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3,6-Dimethyl-*o*-phenylenedimethanol

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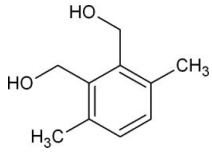
Key indicators: single-crystal X-ray study; T = 296 K; mean σ(C–C) = 0.005 Å; R factor = 0.047; wR factor = 0.121; data-to-parameter ratio = 11.0.

The title compound, $C_{10}H_{14}O_2$, synthesized by reduction of 4,7-dimethyl-2-benzofuran-1,3-dione, crystallizes with two independant molecules in the asymmetric unit, both showing an intramolecular O—H···O hydrogen bond. The crystal packing is stabilized by O—H···O hydrogen bonds.

Related literature

For the influence of chelation to (semi-)metals on the geometry of bifunctional alcohols, see: Klüfers & Vogler (2007). For a related compound, see: Betz *et al.* (2009).



Experimental

Crystal data

$C_{10}H_{14}O_2$
M_r = 166.21
Monoclinic, $P2_1$
a = 9.5821 (7) Å
b = 8.7184 (7) Å
c = 11.7522 (9) Å
β = 107.810 (4)°
V = 934.73 (12) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.08 mm^{-1}
T = 296 K
0.33 × 0.10 × 0.07 mm

Data collection

Bruker APEXII CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1997)
T_{min} = 0.974, T_{max} = 0.994
10452 measured reflections
2468 independent reflections
1296 reflections with $I > 2\sigma(I)$
R_{int} = 0.041

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.047
$wR(F^2)$ = 0.121
S = 0.99
2468 reflections
225 parameters
1 restraint
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.11 e Å^{-3}
$\Delta\rho_{min}$ = −0.12 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1···O2^{i}	0.82	1.89	2.706 (3)	174
O2—H2···O1	0.82	1.97	2.713 (4)	151
O3—H3···O4^{ii}	0.82	1.90	2.709 (4)	167
O4—H4···O3	0.82	1.98	2.717 (4)	150

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

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* (Farrugia, 1999) and *Mercury* (Macrae *et al.*, 2006); software used to prepare material for publication: *SHELXL97* and *PLATON* (Spek, 2009).

The authors are grateful to the Higher Education Commission of Pakistan for the X-ray analysis.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BT5136).

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supporting information

Acta Cryst. (2010). E**66**, o189 [doi:10.1107/S1600536809053513]

3,6-Dimethyl-*o*-phenylenedimethanol

Humaira Yasmeen Gondal, Muhammad Ali, Alain Krief and Muhammad Zia-ur-Rehman

S1. Comment

In continuation of our work regarding the synthesis of various hetrocycles, structure of (3,6-dimethylbenzene-1,2-diyl) dimethanol has been determined. Such diols may act as good ligands for the chelation of (semi-)metals (Klüfers & Vogler, 2007). Bond lengths and bond angles of the title molecule (Scheme 1; Fig. 1) are almost similar to those in the related molecules (Betz *et al.*, 2009).

Methyl groups at C7 & C10 are displaced by 0.71 (2)° and 0.85 (1)°, respectively, from the plane of the aromatic ring. Two independant asymmetric molecules exist in a unit cell and the benzylic oxygen of each molecule is involved in an intramolecular O—H···O hydrogen bond, forming a seven-membered hydrogen-bonded ring. Each molecule is centrosymmetrically linked to their adjacent ones through O—H···O hydrogen bonds (Table 1; Fig. 2).

S2. Experimental

A mixture of 4,7-dimethyl-2-benzofuran-1,3-dione (0.176 g; 1.0 mmole), lithium aluminium hydride (0.042; 1.1 mmole), diethyl ether (20 ml) and tetrahydrofuran (20 ml) was refluxed for 15 h. Reaction mixture was than cooled and quenched with ice cooled water followed by the addition of aqueous sodium hydroxide (15%) to make the contents alkaline. Resulting solid was filtered off and washed with ether. Filtrate was concentrated to obtain (3,6-dimethylbenzene-1,2-diyl) dimethanol followed by its purification on silica gel column eluted by 60% diethyl ether in pentane.

S3. Refinement

All H atoms were identified in a difference map and then were treated as riding (O—H = 0.82, C—H = 0.93 or 0.97 Å), with U_{iso}(H) = 1.2U_{eq}(C,O). In the absence of significant anomalous dispersion effects, Friedel pairs were merged.

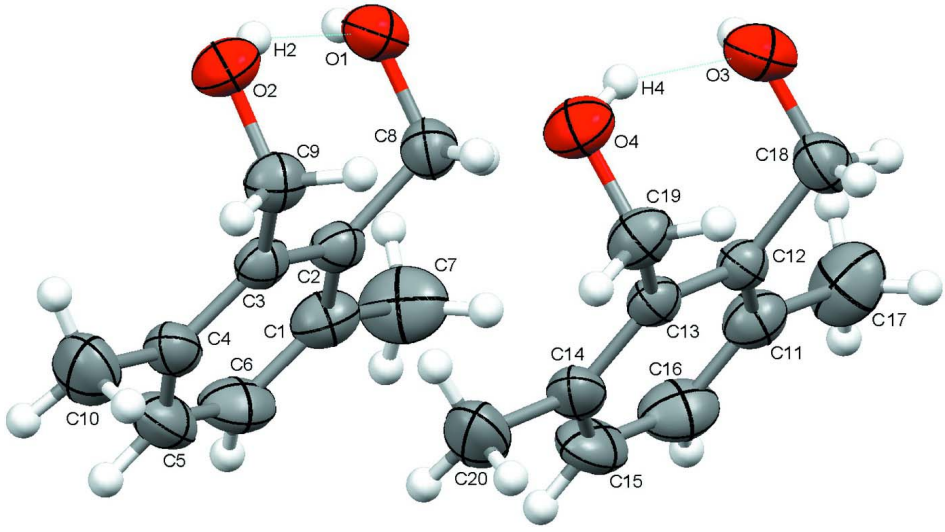

Figure 1

The molecular structure of (**I**), with displacement ellipsoids at the 50% probability level.

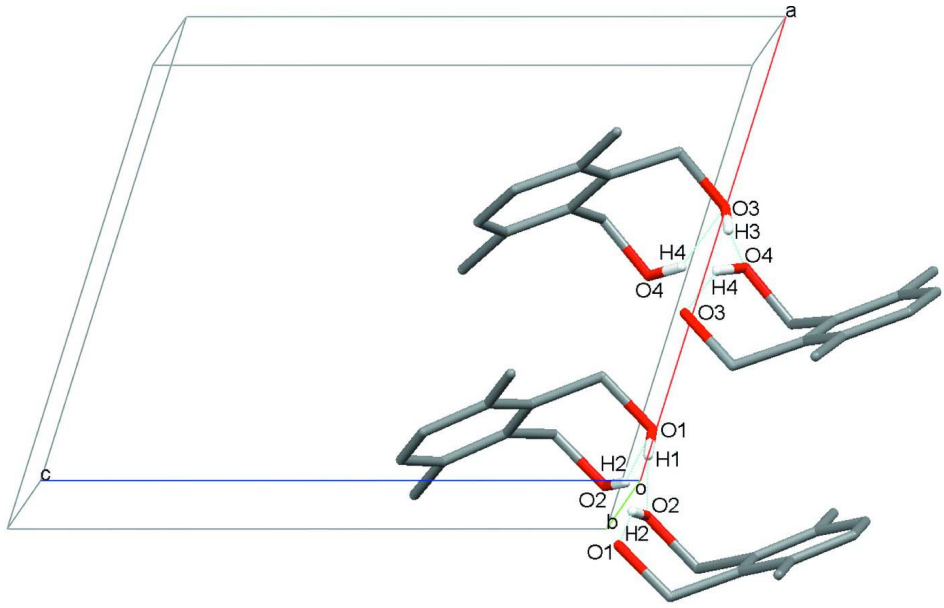

Figure 2

Perspective view of the three-dimensional crystal packing showing hydrogen-bonded interactions (dashed lines). H atoms not involved in hydrogen bonding have been omitted for clarity.

3,6-Dimethyl-*o*-phenylenedimethanol

Crystal data

$C_{10}H_{14}O_2$
M_r = 166.21
Monoclinic, $P2_1$
Hall symbol: P 2yb
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c = 11.7522 (9) Å
β = 107.810 (4)°
V = 934.73 (12) Å^3
Z = 4
F(000) = 360
D_x = 1.181 Mg m^{-3}

Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 1602 reflections
θ = 3.0–19.6°
μ = 0.08 mm^{-1}
T = 296 K
Needle, colorless
0.33 × 0.10 × 0.07 mm

Data collection

Bruker APEXII CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1997)
T_{min} = 0.974, T_{max} = 0.994
10452 measured reflections
2468 independent reflections
1296 reflections with $I > 2\sigma(I)$
R_{int} = 0.041
θ_{max} = 28.5°, θ_{min} = 2.2°
h = −7→12
k = −11→11
l = −15→15

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.047
$wR(F^2)$ = 0.121
S = 0.99
2468 reflections
225 parameters
1 restraint
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0538P)^2 + 0.0276P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ < 0.001
$\Delta\rho_{max}$ = 0.11 e Å^{-3}
$\Delta\rho_{min}$ = −0.12 e Å^{-3}

Special details

Geometry. All s.u.'s (except the s.u. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell s.u.'s are taken into account individually in the estimation of s.u.'s in distances, angles and torsion angles; correlations between s.u.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell s.u.'s is used for estimating s.u.'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 $F^2 > 2\sigma(F^2)$ 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 (Å²)

	x	y	z	U_{iso}*/U_{eq}
C1	0.1958 (4)	0.2892 (4)	0.2857 (3)	0.0643 (10)
C2	0.2068 (3)	0.4103 (4)	0.2113 (3)	0.0511 (8)
C3	0.1604 (3)	0.5579 (4)	0.2305 (2)	0.0492 (8)
C4	0.1010 (3)	0.5855 (4)	0.3226 (3)	0.0587 (9)
C5	0.0928 (4)	0.4638 (5)	0.3960 (3)	0.0776 (12)
H5	0.0555	0.4804	0.4593	0.093*
C6	0.1379 (4)	0.3208 (5)	0.3776 (3)	0.0747 (11)
H6	0.1297	0.2418	0.4283	0.090*
C7	0.2426 (5)	0.1270 (4)	0.2686 (4)	0.0982 (14)
H7A	0.2343	0.0635	0.3329	0.147*
H7B	0.3426	0.1276	0.2679	0.147*
H7C	0.1808	0.0872	0.1940	0.147*

C8	0.2641 (3)	0.3817 (4)	0.1068 (3)	0.0619 (9)
H8A	0.3412	0.4550	0.1094	0.074*
H8B	0.3063	0.2797	0.1137	0.074*
C9	0.1713 (3)	0.6851 (4)	0.1473 (3)	0.0590 (8)
H9A	0.1653	0.7829	0.1849	0.071*
H9B	0.2660	0.6798	0.1336	0.071*
C10	0.0458 (4)	0.7410 (5)	0.3464 (4)	0.0881 (12)
H10A	−0.0084	0.7303	0.4025	0.132*
H10B	−0.0169	0.7830	0.2730	0.132*
H10C	0.1275	0.8084	0.3788	0.132*
C11	0.7091 (4)	0.3069 (4)	0.2561 (3)	0.0623 (9)
C12	0.7047 (3)	0.4486 (3)	0.2009 (3)	0.0468 (8)
C13	0.6475 (3)	0.5778 (4)	0.2417 (2)	0.0492 (8)
C14	0.5941 (4)	0.5662 (5)	0.3388 (3)	0.0637 (9)
C15	0.6017 (4)	0.4238 (6)	0.3923 (3)	0.0825 (13)
H15	0.5667	0.4128	0.4575	0.099*
C16	0.6584 (4)	0.2998 (5)	0.3527 (3)	0.0823 (12)
H16	0.6630	0.2069	0.3926	0.099*
C17	0.7680 (5)	0.1632 (5)	0.2167 (4)	0.0967 (13)
H17A	0.7070	0.1350	0.1383	0.145*
H17B	0.7684	0.0817	0.2718	0.145*
H17C	0.8661	0.1812	0.2150	0.145*
C18	0.7569 (4)	0.4641 (4)	0.0932 (3)	0.0666 (10)
H18A	0.8277	0.5468	0.1065	0.080*
H18B	0.8060	0.3701	0.0830	0.080*
C19	0.6393 (4)	0.7281 (4)	0.1778 (3)	0.0647 (9)
H19A	0.6300	0.8108	0.2302	0.078*
H19B	0.7293	0.7441	0.1578	0.078*
C20	0.5287 (4)	0.7007 (6)	0.3852 (3)	0.0961 (14)
H20A	0.6055	0.7695	0.4271	0.144*
H20B	0.4777	0.6646	0.4388	0.144*
H20C	0.4614	0.7536	0.3195	0.144*
O1	0.1514 (2)	0.3950 (3)	−0.00537 (16)	0.0669 (7)
H1	0.0877	0.3306	−0.0091	0.100*
O2	0.0586 (2)	0.6779 (3)	0.03506 (18)	0.0690 (7)
H2	0.0557	0.5913	0.0072	0.103*
O3	0.6404 (3)	0.4941 (3)	−0.01344 (18)	0.0737 (7)
H3	0.5828	0.4219	−0.0275	0.110*
O4	0.5173 (2)	0.7319 (3)	0.07073 (19)	0.0743 (7)
H4	0.5311	0.6707	0.0223	0.111*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.069 (2)	0.057 (2)	0.059 (2)	−0.0083 (18)	0.0079 (18)	0.0049 (17)
C2	0.0445 (17)	0.059 (2)	0.0453 (16)	−0.0068 (16)	0.0071 (14)	−0.0018 (15)
C3	0.0408 (17)	0.055 (2)	0.0472 (16)	−0.0070 (15)	0.0069 (14)	−0.0022 (15)
C4	0.0525 (19)	0.074 (2)	0.0494 (17)	−0.0070 (17)	0.0154 (15)	−0.0104 (19)

C5	0.076 (3)	0.110 (4)	0.054 (2)	−0.017 (2)	0.031 (2)	−0.009 (2)
C6	0.088 (3)	0.084 (3)	0.052 (2)	−0.018 (2)	0.0213 (19)	0.012 (2)
C7	0.127 (4)	0.061 (3)	0.099 (3)	−0.002 (2)	0.024 (3)	0.007 (2)
C8	0.056 (2)	0.069 (2)	0.0629 (19)	0.0007 (18)	0.0216 (17)	−0.0039 (18)
C9	0.0588 (19)	0.056 (2)	0.0604 (18)	−0.0109 (16)	0.0156 (16)	−0.0021 (16)
C10	0.088 (3)	0.091 (3)	0.089 (3)	0.003 (2)	0.033 (2)	−0.026 (2)
C11	0.060 (2)	0.058 (2)	0.063 (2)	−0.0066 (17)	0.0096 (17)	0.0018 (18)
C12	0.0415 (17)	0.051 (2)	0.0468 (16)	−0.0064 (14)	0.0112 (14)	−0.0044 (14)
C13	0.0426 (17)	0.056 (2)	0.0446 (16)	−0.0077 (15)	0.0077 (14)	−0.0071 (15)
C14	0.054 (2)	0.086 (3)	0.0487 (17)	−0.007 (2)	0.0122 (16)	−0.017 (2)
C15	0.084 (3)	0.119 (4)	0.051 (2)	−0.019 (3)	0.030 (2)	0.012 (2)
C16	0.094 (3)	0.077 (3)	0.069 (2)	−0.016 (2)	0.016 (2)	0.018 (2)
C17	0.099 (3)	0.060 (3)	0.119 (3)	0.009 (2)	0.016 (2)	−0.006 (2)
C18	0.061 (2)	0.081 (3)	0.0633 (19)	−0.0088 (19)	0.0273 (18)	−0.0105 (18)
C19	0.062 (2)	0.057 (2)	0.067 (2)	−0.0059 (17)	0.0078 (17)	−0.0033 (17)
C20	0.079 (3)	0.131 (4)	0.078 (2)	0.002 (3)	0.024 (2)	−0.039 (3)
O1	0.0763 (16)	0.0749 (17)	0.0522 (12)	−0.0081 (13)	0.0237 (12)	−0.0041 (11)
O2	0.0688 (14)	0.0659 (15)	0.0631 (13)	0.0045 (12)	0.0067 (11)	0.0110 (12)
O3	0.0899 (19)	0.0789 (17)	0.0551 (13)	−0.0164 (14)	0.0266 (13)	−0.0036 (12)
O4	0.0759 (15)	0.0693 (16)	0.0693 (14)	0.0096 (12)	0.0097 (13)	0.0111 (12)

Geometric parameters (Å, º)

C1—C6	1.384 (5)	C11—C17	1.504 (5)
C1—C2	1.396 (5)	C12—C13	1.400 (4)
C1—C7	1.515 (5)	C12—C18	1.503 (4)
C2—C3	1.402 (5)	C13—C14	1.390 (5)
C2—C8	1.512 (4)	C13—C19	1.500 (5)
C3—C4	1.389 (4)	C14—C15	1.384 (6)
C3—C9	1.503 (4)	C14—C20	1.508 (6)
C4—C5	1.385 (5)	C15—C16	1.355 (6)
C4—C10	1.512 (5)	C15—H15	0.9300
C5—C6	1.358 (6)	C16—H16	0.9300
C5—H5	0.9300	C17—H17A	0.9600
C6—H6	0.9300	C17—H17B	0.9600
C7—H7A	0.9600	C17—H17C	0.9600
C7—H7B	0.9600	C18—O3	1.425 (4)
C7—H7C	0.9600	C18—H18A	0.9700
C8—O1	1.431 (3)	C18—H18B	0.9700
C8—H8A	0.9700	C19—O4	1.432 (3)
C8—H8B	0.9700	C19—H19A	0.9700
C9—O2	1.428 (3)	C19—H19B	0.9700
C9—H9A	0.9700	C20—H20A	0.9600
C9—H9B	0.9700	C20—H20B	0.9600
C10—H10A	0.9600	C20—H20C	0.9600
C10—H10B	0.9600	O1—H1	0.8200
C10—H10C	0.9600	O2—H2	0.8200
C11—C16	1.366 (5)	O3—H3	0.8200

C11—C12	1.391 (4)	O4—H4	0.8200
C6—C1—C2	117.6 (3)	C12—C11—C17	123.8 (3)
C6—C1—C7	119.7 (3)	C11—C12—C13	120.9 (3)
C2—C1—C7	122.7 (3)	C11—C12—C18	120.2 (3)
C1—C2—C3	120.3 (3)	C13—C12—C18	118.8 (3)
C1—C2—C8	120.1 (3)	C14—C13—C12	120.2 (3)
C3—C2—C8	119.6 (3)	C14—C13—C19	119.9 (3)
C4—C3—C2	120.7 (3)	C12—C13—C19	119.8 (3)
C4—C3—C9	120.4 (3)	C15—C14—C13	117.2 (3)
C2—C3—C9	119.0 (3)	C15—C14—C20	120.2 (3)
C5—C4—C3	117.9 (3)	C13—C14—C20	122.6 (4)
C5—C4—C10	118.8 (3)	C16—C15—C14	122.1 (3)
C3—C4—C10	123.3 (3)	C16—C15—H15	119.0
C6—C5—C4	121.5 (3)	C14—C15—H15	119.0
C6—C5—H5	119.2	C15—C16—C11	122.1 (4)
C4—C5—H5	119.2	C15—C16—H16	119.0
C5—C6—C1	122.0 (3)	C11—C16—H16	119.0
C5—C6—H6	119.0	C11—C17—H17A	109.5
C1—C6—H6	119.0	C11—C17—H17B	109.5
C1—C7—H7A	109.5	H17A—C17—H17B	109.5
C1—C7—H7B	109.5	C11—C17—H17C	109.5
H7A—C7—H7B	109.5	H17A—C17—H17C	109.5
C1—C7—H7C	109.5	H17B—C17—H17C	109.5
H7A—C7—H7C	109.5	O3—C18—C12	112.6 (3)
H7B—C7—H7C	109.5	O3—C18—H18A	109.1
O1—C8—C2	112.0 (3)	C12—C18—H18A	109.1
O1—C8—H8A	109.2	O3—C18—H18B	109.1
C2—C8—H8A	109.2	C12—C18—H18B	109.1
O1—C8—H8B	109.2	H18A—C18—H18B	107.8
C2—C8—H8B	109.2	O4—C19—C13	111.3 (2)
H8A—C8—H8B	107.9	O4—C19—H19A	109.4
O2—C9—C3	112.7 (2)	C13—C19—H19A	109.4
O2—C9—H9A	109.1	O4—C19—H19B	109.4
C3—C9—H9A	109.1	C13—C19—H19B	109.4
O2—C9—H9B	109.1	H19A—C19—H19B	108.0
C3—C9—H9B	109.1	C14—C20—H20A	109.5
H9A—C9—H9B	107.8	C14—C20—H20B	109.5
C4—C10—H10A	109.5	H20A—C20—H20B	109.5
C4—C10—H10B	109.5	C14—C20—H20C	109.5
H10A—C10—H10B	109.5	H20A—C20—H20C	109.5
C4—C10—H10C	109.5	H20B—C20—H20C	109.5
H10A—C10—H10C	109.5	C8—O1—H1	109.5
H10B—C10—H10C	109.5	C9—O2—H2	109.5
C16—C11—C12	117.4 (3)	C18—O3—H3	109.5
C16—C11—C17	118.7 (3)	C19—O4—H4	109.5
C6—C1—C2—C3	0.1 (4)	C16—C11—C12—C13	−1.4 (5)

C7—C1—C2—C3	179.4 (3)	C17—C11—C12—C13	179.6 (3)
C6—C1—C2—C8	−177.9 (3)	C16—C11—C12—C18	−179.2 (3)
C7—C1—C2—C8	1.4 (5)	C17—C11—C12—C18	1.8 (5)
C1—C2—C3—C4	−1.0 (4)	C11—C12—C13—C14	0.1 (4)
C8—C2—C3—C4	177.0 (3)	C18—C12—C13—C14	178.0 (3)
C1—C2—C3—C9	−178.9 (3)	C11—C12—C13—C19	−177.9 (3)
C8—C2—C3—C9	−0.9 (4)	C18—C12—C13—C19	0.0 (4)
C2—C3—C4—C5	1.6 (4)	C12—C13—C14—C15	0.6 (4)
C9—C3—C4—C5	179.5 (3)	C19—C13—C14—C15	178.6 (3)
C2—C3—C4—C10	−178.6 (3)	C12—C13—C14—C20	−178.9 (3)
C9—C3—C4—C10	−0.7 (5)	C19—C13—C14—C20	−0.9 (5)
C3—C4—C5—C6	−1.5 (5)	C13—C14—C15—C16	0.0 (5)
C10—C4—C5—C6	178.7 (4)	C20—C14—C15—C16	179.5 (4)
C4—C5—C6—C1	0.7 (6)	C14—C15—C16—C11	−1.3 (6)
C2—C1—C6—C5	0.0 (5)	C12—C11—C16—C15	2.0 (6)
C7—C1—C6—C5	−179.2 (4)	C17—C11—C16—C15	−179.0 (4)
C1—C2—C8—O1	109.7 (3)	C11—C12—C18—O3	110.9 (3)
C3—C2—C8—O1	−68.3 (4)	C13—C12—C18—O3	−67.0 (4)
C4—C3—C9—O2	−101.5 (3)	C14—C13—C19—O4	−99.6 (3)
C2—C3—C9—O2	76.5 (3)	C12—C13—C19—O4	78.4 (4)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1···O2^{i}	0.82	1.89	2.706 (3)	174
O2—H2···O1	0.82	1.97	2.713 (4)	151
O3—H3···O4^{ii}	0.82	1.90	2.709 (4)	167
O4—H4···O3	0.82	1.98	2.717 (4)	150

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