
O3—B3—O34—B4	167.68 (15)	O2^{i}—Co1—O4—B4^{i}	45.69 (9)
O45—B4—O34—B3	151.66 (14)	O1—Co1—O4—B4^{i}	136.92 (10)
O4^{i}—B4—O34—B3	−84.90 (16)	O1^{i}—Co1—O4—B4^{i}	−43.08 (10)
O124—B4—O34—B3	32.44 (19)	O4^{i}—Co1—O4—B4^{i}	10 (100)
O26—B6—O16—B1	−7.6 (3)	O6—B6—O26—B2	174.61 (15)
O6—B6—O16—B1	172.53 (15)	O16—B6—O26—B2	−5.2 (2)
O15—B1—O16—B6	−129.57 (16)	O23—B2—O26—B6	152.56 (14)
O1—B1—O16—B6	106.99 (17)	O2—B2—O26—B6	−83.94 (17)
O124—B1—O16—B6	−10.0 (2)	O124—B2—O26—B6	33.05 (19)
O5—B5—O15—B1	174.55 (16)	C2—N1—C1—C2^{ii}	−59.8 (3)
O45—B5—O15—B1	−4.2 (3)	C1—N1—C2—C1^{ii}	59.9 (3)
O16—B1—O15—B5	147.91 (15)		

Symmetry codes: (i) −*x*+1, −*y*+1, −*z*+1; (ii) −*x*+2, −*y*+2, −*z*.

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1···O2*W*	0.82 (1)	2.00 (2)	2.7525 (19)	153 (3)
O2—H2···O6^{iii}	0.81 (1)	2.11 (1)	2.876 (2)	157 (3)
O3—H3···O23^{iv}	0.82	1.93	2.745 (2)	172
O4—H4···O2*W*	0.81 (1)	2.08 (1)	2.864 (2)	164 (3)
O5—H5···O45^{v}	0.82	1.91	2.7159 (18)	169
O6—H6···O4^{iii}	0.82	1.95	2.734 (2)	160
O1*W*—H1*W*1···O5	0.86 (1)	1.96 (2)	2.771 (2)	158 (4)
O1*W*—H2*W*1···O26^{vi}	0.86 (1)	2.27 (1)	3.108 (3)	167 (3)
O1*W*—H2*W*1···O23^{vi}	0.86 (1)	2.51 (3)	3.158 (3)	133 (3)
O2*W*—H1*W*2···O3^{vii}	0.85 (1)	2.05 (2)	2.861 (2)	159 (3)
O2*W*—H2*W*2···O1*W*^{viii}	0.85 (1)	2.01 (1)	2.838 (3)	164 (3)
O3*W*—H2*W*3···O1*W*^{ii}	0.85 (1)	2.05 (2)	2.842 (3)	155 (3)
O3*W*—H1*W*3···O1^{ix}	0.85 (1)	2.24 (1)	3.088 (3)	179 (1)
N1—H1*A*···O16	0.90	1.78	2.654 (2)	165
N1—H1*A*···O6	0.90	2.46	2.986 (3)	117
N1—H1*B*···O3*W*	0.90	1.98	2.836 (3)	157
C1—H1*C*···O34^{vii}	0.97	2.56	3.321 (3)	136

Symmetry codes: (ii) −*x*+2, −*y*+2, −*z*; (iii) −*x*+2, −*y*+1, −*z*+1; (iv) −*x*+2, −*y*, −*z*+1; (v) −*x*+1, −*y*+1, −*z*; (vi) −*x*+2, −*y*+1, −*z*; (vii) *x*, *y*+1, *z*; (viii) −*x*+1, −*y*+2, −*z*; (ix) *x*+1, *y*, *z*.