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4α,6α-Dihydroxy-1β-methylsulfonyl-8α,9α-epoxy-2β,12-epoxymethano-β-dihydroagarofuran

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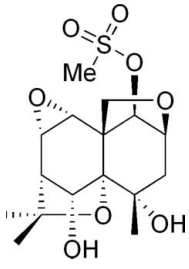
Key indicators: single-crystal X-ray study; T = 296 K; mean σ(C–C) = 0.004 Å; R factor = 0.039; wR factor = 0.085; data-to-parameter ratio = 13.6.

The title molecule, $C_{16}H_{24}O_8S$, is a dihydroagrofuran derivative and has a heteropolycyclic structure. One cyclohexane ring exhibits a chair conformation and the other a non-chair conformation. In the crystal structure there is an intermolecular C—H···O hydrogen-bonding interaction to stabilize the packing.

Related literature

For general background, see: Gao *et al.* (2007); Spivey *et al.* (2002).



Experimental

Crystal data

$C_{16}H_{24}O_8S$
M_r = 376.41
Orthorhombic, $P2_12_12_1$
a = 9.530 (3) Å
b = 10.228 (3) Å
c = 17.424 (5) Å
V = 1698.3 (9) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.23 mm^{-1}
T = 296 K
0.25 × 0.22 × 0.21 mm

Data collection

Bruker APEXII CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.944, T_{max} = 0.953
8175 measured reflections
3151 independent reflections
2633 reflections with $I > 2\sigma(I)$
R_{int} = 0.034

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.039
$wR(F^2)$ = 0.085
S = 1.06
3151 reflections
232 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.19 e Å^{-3}
$\Delta\rho_{min}$ = −0.20 e Å^{-3}
Absolute structure: Flack (1983), 1325 Friedel pairs
Flack parameter: 0.13 (9)

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

D—H···A	D—H	H···A	D···A	D—H···A
C16—H16C···O2^{i}	0.96	2.32	3.218 (4)	156

Symmetry code: (i) $x, y+1, z$.

Data collection: *APEX2* (Bruker, 2005); cell refinement: *SAINT* (Bruker, 2001); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: QM2023).

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supporting information

Acta Cryst. (2011). E**67**, o2496 [doi:10.1107/S1600536811034179]

4*α*,6*α*-Dihydroxy-1*β*-methylsulfonyl-8*α*,9*α*-epoxy-2*β*,12-epoxymethano-*β*-dihydroagarofuran

Jiwen Zhang, Peng Gao, Longbo Li and Wenjun Wu

S1. Comment

Dihydroagrofuran esters and their derivatives have been widely explored as insecticidal medicine (Gao *et al.* 2007; Spivey *et al.* 2002). As a result of our program of screening insecticidal activity constituents from plants of China, some insecticidal *β*-dihydroagrofuran sesquiterpene polyol esters were isolated from the root bark of Chinese bittersweet, *Celastrus angulatus* Max. In order to find a new synthetic insecticide, the /b-dihydroagrofuran sesquiterpene polyol ester was optimized as a lead compound and we obtained an intermediate compound $C_{16}H_{24}O_8S$ (I) and the synthesis and structure are reported here.

The title compound has a hetero-polycyclic structure. The 6-membering ring (C1–C6) exhibits a chair conformation. However, the other 6-membering ring (C1, C6–C10) exhibits neither a chair nor a boat conformation. The five atoms C1, C6, C8, C9 and C10 lie approximately in a plane, and the distance from C7 to the plane is 0.929 (3) Å.

The molecules of **I** crystalized in the $P2_12_12_1$ space group. In the crystal structure there is an intermolecular C—H···O hydrogen-bonding interaction (Table 1), which is helpful to the stabilization of the packing. Symmetry code: *x*, 1+*y*, *z*.

S2. Experimental

A mixture of dihydroagarofuran (3.34 g, 10 mmol) and methanesulfonyl chloride (3.5 mL, 44 mmol) in dry Pyridine (20 mL) was stirred over night at room temperature. When the reaction was completed, 2 mL methol was added to the reaction mixture to quench the reaction, then 50 mL water was added to the mixture and it was extracted with ethyl acetate. The ethyl acetate layer was washed with 50 mL of water, 15 mL of saturated sodium chloride and dried over anhydrous sodium sulfate and was separated on a silica gel column chromatography with a gradient of petroleum ether and ethyl acetate as eluent to yield 1.87 g of the title compound. The compound was then dissolved in THF, and colorless crystals were formed on slow evaporation at room temperature over one week.

S3. Refinement

All H atoms were placed in geometrically calculated positions and refined using a riding model with C—H = 0.93 Å and N—H = 0.86 Å and with U_{iso}(H) = 1.2U_{eq}(C, N).

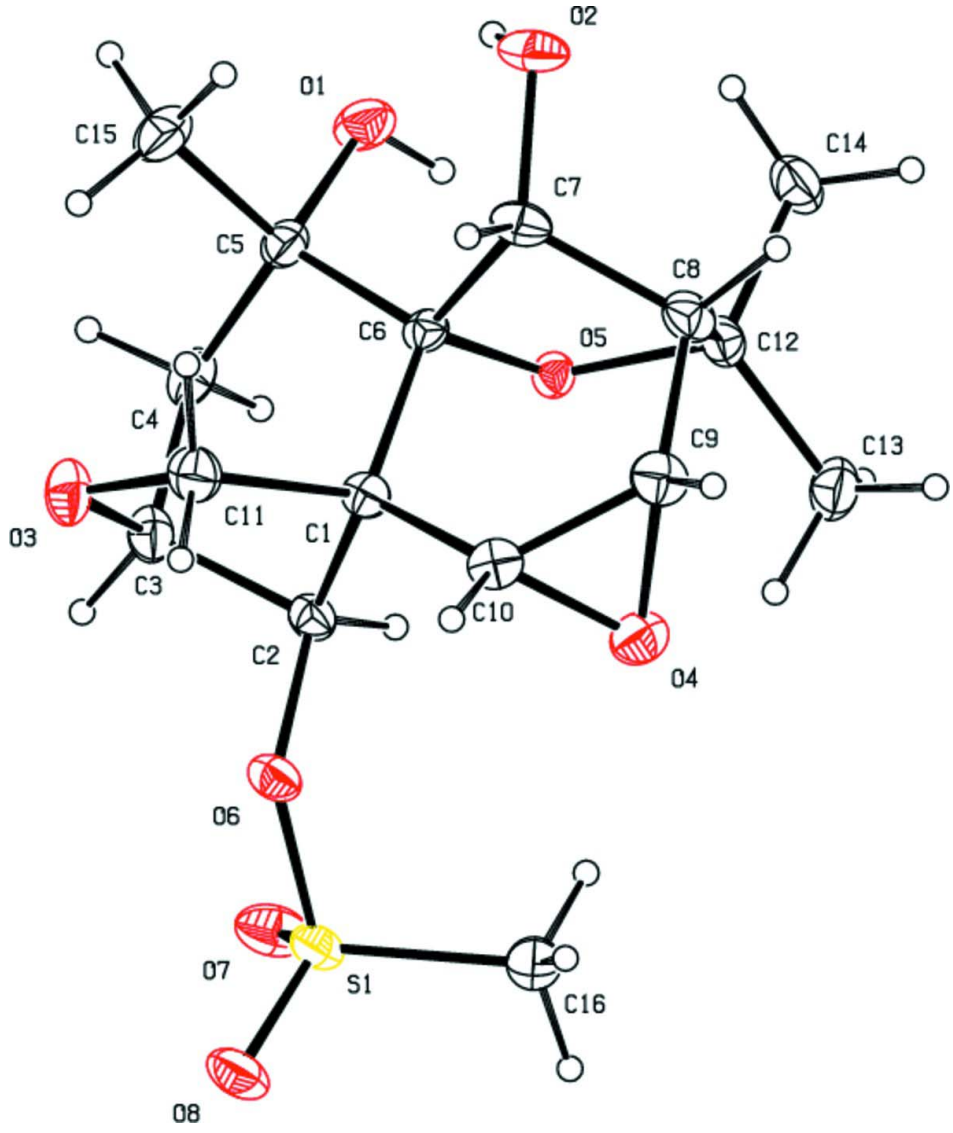

Figure 1

The molecular structure of the title compound with the atom numbering scheme. Displacement ellipsoids are drawn at the 30% probability level.

4*α*,6*α*-Dihydroxy-1*β*-methylsulfonyl-8*α*,9*α*-epoxy-2*β*,12-epoxymethano- *β*-dihydroagarofuran

Crystal data

$C_{16}H_{24}O_8S$
$M_r = 376.41$
Orthorhombic, $P2_12_12_1$
Hall symbol: P 2ac 2ab
$a = 9.530$ (3) Å
$b = 10.228$ (3) Å
$c = 17.424$ (5) Å
$V = 1698.3$ (9) Å^3
$Z = 4$
$F(000) = 800$
$D_x = 1.472$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 2687 reflections
$\theta = 2.3$–22.5°
$\mu = 0.23$ mm^{-1}
$T = 296$ K
Block, colorless
0.25 × 0.22 × 0.21 mm

Data collection

Bruker APEXII CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.944, T_{max} = 0.953
8175 measured reflections
3151 independent reflections
2633 reflections with $I > 2\sigma(I)$
R_{int} = 0.034
θ_{max} = 25.5°, θ_{min} = 2.3°
h = −11→7
k = −12→12
l = −21→20

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.039
$wR(F^2)$ = 0.085
S = 1.06
3151 reflections
232 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-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0384P)^2 + 0.135P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.19 e Å^{-3}
$\Delta\rho_{min}$ = −0.20 e Å^{-3}
Absolute structure: Flack (1983), 1325 Friedel pairs
Absolute structure parameter: 0.13 (9)

Special details

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

	x	*y*	*z*	U_{iso}*/U_{eq}
C1	0.8202 (3)	0.4554 (2)	0.91912 (13)	0.0328 (6)
C2	0.9087 (3)	0.5765 (2)	0.90120 (14)	0.0346 (6)
H2	0.8965	0.6079	0.8485	0.042*
C3	1.0539 (3)	0.5224 (3)	0.91630 (14)	0.0426 (7)
H3	1.1223	0.5932	0.9220	0.051*
C4	1.0957 (3)	0.4311 (3)	0.85095 (16)	0.0463 (7)
H4A	1.1915	0.4021	0.8590	0.056*
H4B	1.0930	0.4793	0.8030	0.056*
C5	1.0002 (3)	0.3113 (3)	0.84427 (14)	0.0390 (6)
C6	0.8443 (3)	0.3563 (2)	0.85189 (13)	0.0303 (6)
C7	0.7308 (3)	0.2501 (3)	0.85700 (16)	0.0423 (7)
H7	0.7108	0.2316	0.9111	0.051*
C8	0.6076 (3)	0.3248 (3)	0.82229 (14)	0.0422 (7)
H8	0.5317	0.2652	0.8077	0.051*
C9	0.5590 (3)	0.4210 (3)	0.88392 (16)	0.0444 (7)

H9	0.4683	0.4023	0.9081	0.053*
C10	0.6664 (3)	0.4827 (2)	0.93331 (15)	0.0388 (6)
H10	0.6393	0.4986	0.9867	0.047*
C11	0.8932 (3)	0.4131 (3)	0.99432 (15)	0.0477 (7)
H11A	0.8498	0.4555	1.0381	0.057*
H11B	0.8863	0.3192	1.0010	0.057*
C12	0.6735 (3)	0.3883 (3)	0.75151 (14)	0.0382 (6)
C13	0.6056 (3)	0.5133 (3)	0.72187 (17)	0.0538 (8)
H13A	0.6224	0.5830	0.7576	0.081*
H13B	0.5063	0.5000	0.7164	0.081*
H13C	0.6452	0.5356	0.6729	0.081*
C14	0.6857 (3)	0.2946 (3)	0.68275 (15)	0.0531 (8)
H14A	0.7452	0.3329	0.6444	0.080*
H14B	0.5943	0.2793	0.6615	0.080*
H14C	0.7254	0.2132	0.6995	0.080*
C15	1.0454 (4)	0.2017 (3)	0.89920 (18)	0.0582 (9)
H15A	0.9702	0.1399	0.9047	0.087*
H15B	1.0677	0.2384	0.9484	0.087*
H15C	1.1266	0.1582	0.8788	0.087*
C16	0.7165 (3)	0.8404 (3)	0.88369 (19)	0.0586 (8)
H16A	0.6393	0.8104	0.9143	0.088*
H16B	0.7223	0.7891	0.8377	0.088*
H16C	0.7025	0.9306	0.8705	0.088*
O1	1.0156 (2)	0.2516 (2)	0.76988 (11)	0.0515 (5)
H1	0.9832	0.3003	0.7370	0.077*
O2	0.7634 (3)	0.13165 (18)	0.81877 (13)	0.0598 (6)
H2A	0.8383	0.1396	0.7961	0.090*
O3	1.0372 (2)	0.4519 (2)	0.98764 (10)	0.0540 (6)
O4	0.59795 (19)	0.56021 (18)	0.87714 (11)	0.0489 (5)
O5	0.81435 (16)	0.42256 (15)	0.77981 (8)	0.0310 (4)
O6	0.87426 (18)	0.67549 (17)	0.95895 (9)	0.0407 (4)
O7	0.9879 (2)	0.85121 (19)	0.88633 (12)	0.0590 (6)
O8	0.8610 (2)	0.89333 (19)	1.00595 (11)	0.0558 (5)
S1	0.87153 (7)	0.82442 (6)	0.93543 (4)	0.04001 (18)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0404 (14)	0.0302 (13)	0.0278 (13)	−0.0028 (12)	0.0013 (11)	0.0036 (11)
C2	0.0408 (15)	0.0339 (14)	0.0293 (12)	−0.0035 (12)	−0.0021 (11)	−0.0016 (12)
C3	0.0402 (16)	0.0470 (17)	0.0406 (15)	−0.0038 (14)	−0.0085 (12)	0.0057 (14)
C4	0.0324 (15)	0.0525 (19)	0.0539 (17)	0.0080 (14)	−0.0023 (13)	0.0076 (15)
C5	0.0423 (15)	0.0369 (15)	0.0378 (14)	0.0094 (14)	−0.0046 (12)	0.0021 (13)
C6	0.0372 (15)	0.0265 (13)	0.0273 (12)	0.0023 (11)	−0.0007 (11)	0.0044 (10)
C7	0.0555 (17)	0.0296 (14)	0.0418 (16)	−0.0075 (14)	0.0082 (14)	−0.0024 (13)
C8	0.0367 (15)	0.0397 (16)	0.0502 (15)	−0.0110 (14)	0.0013 (12)	−0.0043 (14)
C9	0.0360 (14)	0.0453 (17)	0.0518 (16)	−0.0074 (13)	0.0099 (13)	−0.0013 (14)
C10	0.0430 (16)	0.0378 (15)	0.0355 (13)	−0.0011 (12)	0.0092 (13)	0.0052 (13)

C11	0.0603 (19)	0.0474 (17)	0.0353 (14)	0.0002 (15)	−0.0053 (14)	0.0032 (13)
C12	0.0309 (14)	0.0440 (17)	0.0396 (15)	−0.0021 (13)	−0.0042 (12)	−0.0073 (12)
C13	0.0502 (19)	0.064 (2)	0.0476 (16)	0.0101 (16)	−0.0130 (15)	0.0021 (16)
C14	0.0508 (17)	0.062 (2)	0.0463 (17)	−0.0026 (16)	−0.0084 (14)	−0.0189 (15)
C15	0.065 (2)	0.0468 (19)	0.063 (2)	0.0182 (16)	−0.0101 (16)	0.0088 (17)
C16	0.061 (2)	0.0390 (18)	0.076 (2)	−0.0010 (16)	−0.0203 (16)	0.0003 (17)
O1	0.0583 (13)	0.0482 (13)	0.0481 (12)	0.0175 (11)	0.0052 (11)	−0.0063 (10)
O2	0.0803 (16)	0.0256 (10)	0.0734 (15)	−0.0025 (11)	0.0017 (12)	−0.0087 (10)
O3	0.0535 (13)	0.0666 (14)	0.0420 (11)	0.0020 (11)	−0.0171 (10)	0.0074 (11)
O4	0.0431 (11)	0.0423 (12)	0.0614 (12)	0.0022 (10)	0.0045 (9)	0.0029 (10)
O5	0.0323 (9)	0.0312 (9)	0.0294 (8)	−0.0006 (8)	−0.0029 (7)	0.0035 (8)
O6	0.0544 (11)	0.0357 (10)	0.0318 (9)	−0.0046 (10)	−0.0022 (8)	−0.0062 (8)
O7	0.0615 (13)	0.0448 (13)	0.0707 (13)	−0.0125 (11)	0.0216 (11)	−0.0122 (11)
O8	0.0592 (13)	0.0517 (12)	0.0565 (12)	−0.0056 (11)	−0.0002 (11)	−0.0267 (10)
S1	0.0402 (4)	0.0345 (4)	0.0453 (4)	−0.0067 (3)	0.0010 (3)	−0.0108 (3)

Geometric parameters (Å, º)

C1—C10	1.512 (3)	C10—O4	1.419 (3)
C1—C2	1.531 (4)	C10—H10	0.9800
C1—C11	1.545 (3)	C11—O3	1.433 (3)
C1—C6	1.566 (3)	C11—H11A	0.9700
C2—O6	1.465 (3)	C11—H11B	0.9700
C2—C3	1.513 (4)	C12—O5	1.472 (3)
C2—H2	0.9800	C12—C13	1.523 (4)
C3—O3	1.446 (3)	C12—C14	1.538 (4)
C3—C4	1.525 (4)	C13—H13A	0.9600
C3—H3	0.9800	C13—H13B	0.9600
C4—C5	1.531 (4)	C13—H13C	0.9600
C4—H4A	0.9700	C14—H14A	0.9600
C4—H4B	0.9700	C14—H14B	0.9600
C5—O1	1.440 (3)	C14—H14C	0.9600
C5—C15	1.536 (4)	C15—H15A	0.9600
C5—C6	1.561 (3)	C15—H15B	0.9600
C6—O5	1.455 (3)	C15—H15C	0.9600
C6—C7	1.535 (4)	C16—S1	1.738 (3)
C7—O2	1.417 (3)	C16—H16A	0.9600
C7—C8	1.526 (4)	C16—H16B	0.9600
C7—H7	0.9800	C16—H16C	0.9600
C8—C9	1.528 (4)	O1—H1	0.8200
C8—C12	1.529 (4)	O2—H2A	0.8200
C8—H8	0.9800	O6—S1	1.5777 (19)
C9—O4	1.476 (3)	O7—S1	1.427 (2)
C9—C10	1.478 (4)	O8—S1	1.4201 (18)
C9—H9	0.9800		
C10—C1—C2	114.7 (2)	O4—C10—C9	61.24 (17)
C10—C1—C11	110.5 (2)	O4—C10—C1	115.9 (2)

C2—C1—C11	98.7 (2)	C9—C10—C1	119.8 (2)
C10—C1—C6	112.6 (2)	O4—C10—H10	116.2
C2—C1—C6	106.88 (19)	C9—C10—H10	116.2
C11—C1—C6	112.8 (2)	C1—C10—H10	116.2
O6—C2—C3	109.8 (2)	O3—C11—C1	106.6 (2)
O6—C2—C1	107.20 (19)	O3—C11—H11A	110.4
C3—C2—C1	99.9 (2)	C1—C11—H11A	110.4
O6—C2—H2	113.0	O3—C11—H11B	110.4
C3—C2—H2	113.0	C1—C11—H11B	110.4
C1—C2—H2	113.0	H11A—C11—H11B	108.6
O3—C3—C2	103.4 (2)	O5—C12—C13	107.5 (2)
O3—C3—C4	111.4 (2)	O5—C12—C8	101.85 (19)
C2—C3—C4	109.5 (2)	C13—C12—C8	117.1 (2)
O3—C3—H3	110.8	O5—C12—C14	109.9 (2)
C2—C3—H3	110.8	C13—C12—C14	106.9 (2)
C4—C3—H3	110.8	C8—C12—C14	113.3 (2)
C3—C4—C5	113.0 (2)	C12—C13—H13A	109.5
C3—C4—H4A	109.0	C12—C13—H13B	109.5
C5—C4—H4A	109.0	H13A—C13—H13B	109.5
C3—C4—H4B	109.0	C12—C13—H13C	109.5
C5—C4—H4B	109.0	H13A—C13—H13C	109.5
H4A—C4—H4B	107.8	H13B—C13—H13C	109.5
O1—C5—C4	110.3 (2)	C12—C14—H14A	109.5
O1—C5—C15	102.9 (2)	C12—C14—H14B	109.5
C4—C5—C15	111.7 (2)	H14A—C14—H14B	109.5
O1—C5—C6	107.38 (19)	C12—C14—H14C	109.5
C4—C5—C6	108.9 (2)	H14A—C14—H14C	109.5
C15—C5—C6	115.4 (2)	H14B—C14—H14C	109.5
O5—C6—C7	103.96 (19)	C5—C15—H15A	109.5
O5—C6—C5	104.51 (18)	C5—C15—H15B	109.5
C7—C6—C5	117.8 (2)	H15A—C15—H15B	109.5
O5—C6—C1	108.37 (17)	C5—C15—H15C	109.5
C7—C6—C1	108.1 (2)	H15A—C15—H15C	109.5
C5—C6—C1	113.21 (19)	H15B—C15—H15C	109.5
O2—C7—C8	114.2 (2)	S1—C16—H16A	109.5
O2—C7—C6	115.0 (2)	S1—C16—H16B	109.5
C8—C7—C6	99.5 (2)	H16A—C16—H16B	109.5
O2—C7—H7	109.2	S1—C16—H16C	109.5
C8—C7—H7	109.2	H16A—C16—H16C	109.5
C6—C7—H7	109.2	H16B—C16—H16C	109.5
C7—C8—C9	106.1 (2)	C5—O1—H1	109.5
C7—C8—C12	102.5 (2)	C7—O2—H2A	109.5
C9—C8—C12	114.7 (2)	C11—O3—C3	108.27 (19)
C7—C8—H8	111.0	C10—O4—C9	61.38 (17)
C9—C8—H8	111.0	C6—O5—C12	110.91 (17)
C12—C8—H8	111.0	C2—O6—S1	119.51 (14)
O4—C9—C10	57.38 (16)	O8—S1—O7	118.56 (12)
O4—C9—C8	119.2 (2)	O8—S1—O6	104.81 (11)

C10—C9—C8	118.3 (2)	O7—S1—O6	109.17 (11)
O4—C9—H9	116.3	O8—S1—C16	110.00 (15)
C10—C9—H9	116.3	O7—S1—C16	109.34 (14)
C8—C9—H9	116.3	O6—S1—C16	103.88 (12)
C10—C1—C2—O6	48.0 (3)	O2—C7—C8—C12	−77.3 (3)
C11—C1—C2—O6	−69.4 (2)	C6—C7—C8—C12	45.7 (2)
C6—C1—C2—O6	173.55 (17)	C7—C8—C9—O4	102.8 (3)
C10—C1—C2—C3	162.4 (2)	C12—C8—C9—O4	−9.5 (3)
C11—C1—C2—C3	45.1 (2)	C7—C8—C9—C10	36.4 (3)
C6—C1—C2—C3	−72.0 (2)	C12—C8—C9—C10	−76.0 (3)
O6—C2—C3—O3	67.6 (2)	C8—C9—C10—O4	108.3 (3)
C1—C2—C3—O3	−44.9 (2)	O4—C9—C10—C1	−105.0 (3)
O6—C2—C3—C4	−173.6 (2)	C8—C9—C10—C1	3.3 (4)
C1—C2—C3—C4	74.0 (2)	C2—C1—C10—O4	50.3 (3)
O3—C3—C4—C5	50.7 (3)	C11—C1—C10—O4	160.8 (2)
C2—C3—C4—C5	−63.0 (3)	C6—C1—C10—O4	−72.2 (3)
C3—C4—C5—O1	162.3 (2)	C2—C1—C10—C9	120.5 (3)
C3—C4—C5—C15	−84.0 (3)	C11—C1—C10—C9	−129.0 (3)
C3—C4—C5—C6	44.7 (3)	C6—C1—C10—C9	−2.0 (3)
O1—C5—C6—O5	−46.7 (2)	C10—C1—C11—O3	−151.7 (2)
C4—C5—C6—O5	72.7 (2)	C2—C1—C11—O3	−31.1 (3)
C15—C5—C6—O5	−160.7 (2)	C6—C1—C11—O3	81.4 (3)
O1—C5—C6—C7	68.1 (3)	C7—C8—C12—O5	−37.4 (2)
C4—C5—C6—C7	−172.5 (2)	C9—C8—C12—O5	77.1 (2)
C15—C5—C6—C7	−46.0 (3)	C7—C8—C12—C13	−154.3 (2)
O1—C5—C6—C1	−164.40 (19)	C9—C8—C12—C13	−39.8 (3)
C4—C5—C6—C1	−45.0 (3)	C7—C8—C12—C14	80.6 (2)
C15—C5—C6—C1	81.6 (3)	C9—C8—C12—C14	−165.0 (2)
C10—C1—C6—O5	73.0 (2)	C1—C11—O3—C3	3.9 (3)
C2—C1—C6—O5	−53.8 (2)	C2—C3—O3—C11	25.7 (3)
C11—C1—C6—O5	−161.2 (2)	C4—C3—O3—C11	−91.7 (3)
C10—C1—C6—C7	−39.1 (3)	C1—C10—O4—C9	111.3 (3)
C2—C1—C6—C7	−165.9 (2)	C8—C9—O4—C10	−106.7 (3)
C11—C1—C6—C7	86.7 (3)	C7—C6—O5—C12	14.6 (2)
C10—C1—C6—C5	−171.5 (2)	C5—C6—O5—C12	138.72 (19)
C2—C1—C6—C5	61.7 (2)	C1—C6—O5—C12	−100.3 (2)
C11—C1—C6—C5	−45.7 (3)	C13—C12—O5—C6	137.7 (2)
O5—C6—C7—O2	85.7 (3)	C8—C12—O5—C6	14.1 (2)
C5—C6—C7—O2	−29.4 (3)	C14—C12—O5—C6	−106.2 (2)
C1—C6—C7—O2	−159.3 (2)	C3—C2—O6—S1	107.6 (2)
O5—C6—C7—C8	−36.8 (2)	C1—C2—O6—S1	−144.83 (16)
C5—C6—C7—C8	−151.9 (2)	C2—O6—S1—O8	−169.57 (16)
C1—C6—C7—C8	78.2 (2)	C2—O6—S1—O7	−41.58 (19)
O2—C7—C8—C9	162.0 (2)	C2—O6—S1—C16	75.0 (2)
C6—C7—C8—C9	−74.9 (2)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C16—H16*C*···O2^{i}	0.96	2.32	3.218 (4)	156

Symmetry code: (i) *x*, *y*+1, *z*.