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# Acetato(aqua){6,6′-dimethoxy-2,2′-[ethane-1,2-diylbis(nitrilomethanylylidene)]diphenolato}cobalt(III) methanol disolvate

**Gervas Assey,[a] Ray J. Butcher[b]* and Yilma Gultneh[b]**

[a]Nelson Mandela African Institute of Science and Technology, Department of Materials Science and Engineering, PO Box 447, Arusha, Tanzania, and [b]Department of Chemistry, Howard University, 525 College Street, NW, Washington, DC 2059, USA
Correspondence e-mail: rbutcher99@yahoo.com

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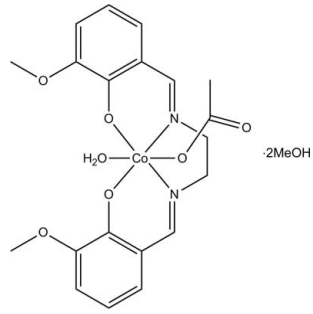
Key indicators: single-crystal X-ray study; $T$ = 115 K; mean $\sigma$(C–C) = 0.002 Å; $R$ factor = 0.040; $wR$ factor = 0.106; data-to-parameter ratio = 23.8.

In the title complex, $[Co(C_{18}H_{18}N_2O_4)(C_2H_3O_2)(H_2O)]\cdot 2CH_3OH$, the $Co^{III}$ atom is hexacoordinated by water and acetate groups in the axial positions and by the tetradentate Schiff base occupying equatorial positions. These axial bonds are longer than the equatorial bonds to the tetradentate Schiff base. Two molecules form a dimer through strong hydrogen bonds from the coordinated water of one molecule to the methoxy O atoms of an adjoining molecule. There is extensive intra- and intermolecular O—H···O hydrogen bonding between the coordinated water and acetate ligands and the methanol solvent molecules. In addition, there are weak intermolecular C—H···O interactions, which link the molecules into a three-dimensional array.

## Related literature

For reports on $O_2$ binding of related cobalt complexes, see: Huie *et al.* (1979); Lindblom *et al.* (1971). For related dimeric structures formed through hydrogen bonding, see: Huie *et al.* (1979); Assey *et al.* (2010*b*). For structurally related complexes with included hydrogen-bonded solvent molecules, see: Assey *et al.* (2010*a*,*b*); Ayikoe *et al.* (2010); Bao *et al.* (2009); Ayikoé *et al.* (2011). For the use of cobalt(III)–salen complexes as catalysts, see: Morandi *et al.* (2011); Haak *et al.* (2010) and for the potential applications of cobalt–Schiff base complexes for magnetic and/or conducting devices, see: Nabei *et al.* (2009); Lin *et al.* (2011).




## Experimental

### Crystal data

$[Co(C_{18}H_{18}N_2O_4)(C_2H_3O_2)(H_2O)]\cdot 2CH_4O$
$M_r$ = 526.42
Monoclinic, $P2_1/c$
$a$ = 9.6306 (3) Å
$b$ = 13.4129 (5) Å
$c$ = 17.9746 (7) Å
$\beta$ = 90.716 (3)°
$V$ = 2321.67 (15) Å$^3$
$Z$ = 4
Mo $K\alpha$ radiation
$\mu$ = 0.80 mm$^{-1}$
$T$ = 115 K
0.49 × 0.45 × 0.38 mm

### Data collection

Oxford Diffraction Xcalibur diffractometer with a Ruby (Gemini Mo) detector
Absorption correction: multi-scan (*CrysAlis RED*; Oxford Diffraction, 2007)
$T_{min}$ = 0.916, $T_{max}$ = 1.000
16513 measured reflections
7669 independent reflections
5549 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.027

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.040
$wR(F^2)$ = 0.106
$S$ = 1.00
7669 reflections
322 parameters
3 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.86 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.45 e Å$^{-3}$

**Table 1**
Selected bond lengths (Å).

| | | | |
|---|---|---|---|
| Co—O2 | 1.8839 (8) | Co—N2 | 1.8910 (10) |
| Co—N1 | 1.8870 (10) | Co—O11 | 1.8995 (8) |
| Co—O1 | 1.8892 (8) | Co—O1*W* | 1.9454 (8) |

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

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| O1*S*—H1*S*···O12 | 0.84 | 1.83 | 2.6671 (14) | 174 |
| O2*S*—H2*S*···O1*S* | 0.84 | 1.95 | 2.7682 (17) | 165 |
| O1*W*—H1*W*1···O1$^{i}$ | 0.80 (1) | 1.99 (1) | 2.7334 (11) | 153 (1) |
| O1*W*—H1*W*1···O3$^{i}$ | 0.80 (1) | 2.32 (1) | 2.9124 (13) | 131 (1) |
| O1*W*—H1*W*2···O2$^{i}$ | 0.80 (1) | 2.18 (2) | 2.8071 (11) | 136 (1) |
| O1*W*—H1*W*2···O4$^{i}$ | 0.80 (1) | 2.17 (1) | 2.8840 (12) | 148 (2) |
| C9—H9*A*···O1*S*$^{ii}$ | 0.99 | 2.52 | 3.2610 (16) | 132 |
| C13—H13*A*···O11$^{iii}$ | 0.95 | 2.61 | 3.5380 (15) | 165 |
| C12*A*—H12*B*···O1 | 0.98 | 2.38 | 3.1807 (15) | 139 |
| C8—H8*A*···O2*S*$^{iv}$ | 0.95 | 2.55 | 3.4335 (16) | 155 |
| C10—H10*A*···O2*S*$^{ii}$ | 0.99 | 2.61 | 3.5119 (17) | 151 |
| C12*A*—H12*C*···O2*S*$^{v}$ | 0.98 | 2.62 | 3.5541 (19) | 161 |

Symmetry codes: (i) $-x+1, -y+1, -z+1$; (ii) $x-1, y, z$; (iii) $-x+1, y+\frac{1}{2}, -z+\frac{3}{2}$; (iv) $-x+1, y-\frac{1}{2}, -z+\frac{3}{2}$; (v) $-x+2, y-\frac{1}{2}, -z+\frac{3}{2}$.

Data collection: *CrysAlis PRO* (Oxford Diffraction, 2007); cell refinement: *CrysAlis PRO*; data reduction: *CrysAlis PRO*;

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: JJ2140).

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# supporting information

*Acta Cryst.* (2012). E**68**, m962–m963 [https://doi.org/10.1107/S1600536812027687]

## Acetato(aqua){6,6′-dimethoxy-2,2′-[ethane-1,2-diylbis(nitrilomethanylylidene)]diphenolato}cobalt(III) methanol disolvate

**Gervas Assey, Ray J. Butcher and Yilma Gultneh**

### S1. Comment

Cobalt Schiff base complexes are of great importance because of their involvement in biological systems. One of their reactions of biological importance is that of binding $O_2$ to a metal chelate (Lindblom *et al.* 1971). In recent years, there have been reports about many studies of metal complexes with di-oxygen as one ligand (Huie *et al.*, 1979). The reason behind these studies is to understand the binding between oxygen and transition metals in the proteins that are involved in oxygen transport in living creatures. Another area where the cobalt Schiff bases have find application is that of organic reactions catalysis (Haak *et al.* 2010). Cobalt(III) salen complexes have been described in the literature as catalysts for enantioselective cyclopropagation with diazoacetates in organic media (Morandi *et al.* 2011). Cobalt Schiff base complexes have also been investigated with respect to their potential application for magnetic and/or conducting devices (Nabei *et al.*, 2009; Lin *et al.*, 2011).

In view of the importance of cobalt Schiff base complexes the structure of the title compound, $CoC_{20}H_{23}N_2O_7{\cdot}2(CH_3OH)$, has been determined. Schiff base ligands containing a methoxy or ethoxy substituent in the 3 position in the aromatic ring and in a *cis* conformation about the central metal are often involved in interactions where these substituent are either coordinated to a metal (Assey *et al.*, 2010*a*,*b*; Ayikoe, *et al.*, 2010) or form strong hydrogen bonds to a water molecule (or some other suitable solvent such as dimethylformamide) in the cavity created by this conformation (Bao *et al.*, 2009; Ayikoé *et al.*, 2011). In this case, as is found in related Mn and Co complexes (Assey *et al.*, 2010*b*; Huie, *et al.*, 1979), this is achieved by two metal complexes coming together to form a hydrogen bonded dimer. The axially coordinated water molecules of each metal complex form strong hydrogen bonds to the two methoxy groups of the adjoining complex (O1W···O1 2.7335 (11), O1W···O3 2.9124 (13), O1W··· O2 2.8071 (11), O1W···O4 2.8840 (12) Å).

The structure consists of six coordinate Co(III) in a slightly distorted octahedral geometry with both methanol and water occupying the axial positions and a tetradentate Schiff base ($N_2O_2$) which is in the equatorial plane. In addition there are two molecules of solvate methanol in the lattice (Fig. 1). From Table 1 it can be seen that the equatorial metal ligand bond lengths are very similar and vary from 1.8839 (8)Å to 1.8910 (10)Å while the axial bond lengths to the water and acetate moieties are slightly longer at 1.9454 (8)Å and 1.8995 (8)Å respectively. The only slightly distorted nature of the coordination sphere about the Co is emphasized by the fact that the *cis* angles vary from 78.40 (4)° to 94.18 (4)° while the *trans* angles range from 173.73 (3)° to 178.40 (4)°.

There is extensive O—H···O intra- and intermolecular hydrogen bonding between the coordinated water and acetate moieties and the methanol solvate molecules (Fig. 2). In addition there are weak C—H···O intermolecular interactions. These link the structure into a three-dimensional array.

## S2. Experimental

The synthesis of the ligand 3-methoxyethylenediaminebissalicylaldimine was accomplished by the reaction of the solution of (2 g, 33.3 mmol) of ethylenediamine in 10 ml methanol which was added to the solution of *o*-vanillin in 40 ml methanol dropwise using a glass pipette. The mixture was refluxed for 24 h. After solvent evaporation under reduced pressure yellow solids were obtained.

The complex was synthesized by mixing a solution of (0.25 g, 1 mmol) of $Co(CH_3COO)_2{\cdot}4H_2O$ in 5 ml me thanol with a solution of (0.33 g, 1 mmol) 3-methoxyethylenediaminebissalicylaldimine in 3 ml of dichloromethene. The mixture was stirred for 1 h at room temperature, filtered and layered with diethyl ether for crystallization. Crystals suitable for single-crystal X-ray diffraction were obtained by slow evaporation.

## S3. Refinement

H atoms were placed in geometrically idealized positions and constrained to ride on their parent atoms with a C—H distances of 0.95 and 0.99 Å $U_{iso}$(H) = 1.2$U_{eq}$(C) and 0.98 Å for $CH_3$ [$U_{iso}$(H) = 1.5$U_{eq}$(C)]. The H atoms attached to methanol O were idealized with an O–H distance of 0.84 Å. The water H's were constrained to have a bond length of 0.82 Å and bond angle of 104.5°.

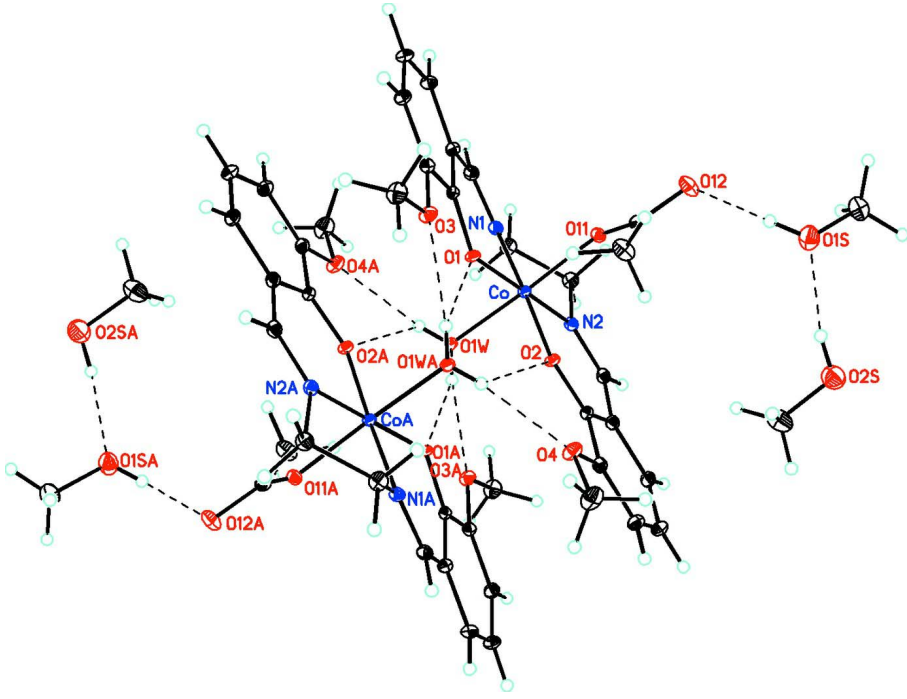


**Figure 1**

Molecular Structure of the title compound (dimer) along with hydrogen bonding interactions between the coordinated water molecule of one molecule and adjoining oxygen atoms of an adjacent molecule (generated by symmetry codes 1 - *x*, 1 - *y*, 1 - *z*). Hydrogen bonding and weak C—H···O intermolecular interactions are shown by dashed lines.

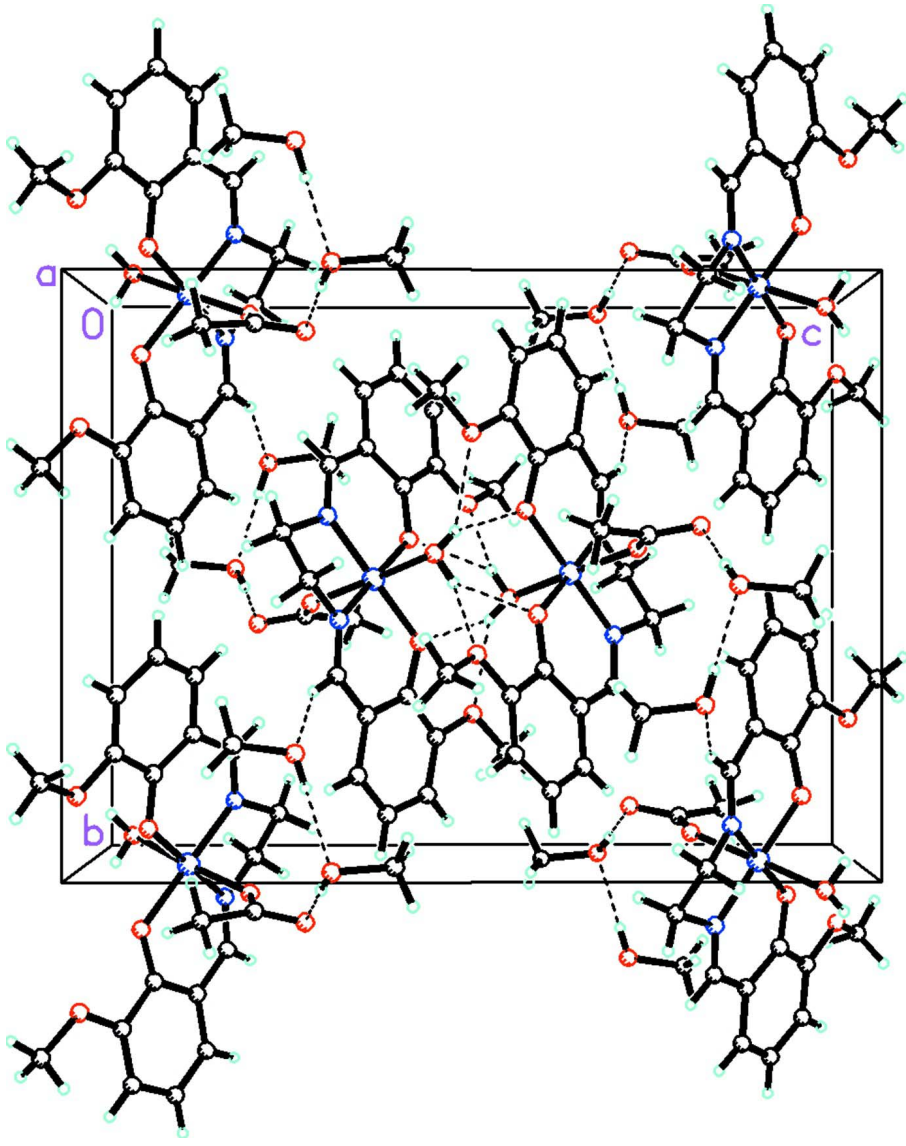


**Figure 2**

The molecular packing for $C_{22}H_{31}CoN_2O_9$ viewed along the *a* axis. O—H···O hydrogen bonding and weak C—H···O intermolecular interactions are shown by dashed lines.

## Acetato(aqua){6,6′-dimethoxy-2,2′-[ethane-1,2- diylbis(nitrilomethanylylidene)]diphenolato}cobalt(III) methanol disolvate

*Crystal data*

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$M_r = 526.42$
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
$a = 9.6306$ (3) Å
$b = 13.4129$ (5) Å
$c = 17.9746$ (7) Å
$\beta = 90.716$ (3)°
$V = 2321.67$ (15) Å$^3$
$Z = 4$
$F(000) = 1104$
$D_x = 1.506$ Mg m$^{-3}$
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 8159 reflections
$\theta = 4.6$–$32.6$°
$\mu = 0.80$ mm$^{-1}$

$T$ = 115 K
Block, black

0.49 × 0.45 × 0.38 mm

*Data collection*

Oxford Diffraction Xcalibur diffractometer with a Ruby (Gemini Mo) detector
Radiation source: Enhance (Mo) X-ray Source
Graphite monochromator
Detector resolution: 10.5081 pixels mm$^{-1}$
$\omega$ scans
Absorption correction: multi-scan (*CrysAlis RED*; Oxford Diffraction, 2007)

$T_{min}$ = 0.916, $T_{max}$ = 1.000
16513 measured reflections
7669 independent reflections
5549 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.027
$\theta_{max}$ = 32.7°, $\theta_{min}$ = 4.6°
$h$ = −14→10
$k$ = −19→19
$l$ = −26→24

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.040
$wR(F^2)$ = 0.106
$S$ = 1.00
7669 reflections
322 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 atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0609P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.003
$\Delta\rho_{max}$ = 0.86 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.45 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 (Å$^2$)*

| | $x$ | $y$ | $z$ | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| Co | 0.466441 (15) | 0.494930 (12) | 0.628307 (8) | 0.01070 (3) |
| O1 | 0.51899 (8) | 0.38488 (6) | 0.56942 (4) | 0.01284 (17) |
| O2 | 0.61286 (8) | 0.56561 (6) | 0.58402 (4) | 0.01292 (17) |
| O3 | 0.66160 (8) | 0.25427 (7) | 0.49906 (5) | 0.01703 (19) |
| O4 | 0.81315 (8) | 0.63147 (7) | 0.50542 (5) | 0.0193 (2) |
| O11 | 0.57142 (8) | 0.45215 (7) | 0.71259 (4) | 0.01444 (18) |
| O12 | 0.74146 (9) | 0.41453 (8) | 0.78855 (5) | 0.0254 (2) |
| O1S | 0.97081 (11) | 0.51409 (8) | 0.82748 (6) | 0.0316 (3) |
| H1S | 0.9021 | 0.4805 | 0.8128 | 0.038* |
| O2S | 1.00189 (11) | 0.71051 (10) | 0.78342 (6) | 0.0372 (3) |
| H2S | 0.9767 | 0.6530 | 0.7959 | 0.045* |
| O1W | 0.34122 (8) | 0.53835 (7) | 0.54896 (4) | 0.01342 (17) |
| H1W1 | 0.3795 (14) | 0.5775 (9) | 0.5223 (8) | 0.033 (4)* |

| | | | | |
|---|---|---|---|---|
| H1W2 | 0.3269 (17) | 0.4892 (8) | 0.5248 (9) | 0.035 (5)* |
| N1 | 0.31519 (9) | 0.42594 (8) | 0.66977 (5) | 0.0138 (2) |
| N2 | 0.40860 (9) | 0.60406 (8) | 0.68688 (5) | 0.0133 (2) |
| C1 | 0.49094 (12) | 0.29163 (9) | 0.58520 (6) | 0.0132 (2) |
| C2 | 0.56595 (12) | 0.21670 (9) | 0.54734 (6) | 0.0149 (2) |
| C3 | 0.73547 (13) | 0.18472 (10) | 0.45519 (7) | 0.0221 (3) |
| H3A | 0.7886 | 0.1398 | 0.4878 | 0.033* |
| H3B | 0.7992 | 0.2205 | 0.4225 | 0.033* |
| H3C | 0.6697 | 0.1458 | 0.4249 | 0.033* |
| C4 | 0.54031 (13) | 0.11683 (9) | 0.55913 (7) | 0.0186 (3) |
| H4A | 0.5914 | 0.0680 | 0.5327 | 0.022* |
| C5 | 0.43877 (13) | 0.08716 (10) | 0.61010 (7) | 0.0209 (3) |
| H5A | 0.4220 | 0.0184 | 0.6188 | 0.025* |
| C6 | 0.36441 (12) | 0.15766 (10) | 0.64706 (7) | 0.0192 (3) |
| H6A | 0.2953 | 0.1372 | 0.6811 | 0.023* |
| C7 | 0.38811 (12) | 0.26038 (9) | 0.63580 (6) | 0.0151 (2) |
| C8 | 0.30021 (12) | 0.33125 (10) | 0.67197 (6) | 0.0162 (3) |
| H8A | 0.2248 | 0.3058 | 0.6998 | 0.019* |
| C9 | 0.21663 (12) | 0.49324 (10) | 0.70532 (7) | 0.0180 (3) |
| H9A | 0.1627 | 0.4573 | 0.7434 | 0.022* |
| H9B | 0.1512 | 0.5215 | 0.6680 | 0.022* |
| C10 | 0.30322 (12) | 0.57550 (10) | 0.74114 (7) | 0.0172 (3) |
| H10A | 0.2439 | 0.6334 | 0.7533 | 0.021* |
| H10B | 0.3481 | 0.5511 | 0.7875 | 0.021* |
| C11 | 0.45679 (12) | 0.69332 (9) | 0.68597 (6) | 0.0148 (2) |
| H11A | 0.4160 | 0.7408 | 0.7183 | 0.018* |
| C12 | 0.56841 (12) | 0.72658 (9) | 0.63936 (6) | 0.0145 (2) |
| C13 | 0.60648 (12) | 0.82845 (9) | 0.64321 (7) | 0.0178 (3) |
| H13A | 0.5585 | 0.8722 | 0.6756 | 0.021* |
| C14 | 0.71224 (13) | 0.86428 (10) | 0.60043 (7) | 0.0209 (3) |
| H14A | 0.7367 | 0.9328 | 0.6029 | 0.025* |
| C15 | 0.78416 (13) | 0.80023 (10) | 0.55325 (7) | 0.0197 (3) |
| H15A | 0.8576 | 0.8254 | 0.5239 | 0.024* |
| C16 | 0.74939 (12) | 0.70131 (10) | 0.54911 (6) | 0.0153 (3) |
| C17 | 0.93798 (13) | 0.66034 (12) | 0.46918 (8) | 0.0283 (3) |
| H17A | 0.9178 | 0.7145 | 0.4341 | 0.042* |
| H17B | 0.9758 | 0.6031 | 0.4422 | 0.042* |
| H17C | 1.0060 | 0.6832 | 0.5064 | 0.042* |
| C18 | 0.63880 (11) | 0.66078 (9) | 0.59181 (6) | 0.0127 (2) |
| C11A | 0.69919 (12) | 0.43003 (10) | 0.72351 (7) | 0.0168 (3) |
| C12A | 0.79963 (13) | 0.42151 (12) | 0.66052 (7) | 0.0244 (3) |
| H12A | 0.8400 | 0.4871 | 0.6503 | 0.037* |
| H12B | 0.7507 | 0.3973 | 0.6160 | 0.037* |
| H12C | 0.8737 | 0.3746 | 0.6742 | 0.037* |
| C1S | 0.96778 (15) | 0.52329 (12) | 0.90478 (8) | 0.0308 (4) |
| H1S3 | 1.0350 | 0.5740 | 0.9209 | 0.046* |
| H1S1 | 0.9917 | 0.4592 | 0.9277 | 0.046* |
| H1S2 | 0.8745 | 0.5432 | 0.9200 | 0.046* |

| | | | | |
|---|---|---|---|---|
| C2S | 0.97663 (17) | 0.72400 (13) | 0.70700 (9) | 0.0356 (4) |
| H2S1 | 0.9926 | 0.7940 | 0.6939 | 0.053* |
| H2S2 | 0.8802 | 0.7061 | 0.6951 | 0.053* |
| H2S3 | 1.0395 | 0.6814 | 0.6786 | 0.053* |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| Co | 0.01352 (6) | 0.00968 (7) | 0.00896 (6) | −0.00053 (6) | 0.00239 (5) | −0.00046 (6) |
| O1 | 0.0197 (4) | 0.0074 (4) | 0.0115 (3) | −0.0009 (3) | 0.0038 (3) | 0.0000 (3) |
| O2 | 0.0161 (3) | 0.0090 (4) | 0.0138 (4) | −0.0018 (3) | 0.0036 (3) | −0.0012 (3) |
| O3 | 0.0225 (4) | 0.0118 (4) | 0.0169 (4) | 0.0007 (3) | 0.0048 (3) | −0.0034 (3) |
| O4 | 0.0208 (4) | 0.0178 (4) | 0.0195 (4) | −0.0061 (3) | 0.0090 (3) | −0.0042 (4) |
| O11 | 0.0165 (3) | 0.0155 (4) | 0.0114 (4) | 0.0009 (3) | 0.0014 (3) | 0.0005 (3) |
| O12 | 0.0227 (4) | 0.0368 (6) | 0.0167 (4) | 0.0030 (4) | −0.0017 (3) | 0.0068 (4) |
| O1S | 0.0299 (5) | 0.0407 (7) | 0.0243 (5) | −0.0068 (4) | 0.0029 (4) | −0.0023 (5) |
| O2S | 0.0404 (6) | 0.0390 (7) | 0.0321 (6) | 0.0006 (5) | −0.0006 (5) | 0.0016 (5) |
| O1W | 0.0178 (4) | 0.0106 (4) | 0.0118 (4) | −0.0020 (3) | 0.0015 (3) | −0.0002 (3) |
| N1 | 0.0145 (4) | 0.0156 (5) | 0.0114 (4) | −0.0009 (4) | 0.0023 (3) | 0.0013 (4) |
| N2 | 0.0159 (4) | 0.0134 (5) | 0.0107 (4) | 0.0016 (4) | 0.0018 (3) | −0.0014 (4) |
| C1 | 0.0180 (5) | 0.0107 (5) | 0.0109 (5) | −0.0016 (4) | −0.0023 (4) | −0.0003 (4) |
| C2 | 0.0183 (5) | 0.0125 (5) | 0.0138 (5) | −0.0004 (4) | −0.0019 (4) | 0.0004 (5) |
| C3 | 0.0238 (6) | 0.0196 (6) | 0.0231 (6) | 0.0053 (5) | 0.0041 (5) | −0.0066 (5) |
| C4 | 0.0255 (6) | 0.0103 (6) | 0.0200 (6) | 0.0009 (5) | −0.0032 (5) | −0.0017 (5) |
| C5 | 0.0288 (6) | 0.0103 (6) | 0.0236 (6) | −0.0034 (5) | −0.0043 (5) | 0.0035 (5) |
| C6 | 0.0220 (5) | 0.0167 (6) | 0.0188 (6) | −0.0055 (5) | −0.0002 (5) | 0.0048 (5) |
| C7 | 0.0184 (5) | 0.0128 (5) | 0.0141 (5) | −0.0023 (4) | −0.0003 (4) | 0.0005 (5) |
| C8 | 0.0168 (5) | 0.0196 (6) | 0.0122 (5) | −0.0048 (5) | 0.0029 (4) | 0.0020 (5) |
| C9 | 0.0148 (5) | 0.0204 (6) | 0.0189 (5) | 0.0003 (5) | 0.0049 (4) | −0.0020 (5) |
| C10 | 0.0187 (5) | 0.0191 (6) | 0.0138 (5) | 0.0005 (5) | 0.0052 (4) | −0.0030 (5) |
| C11 | 0.0168 (5) | 0.0153 (6) | 0.0124 (5) | 0.0025 (4) | 0.0000 (4) | −0.0031 (5) |
| C12 | 0.0172 (5) | 0.0127 (5) | 0.0135 (5) | 0.0011 (4) | −0.0010 (4) | −0.0019 (4) |
| C13 | 0.0238 (5) | 0.0117 (5) | 0.0177 (5) | 0.0014 (5) | −0.0027 (4) | −0.0035 (5) |
| C14 | 0.0289 (6) | 0.0115 (6) | 0.0223 (6) | −0.0042 (5) | −0.0031 (5) | 0.0000 (5) |
| C15 | 0.0233 (5) | 0.0177 (6) | 0.0181 (6) | −0.0070 (5) | 0.0010 (5) | 0.0008 (5) |
| C16 | 0.0183 (5) | 0.0157 (6) | 0.0119 (5) | −0.0016 (4) | 0.0007 (4) | −0.0017 (5) |
| C17 | 0.0224 (6) | 0.0340 (8) | 0.0287 (7) | −0.0086 (6) | 0.0114 (5) | −0.0055 (6) |
| C18 | 0.0153 (5) | 0.0110 (5) | 0.0118 (5) | −0.0013 (4) | −0.0014 (4) | −0.0006 (4) |
| C11A | 0.0192 (5) | 0.0145 (6) | 0.0167 (5) | −0.0020 (5) | 0.0010 (4) | 0.0014 (5) |
| C12A | 0.0183 (5) | 0.0338 (8) | 0.0211 (6) | 0.0070 (5) | 0.0044 (5) | 0.0040 (6) |
| C1S | 0.0294 (7) | 0.0370 (9) | 0.0260 (7) | 0.0033 (6) | −0.0021 (6) | −0.0010 (7) |
| C2S | 0.0403 (8) | 0.0391 (9) | 0.0275 (7) | 0.0132 (7) | 0.0039 (6) | 0.0047 (7) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| Co—O2 | 1.8839 (8) | C6—C7 | 1.4115 (18) |
| Co—N1 | 1.8870 (10) | C6—H6A | 0.9500 |
| Co—O1 | 1.8892 (8) | C7—C8 | 1.4342 (17) |

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|---|---|---|---|
| Co—N2 | 1.8910 (10) | C8—H8A | 0.9500 |
| Co—O11 | 1.8995 (8) | C9—C10 | 1.5211 (18) |
| Co—O1W | 1.9454 (8) | C9—H9A | 0.9900 |
| O1—C1 | 1.3113 (14) | C9—H9B | 0.9900 |
| O2—C18 | 1.3079 (14) | C10—H10A | 0.9900 |
| O3—C2 | 1.3696 (14) | C10—H10B | 0.9900 |
| O3—C3 | 1.4185 (15) | C11—C12 | 1.4419 (16) |
| O4—C16 | 1.3723 (15) | C11—H11A | 0.9500 |
| O4—C17 | 1.4279 (15) | C12—C18 | 1.4083 (16) |
| O11—C11A | 1.2786 (14) | C12—C13 | 1.4162 (17) |
| O12—C11A | 1.2505 (15) | C13—C14 | 1.3708 (18) |
| O1S—C1S | 1.3956 (18) | C13—H13A | 0.9500 |
| O1S—H1S | 0.8400 | C14—C15 | 1.3970 (19) |
| O2S—C2S | 1.4038 (18) | C14—H14A | 0.9500 |
| O2S—H2S | 0.8400 | C15—C16 | 1.3702 (18) |
| O1W—H1W1 | 0.803 (11) | C15—H15A | 0.9500 |
| O1W—H1W2 | 0.801 (11) | C16—C18 | 1.4281 (16) |
| N1—C8 | 1.2789 (17) | C17—H17A | 0.9800 |
| N1—C9 | 1.4625 (16) | C17—H17B | 0.9800 |
| N2—C11 | 1.2842 (16) | C17—H17C | 0.9800 |
| N2—C10 | 1.4672 (15) | C11A—C12A | 1.5027 (17) |
| C1—C7 | 1.4164 (16) | C12A—H12A | 0.9800 |
| C1—C2 | 1.4168 (17) | C12A—H12B | 0.9800 |
| C2—C4 | 1.3790 (17) | C12A—H12C | 0.9800 |
| C3—H3A | 0.9800 | C1S—H1S3 | 0.9800 |
| C3—H3B | 0.9800 | C1S—H1S1 | 0.9800 |
| C3—H3C | 0.9800 | C1S—H1S2 | 0.9800 |
| C4—C5 | 1.4058 (18) | C2S—H2S1 | 0.9800 |
| C4—H4A | 0.9500 | C2S—H2S2 | 0.9800 |
| C5—C6 | 1.3640 (19) | C2S—H2S3 | 0.9800 |
| C5—H5A | 0.9500 | | |

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|---|---|---|---|
| O2—Co—N1 | 177.81 (4) | N1—C9—H9A | 110.5 |
| O2—Co—O1 | 87.09 (3) | C10—C9—H9A | 110.5 |
| N1—Co—O1 | 92.96 (4) | N1—C9—H9B | 110.5 |
| O2—Co—N2 | 94.18 (4) | C10—C9—H9B | 110.5 |
| N1—Co—N2 | 85.73 (4) | H9A—C9—H9B | 108.7 |
| O1—Co—N2 | 178.40 (4) | N2—C10—C9 | 106.75 (9) |
| O2—Co—O11 | 95.47 (3) | N2—C10—H10A | 110.4 |
| N1—Co—O11 | 86.71 (4) | C9—C10—H10A | 110.4 |
| O1—Co—O11 | 93.85 (4) | N2—C10—H10B | 110.4 |
| N2—Co—O11 | 86.98 (4) | C9—C10—H10B | 110.4 |
| O2—Co—O1W | 90.00 (3) | H10A—C10—H10B | 108.6 |
| N1—Co—O1W | 87.81 (4) | N2—C11—C12 | 124.61 (11) |
| O1—Co—O1W | 89.49 (4) | N2—C11—H11A | 117.7 |
| N2—Co—O1W | 89.55 (4) | C12—C11—H11A | 117.7 |
| O11—Co—O1W | 173.73 (3) | C18—C12—C13 | 120.53 (11) |
| C1—O1—Co | 124.52 (7) | C18—C12—C11 | 121.78 (11) |

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| C18—O2—Co | 126.08 (7) | C13—C12—C11 | 117.68 (11) |
| C2—O3—C3 | 117.14 (10) | C14—C13—C12 | 120.30 (12) |
| C16—O4—C17 | 117.47 (10) | C14—C13—H13A | 119.8 |
| C11A—O11—Co | 133.96 (8) | C12—C13—H13A | 119.8 |
| C1S—O1S—H1S | 109.5 | C13—C14—C15 | 120.16 (12) |
| C2S—O2S—H2S | 109.5 | C13—C14—H14A | 119.9 |
| Co—O1W—H1W1 | 110.4 (11) | C15—C14—H14A | 119.9 |
| Co—O1W—H1W2 | 104.6 (11) | C16—C15—C14 | 120.38 (12) |
| H1W1—O1W—H1W2 | 107.0 (14) | C16—C15—H15A | 119.8 |
| C8—N1—C9 | 121.69 (10) | C14—C15—H15A | 119.8 |
| C8—N1—Co | 125.95 (8) | C15—C16—O4 | 125.54 (11) |
| C9—N1—Co | 112.23 (8) | C15—C16—C18 | 121.52 (11) |
| C11—N2—C10 | 120.33 (10) | O4—C16—C18 | 112.94 (11) |
| C11—N2—Co | 127.27 (8) | O4—C17—H17A | 109.5 |
| C10—N2—Co | 112.27 (8) | O4—C17—H17B | 109.5 |
| O1—C1—C7 | 124.67 (11) | H17A—C17—H17B | 109.5 |
| O1—C1—C2 | 117.72 (10) | O4—C17—H17C | 109.5 |
| C7—C1—C2 | 117.59 (11) | H17A—C17—H17C | 109.5 |
| O3—C2—C4 | 125.31 (11) | H17B—C17—H17C | 109.5 |
| O3—C2—C1 | 113.22 (10) | O2—C18—C12 | 125.72 (10) |
| C4—C2—C1 | 121.46 (11) | O2—C18—C16 | 117.18 (10) |
| O3—C3—H3A | 109.5 | C12—C18—C16 | 117.10 (11) |
| O3—C3—H3B | 109.5 | O12—C11A—O11 | 118.92 (11) |
| H3A—C3—H3B | 109.5 | O12—C11A—C12A | 119.12 (11) |
| O3—C3—H3C | 109.5 | O11—C11A—C12A | 121.96 (11) |
| H3A—C3—H3C | 109.5 | C11A—C12A—H12A | 109.5 |
| H3B—C3—H3C | 109.5 | C11A—C12A—H12B | 109.5 |
| C2—C4—C5 | 120.17 (12) | H12A—C12A—H12B | 109.5 |
| C2—C4—H4A | 119.9 | C11A—C12A—H12C | 109.5 |
| C5—C4—H4A | 119.9 | H12A—C12A—H12C | 109.5 |
| C6—C5—C4 | 119.66 (12) | H12B—C12A—H12C | 109.5 |
| C6—C5—H5A | 120.2 | O1S—C1S—H1S3 | 109.5 |
| C4—C5—H5A | 120.2 | O1S—C1S—H1S1 | 109.5 |
| C5—C6—C7 | 121.33 (11) | H1S3—C1S—H1S1 | 109.5 |
| C5—C6—H6A | 119.3 | O1S—C1S—H1S2 | 109.5 |
| C7—C6—H6A | 119.3 | H1S3—C1S—H1S2 | 109.5 |
| C6—C7—C1 | 119.78 (11) | H1S1—C1S—H1S2 | 109.5 |
| C6—C7—C8 | 118.98 (11) | O2S—C2S—H2S1 | 109.5 |
| C1—C7—C8 | 121.08 (11) | O2S—C2S—H2S2 | 109.5 |
| N1—C8—C7 | 125.23 (11) | H2S1—C2S—H2S2 | 109.5 |
| N1—C8—H8A | 117.4 | O2S—C2S—H2S3 | 109.5 |
| C7—C8—H8A | 117.4 | H2S1—C2S—H2S3 | 109.5 |
| N1—C9—C10 | 106.10 (9) | H2S2—C2S—H2S3 | 109.5 |

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|---|---|---|---|
| O2—Co—O1—C1 | 156.99 (9) | C5—C6—C7—C1 | 0.00 (18) |
| N1—Co—O1—C1 | −25.20 (9) | C5—C6—C7—C8 | 175.51 (11) |
| O11—Co—O1—C1 | 61.70 (9) | O1—C1—C7—C6 | 178.37 (11) |
| O1W—Co—O1—C1 | −112.98 (9) | C2—C1—C7—C6 | 0.33 (16) |

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| O1—Co—O2—C18 | 172.53 (9) | O1—C1—C7—C8 | 2.96 (17) |
| N2—Co—O2—C18 | −6.52 (9) | C2—C1—C7—C8 | −175.08 (10) |
| O11—Co—O2—C18 | −93.88 (9) | C9—N1—C8—C7 | 176.95 (11) |
| O1W—Co—O2—C18 | 83.04 (9) | Co—N1—C8—C7 | −7.49 (17) |
| O2—Co—O11—C11A | −31.86 (12) | C6—C7—C8—N1 | 175.92 (11) |
| N1—Co—O11—C11A | 148.33 (12) | C1—C7—C8—N1 | −8.64 (18) |
| O1—Co—O11—C11A | 55.58 (12) | C8—N1—C9—C10 | 139.65 (11) |
| N2—Co—O11—C11A | −125.78 (12) | Co—N1—C9—C10 | −36.47 (11) |
| O1—Co—N1—C8 | 20.37 (10) | C11—N2—C10—C9 | 150.81 (11) |
| N2—Co—N1—C8 | −160.54 (10) | Co—N2—C10—C9 | −33.08 (11) |
| O11—Co—N1—C8 | −73.33 (10) | N1—C9—C10—N2 | 43.52 (12) |
| O1W—Co—N1—C8 | 109.74 (10) | C10—N2—C11—C12 | 174.50 (10) |
| O1—Co—N1—C9 | −163.71 (8) | Co—N2—C11—C12 | −0.97 (17) |
| N2—Co—N1—C9 | 15.38 (8) | N2—C11—C12—C18 | −2.50 (18) |
| O11—Co—N1—C9 | 102.60 (8) | N2—C11—C12—C13 | 177.98 (11) |
| O1W—Co—N1—C9 | −74.34 (8) | C18—C12—C13—C14 | 0.19 (18) |
| O2—Co—N2—C11 | 4.50 (10) | C11—C12—C13—C14 | 179.72 (11) |
| N1—Co—N2—C11 | −173.30 (10) | C12—C13—C14—C15 | −0.64 (19) |
| O11—Co—N2—C11 | 99.77 (10) | C13—C14—C15—C16 | 0.24 (19) |
| O1W—Co—N2—C11 | −85.47 (10) | C14—C15—C16—O4 | −179.43 (11) |
| O2—Co—N2—C10 | −171.28 (7) | C14—C15—C16—C18 | 0.62 (18) |
| N1—Co—N2—C10 | 10.92 (8) | C17—O4—C16—C15 | 9.33 (17) |
| O11—Co—N2—C10 | −76.01 (8) | C17—O4—C16—C18 | −170.72 (10) |
| O1W—Co—N2—C10 | 98.75 (8) | Co—O2—C18—C12 | 5.24 (16) |
| Co—O1—C1—C7 | 17.82 (15) | Co—O2—C18—C16 | −175.66 (7) |
| Co—O1—C1—C2 | −164.14 (8) | C13—C12—C18—O2 | 179.73 (11) |
| C3—O3—C2—C4 | 3.12 (16) | C11—C12—C18—O2 | 0.22 (18) |
| C3—O3—C2—C1 | −176.12 (10) | C13—C12—C18—C16 | 0.62 (16) |
| O1—C1—C2—O3 | 1.04 (15) | C11—C12—C18—C16 | −178.88 (10) |
| C7—C1—C2—O3 | 179.22 (10) | C15—C16—C18—O2 | 179.78 (11) |
| O1—C1—C2—C4 | −178.23 (10) | O4—C16—C18—O2 | −0.17 (14) |
| C7—C1—C2—C4 | −0.05 (16) | C15—C16—C18—C12 | −1.04 (17) |
| O3—C2—C4—C5 | −179.75 (11) | O4—C16—C18—C12 | 179.01 (10) |
| C1—C2—C4—C5 | −0.56 (18) | Co—O11—C11A—O12 | 172.02 (9) |
| C2—C4—C5—C6 | 0.90 (18) | Co—O11—C11A—C12A | −8.37 (19) |
| C4—C5—C6—C7 | −0.62 (18) | | |

*Hydrogen-bond geometry (Å, º)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| O1*S*—H1*S*···O12 | 0.84 | 1.83 | 2.6671 (14) | 174 |
| O2*S*—H2*S*···O1*S* | 0.84 | 1.95 | 2.7682 (17) | 165 |
| O1*W*—H1*W*1···O1$^{i}$ | 0.80 (1) | 1.99 (1) | 2.7334 (11) | 153 (1) |
| O1*W*—H1*W*1···O3$^{i}$ | 0.80 (1) | 2.32 (1) | 2.9124 (13) | 131 (1) |
| O1*W*—H1*W*2···O2$^{i}$ | 0.80 (1) | 2.18 (2) | 2.8071 (11) | 136 (1) |
| O1*W*—H1*W*2···O4$^{i}$ | 0.80 (1) | 2.17 (1) | 2.8840 (12) | 148 (2) |
| C9—H9*A*···O1*S*$^{ii}$ | 0.99 | 2.52 | 3.2610 (16) | 132 |
| C13—H13*A*···O11$^{iii}$ | 0.95 | 2.61 | 3.5380 (15) | 165 |

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|---|---|---|---|---|
| C12*A*—H12*B*···O1 | 0.98 | 2.38 | 3.1807 (15) | 139 |
| C8—H8*A*···O2*S*$^{iv}$ | 0.95 | 2.55 | 3.4335 (16) | 155 |
| C10—H10*A*···O2*S*$^{ii}$ | 0.99 | 2.61 | 3.5119 (17) | 151 |
| C12*A*—H12*C*···O2*S*$^{v}$ | 0.98 | 2.62 | 3.5541 (19) | 161 |

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