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Poly[(μ-2-acetoxybenzoato)(2-acetoxybenzoato)-μ-aqua-mercury(II)]

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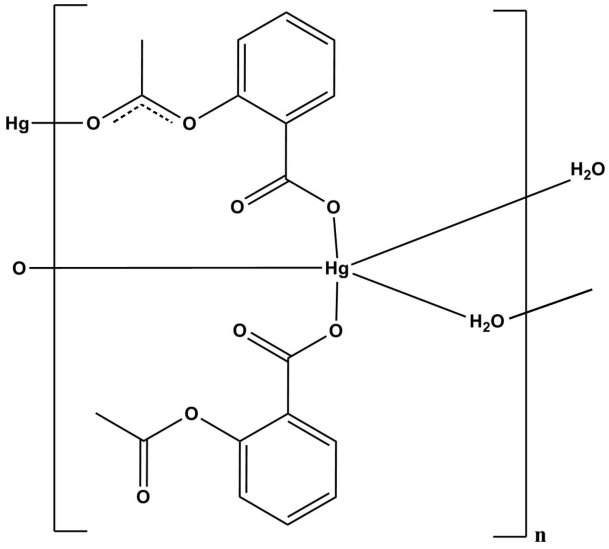
Key indicators: single-crystal X-ray study; T = 120 K; mean σ(C–C) = 0.009 Å; R factor = 0.040; wR factor = 0.092; data-to-parameter ratio = 20.9.

In the title compound, $[Hg(C_9H_7O_4)_2(H_2O)]_n$, the Hg^{II} ion is five-coordinated by three acetylsalicylate anions and water leading to the formation of a coordination polymer extending parallel to (001). O—H···O and C—H···O hydrogen bonds are effective in the stabilization of the crystal structure.

Related literature

For general background to metal complexes with acetylsalicylate as a ligand, see: Manojlović-Muir (1973); Garcia *et al.* (2003); Greenaway *et al.* (1984); Fujimori *et al.* (2005); James *et al.* (1998); Vasquez-Arciga *et al.* (2004); Ma & Moulton (2007).



Experimental

Crystal data

$[Hg(C_9H_7O_4)_2(H_2O)]$
M_r = 1153.80
Triclinic, $P\overline{1}$
a = 6.1851 (9) Å
b = 10.1359 (17) Å
c = 15.453 (2) Å
α = 100.308 (7)°
β = 98.700 (8)°
γ = 100.667 (7)°
V = 919.5 (2) Å^3
Z = 1
Mo $K\alpha$ radiation
μ = 8.42 mm^{-1}
T = 120 K
0.21 × 0.17 × 0.02 mm

Data collection

Bruker Kappa APEXII diffractometer
Absorption correction: analytical (De Meulenaer & Tompa, 1965)
T_{min} = 0.24, T_{max} = 0.83
9510 measured reflections
5293 independent reflections
4404 reflections with $I > 2\sigma(I)$
R_{int} = 0.037

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.040
$wR(F^2)$ = 0.092
S = 0.97
5293 reflections
253 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 1.88 e Å^{-3}
$\Delta\rho_{min}$ = −2.19 e Å^{-3}

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
O9—H2···O2^{i}	0.82	2.01	2.835 (7)	180 (1)
O9—H1···O5^{i}	0.82	1.93	2.758 (5)	179 (1)
C9—H92···O1^{ii}	0.95	2.49	3.409 (9)	163
C15—H151···O4^{iii}	0.95	2.51	3.221 (8)	132
C18—H181···O5^{iii}	0.95	2.59	3.530 (9)	169

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

Data collection: *APEX2* (Bruker, 2006); cell refinement: *SAINT* (Bruker, 2006); data reduction: *SAINT*; program(s) used to solve structure: *SIR92* (Altomare *et al.*, 1994); program(s) used to refine structure: *CRYSTALS* (Betteridge *et al.*, 2003); molecular graphics: *Mercury* (Macrae *et al.*, 2006); software used to prepare material for publication: *CRYSTALS*.

The author thank Bruce Foxman for his generous support in providing single-crystal data and valuable suggestions.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: DN2701).

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supporting information

Acta Cryst. (2011). E**67**, m1151 [doi:10.1107/S1600536811029278]

Poly[(*μ*-2-acetoxybenzoato)(2-acetoxybenzoato)-*μ*-aqua-mercury(II)]

J. PrakashaReddy

S1. Comment

First crystal structure of copper and acetylsalicylic acid (**ASA**) metal complex was reported by Manojlović-Muir (1973) which was reinvestigated by Garcia *et al.* (2003). Various other metal complexes of **ASA** have been also reported (Greenaway *et al.*, 1984; Fujimori *et al.*, 2005; James *et al.*, 1998; Ma & Moulton, 2007; Vásquez-Árciga *et al.*, 2004). For further investigation of the **ASA** complexes, we synthesized the title compound.

The asymmetric unit of the title compound contains two molecules of **ASA**, and a bridging water molecule coordinated to the Hg^{II} ion. The molecular arrangement around Hg^{II} is shown in Fig. 1. Crystal structure analysis shows that the carboxylate of the **ASA** molecules interacts with Hg^{II} in a monodentate fashion while acetyl group O atom of one of the **ASA** molecules coordinated to Hg^{II} ion forming a coordination polymer. The uncoordinated O atom of the carboxylate form intermolecular O—H···O hydrogen bonds with bridging water molecule resulting in the build up of a two-dimensional network parallel to the (001) plane (Fig. 2 and Table 1). Within this layer exist also weak C—H···O interactions (Table 1).

S2. Experimental

The title compound was synthesized by adding a solution of acetylsalicylic acid (36 mg, 0.2 mmol) dissolved in methanol (5 ml) to a mercuric chloride (27 mg, 0.1 mmol) dissolved in methanol (5 ml) in a 2:1 ratio respectively. After 3–4 days, colourless crystals of the title compound were obtained on slow evaporation of the solvent.

S3. Refinement

H atoms bound to the C and O were positioned geometrically and refined as riding atoms,with respective C—H and O—H distances of 0.95 Å and 0.82 Å and with U_{iso}(H) = 1.2Ueq(C, N).

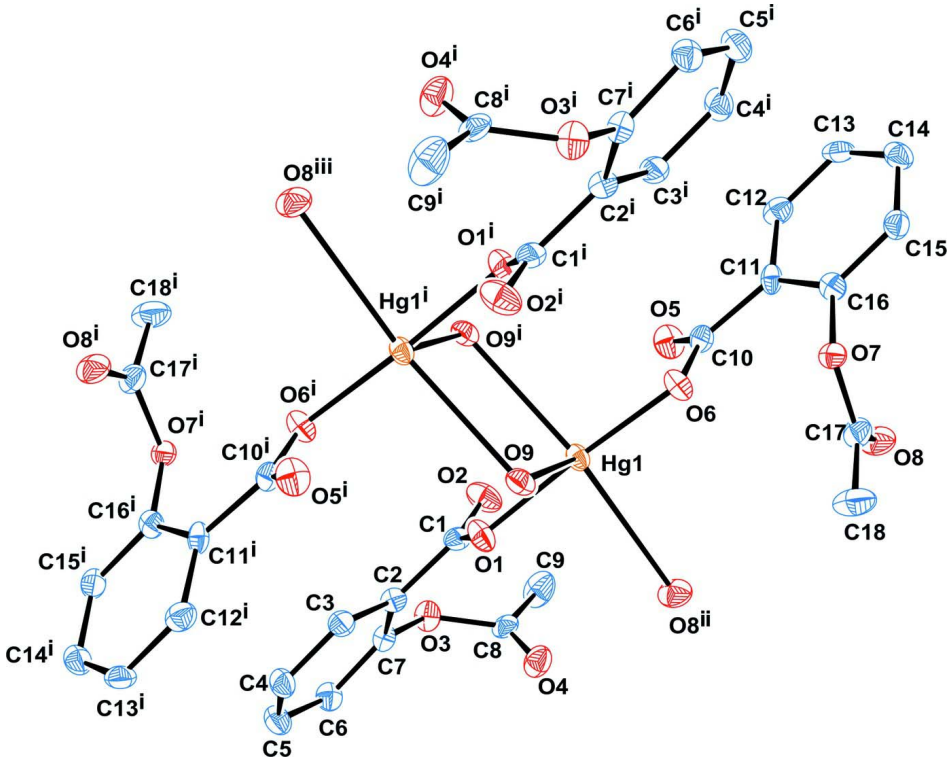

Figure 1

The title compound with the atom labeling scheme. Displacement ellipsoids are drawn at the 50% probability level. H atoms have been omitted for clarity. [Symmetry codes: (i) 2 - *x*, 1 - *y*, 1 - *z*; (ii) 2 - *x*, 2 - *y*, 1 - *z*; (iii) 1 + *x*,*y*,*z*

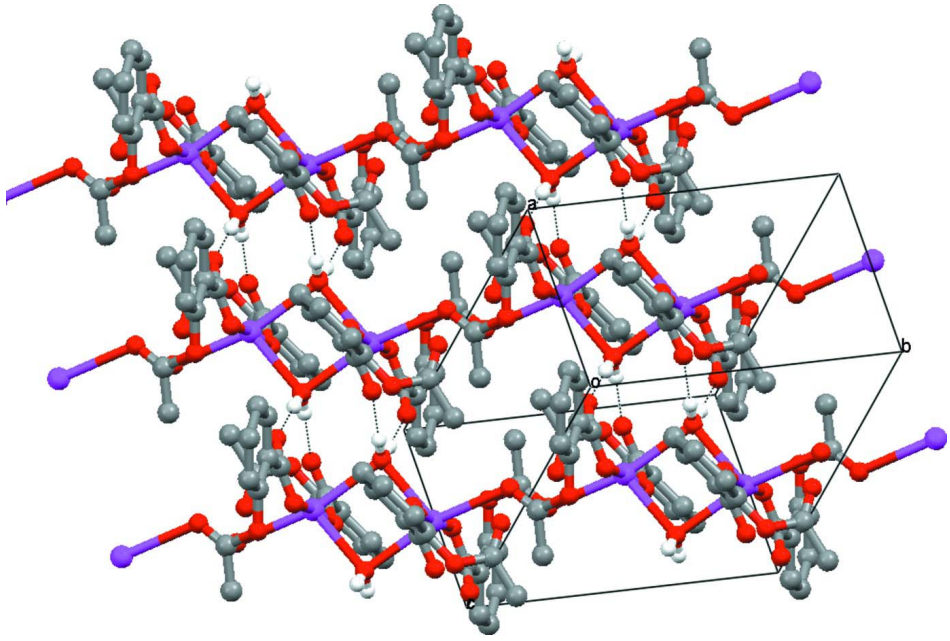

Figure 2

Packing diagram of the title compound. Hydrogen-bond interactions are drawn with dashed lines. H atoms not involved in hydrogen bondings have been omitted for clarity.

Poly[(*μ*-2-acetoxybenzoato)(2-acetoxybenzoato)-*μ*-aqua-mercury(II)]

Crystal data

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$\alpha = 100.308\ (7)°$
$\beta = 98.700\ (8)°$
$\gamma = 100.667\ (7)°$
$V = 919.5\ (2)$ Å^3
$Z = 1$
$F(000) = 552$
$D_x = 2.084$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 3872 reflections
$\theta = 3–30°$
$\mu = 8.42$ mm^{-1}
$T = 120$ K
Plate, colorless
0.21 × 0.17 × 0.02 mm

Data collection

Bruker Kappa APEXII diffractometer
Graphite monochromator
φ & ω scans
Absorption correction: analytical (De Meulenaer & Tompa, 1965)
$T_{min} = 0.24$, $T_{max} = 0.83$
9510 measured reflections
5293 independent reflections
4404 reflections with $I > 2\sigma(I)$
$R_{int} = 0.037$
$\theta_{max} = 30.0°$, $\theta_{min} = 2.2°$
$h = -8\rightarrow7$
$k = -14\rightarrow13$
$l = -21\rightarrow21$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.040$
$wR(F^2) = 0.092$
$S = 0.97$
5293 reflections
253 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
Method = Modified Sheldrick $w = 1/[\sigma^2(F^2) + (0.04P)^2 + 6.15P]$, where $P = [\max(F_o^2,0) + 2F_c^2]/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 1.88$ e Å^{-3}
$\Delta\rho_{min} = -2.19$ e Å^{-3}

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
Hg1	0.89515 (4)	0.65817 (2)	0.467447 (16)	0.0168
O1	0.8495 (8)	0.5346 (4)	0.3440 (3)	0.0248
O2	0.4800 (8)	0.5246 (5)	0.3271 (3)	0.0285
O3	0.2895 (7)	0.4772 (4)	0.1441 (3)	0.0215
O4	0.5203 (8)	0.6855 (4)	0.1796 (4)	0.0281
O5	0.6204 (8)	0.7673 (5)	0.5843 (3)	0.0270
O6	0.9879 (7)	0.7872 (4)	0.5911 (3)	0.0222
O7	1.2498 (7)	1.0048 (4)	0.7117 (3)	0.0174
O8	1.0778 (8)	1.1274 (5)	0.6272 (3)	0.0268
O9	1.2672 (7)	0.5721 (4)	0.4763 (3)	0.0198
C1	0.6439 (11)	0.4964 (6)	0.2984 (4)	0.0198
C2	0.6323 (10)	0.4156 (6)	0.2068 (4)	0.0165
C3	0.7982 (11)	0.3423 (6)	0.1913 (4)	0.0205

C4	0.7977 (11)	0.2696 (6)	0.1066 (5)	0.0231
C5	0.6320 (11)	0.2710 (6)	0.0339 (5)	0.0249
C6	0.4648 (11)	0.3435 (6)	0.0472 (4)	0.0216
C7	0.4668 (10)	0.4133 (6)	0.1336 (4)	0.0178
C8	0.3385 (11)	0.6172 (6)	0.1734 (4)	0.0207
C9	0.1367 (13)	0.6643 (7)	0.1952 (6)	0.0365
C10	0.8163 (11)	0.8122 (6)	0.6245 (4)	0.0195
C11	0.8677 (10)	0.8985 (5)	0.7175 (4)	0.0171
C12	0.7009 (11)	0.8886 (6)	0.7696 (5)	0.0223
C13	0.7399 (12)	0.9606 (6)	0.8567 (4)	0.0238
C14	0.9507 (11)	1.0455 (6)	0.8963 (4)	0.0227
C15	1.1151 (11)	1.0597 (6)	0.8456 (4)	0.0204
C16	1.0744 (10)	0.9876 (6)	0.7573 (4)	0.0174
C17	1.2367 (11)	1.0780 (6)	0.6470 (4)	0.0224
C18	1.4387 (13)	1.0861 (8)	0.6063 (5)	0.0333
H31	0.9129	0.3424	0.2398	0.0255*
H41	0.9097	0.2185	0.0975	0.0281*
H51	0.6341	0.2225	−0.0244	0.0287*
H61	0.3524	0.3452	−0.0016	0.0251*
H91	0.1725	0.7613	0.2154	0.0468*
H92	0.0862	0.6224	0.2410	0.0468*
H93	0.0218	0.6394	0.1432	0.0468*
H121	0.5576	0.8309	0.7441	0.0281*
H131	0.6235	0.9526	0.8904	0.0321*
H141	0.9795	1.0926	0.9572	0.0282*
H151	1.2569	1.1192	0.8710	0.0242*
H181	1.4269	1.1379	0.5610	0.0441*
H182	1.5677	1.1294	0.6511	0.0441*
H183	1.4512	0.9960	0.5807	0.0441*
H2	1.3284	0.5582	0.4330	0.0237*
H1	1.3720	0.6302	0.5086	0.0237*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Hg1	0.01839 (11)	0.01710 (10)	0.01515 (12)	0.00792 (7)	0.00211 (8)	0.00097 (7)
O1	0.028 (2)	0.025 (2)	0.021 (2)	0.0116 (18)	0.0052 (19)	−0.0016 (18)
O2	0.027 (3)	0.042 (3)	0.022 (2)	0.018 (2)	0.007 (2)	0.005 (2)
O3	0.015 (2)	0.022 (2)	0.028 (3)	0.0090 (16)	0.0011 (18)	0.0050 (18)
O4	0.026 (2)	0.021 (2)	0.040 (3)	0.0077 (18)	0.012 (2)	0.009 (2)
O5	0.024 (2)	0.029 (2)	0.026 (3)	0.0072 (18)	−0.002 (2)	0.0028 (19)
O6	0.022 (2)	0.025 (2)	0.017 (2)	0.0076 (17)	0.0018 (18)	−0.0020 (17)
O7	0.020 (2)	0.0172 (18)	0.019 (2)	0.0097 (15)	0.0057 (17)	0.0068 (16)
O8	0.032 (3)	0.029 (2)	0.027 (3)	0.0148 (19)	0.008 (2)	0.015 (2)
O9	0.021 (2)	0.023 (2)	0.014 (2)	0.0036 (16)	0.0030 (17)	0.0014 (16)
C1	0.025 (3)	0.020 (3)	0.017 (3)	0.007 (2)	0.005 (2)	0.008 (2)
C2	0.014 (3)	0.019 (3)	0.018 (3)	0.005 (2)	0.002 (2)	0.006 (2)
C3	0.026 (3)	0.020 (3)	0.018 (3)	0.009 (2)	0.004 (3)	0.007 (2)

C4	0.024 (3)	0.020 (3)	0.026 (4)	0.008 (2)	0.009 (3)	0.002 (2)
C5	0.029 (3)	0.024 (3)	0.020 (3)	0.004 (2)	0.005 (3)	−0.001 (2)
C6	0.022 (3)	0.022 (3)	0.019 (3)	0.005 (2)	−0.001 (2)	0.003 (2)
C7	0.016 (3)	0.015 (2)	0.022 (3)	0.003 (2)	0.002 (2)	0.004 (2)
C8	0.025 (3)	0.019 (3)	0.022 (3)	0.009 (2)	0.006 (3)	0.012 (2)
C9	0.031 (4)	0.029 (3)	0.056 (5)	0.015 (3)	0.013 (4)	0.016 (3)
C10	0.025 (3)	0.015 (2)	0.021 (3)	0.008 (2)	0.005 (2)	0.005 (2)
C11	0.017 (3)	0.012 (2)	0.021 (3)	0.006 (2)	−0.001 (2)	0.001 (2)
C12	0.021 (3)	0.022 (3)	0.027 (4)	0.006 (2)	0.008 (3)	0.009 (3)
C13	0.034 (4)	0.026 (3)	0.020 (3)	0.015 (3)	0.014 (3)	0.013 (3)
C14	0.032 (4)	0.023 (3)	0.016 (3)	0.013 (3)	0.003 (3)	0.004 (2)
C15	0.024 (3)	0.016 (2)	0.021 (3)	0.005 (2)	0.002 (2)	0.003 (2)
C16	0.019 (3)	0.018 (2)	0.019 (3)	0.011 (2)	0.003 (2)	0.005 (2)
C17	0.028 (3)	0.018 (3)	0.023 (3)	0.007 (2)	0.003 (3)	0.007 (2)
C18	0.036 (4)	0.041 (4)	0.034 (4)	0.013 (3)	0.019 (3)	0.020 (3)

Geometric parameters (Å, º)

Hg1—O9^{i}	2.708 (4)	C5—C6	1.394 (9)
Hg1—O8^{ii}	2.823 (4)	C5—H51	0.950
Hg1—O1	2.034 (4)	C6—C7	1.393 (9)
Hg1—O6	2.046 (4)	C6—H61	0.950
Hg1—O9	2.601 (4)	C8—C9	1.479 (10)
O1—C1	1.309 (8)	C9—H91	0.950
O2—C1	1.226 (8)	C9—H92	0.950
O3—C7	1.388 (7)	C9—H93	0.950
O3—C8	1.372 (7)	C10—C11	1.497 (8)
O4—C8	1.187 (8)	C11—C12	1.402 (9)
O5—C10	1.236 (8)	C11—C16	1.401 (8)
O6—C10	1.295 (7)	C12—C13	1.373 (9)
O7—C16	1.382 (7)	C12—H121	0.950
O7—C17	1.348 (8)	C13—C14	1.403 (9)
O8—C17	1.207 (8)	C13—H131	0.950
O9—H2	0.820	C14—C15	1.377 (9)
O9—H1	0.820	C14—H141	0.950
C1—C2	1.488 (9)	C15—C16	1.389 (9)
C2—C3	1.398 (8)	C15—H151	0.950
C2—C7	1.400 (8)	C17—C18	1.477 (10)
C3—C4	1.382 (9)	C18—H181	0.950
C3—H31	0.950	C18—H182	0.950
C4—C5	1.406 (10)	C18—H183	0.950
C4—H41	0.950		
O9—Hg1—O8	107.12 (11)	O4—C8—O3	121.8 (5)
O9—Hg1—O6	94.68 (16)	O4—C8—C9	127.9 (5)
O1—Hg1—O6	171.97 (18)	O3—C8—C9	110.3 (5)
O1—Hg1—O9	78.28 (14)	O5—C10—C11	121.1 (5)
C1—O1—Hg1	116.6 (3)	O6—C10—C11	116.1 (5)

C8—O3—C7	118.1 (4)	C12—C11—C16	117.2 (5)
C17—O7—C16	117.7 (4)	C12—C11—C10	118.4 (5)
O2—C1—O1	124.4 (5)	C16—C11—C10	124.4 (5)
O2—C1—C2	123.5 (5)	C13—C12—C11	121.9 (5)
O1—C1—C2	112.1 (5)	C12—C13—C14	120.1 (5)
C3—C2—C7	117.5 (5)	C15—C14—C13	118.9 (5)
C3—C2—C1	119.1 (5)	C16—C15—C14	120.2 (5)
C7—C2—C1	123.4 (5)	C15—C16—O7	116.4 (5)
C4—C3—C2	121.0 (5)	C15—C16—C11	121.6 (5)
C5—C4—C3	120.1 (5)	O7—C16—C11	122.0 (5)
C4—C5—C6	120.4 (5)	O8—C17—O7	123.1 (5)
C7—C6—C5	118.6 (5)	O8—C17—C18	126.5 (6)
C6—C7—O3	116.2 (5)	O7—C17—C18	110.4 (5)
C6—C7—C2	122.4 (5)	H181—C18—H183	110.00
O3—C7—C2	121.3 (5)	H182—C18—H183	109.00

O9—Hg1—O1—C1	163.5 (4)	C7—O3—C8—O4	9.0 (8)
O9—Hg1—O6—C10	−156.3 (3)	C7—O3—C8—C9	−170.8 (5)
Hg1—O1—C1—O2	−3.7 (7)	Hg1—O6—C10—O5	−3.0 (6)
Hg1—O1—C1—C2	175.2 (3)	Hg1—O6—C10—C11	176.3 (3)
O2—C1—C2—C3	−154.5 (5)	O5—C10—C11—C12	22.0 (8)
O1—C1—C2—C3	26.5 (7)	O6—C10—C11—C12	−157.4 (5)
O2—C1—C2—C7	27.9 (8)	O5—C10—C11—C16	−159.3 (5)
O1—C1—C2—C7	−151.1 (5)	O6—C10—C11—C16	21.3 (7)
C7—C2—C3—C4	−0.3 (8)	C16—C11—C12—C13	−1.9 (8)
C1—C2—C3—C4	−178.0 (5)	C10—C11—C12—C13	176.9 (5)
C2—C3—C4—C5	1.1 (8)	C11—C12—C13—C14	−0.3 (8)
C3—C4—C5—C6	−0.6 (8)	C12—C13—C14—C15	2.8 (8)
C4—C5—C6—C7	−0.5 (8)	C14—C15—C16—O7	−177.9 (5)
C5—C6—C7—O3	−176.4 (4)	C17—O7—C16—C15	−108.1 (5)
C5—C6—C7—C2	1.3 (8)	C17—O7—C16—C11	73.3 (6)
C8—O3—C7—C6	−118.6 (5)	C12—C11—C16—C15	1.8 (7)
C8—O3—C7—C2	63.6 (7)	C10—C11—C16—C15	−177.0 (5)
C3—C2—C7—C6	−0.9 (8)	C12—C11—C16—O7	−179.7 (4)
C1—C2—C7—C6	176.7 (5)	C10—C11—C16—O7	1.5 (7)
C3—C2—C7—O3	176.7 (4)	C16—O7—C17—O8	−0.4 (7)
C1—C2—C7—O3	−5.7 (8)	C16—O7—C17—C18	180.0 (4)

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

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O9—H2···O2^{iii}	0.82	2.01	2.835 (7)	180 (1)
O9—H1···O5^{iii}	0.82	1.93	2.758 (5)	179 (1)
C9—H92···O1^{iv}	0.95	2.49	3.409 (9)	163

C15—H151···O4^{ii}	0.95	2.51	3.221 (8)	132
C18—H181···O5^{ii}	0.95	2.59	3.530 (9)	169

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