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7,7-[Ethane-1,2-diylbis(oxy)]-2-[hydroxy(phenyl)methyl]bicyclo[3.3.1]nonan-3-one

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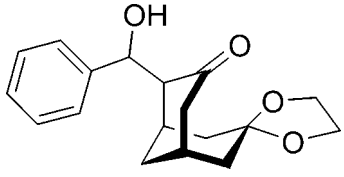
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.004 Å; R factor = 0.039; wR factor = 0.096; data-to-parameter ratio = 8.5.

In the title compound, $C_{18}H_{22}O_4$, the cyclohexane and cyclohexanone rings adopt normal chair and half-chair conformations, respectively. The dioxolane ring is almost planar, with an r.m.s. deviation of 0.094 (3) Å. In the crystal, molecules are connected by O—H···O hydrogen bonds, forming 2_1 helical chains along the a-axis direction. The chains are further connected by C—H···O hydrogen bonds.

Related literature

For related structures having condensed cyclohexanone rings, see: Li *et al.* (2002); Lopez-Alvarado *et al.* (2002). For a related structure with a cyclohexanone ring, see: Shallard-Brown *et al.* (2005). For the synthesis, see: Tomizawa *et al.* (2009).



Experimental

Crystal data

$C_{18}H_{22}O_4$ M_r = 302.36
Orthorhombic, $P2_12_12_1$
a = 9.1465 (3) Å
b = 10.0346 (4) Å
c = 16.6469 (6) Å
V = 1527.88 (10) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.09 mm^{-1}
T = 293 K
0.35 × 0.30 × 0.29 mm

Data collection

Bruker SMART CCD area detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2000)
T_{min} = 0.951, T_{max} = 0.962
12383 measured reflections
1734 independent reflections
1560 reflections with $I > 2\sigma(I)$
R_{int} = 0.026

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.039
$wR(F^2)$ = 0.096
S = 1.03
1734 reflections
203 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.20 e Å^{-3}
$\Delta\rho_{min}$ = −0.17 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O4—H4···O3^{i}	0.86 (4)	2.03 (4)	2.857 (3)	163 (3)
C16—H16···O3^{ii}	0.93	2.59	3.473 (4)	159

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

Data collection: *SMART* (Bruker, 2000); cell refinement: *SAINT* (Bruker, 2000); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 2008); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

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Supporting information for this paper is available from the IUCr electronic archives (Reference: IS5345).

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supporting information

Acta Cryst. (2014). E**70**, o665 [doi:10.1107/S1600536814009040]

7,7-[Ethane-1,2-diylbis(oxy)]-2-[hydroxy(phenyl)methyl]bicyclo[3.3.1]nonan-3-one

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S1. Comment

2-(Hydroxyphenylmethyl)-7,7-ethylenedioxybicyclo[3.3.1]nonan-3-one is a key intermediate of the known asymmetrical catalysis of adamantane derivatives that is used in kinetic resolution of secondary alcohols (Tomizawa *et al.*, 2009). Recently. it was synthesized in our lab and the structure was determined.

In the compound (Fig. 1), the C1/C4 cyclohexyl ring adopts a normal chair conformation. The O1/O2 dioxolane ring is almost planar, with a maximum deviation 0.086 (4) Å at the O2 atom. Atoms C3, C7, C8, C9, C5 and O3 are arranged roughly on a plane, with the maximum deviation 0.171 (4) Å at C7 atom. Therefore, the C4/C8 cyclohexanone ring adopts a half-chair conformation, which is different from most known condensed cyclohexanone ring that is part of the complex structure (Lopez-Alvarado *et al.*, 2002; Li *et al.*, 2002), and from free cyclohexanone in solid state (Shallard-Brown *et al.*, 2005).

In the crystal, molecules are linked by O4—H4···O3^{i} hydrogen bonds (Fig. 2 and Table 1) to form chiral chains. In addition, C—H···O hydrogen bonds help the stability of the crystal. No π–π packing and C—H···π contacts are observed.

S2. Experimental

2-(Hydroxyphenylmethyl)-7,7-ethylenedioxybicyclo[3.3.1]nonan-3-one was synthesized through a known procedure (Tomizawa *et al.*, 2009) and obtained as a white solid in a yield of 61% and a purity of 96%. Single crystals were obtained by recrystalization from anhydrous ethanol. MS (ESI) 325.1 (*M*+Na+) m/*z*.

S3. Refinement

The hydroxyl H atom was located in a difference Fourier map and was refined freely. Other H atoms were placed in calculated positions and allowed to ride on their parent atoms at distances 0.93 Å for phenyl, 0.97 Å for methylene and 0.98 Å for methine with U_{iso}(H) = 1.2U_{eq}(C). In the absence of significant anomalous scattering effects, Friedel pairs have been merged.

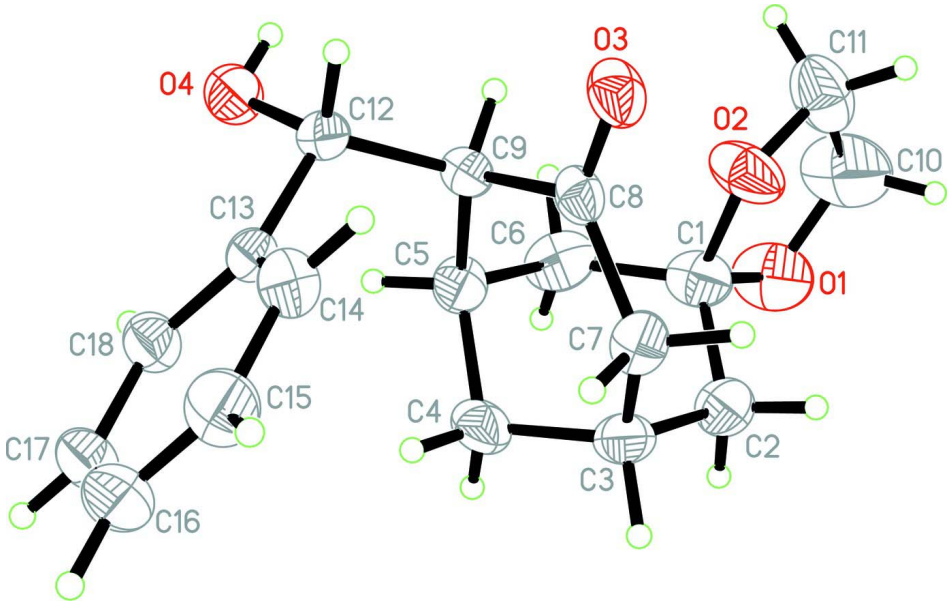

Figure 1

The molecular structure of the title compound with atom labels, showing 40% probability displacement ellipsoids.

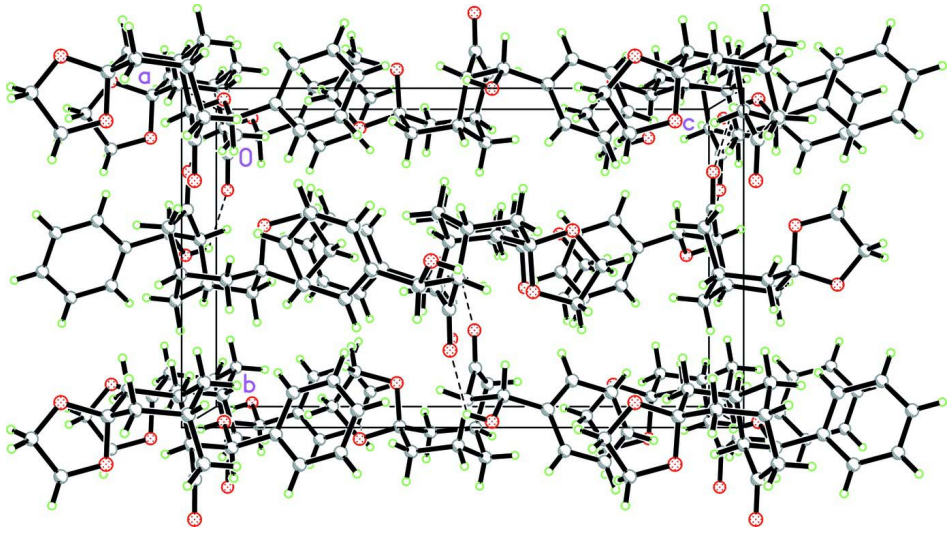

Figure 2

The packing diagram of the title compound viewed down along the *a* axis. O—H···O hydrogen bonds are shown by thin dashed lines.

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b = 10.0346 (4) Å
c = 16.6469 (6) Å
V = 1527.88 (10) Å^3
Z = 4
$F(000)$ = 648
D_x = 1.314 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 1165 reflections
θ = 2.4–24.4°
μ = 0.09 mm^{-1}

T = 293 K
Prism, colorless

0.35 × 0.30 × 0.29 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, 2000)
T_{min} = 0.951, T_{max} = 0.962

12383 measured reflections
1734 independent reflections
1560 reflections with $I > 2\sigma(I)$
R_{int} = 0.026
θ_{max} = 26.0°, θ_{min} = 3.3°
h = −10→11
k = −12→12
l = −20→20

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.039
$wR(F^2)$ = 0.096
S = 1.03
1734 reflections
203 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
$w = 1/[\sigma^2(F_o^2) + (0.0446P)^2 + 0.4409P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.20 e Å^{-3}
$\Delta\rho_{min}$ = −0.17 e Å^{-3}

Special details

Experimental. IR (KBr) 3488, 2929, 2901, 2875, 1685, 1455, 1332, 1268, 1215, 1145, 1094, 1072, 1044, 1024, 948, 715 cm$^{-1.}$ ^{1}NMR (CDCl3) 7.28–7.39 (m, 5H), 4.68–4.70(m, 1H), 3.92–3.95(m, 2H), 3.89 (d, J = 1.5 Hz, 1H), 3.80–3.87 (m, 2H), 2.59–2.63 (m, 2H), 2.51–2.55 (m, 2H), 1.96 (s, 1H), 1.80–1.83 (m, 3H), 1.64–1.67 (m, 1H), 1.52–1.57 (m, 2H) p.p.m.. ^{13}CNMR (CDCl3) 213.2, 141.3, 128.6, 128.2, 127.1, 107.3, 74.6, 64.4, 63.4, 60.1, 45.1, 41.0, 40.1, 30.5, 29.2, 28.4 p.p.m..

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}
O1	0.6491 (3)	0.0825 (2)	0.69986 (12)	0.0753 (7)
O2	0.5859 (3)	−0.1011 (2)	0.62676 (11)	0.0652 (6)
O3	0.4901 (2)	−0.27188 (15)	0.47755 (10)	0.0465 (5)
O4	0.1336 (2)	−0.00830 (19)	0.44707 (11)	0.0497 (5)
C1	0.6058 (3)	0.0396 (3)	0.62152 (15)	0.0506 (7)
C2	0.7289 (3)	0.0663 (3)	0.56347 (16)	0.0496 (7)
H2A	0.8089	0.0059	0.5752	0.060*
H2B	0.7640	0.1565	0.5717	0.060*
C3	0.6849 (3)	0.0497 (3)	0.47526 (15)	0.0454 (6)

H3	0.7658	0.0822	0.4420	0.054*
C4	0.5513 (3)	0.1339 (3)	0.45651 (16)	0.0484 (6)
H4A	0.5262	0.1253	0.4001	0.058*
H4B	0.5720	0.2269	0.4675	0.058*
C5	0.4239 (3)	0.0869 (2)	0.50846 (16)	0.0428 (6)
H5	0.3392	0.1433	0.4965	0.051*
C6	0.4659 (3)	0.1088 (3)	0.59727 (17)	0.0550 (7)
H6A	0.4764	0.2037	0.6069	0.066*
H6B	0.3869	0.0767	0.6310	0.066*
C7	0.6542 (3)	−0.0947 (3)	0.45113 (15)	0.0431 (6)
H7A	0.6618	−0.1010	0.3931	0.052*
H7B	0.7305	−0.1503	0.4738	0.052*
C8	0.5093 (3)	−0.1518 (2)	0.47572 (13)	0.0351 (5)
C9	0.3807 (3)	−0.0595 (2)	0.49186 (13)	0.0340 (5)
H9	0.3354	−0.0919	0.5415	0.041*
C10	0.6360 (6)	−0.0235 (4)	0.75276 (19)	0.0986 (15)
H10A	0.5687	−0.0013	0.7958	0.118*
H10B	0.7303	−0.0448	0.7762	0.118*
C11	0.5806 (4)	−0.1374 (4)	0.70659 (17)	0.0695 (10)
H11A	0.6407	−0.2155	0.7160	0.083*
H11B	0.4809	−0.1578	0.7222	0.083*
C12	0.2635 (2)	−0.0783 (2)	0.42468 (14)	0.0361 (5)
H12	0.2395	−0.1734	0.4220	0.043*
C13	0.3099 (2)	−0.0343 (2)	0.34160 (13)	0.0351 (5)
C14	0.3927 (3)	−0.1185 (3)	0.29428 (14)	0.0445 (6)
H14	0.4169	−0.2028	0.3133	0.053*
C15	0.4402 (3)	−0.0792 (3)	0.21877 (16)	0.0559 (7)
H15	0.4965	−0.1369	0.1878	0.067*
C16	0.4044 (3)	0.0444 (3)	0.18965 (17)	0.0598 (8)
H16	0.4362	0.0709	0.1391	0.072*
C17	0.3212 (3)	0.1284 (3)	0.23589 (17)	0.0541 (7)
H17	0.2968	0.2123	0.2163	0.065*
C18	0.2731 (3)	0.0903 (3)	0.31126 (15)	0.0437 (6)
H18	0.2161	0.1481	0.3417	0.052*
H4	0.078 (4)	−0.061 (4)	0.474 (2)	0.085 (12)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.1027 (18)	0.0848 (16)	0.0384 (10)	−0.0320 (15)	−0.0114 (11)	−0.0115 (11)
O2	0.1016 (17)	0.0530 (12)	0.0411 (10)	−0.0264 (12)	−0.0194 (11)	0.0094 (9)
O3	0.0556 (11)	0.0299 (9)	0.0539 (10)	0.0049 (8)	−0.0135 (9)	−0.0010 (8)
O4	0.0375 (9)	0.0539 (12)	0.0576 (11)	0.0058 (9)	0.0073 (9)	0.0130 (9)
C1	0.0665 (18)	0.0489 (15)	0.0363 (12)	−0.0176 (14)	−0.0052 (12)	−0.0066 (11)
C2	0.0489 (15)	0.0500 (15)	0.0500 (14)	−0.0117 (13)	−0.0108 (12)	−0.0009 (12)
C3	0.0436 (13)	0.0515 (15)	0.0411 (12)	−0.0118 (12)	0.0011 (11)	0.0048 (12)
C4	0.0596 (15)	0.0357 (13)	0.0499 (14)	−0.0120 (12)	−0.0102 (12)	0.0089 (11)
C5	0.0437 (13)	0.0309 (12)	0.0538 (14)	0.0018 (11)	−0.0048 (11)	−0.0021 (11)

C6	0.0579 (17)	0.0506 (16)	0.0564 (16)	−0.0087 (14)	0.0072 (13)	−0.0189 (13)
C7	0.0390 (13)	0.0511 (15)	0.0391 (12)	0.0030 (12)	−0.0009 (10)	−0.0044 (11)
C8	0.0421 (12)	0.0352 (12)	0.0281 (10)	0.0014 (10)	−0.0074 (10)	0.0013 (9)
C9	0.0390 (12)	0.0311 (11)	0.0320 (10)	−0.0010 (10)	0.0005 (9)	0.0025 (9)
C10	0.128 (4)	0.126 (4)	0.0412 (16)	−0.041 (3)	−0.009 (2)	0.002 (2)
C11	0.082 (2)	0.079 (2)	0.0473 (16)	0.022 (2)	0.0053 (16)	0.0114 (16)
C12	0.0329 (12)	0.0333 (12)	0.0422 (12)	−0.0030 (10)	−0.0008 (10)	0.0050 (10)
C13	0.0329 (12)	0.0359 (12)	0.0365 (11)	−0.0049 (10)	−0.0065 (9)	0.0017 (10)
C14	0.0470 (14)	0.0447 (14)	0.0420 (12)	0.0035 (12)	−0.0029 (11)	−0.0007 (11)
C15	0.0582 (17)	0.0692 (19)	0.0403 (14)	0.0010 (16)	0.0036 (12)	−0.0045 (14)
C16	0.0600 (18)	0.080 (2)	0.0393 (13)	−0.0102 (17)	0.0024 (13)	0.0139 (15)
C17	0.0601 (17)	0.0504 (16)	0.0518 (15)	−0.0063 (14)	−0.0077 (13)	0.0182 (13)
C18	0.0473 (14)	0.0395 (13)	0.0445 (13)	−0.0006 (11)	−0.0043 (11)	0.0046 (11)

Geometric parameters (Å, º)

O1—C10	1.386 (4)	C7—H7A	0.9700
O1—C1	1.429 (3)	C7—H7B	0.9700
O2—C11	1.379 (3)	C8—C9	1.521 (3)
O2—C1	1.425 (3)	C9—C12	1.561 (3)
O3—C8	1.218 (3)	C9—H9	0.9800
O4—C12	1.430 (3)	C10—C11	1.467 (5)
O4—H4	0.86 (4)	C10—H10A	0.9700
C1—C2	1.508 (4)	C10—H10B	0.9700
C1—C6	1.511 (4)	C11—H11A	0.9700
C2—C3	1.532 (4)	C11—H11B	0.9700
C2—H2A	0.9700	C12—C13	1.513 (3)
C2—H2B	0.9700	C12—H12	0.9800
C3—C4	1.518 (4)	C13—C14	1.381 (3)
C3—C7	1.529 (4)	C13—C18	1.390 (3)
C3—H3	0.9800	C14—C15	1.387 (4)
C4—C5	1.526 (4)	C14—H14	0.9300
C4—H4A	0.9700	C15—C16	1.371 (4)
C4—H4B	0.9700	C15—H15	0.9300
C5—C6	1.543 (4)	C16—C17	1.372 (4)
C5—C9	1.546 (3)	C16—H16	0.9300
C5—H5	0.9800	C17—C18	1.384 (4)
C6—H6A	0.9700	C17—H17	0.9300
C6—H6B	0.9700	C18—H18	0.9300
C7—C8	1.500 (3)		
C10—O1—C1	108.9 (2)	O3—C8—C7	120.8 (2)
C11—O2—C1	109.0 (2)	O3—C8—C9	119.1 (2)
C12—O4—H4	109 (2)	C7—C8—C9	119.91 (19)
O2—C1—O1	106.1 (2)	C8—C9—C5	114.35 (19)
O2—C1—C2	108.1 (2)	C8—C9—C12	109.31 (18)
O1—C1—C2	108.9 (2)	C5—C9—C12	114.77 (18)
O2—C1—C6	111.3 (2)	C8—C9—H9	105.9

O1—C1—C6	109.9 (2)	C5—C9—H9	105.9
C2—C1—C6	112.3 (2)	C12—C9—H9	105.9
C1—C2—C3	113.5 (2)	O1—C10—C11	107.1 (3)
C1—C2—H2A	108.9	O1—C10—H10A	110.3
C3—C2—H2A	108.9	C11—C10—H10A	110.3
C1—C2—H2B	108.9	O1—C10—H10B	110.3
C3—C2—H2B	108.9	C11—C10—H10B	110.3
H2A—C2—H2B	107.7	H10A—C10—H10B	108.5
C4—C3—C7	109.0 (2)	O2—C11—C10	106.7 (3)
C4—C3—C2	110.3 (2)	O2—C11—H11A	110.4
C7—C3—C2	113.8 (2)	C10—C11—H11A	110.4
C4—C3—H3	107.8	O2—C11—H11B	110.4
C7—C3—H3	107.8	C10—C11—H11B	110.4
C2—C3—H3	107.8	H11A—C11—H11B	108.6
C3—C4—C5	109.0 (2)	O4—C12—C13	109.15 (19)
C3—C4—H4A	109.9	O4—C12—C9	108.93 (19)
C5—C4—H4A	109.9	C13—C12—C9	115.27 (18)
C3—C4—H4B	109.9	O4—C12—H12	107.7
C5—C4—H4B	109.9	C13—C12—H12	107.7
H4A—C4—H4B	108.3	C9—C12—H12	107.7
C4—C5—C6	108.0 (2)	C14—C13—C18	118.4 (2)
C4—C5—C9	112.8 (2)	C14—C13—C12	119.8 (2)
C6—C5—C9	111.7 (2)	C18—C13—C12	121.8 (2)
C4—C5—H5	108.1	C13—C14—C15	121.0 (3)
C6—C5—H5	108.1	C13—C14—H14	119.5
C9—C5—H5	108.1	C15—C14—H14	119.5
C1—C6—C5	113.7 (2)	C16—C15—C14	120.1 (3)
C1—C6—H6A	108.8	C16—C15—H15	119.9
C5—C6—H6A	108.8	C14—C15—H15	119.9
C1—C6—H6B	108.8	C15—C16—C17	119.4 (3)
C5—C6—H6B	108.8	C15—C16—H16	120.3
H6A—C6—H6B	107.7	C17—C16—H16	120.3
C8—C7—C3	116.9 (2)	C16—C17—C18	121.0 (3)
C8—C7—H7A	108.1	C16—C17—H17	119.5
C3—C7—H7A	108.1	C18—C17—H17	119.5
C8—C7—H7B	108.1	C17—C18—C13	120.1 (3)
C3—C7—H7B	108.1	C17—C18—H18	119.9
H7A—C7—H7B	107.3	C13—C18—H18	119.9

C11—O2—C1—O1	14.4 (4)	O3—C8—C9—C12	−64.0 (3)
C11—O2—C1—C2	131.1 (3)	C7—C8—C9—C12	110.9 (2)
C11—O2—C1—C6	−105.2 (3)	C4—C5—C9—C8	37.9 (3)
C10—O1—C1—O2	−8.1 (4)	C6—C5—C9—C8	−83.9 (3)
C10—O1—C1—C2	−124.2 (3)	C4—C5—C9—C12	−89.6 (2)
C10—O1—C1—C6	112.4 (3)	C6—C5—C9—C12	148.6 (2)
O2—C1—C2—C3	76.3 (3)	C1—O1—C10—C11	−0.8 (5)
O1—C1—C2—C3	−168.8 (2)	C1—O2—C11—C10	−14.8 (4)
C6—C1—C2—C3	−46.9 (3)	O1—C10—C11—O2	9.6 (5)

C1—C2—C3—C4	53.7 (3)	C8—C9—C12—O4	170.56 (19)
C1—C2—C3—C7	−69.2 (3)	C5—C9—C12—O4	−59.4 (3)
C7—C3—C4—C5	64.1 (3)	C8—C9—C12—C13	−66.4 (2)
C2—C3—C4—C5	−61.5 (3)	C5—C9—C12—C13	63.6 (3)
C3—C4—C5—C6	62.2 (3)	O4—C12—C13—C14	−154.8 (2)
C3—C4—C5—C9	−61.7 (3)	C9—C12—C13—C14	82.3 (3)
O2—C1—C6—C5	−72.3 (3)	O4—C12—C13—C18	26.0 (3)
O1—C1—C6—C5	170.5 (2)	C9—C12—C13—C18	−96.9 (3)
C2—C1—C6—C5	49.1 (3)	C18—C13—C14—C15	1.1 (4)
C4—C5—C6—C1	−56.8 (3)	C12—C13—C14—C15	−178.2 (2)
C9—C5—C6—C1	67.8 (3)	C13—C14—C15—C16	−0.5 (4)
C4—C3—C7—C8	−45.7 (3)	C14—C15—C16—C17	0.0 (4)
C2—C3—C7—C8	77.9 (3)	C15—C16—C17—C18	0.0 (4)
C3—C7—C8—O3	−161.2 (2)	C16—C17—C18—C13	0.6 (4)
C3—C7—C8—C9	24.0 (3)	C14—C13—C18—C17	−1.1 (4)
O3—C8—C9—C5	165.8 (2)	C12—C13—C18—C17	178.1 (2)
C7—C8—C9—C5	−19.3 (3)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O4—H4···O3^{i}	0.86 (4)	2.03 (4)	2.857 (3)	163 (3)
C16—H16···O3^{ii}	0.93	2.59	3.473 (4)	159

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