Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

1,2,3,4-Tetramethylcyclopent-2-ene-1,4-diol

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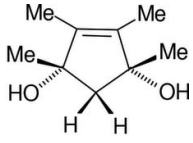
Received 9 July 2008; accepted 29 August 2008

Key indicators: single-crystal X-ray study; T = 133 K; mean σ(C–C) = 0.002 Å; R factor = 0.049; wR factor = 0.142; data-to-parameter ratio = 24.8.

The title compound, $C_9H_{16}O_2$, crystallizes with two molecules in the asymmetric unit. The structure displays intermolecular O—H···O hydrogen bonding.

Related literature

For related literature, see: Etter (1991); Brock & Duncan (1994); Fendrick *et al.* (1988).



Experimental

Crystal data

$C_9H_{16}O_2$
M_r = 156.22
Monoclinic, $P2_1/c$
a = 13.006 (3) Å
b = 10.5279 (16) Å
c = 13.892 (2) Å
β = 107.257 (10)°
V = 1816.6 (6) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 0.08 mm^{-1}
T = 133 (2) K
0.45 × 0.28 × 0.07 mm

Data collection

Bruker SMART CCD diffractometer
Absorption correction: none
20936 measured reflections
5532 independent reflections
3876 reflections with $I > 2\sigma(I)$
R_{int} = 0.048

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.048
$wR(F^2)$ = 0.142
S = 1.03
5532 reflections
223 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.41 e Å^{-3}
$\Delta\rho_{min}$ = −0.23 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O1—H01···O2^{i}	0.95 (2)	1.80 (2)	2.7438 (13)	174.7 (17)
O1′—H01′···O1	0.921 (18)	1.824 (18)	2.7345 (13)	169.3 (16)
O2—H02···O2′^{ii}	0.841 (19)	1.89 (2)	2.7263 (13)	173.0 (18)
O2′—H02′···O1′^{ii}	0.86 (2)	1.89 (2)	2.7333 (13)	166.1 (18)

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

Data collection: *SMART* (Bruker, 1997); cell refinement: *SAINT* (Bruker, 1997); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *XP5* in *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXL97*.

Financial support by the Otto-von-Guericke-Universität Magdeburg is gratefully acknowledged.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BT2745).

References

Brock, C. P. & Duncan, L. L. (1994). *Chem. Mater.* **6**, 1307–1312.
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Fendrick, C. M., Schertz, L. D., Day, V. W. & Marks, T. J. (1988). *Organometallics*, **7**, 1828–1838.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.

supporting information

Acta Cryst. (2008). E**64**, o1881 [doi:10.1107/S160053680802775X]

1,2,3,4-Tetramethylcyclopent-2-ene-1,4-diol

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S1. Comment

In the solid state, alcohols generally form hydrogen-bonded networks resulting in a variety of ring, chain, or helix structures (Brock & Duncan, 1994). The hitherto unknown title compound, 1,2,3,4-tetramethylcyclopen-2-ene-1,4-diol, was obtained in minor quantities (less than 5% isolated yield) in the form of colorless crystals during a preparation of 1,2,3,4-tetramethylcyclopentadiene according to the literature (Fendrick *et al.*, 1988). The structure of the title compound is shown in Figure 1. Dimensions are available in the archived CIF. Especially notable is the hydrogen-bond network in the crystal structure. As depicted in Figure 2, four molecules of 1,2,3,4-tetramethylcyclopen-2-ene-1,4-diol are connected *via* hydrogen-bonds to give cyclic tetramers. Further hydrogen-bonding between adjacent tetrameric units results in an extended hydrogen-bond network.

S2. Experimental

Crystals of the title compound were obtained as a minor by-product during the synthesis of 1,2,3,4-tetramethylcyclo-pentadiene according to the literature preparatio (Fendrick *et al.*, 1988).

S3. Refinement

H atoms bonded to C were refined with fixed individual displacement parameters [U(H) = 1.2 U_{eq}(C) or U(H) = 1.5 U_{eq}(C_{methyl})] using a riding model with C-H(methylen) = 0.99 Å or C-H(methyl) = 0.98Å, respectively. The H atoms bonded to O were refined isotropically.

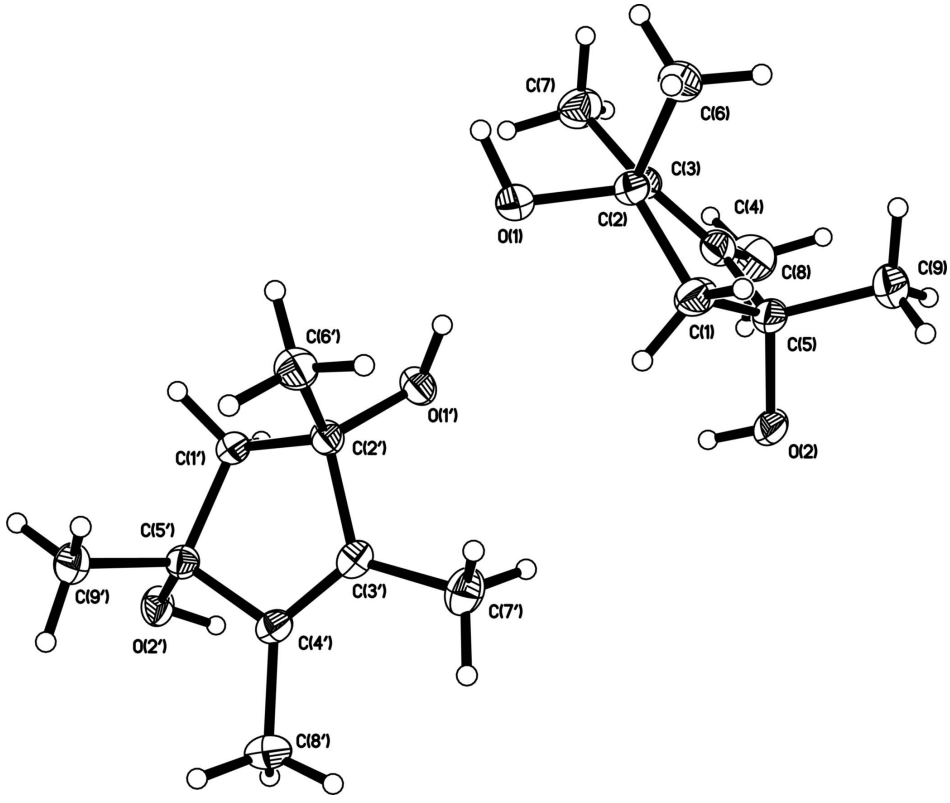

Figure 1

The molecule of the title compound in the crystal. Displacement ellipsoids represent 50% probability levels. H-Atom radii are arbitrary.

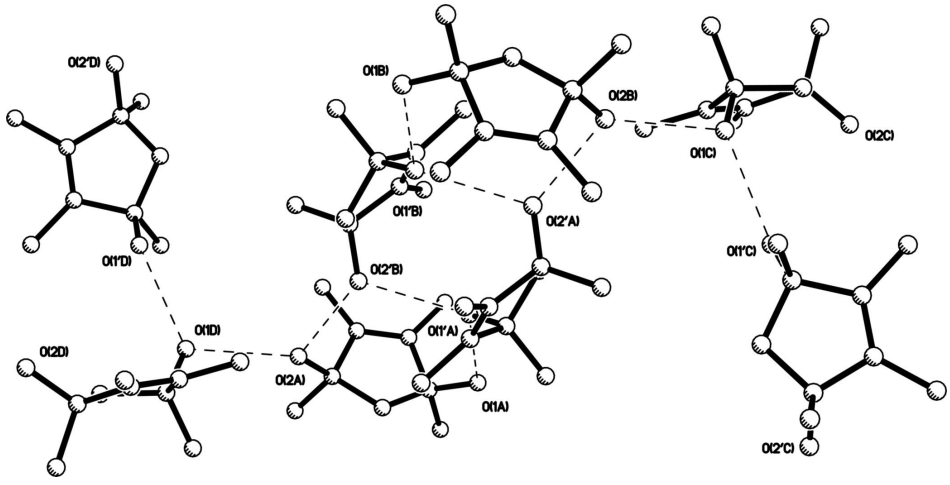

Figure 2

The hydrogen-bond network.

1,2,3,4-Tetramethylcyclopent-2-ene-1,4-diol

Crystal data

$C_9H_{16}O_2$
$M_r = 156.22$
Monoclinic, $P2_1/c$
Hall symbol: -P2ybc
$a = 13.006$ (3) Å
$b = 10.5279$ (16) Å
$c = 13.892$ (2) Å
$\beta = 107.257$ (10)°
$V = 1816.6$ (6) Å^3
$Z = 8$
$F(000) = 688$
$D_x = 1.142$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 5784 reflections
$\theta = 2.5$–30.0°
$\mu = 0.08$ mm^{-1}
$T = 133$ K
Plate, colourless
0.45 × 0.28 × 0.07 mm

Data collection

Bruker SMART CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
Detector resolution: 8.192 pixels mm^{-1}
ω–scans
20936 measured reflections
5532 independent reflections
3876 reflections with $I > 2\sigma(I)$
$R_{int} = 0.048$
$\theta_{max} = 30.5°$, $\theta_{min} = 1.6°$
$h = -18 \rightarrow 18$
$k = -14 \rightarrow 15$
$l = -19 \rightarrow 19$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.048$
$wR(F^2) = 0.142$
$S = 1.03$
5532 reflections
223 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
$w = 1/[\sigma^2(F_o^2) + (0.0812P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.002$
$\Delta\rho_{max} = 0.41$ e Å^{-3}
$\Delta\rho_{min} = -0.23$ 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}
O1	0.16035 (7)	0.34338 (9)	0.59028 (7)	0.0255 (2)
O2	0.16763 (8)	0.21564 (10)	0.28457 (7)	0.0330 (3)
H02	0.2279 (16)	0.2415 (16)	0.3207 (14)	0.048 (5)*
H01	0.1585 (14)	0.3212 (17)	0.6560 (15)	0.055 (5)*
C1	0.08579 (10)	0.28972 (13)	0.41367 (9)	0.0260 (3)

H1A	0.0100	0.3172	0.3852	0.031*
H1B	0.1335	0.3623	0.4115	0.031*
C2	0.10655 (9)	0.24265 (12)	0.52290 (8)	0.0210 (2)
C3	0.17851 (9)	0.12814 (12)	0.52756 (9)	0.0217 (2)
C4	0.17849 (10)	0.09054 (12)	0.43564 (10)	0.0242 (3)
C5	0.11007 (10)	0.17648 (13)	0.35382 (9)	0.0260 (3)
C6	0.00335 (10)	0.20778 (14)	0.54767 (10)	0.0290 (3)
H6C	0.0216	0.1724	0.6159	0.035*
H6B	−0.0368	0.1446	0.4992	0.035*
H6A	−0.0410	0.2840	0.5438	0.035*
C7	0.23648 (11)	0.06809 (14)	0.62666 (10)	0.0312 (3)
H7C	0.2703	−0.0112	0.6148	0.037*
H7B	0.1851	0.0499	0.6641	0.037*
H7A	0.2920	0.1263	0.6659	0.037*
C8	0.23380 (13)	−0.02192 (15)	0.40823 (12)	0.0397 (4)
H8C	0.2779	−0.0635	0.4698	0.048*
H8B	0.2800	0.0058	0.3678	0.048*
H8A	0.1799	−0.0819	0.3691	0.048*
C9	0.00891 (12)	0.11076 (17)	0.28879 (11)	0.0403 (4)
H9C	−0.0333	0.1707	0.2385	0.048*
H9B	−0.0343	0.0814	0.3315	0.048*
H9A	0.0293	0.0379	0.2545	0.048*
O1′	0.34071 (7)	0.44079 (8)	0.55499 (7)	0.0229 (2)
H01′	0.2803 (14)	0.4165 (17)	0.5720 (13)	0.042 (5)*
O2′	0.63799 (7)	0.68485 (9)	0.61022 (7)	0.0229 (2)
H02′	0.6360 (15)	0.6373 (17)	0.5589 (15)	0.053 (5)*
C1′	0.48169 (9)	0.58556 (11)	0.64713 (8)	0.0188 (2)
H1′1	0.5235	0.5089	0.6413	0.023*
H1′2	0.4843	0.5963	0.7186	0.023*
C2′	0.36462 (9)	0.57287 (11)	0.58020 (9)	0.0183 (2)
C3′	0.36529 (9)	0.64743 (11)	0.48658 (9)	0.0195 (2)
C4′	0.45363 (9)	0.71901 (11)	0.50268 (8)	0.0190 (2)
C5′	0.52810 (9)	0.70382 (11)	0.60928 (8)	0.0182 (2)
C6′	0.28221 (10)	0.62512 (13)	0.62934 (10)	0.0258 (3)
H6′C	0.2096	0.6166	0.5823	0.031*
H6′B	0.2974	0.7149	0.6461	0.031*
H6′A	0.2869	0.5772	0.6910	0.031*
C7′	0.27255 (10)	0.63672 (14)	0.39236 (10)	0.0279 (3)
H7′C	0.2824	0.6968	0.3420	0.033*
H7′B	0.2054	0.6563	0.4076	0.033*
H7′A	0.2691	0.5501	0.3658	0.033*
C8′	0.48398 (11)	0.80742 (12)	0.43083 (10)	0.0269 (3)
H8′C	0.4254	0.8108	0.3674	0.032*
H8′B	0.5497	0.7766	0.4178	0.032*
H8′A	0.4966	0.8926	0.4604	0.032*
C9′	0.52987 (11)	0.82140 (12)	0.67418 (10)	0.0251 (3)
H9′C	0.5805	0.8079	0.7414	0.030*
H9′B	0.4576	0.8364	0.6801	0.030*

H9′A	0.5526	0.8953	0.6427	0.030*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0289 (5)	0.0282 (5)	0.0219 (4)	−0.0072 (4)	0.0112 (4)	−0.0031 (4)
O2	0.0267 (5)	0.0570 (7)	0.0158 (4)	−0.0163 (5)	0.0073 (4)	−0.0031 (4)
C1	0.0231 (6)	0.0341 (7)	0.0202 (6)	0.0010 (5)	0.0056 (5)	0.0049 (5)
C2	0.0199 (6)	0.0263 (6)	0.0171 (5)	−0.0033 (5)	0.0058 (4)	0.0005 (4)
C3	0.0188 (6)	0.0260 (6)	0.0205 (6)	−0.0037 (5)	0.0061 (5)	0.0017 (5)
C4	0.0226 (6)	0.0274 (6)	0.0243 (6)	−0.0055 (5)	0.0095 (5)	−0.0036 (5)
C5	0.0208 (6)	0.0402 (7)	0.0173 (6)	−0.0091 (5)	0.0061 (5)	−0.0010 (5)
C6	0.0216 (6)	0.0397 (8)	0.0278 (7)	−0.0046 (5)	0.0106 (5)	−0.0011 (5)
C7	0.0316 (7)	0.0343 (7)	0.0265 (7)	0.0029 (6)	0.0067 (6)	0.0063 (6)
C8	0.0442 (9)	0.0363 (8)	0.0449 (9)	0.0000 (7)	0.0229 (7)	−0.0084 (7)
C9	0.0297 (7)	0.0629 (11)	0.0264 (7)	−0.0213 (7)	0.0055 (6)	−0.0049 (7)
O1′	0.0221 (4)	0.0214 (4)	0.0278 (5)	−0.0045 (3)	0.0114 (4)	−0.0053 (3)
O2′	0.0167 (4)	0.0300 (5)	0.0219 (4)	−0.0034 (3)	0.0057 (3)	−0.0059 (4)
C1′	0.0199 (5)	0.0204 (5)	0.0160 (5)	−0.0008 (4)	0.0053 (4)	0.0006 (4)
C2′	0.0185 (5)	0.0182 (5)	0.0193 (5)	−0.0014 (4)	0.0074 (4)	−0.0025 (4)
C3′	0.0204 (5)	0.0211 (6)	0.0166 (5)	0.0036 (4)	0.0049 (4)	−0.0002 (4)
C4′	0.0227 (6)	0.0192 (5)	0.0161 (5)	0.0025 (4)	0.0071 (4)	0.0009 (4)
C5′	0.0171 (5)	0.0206 (6)	0.0175 (5)	−0.0010 (4)	0.0062 (4)	−0.0009 (4)
C6′	0.0249 (6)	0.0274 (6)	0.0288 (6)	−0.0009 (5)	0.0138 (5)	−0.0038 (5)
C7′	0.0250 (6)	0.0323 (7)	0.0215 (6)	0.0025 (5)	−0.0006 (5)	0.0001 (5)
C8′	0.0320 (7)	0.0270 (6)	0.0241 (6)	0.0014 (5)	0.0119 (5)	0.0067 (5)
C9′	0.0301 (6)	0.0237 (6)	0.0230 (6)	−0.0028 (5)	0.0101 (5)	−0.0054 (5)

Geometric parameters (Å, º)

O1—C2	1.4498 (14)	O1′—C2′	1.4451 (14)
O1—H01	0.95 (2)	O1′—H01′	0.921 (18)
O2—C5	1.4434 (15)	O2′—C5′	1.4394 (14)
O2—H02	0.841 (19)	O2′—H02′	0.86 (2)
C1—C5	1.5388 (19)	C1′—C2′	1.5365 (16)
C1—C2	1.5421 (17)	C1′—C5′	1.5425 (16)
C1—H1A	0.9900	C1′—H1′1	0.9900
C1—H1B	0.9900	C1′—H1′2	0.9900
C2—C3	1.5157 (18)	C2′—C3′	1.5214 (16)
C2—C6	1.5259 (17)	C2′—C6′	1.5334 (17)
C3—C4	1.3369 (17)	C3′—C4′	1.3362 (17)
C3—C7	1.4992 (17)	C3′—C7′	1.4981 (17)
C4—C8	1.492 (2)	C4′—C8′	1.5007 (17)
C4—C5	1.5174 (19)	C4′—C5′	1.5184 (16)
C5—C9	1.5233 (18)	C5′—C9′	1.5275 (16)
C6—H6C	0.9800	C6′—H6′C	0.9800
C6—H6B	0.9800	C6′—H6′B	0.9800
C6—H6A	0.9800	C6′—H6′A	0.9800

C7—H7C	0.9800	C7′—H7′C	0.9800
C7—H7B	0.9800	C7′—H7′B	0.9800
C7—H7A	0.9800	C7′—H7′A	0.9800
C8—H8C	0.9800	C8′—H8′C	0.9800
C8—H8B	0.9800	C8′—H8′B	0.9800
C8—H8A	0.9800	C8′—H8′A	0.9800
C9—H9C	0.9800	C9′—H9′C	0.9800
C9—H9B	0.9800	C9′—H9′B	0.9800
C9—H9A	0.9800	C9′—H9′A	0.9800
C2—O1—H01	107.2 (11)	C2′—O1′—H01′	110.1 (11)
C5—O2—H02	105.7 (13)	C5′—O2′—H02′	106.6 (13)
C5—C1—C2	106.18 (10)	C2′—C1′—C5′	106.36 (9)
C5—C1—H1A	110.5	C2′—C1′—H1′1	110.5
C2—C1—H1A	110.5	C5′—C1′—H1′1	110.5
C5—C1—H1B	110.5	C2′—C1′—H1′2	110.5
C2—C1—H1B	110.5	C5′—C1′—H1′2	110.5
H1A—C1—H1B	108.7	H1′1—C1′—H1′2	108.6
O1—C2—C3	112.37 (10)	O1′—C2′—C3′	110.16 (9)
O1—C2—C6	108.58 (10)	O1′—C2′—C6′	108.94 (10)
C3—C2—C6	111.86 (10)	C3′—C2′—C6′	112.18 (10)
O1—C2—C1	108.08 (10)	O1′—C2′—C1′	109.49 (9)
C3—C2—C1	102.90 (10)	C3′—C2′—C1′	102.50 (9)
C6—C2—C1	112.97 (10)	C6′—C2′—C1′	113.42 (10)
C4—C3—C7	127.58 (12)	C4′—C3′—C7′	128.18 (11)
C4—C3—C2	111.69 (11)	C4′—C3′—C2′	111.76 (10)
C7—C3—C2	120.70 (11)	C7′—C3′—C2′	120.05 (11)
C3—C4—C8	127.96 (13)	C3′—C4′—C8′	128.40 (11)
C3—C4—C5	111.89 (11)	C3′—C4′—C5′	111.83 (10)
C8—C4—C5	120.13 (12)	C8′—C4′—C5′	119.76 (10)
O2—C5—C4	111.39 (11)	O2′—C5′—C4′	111.58 (9)
O2—C5—C9	105.18 (10)	O2′—C5′—C9′	105.43 (9)
C4—C5—C9	112.63 (12)	C4′—C5′—C9′	112.58 (10)
O2—C5—C1	111.66 (11)	O2′—C5′—C1′	111.89 (9)
C4—C5—C1	103.06 (10)	C4′—C5′—C1′	102.51 (9)
C9—C5—C1	113.13 (12)	C9′—C5′—C1′	113.06 (10)
C2—C6—H6C	109.5	C2′—C6′—H6′C	109.5
C2—C6—H6B	109.5	C2′—C6′—H6′B	109.5
H6C—C6—H6B	109.5	H6′C—C6′—H6′B	109.5
C2—C6—H6A	109.5	C2′—C6′—H6′A	109.5
H6C—C6—H6A	109.5	H6′C—C6′—H6′A	109.5
H6B—C6—H6A	109.5	H6′B—C6′—H6′A	109.5
C3—C7—H7C	109.5	C3′—C7′—H7′C	109.5
C3—C7—H7B	109.5	C3′—C7′—H7′B	109.5
H7C—C7—H7B	109.5	H7′C—C7′—H7′B	109.5
C3—C7—H7A	109.5	C3′—C7′—H7′A	109.5
H7C—C7—H7A	109.5	H7′C—C7′—H7′A	109.5
H7B—C7—H7A	109.5	H7′B—C7′—H7′A	109.5

C4—C8—H8C	109.5	C4′—C8′—H8′C	109.5
C4—C8—H8B	109.5	C4′—C8′—H8′B	109.5
H8C—C8—H8B	109.5	H8′C—C8′—H8′B	109.5
C4—C8—H8A	109.5	C4′—C8′—H8′A	109.5
H8C—C8—H8A	109.5	H8′C—C8′—H8′A	109.5
H8B—C8—H8A	109.5	H8′B—C8′—H8′A	109.5
C5—C9—H9C	109.5	C5′—C9′—H9′C	109.5
C5—C9—H9B	109.5	C5′—C9′—H9′B	109.5
H9C—C9—H9B	109.5	H9′C—C9′—H9′B	109.5
C5—C9—H9A	109.5	C5′—C9′—H9′A	109.5
H9C—C9—H9A	109.5	H9′C—C9′—H9′A	109.5
H9B—C9—H9A	109.5	H9′B—C9′—H9′A	109.5
C5—C1—C2—O1	139.28 (10)	C5′—C1′—C2′—O1′	138.54 (9)
C5—C1—C2—C3	20.24 (12)	C5′—C1′—C2′—C3′	21.61 (11)
C5—C1—C2—C6	−100.55 (12)	C5′—C1′—C2′—C6′	−99.55 (11)
O1—C2—C3—C4	−130.31 (11)	O1′—C2′—C3′—C4′	−130.65 (11)
C6—C2—C3—C4	107.25 (12)	C6′—C2′—C3′—C4′	107.81 (12)
C1—C2—C3—C4	−14.31 (13)	C1′—C2′—C3′—C4′	−14.19 (13)
O1—C2—C3—C7	51.62 (15)	O1′—C2′—C3′—C7′	50.55 (14)
C6—C2—C3—C7	−70.82 (14)	C6′—C2′—C3′—C7′	−70.99 (14)
C1—C2—C3—C7	167.63 (11)	C1′—C2′—C3′—C7′	167.00 (10)
C7—C3—C4—C8	1.6 (2)	C7′—C3′—C4′—C8′	−0.3 (2)
C2—C3—C4—C8	−176.35 (12)	C2′—C3′—C4′—C8′	−178.94 (11)
C7—C3—C4—C5	−179.83 (12)	C7′—C3′—C4′—C5′	179.35 (11)
C2—C3—C4—C5	2.27 (15)	C2′—C3′—C4′—C5′	0.67 (14)
C3—C4—C5—O2	130.67 (12)	C3′—C4′—C5′—O2′	133.00 (10)
C8—C4—C5—O2	−50.59 (16)	C8′—C4′—C5′—O2′	−47.36 (14)
C3—C4—C5—C9	−111.43 (13)	C3′—C4′—C5′—C9′	−108.69 (12)
C8—C4—C5—C9	67.31 (16)	C8′—C4′—C5′—C9′	70.96 (14)
C3—C4—C5—C1	10.82 (14)	C3′—C4′—C5′—C1′	13.10 (13)
C8—C4—C5—C1	−170.44 (12)	C8′—C4′—C5′—C1′	−167.25 (10)
C2—C1—C5—O2	−138.72 (10)	C2′—C1′—C5′—O2′	−140.96 (9)
C2—C1—C5—C4	−19.06 (12)	C2′—C1′—C5′—C4′	−21.28 (11)
C2—C1—C5—C9	102.85 (12)	C2′—C1′—C5′—C9′	100.18 (11)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H01···O2^{i}	0.95 (2)	1.80 (2)	2.7438 (13)	174.7 (17)
O1′—H01′···O1	0.921 (18)	1.824 (18)	2.7345 (13)	169.3 (16)
O2—H02···O2′^{ii}	0.841 (19)	1.89 (2)	2.7263 (13)	173.0 (18)
O2′—H02′···O1′^{ii}	0.86 (2)	1.89 (2)	2.7333 (13)	166.1 (18)

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