

## Tetraaquabis[2-(2-nitrophenyl)acetato- $\kappa$ O]cobalt(II)

Muhammad Danish,<sup>a</sup> Muhammad Nawaz Tahir,<sup>b\*</sup> Sana Iftikhar,<sup>a</sup> Muhammad Asam Raza<sup>a</sup> and Muhammad Ashfaq<sup>a</sup>

<sup>a</sup>Department of Chemistry, Institute of Chemical and Biological Sciences, University of Gujrat, Gujrat 50700, Pakistan, and <sup>b</sup>Department of Physics, University of Sargodha, Sargodha, Punjab, Pakistan. \*Correspondence e-mail: dmntahir\_uos@yahoo.com

Received 26 January 2015; accepted 5 February 2015

Edited by M. Weil, Vienna University of Technology, Austria

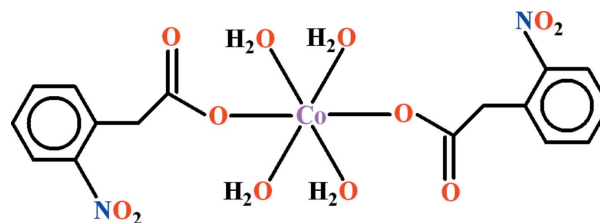
The molecule of the title compound,  $[\text{Co}(\text{C}_8\text{H}_6\text{NO}_4)_2(\text{H}_2\text{O})_4]$ , is centrosymmetric. It is a cobalt(II) complex, bearing two (2-nitrophenyl)acetate and four aqua ligands. The coordination around the  $\text{Co}^{\text{II}}$  atom is distorted octahedral, defined by four O atoms of water molecules in the equatorial plane and by two carboxylate O atoms at axial positions. The dihedral angles between the benzene ring and the acetate and nitro groups are  $61.90(10)$  and  $19.21(11)^\circ$ , respectively. The water molecules form  $\text{O}-\text{H}\cdots\text{O}$  hydrogen bonds with the nitro and carboxylate groups, leading to a layered structural arrangement parallel to (001).

**Keywords:** crystal structure; cobalt(II) complex; hydrogen bonding.

**CCDC reference:** 1047494

### 1. Related literature

The title compound is structurally related to tetraaquabis(acetato- $\kappa$ O)cobalt(II) (Sobolev *et al.*, 2003), tetraaquabis(2-nitrophenoxyethanoato- $\kappa$ O)cobalt(II) dihydrate (Kennard *et al.*, 1985), tetraaquabis((2,4-dichlorophenoxy)acetato- $\kappa$ O)-cobalt(II) dihydrate (Tan *et al.*, 2011), tetraaquabis[2-(6-amino-9H-purin-9-yl)acetato- $\kappa$ O]cobalt(II) (Mishra *et al.*, 2011) and tetraaquabis(3,5-dinitrobenzoato- $\kappa$ O)cobalt(II) tetrahydrate (Tahir *et al.*, 1996).



### 2. Experimental

#### 2.1. Crystal data

$[\text{Co}(\text{C}_8\text{H}_6\text{NO}_4)_2(\text{H}_2\text{O})_4]$   
 $M_r = 491.27$   
 Monoclinic,  $P2_1/n$   
 $a = 5.4431(3) \text{ \AA}$   
 $b = 6.4313(4) \text{ \AA}$   
 $c = 28.5697(15) \text{ \AA}$   
 $\beta = 92.762(2)^\circ$

$V = 998.96(10) \text{ \AA}^3$   
 $Z = 2$   
 Mo  $K\alpha$  radiation  
 $\mu = 0.93 \text{ mm}^{-1}$   
 $T = 296 \text{ K}$   
 $0.32 \times 0.24 \times 0.20 \text{ mm}$

#### 2.2. Data collection

Bruker Kappa APEXII CCD diffractometer  
 Absorption correction: multi-scan (SADABS; Bruker, 2007)  
 $T_{\text{min}} = 0.758$ ,  $T_{\text{max}} = 0.835$

8913 measured reflections  
 2156 independent reflections  
 1937 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.026$

#### 2.3. Refinement

$R[F^2 > 2\sigma(F^2)] = 0.028$   
 $wR(F^2) = 0.070$   
 $S = 1.04$   
 2156 reflections  
 154 parameters

H atoms treated by a mixture of independent and constrained refinement  
 $\Delta\rho_{\text{max}} = 0.27 \text{ e \AA}^{-3}$   
 $\Delta\rho_{\text{min}} = -0.28 \text{ e \AA}^{-3}$

**Table 1**  
Hydrogen-bond geometry ( $\text{\AA}$ ,  $^\circ$ ).

$D-\text{H}\cdots A$	$D-\text{H}$	$\text{H}\cdots A$	$D\cdots A$	$D-\text{H}\cdots A$
$\text{O5}-\text{H5A}\cdots\text{O1}^{\text{i}}$	0.82 (2)	2.00 (2)	2.7984 (16)	166 (2)
$\text{O5}-\text{H5B}\cdots\text{O2}^{\text{ii}}$	0.82 (2)	1.89 (2)	2.6797 (17)	161 (2)
$\text{O6}-\text{H6A}\cdots\text{O2}^{\text{iii}}$	0.78 (2)	1.93 (2)	2.6979 (17)	169 (2)
$\text{O6}-\text{H6B}\cdots\text{O3}$	0.81 (2)	2.22 (2)	2.988 (2)	159 (2)

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

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: *ORTEP-3 for Windows* (Farrugia, 2012) and *PLATON* (Spek, 2009); software used to prepare material for publication: *WinGX* (Farrugia, 2012) and *PLATON*.

### Acknowledgements

The authors acknowledge the provision of funds for the purchase of the diffractometer and encouragement by Dr Muhammad Akram Chaudhary, Vice Chancellor, University of Sargodha, Pakistan.

---

Supporting information for this paper is available from the IUCr electronic archives (Reference: WM5121).

---

### References

Bruker (2007). *APEX2*, *SAINTE* and *SADABS*. Bruker AXS Inc., Madison, Wisconsin, USA.  
Farrugia, L. J. (2012). *J. Appl. Cryst.* **45**, 849–854.

Kennard, C. H. L., Stewart, S. W., O'Reilly, E. J., Smith, G. & White, A. H. (1985). *Polyhedron*, **4**, 697–705.  
Mishra, A. K., Kumar, J., Khanna, S. & Verma, S. (2011). *Cryst. Growth Des.* **11**, 1623–1630.  
Sheldrick, G. M. (2008). *Acta Cryst.* **A64**, 112–122.  
Sobolev, A. N., Miminoshvili, E. B., Miminoshvili, K. E. & Sakvarelidze, T. N. (2003). *Acta Cryst.* **E59**, m836–m837.  
Spek, A. L. (2009). *Acta Cryst.* **D65**, 148–155.  
Tahir, M. N., Ülkü, D. & Mövsümov, E. M. (1996). *Acta Cryst.* **C52**, 1392–1394.  
Tan, X.-W., Li, C.-H., Li, Y.-L. & Zhang, S.-H. (2011). *Z. Kristallogr. New Cryst. Struct.* **226**, 175–176.

## supporting information

*Acta Cryst.* (2015). E71, m59–m60 [doi:10.1107/S2056989015002467]

**Tetraaquabis[2-(2-nitrophenyl)acetato- $\kappa$ O]cobalt(II)**

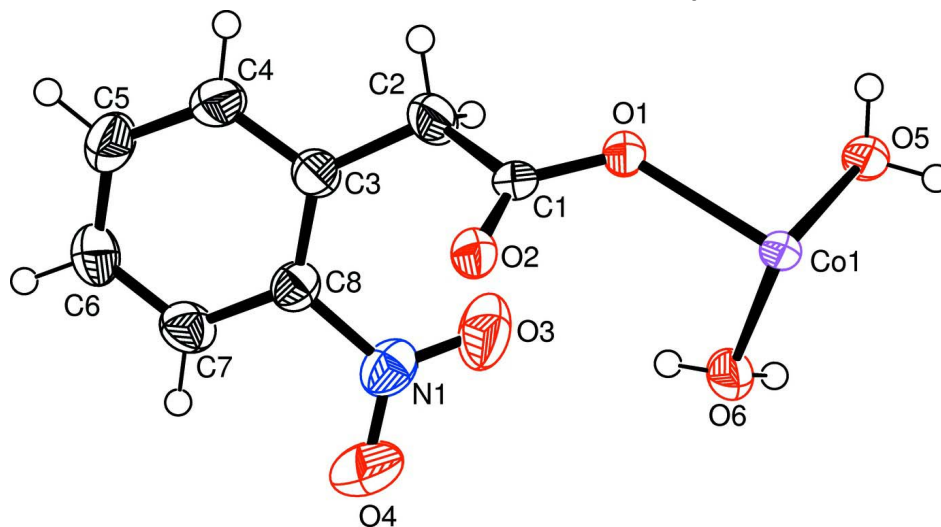
Muhammad Danish, Muhammad Nawaz Tahir, Sana Iftikhar, Muhammad Asam Raza and Muhammad Ashfaq

**S1. Experimental**

The sodium salt of (2-nitrophenyl)acetic acid was prepared by mixing aqueous solutions of (2-nitrophenyl)acetic acid and Na(HCO<sub>3</sub>) in the molar ratio 1:1. To this solution a 0.5 molar equivalent of cobalt(II) acetate was added and the mixture refluxed for 4 h. The resulting solution was evaporated for crystal growth. Light-orange prisms suitable for X-ray data collection were obtained after one week.

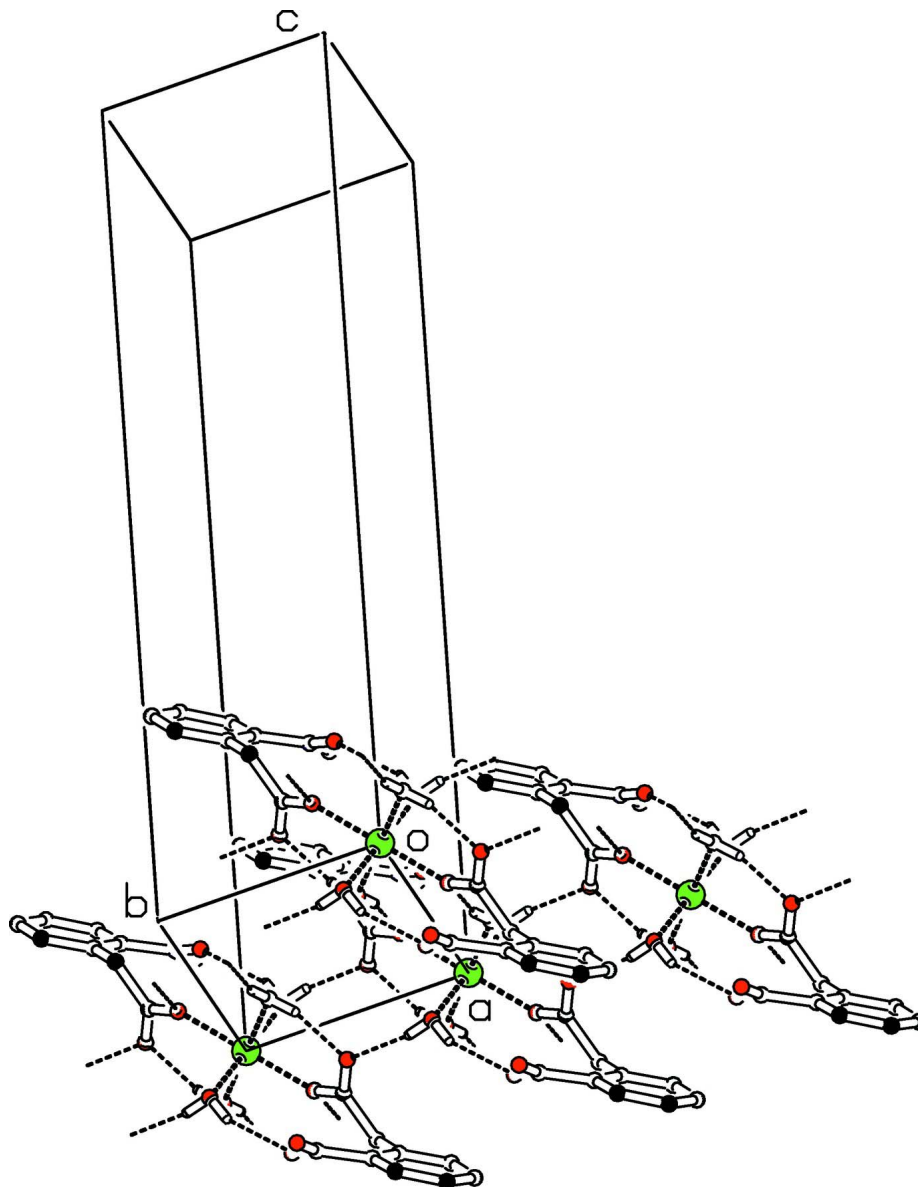
**S2. Refinement**

The coordinates of water H-atoms were refined freely, with  $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{O})$ . The other H-atoms were positioned geometrically (C—H = 0.93–0.97 Å) and refined as riding with  $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$ .



**Figure 1**

View of the asymmetric unit of title compound with the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level. H-atoms are shown as small circles of arbitrary radius.



**Figure 2**

A partial packing diagram of the title compound showing the layered organisation of molecules held together by O—H···O interactions (dashed lines). H atoms not involved in hydrogen bonding are omitted for clarity.

**Tetraaquabis[2-(2-nitrophenyl)acetato- $\kappa$ O]cobalt(II)**

*Crystal data*

$[\text{Co}(\text{C}_8\text{H}_6\text{NO}_4)_2(\text{H}_2\text{O})_4]$

$M_r = 491.27$

Monoclinic,  $P2_1/n$

$a = 5.4431$  (3) Å

$b = 6.4313$  (4) Å

$c = 28.5697$  (15) Å

$\beta = 92.762$  (2)°

$V = 998.96$  (10) Å<sup>3</sup>

$Z = 2$

$F(000) = 506$

$D_x = 1.633$  Mg m<sup>-3</sup>

Mo  $K\alpha$  radiation,  $\lambda = 0.71073$  Å

Cell parameters from 2154 reflections

$\theta = 2.9$ – $27.0$ °

$\mu = 0.93$  mm<sup>-1</sup>

$T = 296$  K

Prism, light-orange

$0.32 \times 0.24 \times 0.20$  mm

*Data collection*

Bruker Kappa APEXII CCD  
diffractometer  
Radiation source: fine-focus sealed tube  
Graphite monochromator  
Detector resolution: 7.80 pixels mm<sup>-1</sup>  
 $\omega$  scans  
Absorption correction: multi-scan  
(*SADABS*; Bruker, 2007)  
 $T_{\min} = 0.758$ ,  $T_{\max} = 0.835$

8913 measured reflections  
2156 independent reflections  
1937 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.026$   
 $\theta_{\max} = 27.0^\circ$ ,  $\theta_{\min} = 2.9^\circ$   
 $h = -6 \rightarrow 5$   
 $k = -8 \rightarrow 8$   
 $l = -36 \rightarrow 36$

*Refinement*

Refinement on  $F^2$   
Least-squares matrix: full  
 $R[F^2 > 2\sigma(F^2)] = 0.028$   
 $wR(F^2) = 0.070$   
 $S = 1.04$   
2156 reflections  
154 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  
 $w = 1/[\sigma^2(F_o^2) + (0.0339P)^2 + 0.3677P]$   
where  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta/\sigma)_{\max} < 0.001$   
 $\Delta\rho_{\max} = 0.27 \text{ e } \text{\AA}^{-3}$   
 $\Delta\rho_{\min} = -0.28 \text{ e } \text{\AA}^{-3}$

*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 ( $\text{\AA}^2$ )*

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
Co1	1.0000	0.0000	0.0000	0.02745 (10)
O1	0.78213 (19)	0.21130 (18)	0.03439 (4)	0.0354 (3)
O2	1.0428 (2)	0.45515 (17)	0.06128 (4)	0.0349 (3)
O3	0.9861 (3)	0.1663 (2)	0.13936 (6)	0.0656 (4)
O4	1.2715 (3)	0.2897 (3)	0.18485 (7)	0.0860 (6)
O5	0.7121 (2)	-0.21593 (19)	-0.00252 (5)	0.0367 (3)
H5A	0.572 (4)	-0.193 (3)	-0.0126 (7)	0.044*
H5B	0.761 (4)	-0.309 (3)	-0.0197 (7)	0.044*
O6	1.1243 (2)	-0.1312 (2)	0.06473 (5)	0.0396 (3)
H6A	1.089 (4)	-0.249 (4)	0.0668 (7)	0.047*
H6B	1.076 (4)	-0.079 (4)	0.0883 (8)	0.047*
N1	1.0723 (3)	0.3042 (2)	0.16413 (5)	0.0449 (4)
C1	0.8429 (3)	0.3604 (2)	0.06134 (5)	0.0302 (3)
C2	0.6512 (3)	0.4255 (4)	0.09495 (7)	0.0465 (5)
H2A	0.5280	0.5076	0.0776	0.056*

H2B	0.5702	0.3010	0.1056	0.056*
C3	0.7378 (3)	0.5481 (3)	0.13750 (6)	0.0360 (4)
C4	0.6146 (4)	0.7320 (3)	0.14716 (7)	0.0477 (5)
H4	0.4881	0.7762	0.1265	0.057*
C5	0.6733 (4)	0.8505 (3)	0.18614 (7)	0.0501 (5)
H5	0.5823	0.9693	0.1920	0.060*
C6	0.8658 (4)	0.7945 (3)	0.21649 (7)	0.0478 (5)
H6	0.9062	0.8753	0.2427	0.057*
C7	0.9977 (3)	0.6180 (3)	0.20765 (6)	0.0419 (4)
H7	1.1312	0.5804	0.2274	0.050*
C8	0.9304 (3)	0.4964 (2)	0.16911 (6)	0.0340 (4)

*Atomic displacement parameters (Å<sup>2</sup>)*

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
Co1	0.01995 (16)	0.02718 (16)	0.03467 (18)	0.00213 (11)	-0.00444 (11)	-0.00896 (12)
O1	0.0242 (5)	0.0371 (6)	0.0445 (7)	0.0033 (5)	-0.0030 (5)	-0.0170 (5)
O2	0.0296 (6)	0.0312 (6)	0.0437 (7)	0.0001 (5)	-0.0005 (5)	-0.0103 (5)
O3	0.0995 (13)	0.0358 (8)	0.0613 (9)	0.0115 (8)	0.0019 (9)	-0.0049 (7)
O4	0.0700 (11)	0.0865 (13)	0.0987 (14)	0.0409 (10)	-0.0245 (10)	-0.0129 (11)
O5	0.0227 (6)	0.0368 (6)	0.0501 (7)	0.0005 (5)	-0.0034 (5)	-0.0142 (6)
O6	0.0452 (7)	0.0307 (6)	0.0417 (7)	0.0038 (5)	-0.0094 (6)	-0.0072 (5)
N1	0.0545 (10)	0.0427 (9)	0.0380 (8)	0.0124 (7)	0.0064 (7)	0.0062 (7)
C1	0.0244 (8)	0.0328 (8)	0.0328 (8)	0.0075 (6)	-0.0058 (6)	-0.0059 (6)
C2	0.0287 (9)	0.0635 (12)	0.0468 (11)	0.0016 (8)	-0.0009 (8)	-0.0240 (9)
C3	0.0286 (9)	0.0451 (9)	0.0345 (9)	0.0011 (7)	0.0027 (7)	-0.0089 (7)
C4	0.0394 (10)	0.0592 (12)	0.0439 (10)	0.0161 (9)	-0.0047 (8)	-0.0120 (9)
C5	0.0569 (12)	0.0461 (11)	0.0473 (11)	0.0134 (9)	0.0030 (9)	-0.0123 (9)
C6	0.0560 (12)	0.0498 (11)	0.0374 (10)	0.0006 (9)	0.0010 (8)	-0.0146 (8)
C7	0.0417 (10)	0.0530 (11)	0.0305 (8)	0.0021 (8)	-0.0034 (7)	-0.0011 (8)
C8	0.0351 (9)	0.0353 (9)	0.0319 (8)	0.0026 (7)	0.0054 (7)	0.0003 (7)

*Geometric parameters (Å, °)*

Co1—O1 <sup>i</sup>	2.0810 (11)	C1—C2	1.511 (2)
Co1—O1	2.0810 (11)	C2—C3	1.505 (2)
Co1—O5	2.0925 (12)	C2—H2A	0.9700
Co1—O5 <sup>i</sup>	2.0925 (12)	C2—H2B	0.9700
Co1—O6	2.1141 (13)	C3—C8	1.391 (2)
Co1—O6 <sup>i</sup>	2.1141 (13)	C3—C4	1.394 (3)
O1—C1	1.2637 (18)	C4—C5	1.374 (3)
O2—C1	1.2473 (19)	C4—H4	0.9300
O3—N1	1.214 (2)	C5—C6	1.376 (3)
O4—N1	1.213 (2)	C5—H5	0.9300
O5—H5A	0.82 (2)	C6—C7	1.373 (3)
O5—H5B	0.82 (2)	C6—H6	0.9300
O6—H6A	0.78 (2)	C7—C8	1.385 (2)
O6—H6B	0.81 (2)	C7—H7	0.9300

N1—C8	1.468 (2)		
O1 <sup>i</sup> —Co1—O1	180.0	O2—C1—C2	119.65 (14)
O1 <sup>i</sup> —Co1—O5	89.61 (5)	O1—C1—C2	115.40 (14)
O1—Co1—O5	90.39 (5)	C3—C2—C1	117.33 (14)
O1 <sup>i</sup> —Co1—O5 <sup>i</sup>	90.39 (5)	C3—C2—H2A	108.0
O1—Co1—O5 <sup>i</sup>	89.61 (5)	C1—C2—H2A	108.0
O5—Co1—O5 <sup>i</sup>	180.0	C3—C2—H2B	108.0
O1 <sup>i</sup> —Co1—O6	89.23 (5)	C1—C2—H2B	108.0
O1—Co1—O6	90.77 (5)	H2A—C2—H2B	107.2
O5—Co1—O6	88.44 (5)	C8—C3—C4	115.41 (16)
O5 <sup>i</sup> —Co1—O6	91.56 (5)	C8—C3—C2	126.60 (16)
O1 <sup>i</sup> —Co1—O6 <sup>i</sup>	90.77 (5)	C4—C3—C2	117.98 (16)
O1—Co1—O6 <sup>i</sup>	89.23 (5)	C5—C4—C3	122.40 (18)
O5—Co1—O6 <sup>i</sup>	91.56 (5)	C5—C4—H4	118.8
O5 <sup>i</sup> —Co1—O6 <sup>i</sup>	88.44 (5)	C3—C4—H4	118.8
O6—Co1—O6 <sup>i</sup>	180.00 (6)	C4—C5—C6	120.38 (18)
C1—O1—Co1	130.14 (10)	C4—C5—H5	119.8
Co1—O5—H5A	125.5 (15)	C6—C5—H5	119.8
Co1—O5—H5B	103.7 (14)	C7—C6—C5	119.33 (17)
H5A—O5—H5B	104 (2)	C7—C6—H6	120.3
Co1—O6—H6A	112.4 (16)	C5—C6—H6	120.3
Co1—O6—H6B	117.5 (16)	C6—C7—C8	119.51 (17)
H6A—O6—H6B	104 (2)	C6—C7—H7	120.2
O4—N1—O3	122.64 (18)	C8—C7—H7	120.2
O4—N1—C8	118.61 (17)	C7—C8—C3	122.90 (16)
O3—N1—C8	118.75 (16)	C7—C8—N1	115.63 (16)
O2—C1—O1	124.94 (15)	C3—C8—N1	121.46 (15)
Co1—O1—C1—O2	25.0 (2)	C6—C7—C8—C3	2.2 (3)
Co1—O1—C1—C2	-156.08 (13)	C6—C7—C8—N1	-176.35 (17)
O2—C1—C2—C3	-20.9 (3)	C4—C3—C8—C7	-0.1 (3)
O1—C1—C2—C3	160.19 (17)	C2—C3—C8—C7	-179.68 (18)
C1—C2—C3—C8	-50.9 (3)	C4—C3—C8—N1	178.29 (16)
C1—C2—C3—C4	129.5 (2)	C2—C3—C8—N1	-1.3 (3)
C8—C3—C4—C5	-2.3 (3)	O4—N1—C8—C7	-19.3 (3)
C2—C3—C4—C5	177.3 (2)	O3—N1—C8—C7	160.92 (17)
C3—C4—C5—C6	2.6 (3)	O4—N1—C8—C3	162.21 (19)
C4—C5—C6—C7	-0.5 (3)	O3—N1—C8—C3	-17.6 (3)
C5—C6—C7—C8	-1.8 (3)		

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

#### 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>
O5—H5A $\cdots$ O1 <sup>ii</sup>	0.82 (2)	2.00 (2)	2.7984 (16)	166 (2)
O5—H5B $\cdots$ O2 <sup>i</sup>	0.82 (2)	1.89 (2)	2.6797 (17)	161 (2)

O6—H6A···O2 <sup>iii</sup>	0.78 (2)	1.93 (2)	2.6979 (17)	169 (2)
O6—H6B···O3	0.81 (2)	2.22 (2)	2.988 (2)	159 (2)

---

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