



Crystal structure of the salt bis(triethanolamine- κ^3N,O,O')cobalt(II) bis[2-(2-oxo-2,3-dihydro-1,3-benzothiazol-3-yl)acetate]

Jamshid M. Ashurov,^{a*} Nodira J. Obidova,^a Hudaybergen B. Abdireymov^b and Bakhtiyar T. Ibragimov^a

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^aInstitute of Bioorganic Chemistry, Academy of Sciences of Uzbekistan, M. Ulugbek Str. 83, Tashkent 700125, Uzbekistan, and ^bKarakalpak State University, Nukus str. Abdirova 1, Karakalpakstan 742012, Uzbekistan.
*Correspondence e-mail: atom.uz@mail.ru

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Keywords: crystal structure; triethanolamine; α -(*N*-benzothiazolin-2-one) acetic acid; hydrogen bonding.

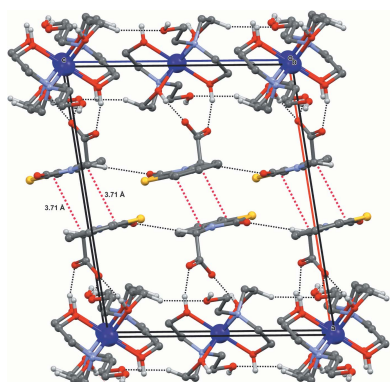
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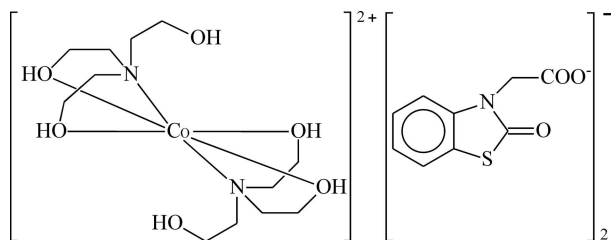
The reaction of 2-(2-oxo-2,3-dihydro-1,3-benzothiazol-3-yl)acetic acid (NBTA) and triethanolamine (TEA) with $\text{Co}(\text{NO}_3)_2$ results in the formation of the title complex, $[\text{Co}(\text{C}_6\text{H}_{15}\text{NO}_3)_2](\text{C}_9\text{H}_6\text{NO}_3\text{S})_2$, which is formed as a result of the association of bis(triethanolamine)cobalt(II) and 2-(2-oxo-2,3-dihydro-1,3-benzothiazol-3-yl)acetate units. It crystallizes in the monoclinic centrosymmetric space group $P2_1/c$, with the Co^{II} ion situated on an inversion centre. In the complex cation, the Co^{II} ion is octahedrally coordinated by two *N,O,O'*-tridentate TEA molecules with a facial distribution and the N atoms in a *trans* arrangement. Two ethanol groups of each TEA molecule form two five-membered chelate rings around the Co^{II} ion, while the third ethanol group does not coordinate to the metal. The free and coordinating hydroxy groups of the TEA molecules are involved in hydrogen bonding with the O atoms of NBTA anions, forming an infinite two-dimensional network extending parallel to the *bc* plane.

1. Chemical context

Triethanolamine (TEA) is used as a corrosion inhibitor in metal-cutting fluids, as a curing agent for epoxy and rubber polymers, adhesives and antistatic agents and as a pharmaceutical intermediate and an ointment emulsifier *etc.* However, TEA is not a substance possessing a specific physiological action (Beyer *et al.*, 1983; Knaak *et al.*, 1997) with exception of its low antibacterial activity. Benzothiazole is a precursor for rubber accelerators, a component of cyanine dyes, a slimicide in the paper and pulp industry, and is used in the production of certain fungicides, herbicides, antifungal agents and pharmaceuticals (Bellavia *et al.*, 2000; Seo *et al.*, 2000). The interaction of metal ions with TEA results in the formation of complexes in which TEA demonstrates monodentate (Kumar *et al.*, 2014), bidentate (Kapteijn *et al.*, 1997), tridentate (Gao *et al.*, 2004; Ucar *et al.*, 2004; Topcu *et al.*, 2001; Krabbes *et al.*, 1999; Haukka *et al.*, 2005; Yeşilel *et al.*, 2004; Mirskova *et al.*, 2013) and tetradentate binding (Zaitsev *et al.*, 2014; Kazak *et al.*, 2003; Yilmaz *et al.*, 2004; Langley *et al.*, 2011; Rickard *et al.*, 1999; Maestri & Brown, 2004; Kovbasyuk *et al.*, 2001; Tudor *et al.*, 2001). In some complexes, TEA can show bridging properties (Atria *et al.*, 2015; Wittick *et al.*, 2006; Sharma *et al.*, 2014; Yang *et al.*, 2014; Funes *et al.*, 2014). Here, we report the synthesis and structure of the title compound, $[\text{Co}(\text{C}_6\text{H}_{15}\text{NO}_3)_2](\text{C}_9\text{H}_6\text{NO}_3\text{S})_2$, (**I**).



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2. Structural commentary

The molecular structure of compound (**I**) is shown in Fig. 1. The structure consists of a complex cation and one 2-(2-oxo-2,3-dihydro-1,3-benzothiazol-3-yl)acetate anion. The asymmetric unit contains a half of the cationic moiety because the Co^{II} ion is located on an inversion centre. The cation and anion are linked by an $\text{O6} \cdots \text{H6} \cdots \text{O2}$ hydrogen bond (Table 1). In the cationic complex, the Co^{II} ion is coordinated by four oxygen and two nitrogen atoms of two ligands. The nitrogen atoms occupy *trans* positions of the coordination polyhedron. The $\text{Co}-\text{N}$ bond lengths [2.151 (3) Å] are equal as a result of symmetry, and the $\text{N}-\text{Co}-\text{N}$ bond angle is 180° . The $\text{Co}-\text{O}$ distances are 2.097 (2) Å and 2.101 (3) Å. One hydroxy group of each ethanol substituent is not involved in the coordination and is directed away from the coordination centre. The $\text{N}-\text{Co}-\text{O}$ bond angles range from 81.60 (10) to 98.40 (10) $^\circ$ and the $\text{O}-\text{Co}-\text{O}$ angles are 89.79 (10) and 90.21 (10) $^\circ$. Thus, the coordination polyhedron of the central atom is a slightly distorted octahedron of the CoN_2O_4 -type. The thiazoline ring (C1/C6/N1/C7/S1) and the bicyclic benzothiazole unit (N1/S1/C1-C7) are close to planar, the largest deviations from the least-squares planes being 0.019 (2) and 0.028 (4) Å, respectively. The dihedral angle between the plane of the carboxylate group and the benzothiazole ring system is 85.6 (2) $^\circ$.

3. Supramolecular features

The crystal structure of (**I**) contains an intricate network of intermolecular $\text{O}-\text{H} \cdots \text{O}$ and $\text{C}-\text{H} \cdots \text{O}$ hydrogen bonds (Table 1). The $[\text{Co}(\text{TEA})_2]^{2+}$ cations play an important role in

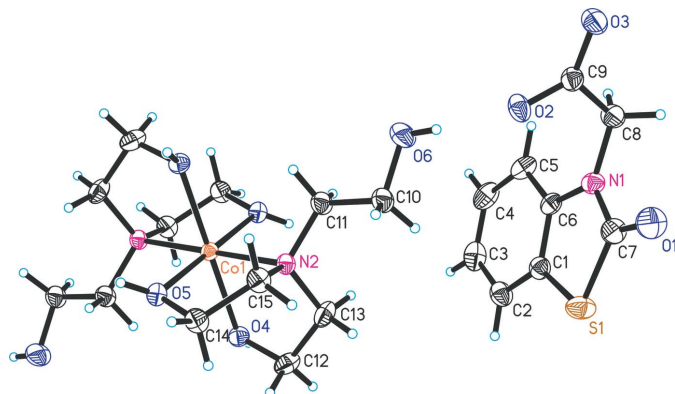


Figure 1
The molecular structure of (**I**), showing the atom-labelling scheme. Unlabelled atoms are generated by the inversion centre.

Table 1
Hydrogen-bond geometry (Å, $^\circ$).

$D-\text{H} \cdots A$	$D-\text{H}$	$\text{H} \cdots A$	$D \cdots A$	$D-\text{H} \cdots A$
$\text{O4}-\text{H4} \cdots \text{O2}^{\text{i}}$	0.88 (3)	1.71 (3)	2.572 (4)	166 (3)
$\text{O5}-\text{H5} \cdots \text{O3}^{\text{ii}}$	0.86 (1)	1.75 (2)	2.577 (4)	159 (3)
$\text{O6}-\text{H6} \cdots \text{O2}$	0.82	1.88	2.697 (4)	173
$\text{C8}-\text{H8A} \cdots \text{O1}^{\text{iii}}$	0.97	2.48	3.432 (6)	167
$\text{C12}-\text{H12B} \cdots \text{O6}^{\text{iv}}$	0.97	2.53	3.455 (6)	159

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

the supramolecular architecture. Each cation is surrounded by four 2-(2-oxo-2,3-dihydro-1,3-benzothiazol-3-yl)acetate anions. The H atoms of the free hydroxy group of the TEA ligand form a hydrogen bond with the carboxylate O atom of the NBTA ion while the coordinating hydroxy H atoms are involved in intermolecular hydrogen bonding with the carboxylate O atoms of the NBTA ions [$\text{H4} \cdots \text{O2}^{\text{i}} = 1.71$ (3) Å and $\text{H5} \cdots \text{O3}^{\text{ii}} = 1.752$ (17) Å; symmetry codes: (i) $x, -1 + y, z$; (ii) $2 - x, 1 - y, 2 - z$]. In addition, there is weak hydrogen bond between the $-\text{CH}_2$ group and the non-coordinating hydroxy-O atoms of the TEA ligand, with a $\text{C} \cdots \text{O}$ distance of 3.455 (6) Å. The above-mentioned hydrogen bonds give rise to $R_4^4(22)$ and $C_4^4(22)$ graph-set motifs. The crystal structure contains layers of hydrogen-bonded cations that are sandwiched between layers of hydrogen-bonded anions. Each layer extends in the bc plane. There is hydrogen bonding within and between these layers. These are arranged along [100] in the sequence $ACA \cdot ACA \cdot ACA$ (where A = anion layer and C = cation layer; Fig. 2) The NBTA anion layers are not linked by hydrogen bonds, but there are $\pi-\pi$ stacking interactions between benzene (centroid $Cg1$) and thiazolin (centroid $Cg2$)

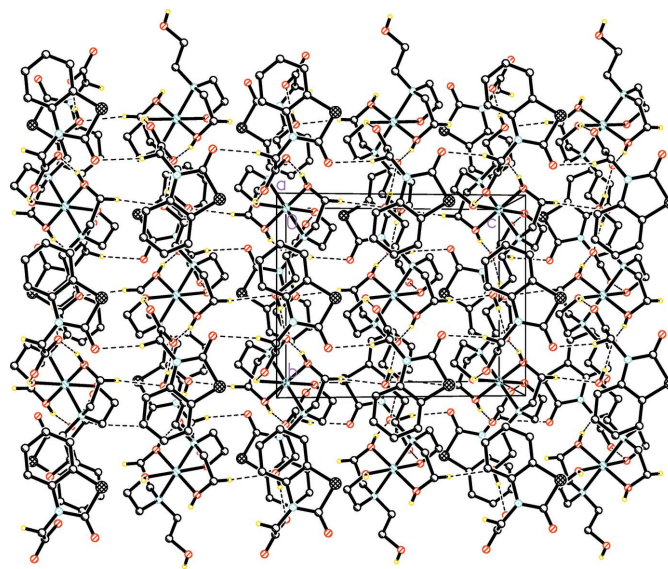


Figure 2
Part of the crystal structure with hydrogen bonds shown as dashed lines. For clarity, H atoms not involved in hydrogen bonding are not shown.

rings [$Cg1 \cdots Cg2(-x, -y, -z) = 3.71 \text{ \AA}$] of adjacent inversion-related molecules (Fig. 3).

4. Database survey

A survey of the Cambridge Structural Database (CSD; Groom & Allen, 2014) showed that coordination complexes of TEA with many metals including those of the *s*-, *d*-, *p*-, and *f*-blocks have been reported. Structures containing the bis(triethanolamine)cobalt(II) cation are described in the CSD entries with refcodes ASUGEA, IGALOR, WEPLIN.

5. Synthesis and crystallization

To an aqueous solution (2.5 ml) of $Co(NO_3)_2$ (0.091 g, 0.5 mmol) was added slowly an ethanol solution (5 ml) containing TEA (132 μ l) and NBTA (0.209 g, 1 mmol) with constant stirring. A light-brown crystalline product was obtained at room temperature by solvent evaporation after four weeks (yield 70%). Elemental analysis calculated for $C_{30}H_{42}CoN_4O_{12}S_2$: C, 46.57; H, 5.47; N, 7.24. Found: C, 46.62; H, 5.41; N, 7.19.

6. Refinement details

Crystal data, data collection and structure refinement details are summarized in Table 2. The coordinating hydroxy H atoms of the TEA ligand were located in a difference Fourier map and freely refined. C-bound H atoms were placed in calculated positions and refined as riding atoms: C–H = 0.93 and 0.97 \AA for aromatic and methylene H, with $U_{iso}(H) = 1.2U_{eq}(C)$.

Table 2
Experimental details.

Crystal data	
Chemical formula	$[Co(C_6H_{15}NO_3)_2](C_9H_6NO_3S)_2$
M_r	773.73
Crystal system, space group	Monoclinic, $P2_1/c$
Temperature (K)	293
a, b, c (\AA)	14.6953 (6), 9.7043 (3), 12.1311 (4)
β ($^\circ$)	98.513 (4)
V (\AA^3)	1710.94 (11)
Z	2
Radiation type	Cu $K\alpha$
μ (mm^{-1})	5.66
Crystal size (mm)	0.28 \times 0.24 \times 0.18
Data collection	
Diffractometer	Oxford Diffraction Xcalibur Ruby
Absorption correction	Multi-scan (SCALE3 ABSPACK in <i>CrysAlis PRO</i> ; Oxford Diffraction, 2009)
T_{min}, T_{max}	0.280, 0.797
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	7096, 3487, 2693
R_{int}	0.048
$(\sin \theta/\lambda)_{max}$ (\AA^{-1})	0.629
Refinement	
$R[F^2 > 2\sigma(F^2)], wR(F^2), S$	0.061, 0.175, 1.03
No. of reflections	3487
No. of parameters	230
No. of restraints	6
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}, \Delta\rho_{min}$ ($e \text{ \AA}^{-3}$)	0.47, -0.53

Computer programs: *CrysAlis PRO* (Oxford Diffraction, 2009), *SHELXS97*, *SHELXL97 XP* and *SHELXTL* (Sheldrick, 2008).

Acknowledgements

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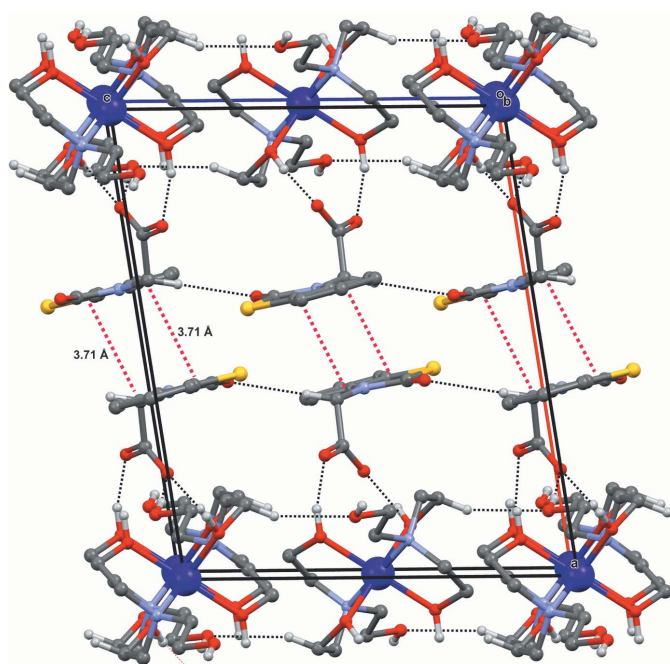


Figure 3

The crystal structure packing of (I). Hydrogen bonds are indicated by black dashed lines and π – π stacking interactions by red dashed lines.

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Crystal structure of the salt bis(triethanolamine- κ^3N,O,O')cobalt(II) bis[2-(2-oxo-2,3-dihydro-1,3-benzothiazol-3-yl)acetate]

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Computing details

Data collection: *CrysAlis PRO* (Oxford Diffraction, 2009); cell refinement: *CrysAlis PRO* (Oxford Diffraction, 2009); data reduction: *CrysAlis PRO* (Oxford Diffraction, 2009); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *XP* in *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL* (Sheldrick, 2008).

Bis(triethanolamine- κ^3N,O,O')cobalt(II) bis[2-(2-oxo-2,3-dihydro-1,3-benzothiazol-3-yl)acetate]

Crystal data

$[\text{Co}(\text{C}_6\text{H}_{15}\text{NO}_3)_2](\text{C}_9\text{H}_6\text{NO}_3\text{S})_2$

$M_r = 773.73$

Monoclinic, $P2_1/c$

Hall symbol: -P 2ybc

$a = 14.6953$ (6) Å

$b = 9.7043$ (3) Å

$c = 12.1311$ (4) Å

$\beta = 98.513$ (4)°

$V = 1710.94$ (11) Å³

$Z = 2$

$F(000) = 810$

$D_x = 1.502$ Mg m⁻³

Cu $K\alpha$ radiation, $\lambda = 1.54184$ Å

Cell parameters from 1414 reflections

$\theta = 3.7\text{--}75.3^\circ$

$\mu = 5.66$ mm⁻¹

$T = 293$ K

Block, dark orange

$0.28 \times 0.24 \times 0.18$ mm

Data collection

Oxford Diffraction Xcalibur Ruby diffractometer

Radiation source: fine-focus sealed tube

Graphite monochromator

Detector resolution: 10.2576 pixels mm⁻¹

ω scans

Absorption correction: multi-scan

(SCALE3 ABSPACK in *CrysAlis PRO*; Oxford Diffraction, 2009)

$T_{\min} = 0.280$, $T_{\max} = 0.797$

7096 measured reflections

3487 independent reflections

2693 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.048$

$\theta_{\max} = 75.8^\circ$, $\theta_{\min} = 5.5^\circ$

$h = -18 \rightarrow 17$

$k = -10 \rightarrow 12$

$l = -12 \rightarrow 15$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.061$

$wR(F^2) = 0.175$

$S = 1.03$

3487 reflections

230 parameters

6 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
 $w = 1/[\sigma^2(F_o^2) + (0.0899P)^2 + 0.4878P]$
where $P = (F_o^2 + 2F_c^2)/3$

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

$$\Delta\rho_{\max} = 0.47 \text{ e } \text{\AA}^{-3}$$

$$\Delta\rho_{\min} = -0.53 \text{ e } \text{\AA}^{-3}$$

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 (\AA^2)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
Co1	1.0000	0.0000	1.0000	0.0321 (2)
S1	1.42643 (10)	0.51313 (12)	1.23063 (9)	0.0613 (3)
O4	1.09939 (16)	-0.1150 (3)	1.1029 (2)	0.0405 (6)
H4	1.1359 (16)	-0.175 (3)	1.078 (2)	0.061*
O2	1.21319 (18)	0.7409 (3)	1.0090 (3)	0.0511 (7)
O5	0.92168 (17)	0.0172 (2)	1.1309 (2)	0.0397 (6)
H5	0.8630 (7)	0.025 (4)	1.130 (2)	0.060*
C4	1.3618 (3)	0.3107 (6)	0.8983 (4)	0.0640 (12)
H4A	1.3469	0.2728	0.8275	0.077*
N2	1.07355 (19)	0.1681 (3)	1.0879 (2)	0.0354 (6)
O6	1.1297 (3)	0.4967 (3)	0.9585 (3)	0.0719 (11)
H6	1.1537	0.5703	0.9793	0.108*
O3	1.25064 (18)	0.9228 (3)	0.9142 (3)	0.0593 (8)
O1	1.4058 (3)	0.7837 (3)	1.1993 (3)	0.0715 (9)
N1	1.3885 (2)	0.6444 (3)	1.0445 (3)	0.0432 (7)
C11	1.0861 (3)	0.2771 (4)	1.0053 (3)	0.0455 (9)
H11A	1.0256	0.3054	0.9693	0.055*
H11B	1.1176	0.2363	0.9484	0.055*
C1	1.4051 (2)	0.4195 (4)	1.1068 (3)	0.0441 (8)
C9	1.2684 (2)	0.8119 (4)	0.9634 (3)	0.0437 (8)
C10	1.1382 (3)	0.4043 (4)	1.0483 (3)	0.0507 (9)
H10A	1.1122	0.4435	1.1102	0.061*
H10B	1.2024	0.3826	1.0731	0.061*
C6	1.3850 (2)	0.5060 (4)	1.0156 (3)	0.0405 (8)
C13	1.1640 (3)	0.1118 (4)	1.1391 (4)	0.0535 (10)
H13A	1.1899	0.1712	1.2002	0.064*
H13B	1.2056	0.1126	1.0841	0.064*
C15	1.0160 (3)	0.2213 (4)	1.1688 (3)	0.0464 (9)
H15A	0.9732	0.2890	1.1321	0.056*
H15B	1.0551	0.2672	1.2292	0.056*
C8	1.3671 (3)	0.7592 (4)	0.9693 (4)	0.0500 (10)

H8A	1.3771	0.7314	0.8952	0.060*
H8B	1.4092	0.8341	0.9928	0.060*
C7	1.4049 (3)	0.6711 (5)	1.1570 (4)	0.0520 (10)
C12	1.1576 (3)	-0.0320 (5)	1.1821 (4)	0.0542 (11)
H12A	1.2186	-0.0725	1.1962	0.065*
H12B	1.1329	-0.0298	1.2520	0.065*
C3	1.3811 (3)	0.2232 (5)	0.9886 (4)	0.0628 (12)
H3	1.3783	0.1283	0.9781	0.075*
C5	1.3638 (3)	0.4522 (5)	0.9094 (3)	0.0522 (10)
H5A	1.3512	0.5095	0.8475	0.063*
C2	1.4045 (3)	0.2764 (4)	1.0941 (4)	0.0540 (10)
H2	1.4195	0.2186	1.1552	0.065*
C14	0.9626 (3)	0.1087 (4)	1.2162 (3)	0.0480 (9)
H14A	1.0035	0.0572	1.2714	0.058*
H14B	0.9148	0.1495	1.2530	0.058*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Co1	0.0309 (4)	0.0303 (4)	0.0344 (4)	0.0010 (3)	0.0022 (3)	0.0001 (3)
S1	0.0879 (9)	0.0538 (7)	0.0408 (5)	0.0058 (5)	0.0049 (5)	0.0012 (4)
O4	0.0378 (12)	0.0369 (14)	0.0464 (13)	0.0066 (10)	0.0050 (10)	0.0020 (11)
O2	0.0412 (13)	0.0348 (14)	0.0799 (19)	0.0011 (11)	0.0180 (13)	0.0036 (13)
O5	0.0371 (12)	0.0378 (14)	0.0445 (14)	-0.0006 (10)	0.0072 (10)	-0.0045 (10)
C4	0.056 (2)	0.075 (3)	0.058 (3)	0.007 (2)	-0.001 (2)	-0.025 (2)
N2	0.0368 (14)	0.0308 (15)	0.0384 (14)	-0.0032 (11)	0.0050 (11)	-0.0025 (12)
O6	0.090 (3)	0.048 (2)	0.072 (2)	-0.0219 (16)	-0.007 (2)	0.0152 (16)
O3	0.0405 (14)	0.0499 (18)	0.089 (2)	0.0076 (13)	0.0143 (14)	0.0197 (16)
O1	0.094 (3)	0.0485 (19)	0.069 (2)	0.0017 (17)	0.0040 (18)	-0.0165 (16)
N1	0.0388 (15)	0.0467 (19)	0.0439 (16)	0.0064 (13)	0.0056 (12)	0.0039 (14)
C11	0.052 (2)	0.039 (2)	0.0442 (19)	-0.0072 (17)	0.0051 (16)	-0.0020 (16)
C1	0.0381 (17)	0.048 (2)	0.046 (2)	0.0000 (16)	0.0090 (15)	-0.0006 (17)
C9	0.0375 (17)	0.041 (2)	0.052 (2)	0.0019 (15)	0.0066 (15)	-0.0002 (17)
C10	0.057 (2)	0.043 (2)	0.051 (2)	-0.0116 (18)	0.0041 (18)	-0.0016 (18)
C6	0.0294 (15)	0.050 (2)	0.0422 (19)	0.0057 (14)	0.0044 (14)	-0.0037 (16)
C13	0.041 (2)	0.049 (2)	0.066 (2)	-0.0023 (17)	-0.0108 (18)	-0.012 (2)
C15	0.055 (2)	0.040 (2)	0.045 (2)	-0.0034 (17)	0.0101 (17)	-0.0086 (17)
C8	0.0390 (18)	0.051 (2)	0.062 (2)	0.0061 (17)	0.0114 (17)	0.011 (2)
C7	0.054 (2)	0.047 (2)	0.054 (2)	0.0028 (18)	0.0059 (18)	-0.003 (2)
C12	0.055 (2)	0.048 (2)	0.053 (2)	0.0105 (18)	-0.0121 (19)	-0.0029 (19)
C3	0.052 (2)	0.051 (3)	0.086 (3)	0.000 (2)	0.014 (2)	-0.017 (2)
C5	0.046 (2)	0.066 (3)	0.043 (2)	0.013 (2)	0.0007 (17)	-0.009 (2)
C2	0.053 (2)	0.044 (2)	0.067 (3)	0.0011 (18)	0.014 (2)	0.003 (2)
C14	0.056 (2)	0.048 (2)	0.0405 (19)	-0.0068 (18)	0.0112 (16)	-0.0064 (17)

Geometric parameters (Å, °)

Co1—O4	2.097 (2)	C11—C10	1.505 (5)
Co1—O4 ⁱ	2.097 (2)	C11—H11A	0.9700
Co1—O5 ⁱ	2.101 (3)	C11—H11B	0.9700
Co1—O5	2.101 (3)	C1—C6	1.386 (5)
Co1—N2 ⁱ	2.151 (3)	C1—C2	1.398 (6)
Co1—N2	2.151 (3)	C9—C8	1.529 (5)
S1—C1	1.744 (4)	C10—H10A	0.9700
S1—C7	1.779 (5)	C10—H10B	0.9700
O4—C12	1.436 (5)	C6—C5	1.382 (5)
O4—H4	0.875 (9)	C13—C12	1.498 (6)
O2—C9	1.254 (4)	C13—H13A	0.9700
O5—C14	1.427 (4)	C13—H13B	0.9700
O5—H5	0.863 (9)	C15—C14	1.509 (5)
C4—C5	1.380 (7)	C15—H15A	0.9700
C4—C3	1.382 (7)	C15—H15B	0.9700
C4—H4A	0.9300	C8—H8A	0.9700
N2—C15	1.480 (4)	C8—H8B	0.9700
N2—C13	1.486 (5)	C12—H12A	0.9700
N2—C11	1.487 (5)	C12—H12B	0.9700
O6—C10	1.401 (5)	C3—C2	1.374 (6)
O6—H6	0.8200	C3—H3	0.9300
O3—C9	1.239 (5)	C5—H5A	0.9300
O1—C7	1.207 (5)	C2—H2	0.9300
N1—C7	1.374 (5)	C14—H14A	0.9700
N1—C6	1.387 (5)	C14—H14B	0.9700
N1—C8	1.445 (5)		
O4—Co1—O4 ⁱ	179.999 (1)	C11—C10—H10A	110.6
O4—Co1—O5 ⁱ	89.79 (10)	O6—C10—H10B	110.6
O4 ⁱ —Co1—O5 ⁱ	90.21 (10)	C11—C10—H10B	110.6
O4—Co1—O5	90.21 (10)	H10A—C10—H10B	108.7
O4 ⁱ —Co1—O5	89.79 (10)	C5—C6—C1	120.5 (4)
O5 ⁱ —Co1—O5	180.00 (14)	C5—C6—N1	126.6 (4)
O4—Co1—N2 ⁱ	98.40 (10)	C1—C6—N1	112.9 (3)
O4 ⁱ —Co1—N2 ⁱ	81.60 (10)	N2—C13—C12	112.9 (3)
O5 ⁱ —Co1—N2 ⁱ	81.74 (10)	N2—C13—H13A	109.0
O5—Co1—N2 ⁱ	98.26 (10)	C12—C13—H13A	109.0
O4—Co1—N2	81.60 (10)	N2—C13—H13B	109.0
O4 ⁱ —Co1—N2	98.40 (10)	C12—C13—H13B	109.0
O5 ⁱ —Co1—N2	98.26 (10)	H13A—C13—H13B	107.8
O5—Co1—N2	81.74 (10)	N2—C15—C14	112.4 (3)
N2 ⁱ —Co1—N2	180.0	N2—C15—H15A	109.1
C1—S1—C7	91.15 (19)	C14—C15—H15A	109.1
C12—O4—Co1	113.2 (2)	N2—C15—H15B	109.1
C12—O4—H4	105.5 (16)	C14—C15—H15B	109.1
Co1—O4—H4	124.2 (16)	H15A—C15—H15B	107.9

C14—O5—Co1	112.2 (2)	N1—C8—C9	113.8 (3)
C14—O5—H5	105.9 (15)	N1—C8—H8A	108.8
Co1—O5—H5	130.5 (18)	C9—C8—H8A	108.8
C5—C4—C3	122.3 (4)	N1—C8—H8B	108.8
C5—C4—H4A	118.8	C9—C8—H8B	108.8
C3—C4—H4A	118.8	H8A—C8—H8B	107.7
C15—N2—C13	114.6 (3)	O1—C7—N1	125.6 (4)
C15—N2—C11	109.8 (3)	O1—C7—S1	125.2 (3)
C13—N2—C11	110.5 (3)	N1—C7—S1	109.2 (3)
C15—N2—Co1	107.4 (2)	O4—C12—C13	110.6 (3)
C13—N2—Co1	106.3 (2)	O4—C12—H12A	109.5
C11—N2—Co1	108.0 (2)	C13—C12—H12A	109.5
C10—O6—H6	109.5	O4—C12—H12B	109.5
C7—N1—C6	115.3 (3)	C13—C12—H12B	109.5
C7—N1—C8	118.2 (3)	H12A—C12—H12B	108.1
C6—N1—C8	126.1 (3)	C2—C3—C4	120.1 (5)
N2—C11—C10	117.2 (3)	C2—C3—H3	120.0
N2—C11—H11A	108.0	C4—C3—H3	120.0
C10—C11—H11A	108.0	C4—C5—C6	117.7 (4)
N2—C11—H11B	108.0	C4—C5—H5A	121.1
C10—C11—H11B	108.0	C6—C5—H5A	121.1
H11A—C11—H11B	107.2	C3—C2—C1	118.2 (4)
C6—C1—C2	121.1 (4)	C3—C2—H2	120.9
C6—C1—S1	111.2 (3)	C1—C2—H2	120.9
C2—C1—S1	127.6 (3)	O5—C14—C15	111.2 (3)
O3—C9—O2	125.8 (3)	O5—C14—H14A	109.4
O3—C9—C8	116.4 (3)	C15—C14—H14A	109.4
O2—C9—C8	117.8 (3)	O5—C14—H14B	109.4
O6—C10—C11	105.9 (3)	C15—C14—H14B	109.4
O6—C10—H10A	110.6	H14A—C14—H14B	108.0
O4 ⁱ —Co1—O4—C12	-139 (11)	C2—C1—C6—N1	179.6 (3)
O5 ⁱ —Co1—O4—C12	103.4 (3)	S1—C1—C6—N1	1.1 (4)
O5—Co1—O4—C12	-76.6 (3)	C7—N1—C6—C5	175.5 (4)
N2 ⁱ —Co1—O4—C12	-175.0 (3)	C8—N1—C6—C5	2.5 (6)
N2—Co1—O4—C12	5.0 (3)	C7—N1—C6—C1	-4.1 (5)
O4—Co1—O5—C14	72.2 (2)	C8—N1—C6—C1	-177.1 (3)
O4 ⁱ —Co1—O5—C14	-107.8 (2)	C15—N2—C13—C12	80.4 (4)
O5 ⁱ —Co1—O5—C14	-141.4 (8)	C11—N2—C13—C12	-154.9 (3)
N2 ⁱ —Co1—O5—C14	170.7 (2)	Co1—N2—C13—C12	-38.0 (4)
N2—Co1—O5—C14	-9.3 (2)	C13—N2—C15—C14	-83.1 (4)
O4—Co1—N2—C15	-105.4 (2)	C11—N2—C15—C14	151.8 (3)
O4 ⁱ —Co1—N2—C15	74.6 (2)	Co1—N2—C15—C14	34.7 (4)
O5 ⁱ —Co1—N2—C15	166.0 (2)	C7—N1—C8—C9	-77.0 (5)
O5—Co1—N2—C15	-14.0 (2)	C6—N1—C8—C9	95.8 (4)
N2 ⁱ —Co1—N2—C15	-5 (14)	O3—C9—C8—N1	169.0 (4)
O4—Co1—N2—C13	17.6 (2)	O2—C9—C8—N1	-10.3 (5)
O4 ⁱ —Co1—N2—C13	-162.4 (2)	C6—N1—C7—O1	-176.0 (4)

O5 ⁱ —Co1—N2—C13	-70.9 (3)	C8—N1—C7—O1	-2.4 (6)
O5—Co1—N2—C13	109.1 (3)	C6—N1—C7—S1	4.9 (4)
N2 ⁱ —Co1—N2—C13	118 (14)	C8—N1—C7—S1	178.5 (3)
O4—Co1—N2—C11	136.3 (2)	C1—S1—C7—O1	177.4 (4)
O4 ⁱ —Co1—N2—C11	-43.7 (2)	C1—S1—C7—N1	-3.5 (3)
O5 ⁱ —Co1—N2—C11	47.7 (2)	Co1—O4—C12—C13	-26.9 (4)
O5—Co1—N2—C11	-132.3 (2)	N2—C13—C12—O4	44.2 (5)
N2 ⁱ —Co1—N2—C11	-123 (13)	C5—C4—C3—C2	-0.9 (7)
C15—N2—C11—C10	64.6 (4)	C3—C4—C5—C6	-0.7 (7)
C13—N2—C11—C10	-62.7 (4)	C1—C6—C5—C4	1.1 (6)
Co1—N2—C11—C10	-178.6 (3)	N1—C6—C5—C4	-178.4 (4)
C7—S1—C1—C6	1.4 (3)	C4—C3—C2—C1	2.0 (6)
C7—S1—C1—C2	-177.0 (4)	C6—C1—C2—C3	-1.6 (6)
N2—C11—C10—O6	-172.3 (4)	S1—C1—C2—C3	176.6 (3)
C2—C1—C6—C5	0.1 (6)	Co1—O5—C14—C15	30.8 (4)
S1—C1—C6—C5	-178.4 (3)	N2—C15—C14—O5	-44.5 (4)

Symmetry code: (i) $-x+2, -y, -z+2$.

Hydrogen-bond geometry ($\text{\AA}, ^\circ$)

<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>
O4—H4 \cdots O2 ⁱⁱ	0.88 (3)	1.71 (3)	2.572 (4)	166 (3)
O5—H5 \cdots O3 ⁱⁱⁱ	0.86 (1)	1.75 (2)	2.577 (4)	159 (3)
O6—H6 \cdots O2	0.82	1.88	2.697 (4)	173
C8—H8 <i>A</i> \cdots O1 ^{iv}	0.97	2.48	3.432 (6)	167
C12—H12 <i>B</i> \cdots O6 ^v	0.97	2.53	3.455 (6)	159

Symmetry codes: (ii) $x, y-1, z$; (iii) $-x+2, -y+1, -z+2$; (iv) $x, -y+3/2, z-1/2$; (v) $x, -y+1/2, z+1/2$.