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Bis[(2-aminophenyl)methanol-κ^2N,O]-bis(nitrato-κO)cobalt(II)

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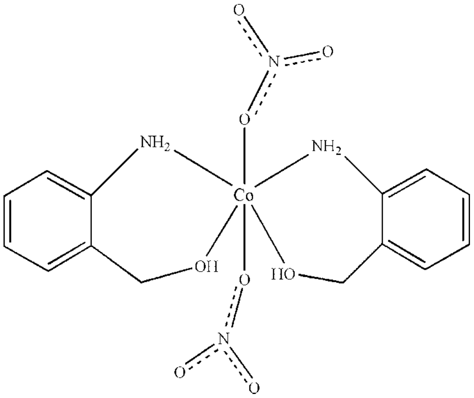
Key indicators: single-crystal X-ray study; T = 120 K; mean σ(C–C) = 0.002 Å; R factor = 0.032; wR factor = 0.088; data-to-parameter ratio = 16.8.

The asymmetric unit of the title compound, $[Co(NO_3)_2(C_7H_9NO)_2]$, contains one-half of the molecule. The Co^{II} atom (site symmetry 2) is six-coordinate in a distorted octahedral configuration bonded by two N and two O atoms from two (2-aminophenyl)methanol ligands and two O atoms from the two nitrate anions. Crystal packing is stabilized by intermolecular N—H$\cdots$O, O—H$\cdots$O and C—H$\cdots$O hydrogen-bonding interactions.

Related literature

For related structures with different metal atoms, see: Bandoli *et al.* (2002); Lewiriski *et al.* (1998); Esmhosseini (2010); Esmhosseini & Maleki (2010). For bond distances and angles, see: Allen (2002).



Experimental

Crystal data

$[Co(NO_3)_2(C_7H_9NO)_2]$
M_r = 429.25
Orthorhombic, *Pnab*
a = 7.2554 (6) Å
b = 10.1685 (7) Å
c = 23.250 (2) Å

V = 1715.3 (3) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 1.05 mm^{-1}
T = 120 K
0.50 × 0.20 × 0.15 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2003)
T_{min} = 0.768, T_{max} = 0.861

6514 measured reflections
2271 independent reflections
2065 reflections with $I > 2\sigma(I)$
R_{int} = 0.046

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.032
$wR(F^2)$ = 0.088
S = 1.08
2271 reflections
135 parameters

H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.46 e Å^{-3}
$\Delta\rho_{min}$ = −0.46 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

O2—Co1	2.1288 (11)	Co1—N1	2.1463 (12)
Co1—O1^i	2.1025 (10)		
O1—Co1—O1^i	84.64 (6)	O1^i—Co1—N1^i	85.27 (4)
O1—Co1—O2	88.90 (4)	O2—Co1—N1^i	94.26 (4)
O1^i—Co1—O2	84.43 (4)	O1—Co1—N1	85.27 (4)
O2—Co1—O2^i	170.98 (5)	O2—Co1—N1	91.22 (5)
O1—Co1—N1^i	169.09 (5)	N1^i—Co1—N1	105.07 (7)

Symmetry code: (i) $-x+\frac{1}{2}, y, -z+1$.

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

D—H$\cdots A$	D—H	H$\cdots A$	$D\cdots A$	D—H$\cdots A$
N1—H1$C\cdots$O3^{ii}	0.88 (2)	2.15 (2)	2.9897 (16)	158 (2)
N1—H1$D\cdots$O4^{iii}	0.84 (3)	2.24 (3)	3.0689 (17)	169 (2)
O1—H1$E\cdots$O2^{iv}	0.84 (2)	1.86 (2)	2.6908 (14)	172 (2)
C1—H1$B\cdots$O4^{iii}	0.97	2.54	3.4145 (18)	151

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

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT* (Bruker, 1998); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 2008); program(s) used to refine structure: *SHELXTL*; molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: JJ2052).

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supporting information

Acta Cryst. (2010). E**66**, m1126 [https://doi.org/10.1107/S1600536810032381]

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Majid Esmhosseini and Mahdokt Rezazadeh

S1. Comment

Only four metal complexes with the (2-aminophenyl)methanol, bidentate ligand have been prepared and include the Re (Bandoli *et al.*, 2002), Al (Lewiriski *et al.*, 1998), Zn (Esmhosseini, 2010) and Mn (Esmhosseini & Maleki, 2010) compounds. We report herein the synthesis and crystal structure of the Co analogue compound, $[Co(C_7H_9NO)_2(NO_3)_2]$.

The asymmetric unit of the title compound, $[Co(C_7H_9NO)_2(NO_3)_2]$, contains one-half of the molecule (Fig. 1). The Co^{II} atom in the cation is six-coordinate in a distorted hexagonal configuration bonded by two N and two O atoms from two (2-aminophenyl)methanol ligands and two O atoms from the two nitrate anions. Bond distances and angles are in normal ranges (Allen, 2002). Intermolecular N—H···O, O—H···O and C—H···O hydrogen bonding stabilize the crystal structure, (Table 2, Fig. 2).

S2. Experimental

For the preparation of the title compound, a solution of (2-aminophenyl)methanol (0.25 g, 2.00 mmol) in methanol (10 ml) was added to a solution of $Co(NO_3)_2.6H_2O$ (0.29 g, 1.00 mmol) in methanol (10 ml) and the resulting colorless solution was stirred for 20 min at 313 K. This solution was left to evaporate slowly at room temperature. After one week, light violet block crystals of the title compound were isolated (yield 0.32 g, 74.5%).

S3. Refinement

The H atoms on the C and N atoms were positioned geometrically, and refined as riding atoms, with C–H = 0.93 Å (CH), C–H = 0.97 Å (CH_2), N–H = 0.88, 0.84 Å (NH_2) and constrained to ride on their parent atoms, with $U_{iso}(H) = 1.2U_{eq}(C)$, $U_{iso}(H) = 1.9U_{eq}(N)$. The H on O1 was located by a Fourier map and refined isotropically.

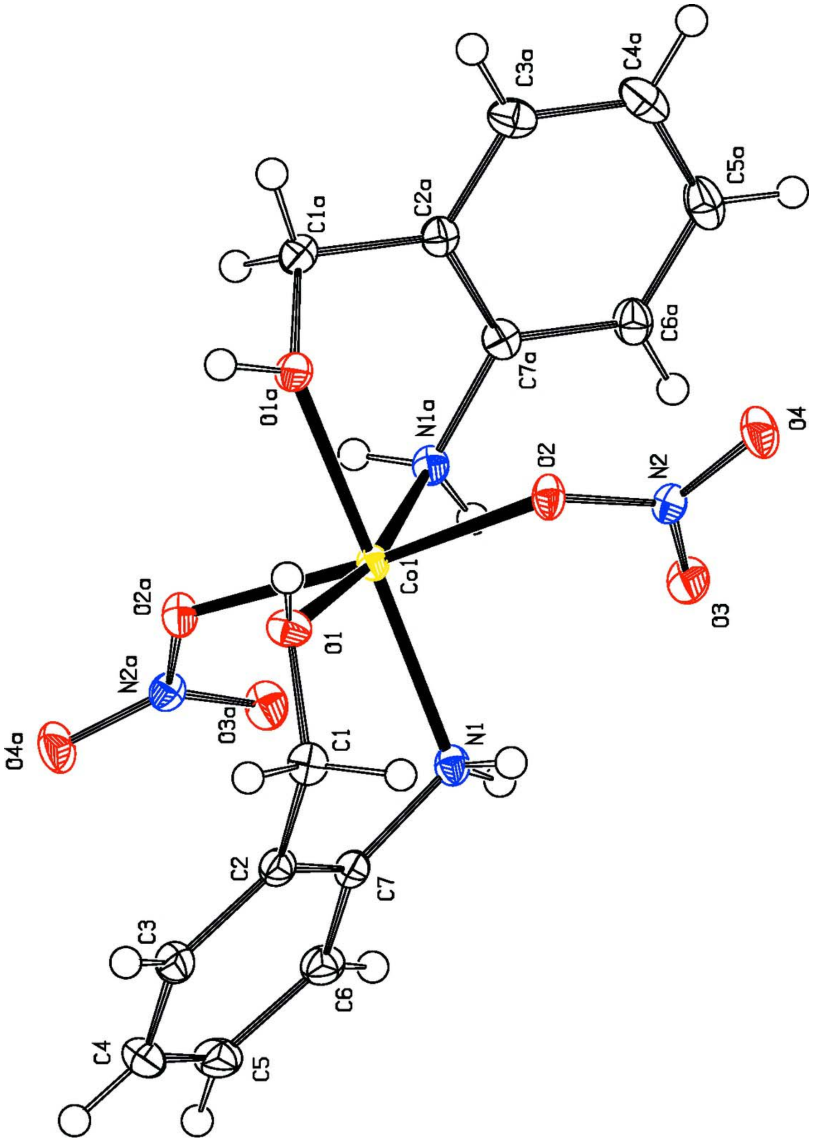

Figure 1

The molecular structure of the title molecule, [Co(C_7H_9NO)$_2$(NO_3)$_2$], with the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level.

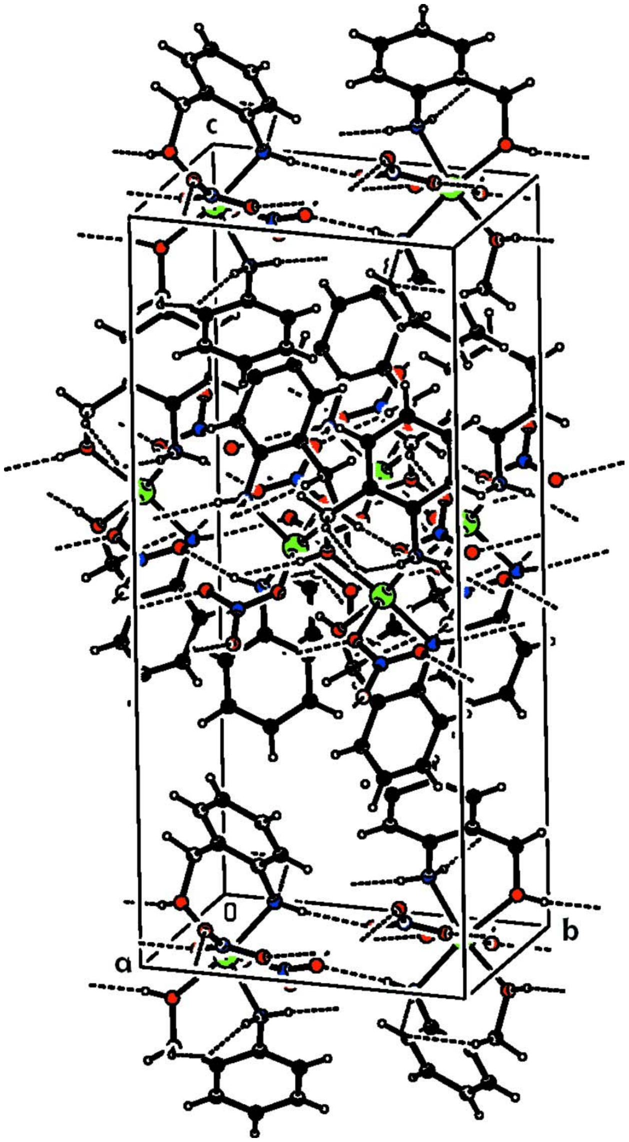

Figure 2

Unit-cell packing diagram for title molecule, [Co(C_7H_9NO)$_2$(NO_3)$_2$]. Hydrogen bonds are shown as dashed lines.

Bis[(2-aminophenyl)methanol-κ^2N,O]bis(nitrato- κO)cobalt(II)

Crystal data

[Co(NO_3)$_2$(C_7H_9NO)$_2$]
M_r = 429.25
Orthorhombic, *Pnab*
Hall symbol: -P 2bc 2n
a = 7.2554 (6) Å
b = 10.1685 (7) Å
c = 23.250 (2) Å
V = 1715.3 (3) Å^3
Z = 4

F(000) = 884
D_x = 1.662 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 1009 reflections
θ = 2.2–29.2°
μ = 1.05 mm^{-1}
T = 120 K
Block, light violet
0.50 × 0.20 × 0.15 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2003)
$T_{\min} = 0.768$, $T_{\max} = 0.861$
6514 measured reflections
2271 independent reflections
2065 reflections with $I > 2\sigma(I)$
$R_{\text{int}} = 0.046$
$\theta_{\max} = 29.2°$, $\theta_{\min} = 2.2°$
$h = -6 \rightarrow 9$
$k = -11 \rightarrow 13$
$l = -26 \rightarrow 31$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.032$
$wR(F^2) = 0.088$
$S = 1.08$
2271 reflections
135 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0456P)^2 + 0.8425P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} = 0.007$
$\Delta\rho_{\max} = 0.46$ e Å^{-3}
$\Delta\rho_{\min} = -0.46$ 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}
O3	−0.06393 (16)	0.10499 (10)	0.53584 (5)	0.0194 (2)
O4	−0.24657 (15)	0.23434 (12)	0.58377 (5)	0.0213 (2)
O1	0.18951 (16)	0.45350 (10)	0.44211 (4)	0.0155 (2)
H1E	0.142 (3)	0.524 (2)	0.4531 (9)	0.029 (6)*
C2	0.2247 (2)	0.32739 (15)	0.35482 (6)	0.0145 (3)
C4	0.4195 (2)	0.26108 (18)	0.27496 (6)	0.0230 (3)
H4	0.4794	0.2816	0.2407	0.028*
N2	−0.11401 (17)	0.21530 (11)	0.55146 (5)	0.0135 (2)
C7	0.23941 (19)	0.19961 (13)	0.37774 (7)	0.0143 (3)
O2	−0.02236 (15)	0.31708 (9)	0.53328 (5)	0.0151 (2)
Co1	0.2500	0.30062 (2)	0.5000	0.01128 (10)
C6	0.3427 (2)	0.10409 (15)	0.34922 (6)	0.0179 (3)
H6	0.3508	0.0195	0.3642	0.022*
C3	0.3146 (2)	0.35577 (15)	0.30337 (6)	0.0188 (3)
H3	0.3044	0.4396	0.2877	0.023*

C5	0.4337 (2)	0.13548 (16)	0.29835 (7)	0.0223 (3)
H5	0.5044	0.0721	0.2798	0.027*
N1	0.15712 (18)	0.17223 (12)	0.43271 (5)	0.0140 (2)
H1C	0.162 (3)	0.088 (2)	0.4413 (9)	0.028 (5)*
H1D	0.044 (4)	0.189 (2)	0.4333 (10)	0.027 (6)*
C1	0.1144 (2)	0.43142 (13)	0.38520 (6)	0.0158 (3)
H1A	0.1181	0.5126	0.3633	0.019*
H1B	−0.0131	0.4036	0.3882	0.019*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O3	0.0226 (5)	0.0110 (4)	0.0246 (5)	−0.0008 (4)	0.0041 (4)	−0.0014 (4)
O4	0.0135 (5)	0.0244 (6)	0.0259 (6)	0.0003 (4)	0.0074 (4)	0.0004 (5)
O1	0.0207 (5)	0.0104 (4)	0.0152 (5)	0.0035 (4)	0.0008 (4)	−0.0007 (4)
C2	0.0126 (6)	0.0153 (6)	0.0155 (6)	−0.0010 (5)	−0.0010 (5)	−0.0010 (5)
C4	0.0208 (7)	0.0333 (8)	0.0149 (6)	−0.0045 (6)	0.0041 (6)	−0.0032 (6)
N2	0.0116 (5)	0.0129 (5)	0.0160 (5)	−0.0006 (4)	−0.0010 (4)	0.0005 (4)
C7	0.0129 (7)	0.0145 (6)	0.0155 (6)	−0.0022 (5)	−0.0001 (5)	−0.0014 (5)
O2	0.0134 (5)	0.0101 (4)	0.0219 (5)	−0.0008 (3)	0.0040 (4)	0.0008 (4)
Co1	0.01166 (16)	0.00913 (15)	0.01306 (15)	0.000	0.00220 (9)	0.000
C6	0.0174 (7)	0.0175 (6)	0.0190 (6)	0.0009 (5)	−0.0002 (5)	−0.0043 (5)
C3	0.0195 (7)	0.0214 (7)	0.0156 (6)	−0.0048 (6)	−0.0004 (6)	0.0016 (5)
C5	0.0195 (7)	0.0267 (8)	0.0206 (7)	0.0012 (6)	0.0027 (6)	−0.0092 (6)
N1	0.0141 (6)	0.0112 (5)	0.0168 (5)	−0.0004 (4)	0.0021 (4)	0.0007 (4)
C1	0.0151 (6)	0.0148 (6)	0.0175 (6)	0.0015 (5)	−0.0011 (5)	0.0016 (5)

Geometric parameters (Å, º)

O3—N2	1.2338 (15)	O2—Co1	2.1288 (11)
O4—N2	1.2356 (16)	Co1—O1^{i}	2.1025 (10)
O1—C1	1.4485 (17)	Co1—O2^{i}	2.1288 (11)
O1—Co1	2.1025 (10)	Co1—N1^{i}	2.1463 (12)
O1—H1E	0.83 (2)	Co1—N1	2.1463 (12)
C2—C3	1.393 (2)	C6—C5	1.392 (2)
C2—C7	1.408 (2)	C6—H6	0.9300
C2—C1	1.503 (2)	C3—H3	0.9300
C4—C5	1.392 (2)	C5—H5	0.9300
C4—C3	1.394 (2)	N1—H1C	0.88 (2)
C4—H4	0.9300	N1—H1D	0.84 (3)
N2—O2	1.3008 (15)	C1—H1A	0.9700
C7—C6	1.394 (2)	C1—H1B	0.9700
C7—N1	1.4378 (19)		
C1—O1—Co1	123.28 (8)	O1—Co1—N1	85.27 (4)
C1—O1—H1E	104.9 (15)	O1^{i}—Co1—N1	169.09 (5)
Co1—O1—H1E	121.7 (14)	O2—Co1—N1	91.22 (5)
C3—C2—C7	118.74 (14)	O2^{i}—Co1—N1	94.26 (4)

C3—C2—C1	120.48 (13)	N1^{i}—Co1—N1	105.07 (7)
C7—C2—C1	120.78 (13)	C5—C6—C7	119.95 (14)
C5—C4—C3	119.28 (14)	C5—C6—H6	120.0
C5—C4—H4	120.4	C7—C6—H6	120.0
C3—C4—H4	120.4	C2—C3—C4	121.30 (15)
O3—N2—O4	123.42 (12)	C2—C3—H3	119.3
O3—N2—O2	118.50 (12)	C4—C3—H3	119.3
O4—N2—O2	118.08 (12)	C6—C5—C4	120.50 (14)
C6—C7—C2	120.22 (14)	C6—C5—H5	119.8
C6—C7—N1	120.72 (13)	C4—C5—H5	119.8
C2—C7—N1	118.92 (13)	C7—N1—Co1	113.56 (9)
N2—O2—Co1	122.01 (8)	C7—N1—H1C	112.0 (14)
O1—Co1—O1^{i}	84.64 (6)	Co1—N1—H1C	114.4 (14)
O1—Co1—O2	88.90 (4)	C7—N1—H1D	112.5 (16)
O1^{i}—Co1—O2	84.43 (4)	Co1—N1—H1D	100.0 (16)
O1—Co1—O2^{i}	84.43 (4)	H1C—N1—H1D	103 (2)
O1^{i}—Co1—O2^{i}	88.90 (4)	O1—C1—C2	109.76 (11)
O2—Co1—O2^{i}	170.98 (5)	O1—C1—H1A	109.7
O1—Co1—N1^{i}	169.09 (5)	C2—C1—H1A	109.7
O1^{i}—Co1—N1^{i}	85.27 (4)	O1—C1—H1B	109.7
O2—Co1—N1^{i}	94.26 (4)	C2—C1—H1B	109.7
O2^{i}—Co1—N1^{i}	91.22 (5)	H1A—C1—H1B	108.2

C3—C2—C7—C6	0.2 (2)	N1—C7—C6—C5	−174.82 (14)
C1—C2—C7—C6	−179.79 (13)	C7—C2—C3—C4	−0.8 (2)
C3—C2—C7—N1	175.93 (13)	C1—C2—C3—C4	179.16 (14)
C1—C2—C7—N1	−4.0 (2)	C5—C4—C3—C2	0.4 (2)
O3—N2—O2—Co1	−18.93 (17)	C7—C6—C5—C4	−1.3 (2)
O4—N2—O2—Co1	160.75 (10)	C3—C4—C5—C6	0.7 (2)
C1—O1—Co1—O1^{i}	−174.89 (13)	C6—C7—N1—Co1	120.28 (12)
C1—O1—Co1—O2	−90.38 (11)	C2—C7—N1—Co1	−55.46 (15)
C1—O1—Co1—O2^{i}	95.70 (11)	O1—Co1—N1—C7	49.56 (10)
C1—O1—Co1—N1^{i}	162.6 (2)	O1^{i}—Co1—N1—C7	72.1 (3)
C1—O1—Co1—N1	0.94 (11)	O2—Co1—N1—C7	138.36 (10)
N2—O2—Co1—O1	145.62 (10)	O2^{i}—Co1—N1—C7	−34.48 (10)
N2—O2—Co1—O1^{i}	−129.65 (10)	N1^{i}—Co1—N1—C7	−126.90 (11)
N2—O2—Co1—N1^{i}	−44.83 (10)	Co1—O1—C1—C2	−49.00 (15)
N2—O2—Co1—N1	60.38 (10)	C3—C2—C1—O1	−119.95 (14)
C2—C7—C6—C5	0.9 (2)	C7—C2—C1—O1	60.01 (17)

Symmetry code: (i) $-x+1/2$, y, $-z+1$.

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1*C*···O3^{ii}	0.88 (2)	2.15 (2)	2.9897 (16)	158 (2)
N1—H1*D*···O4^{iii}	0.84 (3)	2.24 (3)	3.0689 (17)	169 (2)

O1—H1*E*···O2^{iv}	0.84 (2)	1.86 (2)	2.6908 (14)	172 (2)
C1—H1*B*···O4^{iii}	0.97	2.54	3.4145 (18)	151

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