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Bis(3-deoxy-1,2-O-isopropylidenea-D-glucofuranos-3-yl) disulfide

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Key indicators: single-crystal X-ray study; T = 293 K; mean σ (C–C) = 0.002 Å; R factor = 0.029; wR factor = 0.066; data-to-parameter ratio = 18.4.

The title compound, $C_{18}H_{30}O_{10}S_2$, was prepared as a part of a project aimed at the synthesis of potential gelators of organic solvents. In the crystalline state, it forms hydrogen-bonded chains.

Related literature

For low-molecular-mass organogelators see: Terech & Weiss (1997); Luboradzki et al. (2005). For related literature, see: Risbood et al. (1981).



a = 8.7266 (1) Å

b = 14.4778 (4) Å

c = 17.8606 (5) Å

Experimental

Crystal data C18H30O10S2 $M_r = 470.54$ Orthorhombic, P212121 V = 2256.54 (9) Å³ 7 - 4Mo $K\alpha$ radiation

Data collection

Nonius KappaCCD diffractometer Absorption correction: none 22012 measured reflections

Refinement

 $R[F^2 > 2\sigma(F^2)] = 0.029$ $\Delta \rho_{\text{max}} = 0.21 \text{ e} \text{ Å}^{-3}$ $\Delta \rho_{\rm min} = -0.21 \text{ e } \text{\AA}^{-3}$ $wR(F^2) = 0.066$ S = 1.09Absolute structure: Flack (1983), 5134 reflections 279 parameters Flack parameter: 0.02 (5) H-atom parameters constrained

Table 1

Hydrogen-bond geometry (Å, °).

$D - H \cdots A$	D-H	$H \cdot \cdot \cdot A$	$D \cdots A$	$D - \mathbf{H} \cdot \cdot \cdot A$
$O4-H4O\cdots O10^{i}$	0.82	1.94	2.7249 (18)	159
$O5-H5O\cdots O3^{i}$	0.82	1.99	2.8055 (18)	176
$O9-H9O\cdots O5^{ii}$	0.82	2.05	2.8338 (17)	159
$O10-H10O\cdots O9^{iii}$	0.82	2.04	2.8305 (18)	163

Symmetry codes: (i) x - 1, y, z; (ii) x + 1, y, z; (iii) $x + \frac{1}{2}$, $-y + \frac{3}{2}$, -z + 1.

Data collection: COLLECT (Nonius, 1997); cell refinement: DENZO and SCALEPACK (Otwinowski & Minor, 1997); data reduction: DENZO and SCALEPACK; program(s) used to solve structure: SHELXS97 (Sheldrick, 1997); program(s) used to refine structure: SHELXL97 (Sheldrick, 1997); molecular graphics: ORTEP-3 (Farrugia, 1997); software used to prepare material for publication: SHELXL97 and PLATON (Spek, 2003).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: AT2343).

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 $\mu = 0.29 \text{ mm}^{-1}$ T = 293 (2) K

 $R_{\rm int} = 0.032$

 $0.4 \times 0.2 \times 0.1 \text{ mm}$

5134 independent reflections

2211 Friedel pairs

4969 reflections with $I > 2\sigma(I)$

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Bis(3-deoxy-1,2-O-isopropylidene-@-D-glucofuranos-3-yl) disulfide

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Comment

The title compound, (I), was prepared as a part of a project aimed at the synthesis of potential gelators of organic solvents (Luboradzki *et al.*, 2005). The class of saccharide-based gelators having free OH groups and the glucofuranose fragment are able to form gels with huge spectrum of organic solvents. According to the driving forces responsible for molecular aggregation they may be classified as hydrogen-bond-based gelators (Terech & Weiss 1997).

The crystal structure of (I) (Fig. 1) contains one independent molecule of the title compound per asymmetric unit. The molecules are bound into one dimensional hydrogen bond-based chains (generated by the screw axis along the a axis) utilizing all hydroxy H atoms (Fig. 2). Each molecule is involved in four hydrogen bonds as proton donor and in four as acceptor.

Experimental

The title compound (I) was prepared from 1,2-*O*-Isopropylidene-3-thio- α -*D*-glucofuranose by oxidation in hot methanol involving oxygen from the air. Subsequently it was recrystallized by cooling hot methanol solution.

Refinement

All H atoms were geometrically constrained to ride on their parent atom, fixing the bond lengths at 0.82, 0.96, 0.97 and 0.98 Å for hydroxyl, methine, methylene and methyl H atoms, respectively, and with $U_{iso}(H)=1.2U_{eq}(1.5U_{eq})$ for methyl and hydroxyl) of the carrier atom. –OH hydrogen atoms were refined by use of a rotating group refinement (AFIX 147). The absolute configuration determined from anomalous scattering effects is as expected from the synthesis.

Figures



Fig. 1. The molecular structure of (I). Displacement ellipsoids are drawn at the 30% probability level. H atoms are shown as circles of arbitrary radii.



Fig. 2. The packing of (I), viewed down the a axis, with the b axis vertical.

Bis(3-deoxy-1,2-O-isopropylidene-α-D-glucofuranos-3-yl) disulfide

Crystal data	
$C_{18}H_{30}O_{10}S_2$	$F_{000} = 1000$
$M_r = 470.54$	$D_{\rm x} = 1.385 {\rm ~Mg~m}^{-3}$
Orthorhombic, $P2_12_12_1$	Mo K α radiation $\lambda = 0.71073$ Å
Hall symbol: P 2ac 2ab	Cell parameters from 17407 reflections
a = 8.7266 (1) Å	$\theta = 1.0-27.5^{\circ}$
<i>b</i> = 14.4778 (4) Å	$\mu = 0.29 \text{ mm}^{-1}$
c = 17.8606 (5) Å	T = 293 (2) K
$V = 2256.54 (9) \text{ Å}^3$	Plate, colourless
Z = 4	$0.4 \times 0.2 \times 0.1 \text{ mm}$

Data collection

Nonius KappaCCD diffractometer	5134 independent reflections
Radiation source: fine-focus sealed tube	4969 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{\rm int} = 0.032$
Detector resolution: 1242 (horizontal) x 1152 (vertic- al) pixels, CCD pixel size is 22.5 x 22.5 μ m which gives at the imput a pixel of 110 x 110 μ m (with 2 x 2 binning) pixels mm ⁻¹	$\theta_{max} = 27.5^{\circ}$
T = 293(2) K	$\theta_{\min} = 2.6^{\circ}$
189 frames via φ rotation (rotation angle 1.9°) and 2*287 s per frame and 13 frames via ω rotation (rotation angle 1.9°) and 2*287 s per frame scans	$h = -11 \rightarrow 11$
Absorption correction: none	$k = -18 \rightarrow 18$
22012 measured reflections	$l = -23 \rightarrow 23$

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)] = 0.029$	$w = 1/[\sigma^{2}(F_{o}^{2}) + (0.0134P)^{2} + 1.4932P]$ where $P = (F_{o}^{2} + 2F_{c}^{2})/3$
$wR(F^2) = 0.066$	$(\Delta/\sigma)_{\rm max} = 0.001$
<i>S</i> = 1.09	$\Delta \rho_{max} = 0.21 \text{ e } \text{\AA}^{-3}$
5134 reflections	$\Delta \rho_{min} = -0.21 \text{ e } \text{\AA}^{-3}$
279 parameters	Extinction correction: none
Primary atom site location: structure-invariant direct methods	Absolute structure: Flack (1983), 2211 Freidel pairs
Secondary atom site location: difference Fourier map	Flack parameter: 0.02 (5)

Special details

Experimental. Synthesis of 1,2-*O*-Isopropylidene-3-thio- α -*D*-glucofuranose: To a suspension of LiAlH₄ (160 mg, 4.2 m*M*) in THF (25 ml) cooled in ice bath a solution of 5,6-di-*O*-acetyl-1,2-*O*-isopropylidene-3-thiocyanato- α -*D*-glucofuranose (Risbood *et al.*1981) (1, 629 mg, 1.8 m*M*) in THF (5 ml) was slowly added and stirred at room temp. for 3 h under an argon atmosphere. An excess of LiAlH₄ was decomposed by addition of ethyl acetate (1 ml), then the reaction mixture was cautiously acidified by addition of 5% aqueous NH₄Cl and solvents were evaporated to dryness. Column chromatography of the residue (hexane ? ethyl acetate, 5:1 than 1:1, then hexane ? ethyl acetate - methanol, 5:3:1) yielded 301 mg (70%) of the title compound as foam. [α]_D² –9.7 (c 1/2, chloroform ? methanol, 1:1); ¹H NMR (CD₃OD) δ : 5.86 (d, 1H, J_{1,2} 3.5 Hz, H-1), 4.66 (d, 1H, H-2), 4.18 (dd, 1H, J_{4,3} 3.7, J_{4,5} 9.4 Hz, H-4), 3.88 (m, 1H, H-5), 3.75 (dd, 1H, J_{6,5} 2.8, J_{6,6}? 11.6 Hz, H-6), 3.58 (dd, 1H, J_{6,5} 5.7, H-6?), 3.48 (d, 1H, H-3), 3.31 (m, 1H, SH), 1.46 (s, 3H, CH₃), 1.29 (s, 3H, CH₃). ¹³C NMR (CD₃OD) δ : 112.9 (C), 106.0 (C-1), 88.7, 79.7, 71.8, 65.2 (C-6), 46.3 (C-3), 26.8 (CH₃), 26.4 (CH₃). HR—MS (ESI) calc. for C₉H₁₆NaO₅S [*M*+Na]+: 259.0611. Found: 259.0615.

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 (A^2)

	x	У	Ζ	$U_{\rm iso}$ */ $U_{\rm eq}$
S1	0.06709 (5)	0.57977 (3)	0.73252 (2)	0.01991 (9)
S2	0.25277 (5)	0.54599 (3)	0.66943 (2)	0.01858 (9)
01	-0.05475 (13)	0.73533 (8)	0.84580 (6)	0.0182 (2)
O2	0.13077 (14)	0.82781 (9)	0.90160 (7)	0.0221 (3)
O3	0.29050 (13)	0.80305 (8)	0.80408 (7)	0.0193 (3)

04 -0.15521 (16) 0.7003 0.65014 (7) 0.0264 (3) 1H0 -0.2082 0.7303 0.6213 0.040* 05 -0.45500 (14) 0.75117 (9) 0.7178 (7) 0.0227 (3) H5O -0.5321 0.7658 0.7413 0.034* 06 0.35095 (14) 0.49495 (8) 0.50471 (7) 0.0230 (3) 07 0.1544 (15) 0.72871 (8) 0.57326 (7) 0.0230 (3) 08 0.00355 (14) 0.5499 (9) 0.43354 (7) 0.0230 (3) 090 0.41651 (15) 0.72871 (8) 0.57326 (7) 0.0230 (3) 010 0.72117 (14) 0.67699 (10) 0.52755 (7) 0.0254 (3) 1H00 0.7829 0.6932 0.4955 0.038* C1 0.09359 (19) 0.73170 (1) 0.7457 (9) 0.018 (3) H1 0.1045 0.6917 0.9171 (0) 0.0124 (3) H2 0.2750 0.6233 0.8222 0.20* C2 0.07992 (19) 0.73171 (1) 0.7413 (9)					
H40-0.20820.73030.62130.040*05-0.45500 (14)0.75117 (9)0.71783 (7)0.0227 (3)H50-0.53210.76780.74130.034*060.35095 (14)0.49495 (8)0.50471 (7)0.0197 (3)070.15464 (15)0.42656 (10)0.43354 (7)0.0226 (3)080.00365 (14)0.72871 (8)0.57326 (7)0.0230 (3)090.41651 (15)0.72871 (8)0.57326 (7)0.0254 (3)11000.72117 (14)0.67699 (10)0.52755 (7)0.0254 (3)11000.7217 (14)0.67699 (10)0.52755 (7)0.0254 (3)11100.10450.69170.91710.0181 (3)1120.10359 (19)0.73702 (12)0.87676 (9)0.0181 (3)1120.27500.66530.82220.020*C30.1050 (19)0.70371 (11)0.74457 (9)0.0174 (3)1330.15100.73020.69940.021*C4-0.03968 (19)0.7540 (11)0.7571 (19)0.0162 (3)144-0.02040.82270.76160.019* (3)155A-0.2184 (19)0.75140 (11)0.7574 (10)0.0188 (3)16A-0.3190.75240 (11)0.7524 (11)0.022* (26)C5-0.18473 (19)0.7814 (12)0.7540 (11)0.024* (15)155A-0.2040.82170.81040.023*C70.2787 (2)0.87270.81040.023*C6-0.3189 (19)0.7516 (10)0.	O4	-0.15521 (16)	0.76064 (10)	0.65014 (7)	0.0264 (3)
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H900.46790.74500.60940.030*O100.72117 (14)0.67699 (10)0.52755 (7)0.0254 (3)H1000.78290.69320.49550.0318 (3)H10.10450.69170.91710.022*C20.20792 (19)0.71817 (12)0.81233 (9)0.0168 (3)H20.27500.66530.82220.027*C30.10501 (19)0.70371 (11)0.74457 (9)0.0174 (3)H30.15100.73020.6940.021*C4-0.03968 (19)0.75640 (11)0.7611 (9)0.0162 (3)H4-0.02040.82270.76160.019*C5-0.18473 (19)0.73217 (12)0.72500 (9)0.021*C6-0.32189 (19)0.78143 (12)0.7560 (10)0.188 (3)H6A-0.33190.76700.81040.023*H6B-0.30980.84770.75240.0226* (4)C80.4020 (2)0.82149 (14)0.92836 (11)0.265 (4)K80.30610.75780.90880.404*H80.50090.83760.90880.404*H9A0.20200.9548 (13)0.85718 (12)0.0284 (4)H9A0.20200.95860.90270.43*H9B0.37960.97040.83560.023*C110.902 (2)0.5086 (12)0.5764 (9)0.0165 (3)H1A0.22740.5764 (9)0.0158 (3)H1A0.22740.5764 (9)0.0165 (3)H1A<	09	0.41651 (15)	0.72871 (8)	0.57326 (7)	0.0203 (3)
O10 0.72117 (14) 0.67699 (10) 0.52755 (7) 0.0254 (3) H100 0.7829 0.6932 0.4955 0.038* C1 0.09359 (19) 0.73702 (12) 0.87676 (9) 0.0181 (3) H1 0.1045 0.6917 0.9171 0.022* C2 0.20792 (19) 0.71817 (12) 0.81233 (9) 0.0168 (3) H2 0.2750 0.6653 0.8222 0.020* C3 0.10501 (19) 0.70371 (11) 0.74457 (9) 0.0174 (3) H3 0.1510 0.73217 (12) 0.72500 (9) 0.0179 (3) H4 -0.0204 0.8227 0.7616 0.019* C5 -0.18473 (19) 0.73143 (12) 0.75760 (10) 0.188 (3) H5A -0.2013 0.6652 0.7255 0.022* C6 -0.3189 (19) 0.7814 (12) 0.75760 (10) 0.188 (3) H6A -0.3098 0.8477 0.7524 0.022* C7 0.2787 (2) 0.82194 (14) 0.92836 (11) 0.0265 (4)<	H9O	0.4679	0.7450	0.6094	0.030*
H1000.78290.69320.49550.038*C10.09359 (19)0.73702 (12)0.87676 (9)0.0181 (3)H10.10450.69170.91710.0268 (3)C20.20792 (19)0.71817 (12)0.81233 (9)0.0168 (3)H20.27500.66530.82220.020*C30.10501 (19)0.70371 (11)0.74457 (9)0.0174 (3)H30.15100.73020.69940.021*C4-0.03968 (19)0.75640 (11)0.76711 (9)0.0162 (3)H4-0.02040.82270.76160.019*C5-0.18473 (19)0.73217 (12)0.72500 (9)0.0179 (3)H5A-0.20130.66520.72650.022*C6-0.32189 (19)0.78143 (12)0.75760 (10)0.0188 (3)H6B-0.30980.84770.75240.023*C70.2787 (2)0.85227 (12)0.87392 (10)0.0204 (4)C80.4020 (2)0.82149 (14)0.92836 (11)0.0265 (4)H8A0.38690.81160.97570.040*H8B0.50090.83760.90880.043*H9A0.20200.96950.82260.043*H9B0.37960.97040.83560.023*C10.2131 (19)0.44449 (12)0.50562 (10)0.0195 (3)H10A0.22370.38680.90270.046*H9B0.3756 (12)0.5428 (9)0.0188 (3)H10A0.2240.50586 (12)0.5428 (9)	O10	0.72117 (14)	0.67699 (10)	0.52755 (7)	0.0254 (3)
C1 $0.09359 (19)$ $0.73702 (12)$ $0.87676 (9)$ $0.0181 (3)$ H1 0.1045 0.6917 0.9171 $0.022*$ C2 $0.20792 (19)$ $0.71817 (12)$ $0.81233 (9)$ $0.0168 (3)$ H2 0.2750 0.6653 0.8222 $0.020*$ C3 $0.10501 (19)$ $0.73071 (11)$ $0.74457 (9)$ $0.0174 (3)$ H3 0.1510 0.7302 0.6994 $0.021*$ C4 $-0.03968 (19)$ $0.7564 (11)$ $0.76711 (9)$ $0.0162 (3)$ H4 -0.0204 0.8227 0.7616 $0.019*$ C5 $-0.18473 (19)$ $0.73217 (12)$ $0.72500 (9)$ $0.0179 (3)$ H5A -0.2013 0.6652 0.7255 $0.022*$ C6 $-0.32189 (19)$ $0.78143 (12)$ $0.75760 (10)$ $0.188 (3)$ H6A -0.398 0.8477 0.7524 $0.023*$ C7 $0.2787 (2)$ $0.85227 (12)$ $0.87392 (10)$ $0.0264 (4)$ C8 $0.4020 (2)$ $0.82149 (14)$ $0.92836 (11)$ $0.0265 (4)$ H8A 0.3869 0.8516 0.9757 $0.404*$ H8B 0.5009 0.8376 0.9088 0.404° H9A 0.2020 0.99455 0.8226 0.043^{*} H9B 0.3796 0.9774 0.8356 0.043^{*} H9A 0.2020 $0.9586 (12)$ $0.57594 (9)$ $0.0165 (3)$ H1A 0.0274 0.7528 0.9027 0.043^{*} H9B 0.3796 0.977 0.443^{*} <td>H10O</td> <td>0.7829</td> <td>0.6932</td> <td>0.4955</td> <td>0.038*</td>	H10O	0.7829	0.6932	0.4955	0.038*
H1 0.1045 0.6917 0.9171 0.022^* C2 $0.20792 (19)$ $0.71817 (12)$ $0.81233 (9)$ $0.0168 (3)$ H2 0.2750 0.6653 0.8222 0.020^* C3 $0.10501 (19)$ $0.70371 (11)$ $0.74457 (9)$ $0.0174 (3)$ H3 0.1510 0.7302 0.6994 0.021^* C4 $-0.03968 (19)$ $0.75640 (11)$ $0.76711 (9)$ $0.0162 (3)$ H4 -0.0204 0.8227 0.7616 0.019^* C5 $-0.18473 (19)$ $0.73217 (12)$ $0.72500 (9)$ $0.0179 (3)$ H5A -0.2013 0.6652 0.7265 0.022^* C6 $-0.32189 (19)$ $0.78143 (12)$ $0.75760 (10)$ $0.0188 (3)$ H6A -0.3098 0.8477 0.7524 0.023^* C7 $0.2787 (2)$ $0.85227 (12)$ $0.87392 (10)$ $0.0204 (4)$ C8 $0.4020 (2)$ $0.82149 (14)$ $0.92386 (11)$ $0.0265 (4)$ H8A 0.3869 0.8516 0.9757 0.404^* H8B 0.5009 0.8376 0.9088 0.404^* H8B 0.5099 0.8376 0.9274 0.43^* H9A 0.2020 0.9695 0.8226 0.43^* H9B 0.3796 0.9704 0.8356 0.023^* C10 $0.21131 (19)$ $0.44449 (12)$ $0.50562 (10)$ $0.0195 (3)$ H10A 0.2237 $0.3868 (12)$ $0.5736 (9)$ $0.0165 (3)$ H11A 0.0274 $0.5796 (10)$ $0.0195 (3)$	C1	0.09359 (19)	0.73702 (12)	0.87676 (9)	0.0181 (3)
C2 $0.20792 (19)$ $0.71817 (12)$ $0.81233 (9)$ $0.0168 (3)$ H2 0.2750 0.6653 0.8222 0.020^* C3 $0.10501 (19)$ $0.70371 (11)$ $0.74457 (9)$ $0.0174 (3)$ H3 0.1510 0.7302 0.6994 0.021^* C4 $-0.03968 (19)$ $0.75540 (11)$ $0.76711 (9)$ $0.0162 (3)$ H4 -0.0204 0.8227 0.7616 0.019^* C5 $-0.18473 (19)$ $0.73217 (12)$ $0.72500 (9)$ $0.0179 (3)$ H5A -0.2013 0.6652 0.7265 0.022^* C6 $-0.32189 (19)$ $0.78143 (12)$ $0.75760 (10)$ $0.0188 (3)$ H6B -0.3098 0.8477 0.7524 0.023^* C7 $0.2787 (2)$ $0.85227 (12)$ $0.87392 (10)$ $0.0204 (4)$ C8 $0.4020 (2)$ $0.82149 (14)$ $0.92836 (11)$ $0.0265 (4)$ H8A 0.3869 0.8516 0.9757 0.404^* H8B 0.5009 0.8376 0.9088 0.404^* C9 $0.2824 (2)$ $0.9548 (13)$ $0.85718 (12)$ $0.0284 (4)$ H9A 0.2020 0.9695 0.8226 0.043^* H9B 0.3796 0.974 0.8356 0.043^* H9B 0.3796 0.9386 0.9027 0.043^* H9C 0.2679 $0.9866 (12)$ $0.5756 (10)$ $0.0195 (3)$ H10A 0.2237 $0.5866 (12)$ $0.5769 (9)$ 0.023^* C11 $0.0902 (2)$ $0.50586 (12)$ <td< td=""><td>H1</td><td>0.1045</td><td>0.6917</td><td>0.9171</td><td>0.022*</td></td<>	H1	0.1045	0.6917	0.9171	0.022*
H2 0.2750 0.6653 0.8222 0.020^* C3 0.10501 (19) 0.70371 (11) 0.74457 (9) 0.0174 (3)H3 0.1510 0.7302 0.6994 0.021^* C4 -0.03968 (19) 0.75640 (11) 0.76711 (9) 0.0162 (3)H4 -0.0204 0.8227 0.7616 0.019^* C5 -0.18473 (19) 0.73217 (12) 0.72500 (9) 0.0179 (3)H5A -0.2013 0.6652 0.7265 0.022^* C6 -0.32189 (19) 0.78143 (12) 0.75760 (10) 0.0188 (3)H6B -0.3098 0.8477 0.7524 0.023^* C7 0.2787 (2) 0.85227 (12) 0.87392 (10) 0.0204 (4)C8 0.4020 (2) 0.82149 (14) 0.92836 (11) 0.0265 (4)H8A 0.3869 0.8516 0.9757 0.404^* H8B 0.5009 0.8376 0.9088 0.404^* C9 0.2824 (2) 0.9548 (13) 0.85718 (12) 0.0284 (4)H9A 0.2020 0.9695 0.8226 0.043^* H9B 0.3796 0.9704 0.8356 0.023^* C10 0.21131 (19) 0.44449 (12) 0.50562 (10) 0.0195 (3)H1A 0.00274 0.4729 0.5764 (9) 0.0165 (3)H1A 0.0274 0.4729 0.5764 (9) 0.0165 (3)H1A 0.0274 0.6217 0.4760 0.023^* C12 0.18450 (19) 0.58362 (12) 0	C2	0.20792 (19)	0.71817 (12)	0.81233 (9)	0.0168 (3)
C3 $0.10501(19)$ $0.70371(11)$ $0.74457(9)$ $0.0174(3)$ H3 0.1510 0.7302 0.6994 $0.021*$ C4 $-0.03968(19)$ $0.75640(11)$ $0.76711(9)$ $0.0162(3)$ H4 -0.0204 0.8227 0.7616 $0.019*$ C5 $-0.18473(19)$ $0.73217(12)$ $0.72500(9)$ $0.0179(3)$ H5A -0.2013 0.6652 0.7265 $0.022*$ C6 $-0.32189(19)$ $0.78143(12)$ $0.75760(10)$ $0.188(3)$ H6A -0.3319 0.7670 0.8104 $0.023*$ C7 $0.2787(2)$ $0.85227(12)$ $0.87392(10)$ $0.204(4)$ C8 $0.4020(2)$ $0.82149(14)$ $0.9238(11)$ $0.2026(4)$ H8A 0.3809 0.8376 0.9088 $0.40*$ H8B 0.5009 0.8376 0.9088 $0.404*$ H8C 0.3961 0.7558 0.9351 $0.404*$ H9A 0.2020 0.9695 0.8226 $0.43*$ H9B 0.3796 0.9704 0.8356 $0.023*$ C10 $0.21131(19)$ $0.44449(12)$ $0.50562(10)$ $0.0189(3)$ H11A 0.0274 0.4729 0.5796 $0.023*$ C12 $0.18450(19)$ $0.5836(12)$ $0.54282(9)$ $0.0165(3)$ H12 0.1264 0.6114 0.5799 $0.204*$ C13 $0.31752(19)$ $0.59361(1)$ $0.55164(9)$ $0.0165(3)$ H14 0.5000 0.6040 0.5945 $0.204*$ C14 $0.$	H2	0.2750	0.6653	0.8222	0.020*
H3 0.1510 0.7302 0.6994 $0.021*$ C4 -0.03968 (19) 0.75640 (11) 0.76711 (9) 0.0162 (3)H4 -0.0204 0.8227 0.7616 $0.019*$ C5 -0.18473 (19) 0.73217 (12) 0.72500 (9) 0.0179 (3)H5A -0.2013 0.6652 0.7256 $0.022*$ C6 -0.32189 (19) 0.78143 (12) 0.75760 (10) 0.0188 (3)H6A -0.3319 0.7670 0.8104 $0.023*$ C7 0.2787 (2) 0.85227 (12) 0.87392 (10) 0.2044 (4)C8 0.4020 (2) 0.82149 (14) 0.92836 (11) 0.2656 (4)H8A 0.3869 0.8516 0.9757 $0.404*$ H8B 0.5009 0.8376 0.9088 $0.404*$ H8C 0.3961 0.7558 0.9351 $0.404*$ H9A 0.2020 0.9695 0.8226 $0.043*$ H9B 0.3796 0.9704 0.8356 $0.023*$ C10 0.21131 (19) 0.44449 (12) 0.50562 (10) 0.0189 (3)H11A 0.0274 0.4729 0.5796 $0.023*$ C12 0.18450 (19) 0.5386 (12) 0.54282 (9) 0.189 (3)H11A 0.0274 0.6217 0.4760 $0.019*$ C13 0.31752 (19) 0.59043 (11) 0.52161 (9) 0.0166 (3)H14 0.5000 0.6040 0.5945 $0.202*$ C12 0.18450 (19) 0.53717 (11) 0.55074 (9) 0	C3	0.10501 (19)	0.70371 (11)	0.74457 (9)	0.0174 (3)
C4 $-0.03968 (19)$ $0.75640 (11)$ $0.76711 (9)$ $0.0162 (3)$ H4 -0.0204 0.8227 0.7616 $0.019*$ C5 $-0.18473 (19)$ $0.73217 (12)$ $0.72500 (9)$ $0.0179 (3)$ H5A -0.2013 0.6652 0.7265 $0.022*$ C6 $-0.32189 (19)$ $0.78143 (12)$ $0.75760 (10)$ $0.0188 (3)$ H6A -0.3319 0.7670 0.8104 $0.023*$ H6B -0.3098 0.8477 0.7524 $0.023*$ C7 $0.2787 (2)$ $0.85227 (12)$ $0.87392 (10)$ $0.0204 (4)$ C8 $0.4020 (2)$ $0.82149 (14)$ $0.92836 (11)$ $0.0265 (4)$ H8A 0.3869 0.8516 0.9757 $0.040*$ H8B 0.5009 0.8376 0.9088 $0.404*$ C9 $0.2824 (2)$ $0.95448 (13)$ $0.85718 (12)$ $0.0284 (4)$ H9A 0.2020 0.9695 0.8226 $0.043*$ H9B 0.3796 0.9704 0.8356 $0.043*$ H9C 0.2679 0.9886 0.9027 $0.043*$ C10 $0.21131 (19)$ $0.44449 (12)$ $0.50562 (10)$ $0.0195 (3)$ H10A 0.2237 0.3868 0.5336 $0.023*$ C11 $0.0902 (2)$ $0.50586 (12)$ $0.54282 (9)$ $0.189 (3)$ H11A 0.0274 0.6414 0.5799 $0.208*$ C12 $0.18450 (19)$ $0.55836 (12)$ $0.5764 (9)$ $0.0165 (3)$ H11A 0.2287 0.6217 0.4760 <td< td=""><td>H3</td><td>0.1510</td><td>0.7302</td><td>0.6994</td><td>0.021*</td></td<>	H3	0.1510	0.7302	0.6994	0.021*
H4-0.02040.82270.76160.019*C5-0.18473 (19)0.73217 (12)0.72500 (9)0.0179 (3)H5A-0.20130.66520.72650.022*C6-0.32189 (19)0.78143 (12)0.75760 (10)0.0188 (3)H6A-0.33190.76700.81040.023*H6B-0.30980.84770.75240.0204 (4)C70.2787 (2)0.85227 (12)0.87392 (10)0.0204 (4)C80.4020 (2)0.82149 (14)0.9283 (11)0.0265 (4)H8A0.38690.85160.97570.040*H8B0.50090.83760.90880.404*C90.2824 (2)0.95448 (13)0.85718 (12)0.0284 (4)H9A0.20200.96950.82260.043*H9B0.37960.97040.83560.023*C100.21131 (19)0.44449 (12)0.50562 (10)0.0195 (3)H1A0.02740.5086 (12)0.5764 (9)0.0165 (3)H1A0.02740.5086 (12)0.57694 (9)0.0165 (3)H1A0.02740.62170.47600.019*C120.18450 (19)0.58362 (12)0.57694 (9)0.0165 (3)H130.28270.62170.47600.019*C140.46207 (19)0.63771 (11)0.55074 (9)0.0166 (3)H130.28270.62170.47600.019*C140.46207 (19)0.63771 (11)0.55074 (9)0.0166 (3)H140.50000.6	C4	-0.03968 (19)	0.75640 (11)	0.76711 (9)	0.0162 (3)
C5 -0.18473 (19) 0.73217 (12) 0.72500 (9) 0.0179 (3)H5A -0.2013 0.6652 0.7265 $0.022*$ C6 -0.32189 (19) 0.78143 (12) 0.75760 (10) 0.0188 (3)H6A -0.3319 0.7670 0.8104 $0.023*$ H6B -0.3098 0.8477 0.7524 $0.023*$ C7 0.2787 (2) 0.85227 (12) 0.87392 (10) 0.0204 (4)C8 0.4020 (2) 0.82149 (14) 0.92836 (11) 0.0265 (4)H8A 0.3869 0.8376 0.9088 $0.404°$ H8B 0.5009 0.8376 0.9088 $0.404°$ C9 0.2824 (2) 0.95448 (13) 0.85718 (12) 0.0284 (4)H9A 0.2020 0.9695 0.8226 $0.043*$ H9B 0.3796 0.9704 0.8356 $0.023*$ C10 0.21131 (19) 0.44449 (12) 0.50562 (10) 0.0195 (3)H1A 0.227 0.3868 0.5336 $0.023*$ C11 0.9002 (2) 0.50586 (12) 0.57694 (9) 0.0165 (3)H1A 0.274 0.4729 0.5796 $0.023*$ C12 0.18450 (19) 0.5362 (12) 0.57694 (9) 0.0165 (3)H1A 0.2671 0.6414 0.5799 $0.020*$ C13 0.31752 (19) 0.59043 (11) 0.52161 (9) 0.0165 (3)H14 0.5000 0.6416 0.5745 $0.024*$ C15 0.5868 (2) 0.64160 (12) 0.49218	H4	-0.0204	0.8227	0.7616	0.019*
H5A -0.2013 0.6652 0.7265 $0.022*$ C6 $-0.32189(19)$ $0.78143(12)$ $0.75760(10)$ $0.0188(3)$ H6A -0.3319 0.7670 0.8104 $0.023*$ H6B -0.3098 0.8477 0.7524 $0.023*$ C7 $0.2787(2)$ $0.85227(12)$ $0.87392(10)$ $0.0204(4)$ C8 $0.4020(2)$ $0.82149(14)$ $0.92836(11)$ $0.0265(4)$ H8A 0.3869 0.8516 0.9757 $0.040*$ H8B 0.5009 0.8376 0.9088 $0.040*$ C9 $0.2824(2)$ $0.95448(13)$ $0.85718(12)$ $0.0284(4)$ H9A 0.2020 0.9695 0.8226 $0.043*$ H9B 0.3796 0.9704 0.8356 $0.043*$ H9C 0.2679 0.9886 0.9027 $0.443*$ H9A 0.2237 0.3668 0.5336 $0.023*$ C10 $0.21131(19)$ $0.44449(12)$ $0.50562(10)$ $0.195(3)$ H1A 0.0274 0.4729 $0.57964(9)$ $0.0165(3)$ H1A 0.0274 0.6217 0.4760 $0.019*$ C12 $0.18450(19)$ $0.5362(12)$ $0.57694(9)$ $0.0165(3)$ H13 0.2827 0.6217 0.4760 $0.019*$ C14 $0.46207(19)$ $0.63771(11)$ $0.55074(9)$ $0.0166(3)$ H14 0.5000 0.6040 $0.5945(10)$ $0.020*$ C15 $0.5868(2)$ $0.64160(12)$ $0.49218(10)$ $0.020*(3)$ H15A 0.6	C5	-0.18473 (19)	0.73217 (12)	0.72500 (9)	0.0179 (3)
$C6$ $-0.32189(19)$ $0.78143(12)$ $0.75760(10)$ $0.0188(3)$ $H6A$ -0.3319 0.7670 0.8104 $0.023*$ $H6B$ -0.3098 0.8477 0.7524 $0.023*$ $C7$ $0.2787(2)$ $0.85227(12)$ $0.87392(10)$ $0.0204(4)$ $C8$ $0.4020(2)$ $0.82149(14)$ $0.92836(11)$ $0.0265(4)$ $H8A$ 0.3869 0.8516 0.9757 0.404° $H8B$ 0.5009 0.8376 0.9088 0.040° $C9$ $0.2824(2)$ $0.9548(13)$ $0.85718(12)$ $0.0284(4)$ $H9A$ 0.2020 0.9695 0.8226 0.043° $H9B$ 0.3796 0.9704 0.8356 0.0023° $H9B$ 0.3796 0.9704 0.8356 0.043° $H9C$ 0.2679 0.9886 0.9027 0.434° $C10$ $0.21131(19)$ $0.44449(12)$ $0.50562(10)$ $0.1189(3)$ $H10A$ 0.2237 0.3868 0.5336 0.023° $C11$ $0.9092(2)$ $0.50586(12)$ $0.54282(9)$ $0.1189(3)$ $H11A$ 0.0274 0.4729 $0.57964(9)$ $0.0165(3)$ $H12$ 0.1264 0.6414 0.5799 0.202° $C13$ $0.31752(19)$ $0.59043(11)$ $0.52161(9)$ $0.0166(3)$ $H14$ 0.5000 $0.6417(10)$ $0.5974(9)$ $0.0166(3)$ $H14$ 0.5000 $0.64160(12)$ $0.49218(10)$ $0.0207(4)$ $C14$ 0.6663 0.5804	H5A	-0.2013	0.6652	0.7265	0.022*
H6A -0.3319 0.7670 0.8104 0.023^* H6B -0.3098 0.8477 0.7524 0.023^* C7 0.2787 (2) 0.85227 (12) 0.87392 (10) 0.0204 (4)C8 0.4020 (2) 0.82149 (14) 0.92836 (11) 0.0265 (4)H8A 0.3869 0.8516 0.9757 0.040^* H8B 0.5009 0.8376 0.9088 0.404^* C9 0.2824 (2) 0.95448 (13) 0.85718 (12) 0.0284 (4)H9A 0.2020 0.9695 0.8226 0.043^* H9B 0.3796 0.9704 0.8356 0.043^* H9C 0.2679 0.9886 0.9027 0.443^* C10 0.21131 (19) 0.44449 (12) 0.50562 (10) 0.1195 (3)H10A 0.2237 0.3868 0.5336 0.023^* C11 0.902 (2) 0.50586 (12) 0.57694 (9) 0.0189 (3)H11A 0.0274 0.4729 0.57694 (9) 0.0165 (3)H12 0.1264 0.6414 0.5799 0.20^* C13 0.31752 (19) 0.59043 (11) 0.52161 (9) 0.0166 (3)H13 0.2827 0.6217 0.4760 0.019^* C14 0.46207 (19) 0.6371 (11) 0.55074 (9) 0.020^* C15 0.5868 (2) 0.6116 0.4723 0.024^* H15A 0.6063 0.5804 0.4723 0.024^* H15B 0.5552 0.6816 0.4512 0.024^* <t< td=""><td>C6</td><td>-0.32189 (19)</td><td>0.78143 (12)</td><td>0.75760 (10)</td><td>0.0188 (3)</td></t<>	C6	-0.32189 (19)	0.78143 (12)	0.75760 (10)	0.0188 (3)
H6B -0.3098 0.8477 0.7524 0.023^* C7 0.2787 (2) 0.85227 (12) 0.87392 (10) 0.0204 (4)C8 0.4020 (2) 0.82149 (14) 0.92836 (11) 0.0265 (4)H8A 0.3869 0.8516 0.9757 0.040^* H8B 0.5009 0.8376 0.9088 0.404^* H8C 0.3961 0.7558 0.9351 0.404^* C9 0.2824 (2) 0.95448 (13) 0.85718 (12) 0.0284 (4)H9A 0.2020 0.9695 0.8226 0.043^* H9B 0.3796 0.9704 0.8356 0.043^* H9C 0.2679 0.9886 0.9027 0.043^* C10 0.21131 (19) 0.44449 (12) 0.50562 (10) 0.0195 (3)H10A 0.2237 0.3868 0.5336 0.023^* C11 0.902 (2) 0.50586 (12) 0.5796 0.023^* C12 0.18450 (19) 0.58362 (12) 0.57964 (9) 0.0165 (3)H12 0.1264 0.6414 0.5799 0.20^* C13 0.31752 (19) 0.59043 (11) 0.52161 (9) 0.0166 (3)H13 0.2827 0.6217 0.4760 0.019^* C14 0.46207 (19) 0.63771 (11) 0.55074 (9) 0.020^* C15 0.5868 (2) 0.64160 (12) 0.4723 0.024^* H14 0.5000 0.6040 0.5945 0.020^* C15 0.5868 (2) 0.6160 (12) 0.49218 (10) <td< td=""><td>H6A</td><td>-0.3319</td><td>0.7670</td><td>0.8104</td><td>0.023*</td></td<>	H6A	-0.3319	0.7670	0.8104	0.023*
C70.2787 (2)0.85227 (12)0.87392 (10)0.0204 (4)C80.4020 (2)0.82149 (14)0.92836 (11)0.0265 (4)H8A0.38690.85160.97570.040*H8B0.50090.83760.90880.040*H8C0.39610.75580.93510.040*C90.2824 (2)0.95448 (13)0.85718 (12)0.0284 (4)H9A0.20200.96950.82260.043*H9B0.37960.97040.83560.043*H9C0.26790.98860.90270.043*C100.21131 (19)0.44449 (12)0.50562 (10)0.195 (3)H10A0.22370.38680.53360.023*C110.0902 (2)0.50586 (12)0.54282 (9)0.189 (3)H11A0.02740.47290.57694 (9)0.0165 (3)H120.12640.64140.57990.020*C130.31752 (19)0.59043 (11)0.52161 (9)0.0161 (3)H130.28270.62170.47600.019*C140.46207 (19)0.63771 (11)0.55074 (9)0.0166 (3)H140.50000.60400.59450.020*C150.5868 (2)0.64160 (12)0.49218 (10)0.0203 (3)H15A0.60630.58040.47230.024*H15B0.55620.68160.45120.024*C160.0177 (2)0.47929 (12)0.4167 (10)0.0207 (4)C17-0.1173 (2)0.41418 (14)0.451	H6B	-0.3098	0.8477	0.7524	0.023*
C8 0.4020 (2) 0.82149 (14) 0.92836 (11) 0.0265 (4) H8A 0.3869 0.8516 0.9757 0.040* H8B 0.5009 0.8376 0.9088 0.040* H8C 0.3961 0.7558 0.9351 0.040* C9 0.2824 (2) 0.95448 (13) 0.85718 (12) 0.0284 (4) H9A 0.2020 0.9695 0.8226 0.043* H9B 0.3796 0.9704 0.8356 0.043* H9C 0.2679 0.9886 0.9027 0.043* C10 0.21131 (19) 0.44449 (12) 0.50562 (10) 0.0195 (3) H10A 0.2237 0.3868 0.5336 0.023* C11 0.0902 (2) 0.50586 (12) 0.54282 (9) 0.0189 (3) H11A 0.0274 0.4729 0.5764 (9) 0.0165 (3) H12 0.1264 0.6414 0.5799 0.20* C13 0.31752 (19) 0.5914 (11) 0.55074 (9) 0.0166 (3) H13	C7	0.2787 (2)	0.85227 (12)	0.87392 (10)	0.0204 (4)
H8A0.38690.85160.97570.040*H8B0.50090.83760.90880.040*H8C0.39610.75580.93510.040*C90.2824 (2)0.95448 (13)0.85718 (12)0.0284 (4)H9A0.20200.96950.82260.043*H9B0.37960.97040.83560.043*H9C0.26790.98860.90270.043*C100.21131 (19)0.44449 (12)0.50562 (10)0.0195 (3)H10A0.22370.38680.53360.023*C110.0902 (2)0.50586 (12)0.54282 (9)0.0189 (3)H11A0.02740.47290.57960.023*C120.18450 (19)0.58362 (12)0.57694 (9)0.0165 (3)H120.12640.64140.57990.020*C130.31752 (19)0.59043 (11)0.52161 (9)0.0161 (3)H130.28270.62170.47600.019*C140.46207 (19)0.63771 (11)0.55074 (9)0.0166 (3)H140.50000.60400.59450.020*C150.5868 (2)0.64160 (12)0.49218 (10)0.0203 (3)H15A0.60630.58040.47230.024*H15B0.55620.68160.45120.024*C160.0177 (2)0.47929 (12)0.41967 (10)0.0207 (4)C17-0.1173 (2)0.41418 (14)0.41582 (11)0.0288 (4)H17A-0.12260.37870.46110	C8	0.4020 (2)	0.82149 (14)	0.92836 (11)	0.0265 (4)
H8B0.50090.83760.90880.040*H8C0.39610.75580.93510.040*C90.2824 (2)0.95448 (13)0.85718 (12)0.0284 (4)H9A0.20200.96950.82260.043*H9B0.37960.97040.83560.043*H9C0.26790.98860.90270.043*C100.21131 (19)0.44449 (12)0.50562 (10)0.0195 (3)H10A0.22370.38680.53360.023*C110.0902 (2)0.50586 (12)0.54282 (9)0.0189 (3)H11A0.02740.47290.57960.023*C120.18450 (19)0.58362 (12)0.57694 (9)0.0165 (3)H120.12640.64140.57990.020*C130.31752 (19)0.59043 (11)0.52161 (9)0.0166 (3)H140.50000.60400.59450.020*C150.5868 (2)0.64160 (12)0.49218 (10)0.0203 (3)H15A0.60630.58040.47230.024*H15B0.55620.68160.45120.024*C160.0177 (2)0.47929 (12)0.41967 (10)0.0207 (4)C17-0.1173 (2)0.41418 (14)0.41582 (11)0.0288 (4)H17A-0.12260.37870.46110.043*	H8A	0.3869	0.8516	0.9757	0.040*
H8C0.39610.75580.93510.040*C90.2824 (2)0.95448 (13)0.85718 (12)0.0284 (4)H9A0.20200.96950.82260.043*H9B0.37960.97040.83560.043*H9C0.26790.98860.90270.043*C100.21131 (19)0.44449 (12)0.50562 (10)0.0195 (3)H10A0.22370.38680.53360.023*C110.0902 (2)0.50586 (12)0.54282 (9)0.0189 (3)H11A0.02740.47290.57694 (9)0.0165 (3)H120.12640.64140.57990.020*C130.31752 (19)0.59043 (11)0.52161 (9)0.0166 (3)H140.50000.60400.59450.020*C150.5868 (2)0.64160 (12)0.49218 (10)0.0203 (3)H15A0.60630.58040.47230.024*H15B0.55620.68160.45120.024*C160.0177 (2)0.47929 (12)0.41967 (10)0.0207 (4)C17-0.1173 (2)0.41418 (14)0.41582 (11)0.0288 (4)H17A-0.12260.37870.46110.043*	H8B	0.5009	0.8376	0.9088	0.040*
C90.2824 (2)0.95448 (13)0.85718 (12)0.0284 (4)H9A0.20200.96950.82260.043*H9B0.37960.97040.83560.043*H9C0.26790.98860.90270.043*C100.21131 (19)0.44449 (12)0.50562 (10)0.0195 (3)H10A0.22370.38680.53360.023*C110.0902 (2)0.50586 (12)0.54282 (9)0.0189 (3)H11A0.02740.47290.5764 (9)0.0165 (3)H120.18450 (19)0.58362 (12)0.57694 (9)0.0165 (3)H130.28270.62170.47600.019*C140.46207 (19)0.63771 (11)0.55074 (9)0.0166 (3)H140.50000.60400.59450.020*C150.5868 (2)0.64160 (12)0.49218 (10)0.0203 (3)H15A0.60630.58040.47230.024*H15B0.55620.68160.45120.024*C160.0177 (2)0.47929 (12)0.41967 (10)0.0207 (4)C17-0.1173 (2)0.41418 (14)0.41582 (11)0.0288 (4)H17A-0.12260.37870.46110.043*	H8C	0.3961	0.7558	0.9351	0.040*
H9A0.20200.96950.82260.043*H9B0.37960.97040.83560.043*H9C0.26790.98860.90270.043*C100.21131 (19)0.44449 (12)0.50562 (10)0.0195 (3)H10A0.22370.38680.53360.023*C110.0902 (2)0.50586 (12)0.54282 (9)0.0189 (3)H11A0.02740.47290.57960.023*C120.18450 (19)0.58362 (12)0.57694 (9)0.0165 (3)H120.12640.64140.57990.020*C130.31752 (19)0.59043 (11)0.52161 (9)0.0161 (3)H130.28270.62170.47600.019*C140.46207 (19)0.63771 (11)0.55074 (9)0.0166 (3)H140.50000.60400.59450.020*C150.5868 (2)0.64160 (12)0.49218 (10)0.0203 (3)H15A0.60630.58040.47230.024*H15B0.55620.68160.45120.024*C160.0177 (2)0.47929 (12)0.41967 (10)0.0207 (4)C17-0.1173 (2)0.41418 (14)0.41582 (11)0.0288 (4)H17A-0.12260.37870.46110.043*	С9	0.2824 (2)	0.95448 (13)	0.85718 (12)	0.0284 (4)
H9B0.37960.97040.83560.043*H9C0.26790.98860.90270.043*C100.21131 (19)0.44449 (12)0.50562 (10)0.0195 (3)H10A0.22370.38680.53360.023*C110.0902 (2)0.50586 (12)0.54282 (9)0.0189 (3)H11A0.02740.47290.579640.023*C120.18450 (19)0.58362 (12)0.57694 (9)0.0165 (3)H120.12640.64140.57990.020*C130.31752 (19)0.59043 (11)0.52161 (9)0.0161 (3)H130.28270.62170.47600.019*C140.46207 (19)0.63771 (11)0.55074 (9)0.0166 (3)H140.50000.60400.59450.020*C150.5868 (2)0.64160 (12)0.49218 (10)0.0203 (3)H15A0.60630.58040.47230.024*H15B0.55620.68160.45120.024*C160.0177 (2)0.47929 (12)0.41967 (10)0.0207 (4)C17-0.1173 (2)0.41418 (14)0.41582 (11)0.0288 (4)H17A-0.12260.37870.46110.043*	H9A	0.2020	0.9695	0.8226	0.043*
H9C0.26790.98860.90270.043*C100.21131 (19)0.44449 (12)0.50562 (10)0.0195 (3)H10A0.22370.38680.53360.023*C110.0902 (2)0.50586 (12)0.54282 (9)0.0189 (3)H11A0.02740.47290.57960.023*C120.18450 (19)0.58362 (12)0.57694 (9)0.0165 (3)H120.12640.64140.57990.020*C130.31752 (19)0.59043 (11)0.52161 (9)0.0161 (3)H130.28270.62170.47600.019*C140.46207 (19)0.63771 (11)0.55074 (9)0.0166 (3)H140.50000.60400.59450.020*C150.5868 (2)0.64160 (12)0.49218 (10)0.0203 (3)H15A0.60630.58040.47230.024*H15B0.55620.68160.45120.024*C160.0177 (2)0.47929 (12)0.41967 (10)0.0207 (4)C17-0.1173 (2)0.41418 (14)0.41582 (11)0.0288 (4)H17A-0.12260.37870.46110.043*	H9B	0.3796	0.9704	0.8356	0.043*
C100.21131 (19)0.4449 (12)0.50562 (10)0.0195 (3)H10A0.22370.38680.53360.023*C110.0902 (2)0.50586 (12)0.54282 (9)0.0189 (3)H11A0.02740.47290.57960.023*C120.18450 (19)0.58362 (12)0.57694 (9)0.0165 (3)H120.12640.64140.57990.020*C130.31752 (19)0.59043 (11)0.52161 (9)0.0161 (3)H130.28270.62170.47600.019*C140.46207 (19)0.63771 (11)0.55074 (9)0.0166 (3)H140.50000.60400.59450.020*C150.5868 (2)0.64160 (12)0.49218 (10)0.0203 (3)H15A0.60630.58040.47230.024*H15B0.55620.68160.45120.024*C160.0177 (2)0.47929 (12)0.41967 (10)0.0207 (4)C17-0.1173 (2)0.41418 (14)0.41582 (11)0.0288 (4)H17A-0.12260.37870.46110.043*	Н9С	0.2679	0.9886	0.9027	0.043*
H10A 0.2237 0.3868 0.5336 0.023^* C11 $0.0902 (2)$ $0.50586 (12)$ $0.54282 (9)$ $0.0189 (3)$ H11A 0.0274 0.4729 0.5796 0.023^* C12 $0.18450 (19)$ $0.58362 (12)$ $0.57694 (9)$ $0.0165 (3)$ H12 0.1264 0.6414 0.5799 0.020^* C13 $0.31752 (19)$ $0.59043 (11)$ $0.52161 (9)$ $0.0161 (3)$ H13 0.2827 0.6217 0.4760 0.019^* C14 $0.46207 (19)$ $0.63771 (11)$ $0.55074 (9)$ 0.020^* C15 $0.5868 (2)$ $0.64160 (12)$ $0.49218 (10)$ $0.0203 (3)$ H15A 0.6063 0.5804 0.4723 0.024^* H15B 0.5562 0.6816 0.4512 0.024^* C16 $0.0177 (2)$ $0.41418 (14)$ $0.41582 (11)$ $0.0288 (4)$ H17A -0.1226 0.3787 0.4611 0.043^*	C10	0.21131 (19)	0.44449 (12)	0.50562 (10)	0.0195 (3)
C110.0902 (2)0.50586 (12)0.54282 (9)0.0189 (3)H11A0.02740.47290.57960.023*C120.18450 (19)0.58362 (12)0.57694 (9)0.0165 (3)H120.12640.64140.57990.020*C130.31752 (19)0.59043 (11)0.52161 (9)0.0161 (3)H130.28270.62170.47600.019*C140.46207 (19)0.63771 (11)0.55074 (9)0.0166 (3)H140.50000.60400.59450.020*C150.5868 (2)0.64160 (12)0.49218 (10)0.0203 (3)H15A0.60630.58040.47230.024*H15B0.55620.68160.45120.024*C160.0177 (2)0.47929 (12)0.41967 (10)0.0207 (4)C17-0.1173 (2)0.41418 (14)0.41582 (11)0.0288 (4)H17A-0.12260.37870.46110.043*	H10A	0.2237	0.3868	0.5336	0.023*
H11A0.02740.47290.57960.023*C120.18450 (19)0.58362 (12)0.57694 (9)0.0165 (3)H120.12640.64140.57990.020*C130.31752 (19)0.59043 (11)0.52161 (9)0.0161 (3)H130.28270.62170.47600.019*C140.46207 (19)0.63771 (11)0.55074 (9)0.0166 (3)H140.50000.60400.59450.020*C150.5868 (2)0.64160 (12)0.49218 (10)0.0203 (3)H15A0.60630.58040.47230.024*H15B0.55620.68160.45120.0207 (4)C17-0.1173 (2)0.41418 (14)0.41582 (11)0.0288 (4)H17A-0.12260.37870.46110.043*	C11	0.0902 (2)	0.50586 (12)	0.54282 (9)	0.0189 (3)
C120.18450 (19)0.58362 (12)0.57694 (9)0.0165 (3)H120.12640.64140.57990.020*C130.31752 (19)0.59043 (11)0.52161 (9)0.0161 (3)H130.28270.62170.47600.019*C140.46207 (19)0.63771 (11)0.55074 (9)0.0166 (3)H140.50000.60400.59450.020*C150.5868 (2)0.64160 (12)0.49218 (10)0.0203 (3)H15A0.60630.58040.47230.024*H15B0.55620.68160.45120.0207 (4)C17-0.1173 (2)0.41418 (14)0.41582 (11)0.0288 (4)H17A-0.12260.37870.46110.043*	H11A	0.0274	0.4729	0.5796	0.023*
H120.12640.64140.57990.020*C130.31752 (19)0.59043 (11)0.52161 (9)0.0161 (3)H130.28270.62170.47600.019*C140.46207 (19)0.63771 (11)0.55074 (9)0.0166 (3)H140.50000.60400.59450.020*C150.5868 (2)0.64160 (12)0.49218 (10)0.0203 (3)H15A0.60630.58040.47230.024*H15B0.55620.68160.45120.024*C160.0177 (2)0.47929 (12)0.41967 (10)0.0207 (4)C17-0.1173 (2)0.41418 (14)0.41582 (11)0.0288 (4)H17A-0.12260.37870.46110.043*	C12	0.18450 (19)	0.58362 (12)	0.57694 (9)	0.0165 (3)
C130.31752 (19)0.59043 (11)0.52161 (9)0.0161 (3)H130.28270.62170.47600.019*C140.46207 (19)0.63771 (11)0.55074 (9)0.0166 (3)H140.50000.60400.59450.020*C150.5868 (2)0.64160 (12)0.49218 (10)0.0203 (3)H15A0.60630.58040.47230.024*H15B0.55620.68160.45120.0207 (4)C160.0177 (2)0.47929 (12)0.41967 (10)0.0207 (4)C17-0.1173 (2)0.41418 (14)0.41582 (11)0.0288 (4)H17A-0.12260.37870.46110.043*	H12	0.1264	0.6414	0.5799	0.020*
H130.28270.62170.47600.019*C140.46207 (19)0.63771 (11)0.55074 (9)0.0166 (3)H140.50000.60400.59450.020*C150.5868 (2)0.64160 (12)0.49218 (10)0.0203 (3)H15A0.60630.58040.47230.024*H15B0.55620.68160.45120.0207 (4)C160.0177 (2)0.47929 (12)0.41967 (10)0.0207 (4)C17-0.1173 (2)0.41418 (14)0.41582 (11)0.0288 (4)H17A-0.12260.37870.46110.043*	C13	0.31752 (19)	0.59043 (11)	0.52161 (9)	0.0161 (3)
C140.46207 (19)0.63771 (11)0.55074 (9)0.0166 (3)H140.50000.60400.59450.020*C150.5868 (2)0.64160 (12)0.49218 (10)0.0203 (3)H15A0.60630.58040.47230.024*H15B0.55620.68160.45120.0207 (4)C160.0177 (2)0.417929 (12)0.41967 (10)0.0207 (4)C17-0.1173 (2)0.41418 (14)0.41582 (11)0.0288 (4)H17A-0.12260.37870.46110.043*	H13	0.2827	0.6217	0.4760	0.019*
H140.50000.60400.59450.020*C150.5868 (2)0.64160 (12)0.49218 (10)0.0203 (3)H15A0.60630.58040.47230.024*H15B0.55620.68160.45120.024*C160.0177 (2)0.47929 (12)0.41967 (10)0.0207 (4)C17-0.1173 (2)0.41418 (14)0.41582 (11)0.0288 (4)H17A-0.12260.37870.46110.043*	C14	0.46207 (19)	0.63771 (11)	0.55074 (9)	0.0166 (3)
C150.5868 (2)0.64160 (12)0.49218 (10)0.0203 (3)H15A0.60630.58040.47230.024*H15B0.55620.68160.45120.024*C160.0177 (2)0.47929 (12)0.41967 (10)0.0207 (4)C17-0.1173 (2)0.41418 (14)0.41582 (11)0.0288 (4)H17A-0.12260.37870.46110.043*	H14	0.5000	0.6040	0.5945	0.020*
H15A0.60630.58040.47230.024*H15B0.55620.68160.45120.024*C160.0177 (2)0.47929 (12)0.41967 (10)0.0207 (4)C17-0.1173 (2)0.41418 (14)0.41582 (11)0.0288 (4)H17A-0.12260.37870.46110.043*	C15	0.5868 (2)	0.64160 (12)	0.49218 (10)	0.0203 (3)
H15B0.55620.68160.45120.024*C160.0177 (2)0.47929 (12)0.41967 (10)0.0207 (4)C17-0.1173 (2)0.41418 (14)0.41582 (11)0.0288 (4)H17A-0.12260.37870.46110.043*	H15A	0.6063	0.5804	0.4723	0.024*
C160.0177 (2)0.47929 (12)0.41967 (10)0.0207 (4)C17-0.1173 (2)0.41418 (14)0.41582 (11)0.0288 (4)H17A-0.12260.37870.46110.043*	H15B	0.5562	0.6816	0.4512	0.024*
C17-0.1173 (2)0.41418 (14)0.41582 (11)0.0288 (4)H17A-0.12260.37870.46110.043*	C16	0.0177 (2)	0.47929 (12)	0.41967 (10)	0.0207 (4)
H17A -0.1226 0.3787 0.4611 0.043*	C17	-0.1173 (2)	0.41418 (14)	0.41582 (11)	0.0288 (4)
	H17A	-0.1226	0.3787	0.4611	0.043*

H17B	-0.1051	0.3734	0.3739	0.043*
H17C	-0.2100	0.4491	0.4100	0.043*
C18	0.0392 (3)	0.53557 (16)	0.34954 (12)	0.0432 (6)
H18A	-0.0497	0.5734	0.3414	0.065*
H18B	0.0531	0.4950	0.3076	0.065*
H18C	0.1278	0.5743	0.3549	0.065*

Atomic displacement parameters $(Å^2)$

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.0209 (2)	0.01871 (19)	0.02014 (19)	-0.00514 (17)	0.00455 (17)	-0.00471 (16)
S2	0.01921 (19)	0.01991 (18)	0.01661 (18)	0.00203 (17)	0.00090 (17)	-0.00052 (15)
01	0.0146 (6)	0.0254 (6)	0.0145 (5)	-0.0016 (5)	-0.0011 (4)	-0.0011 (5)
O2	0.0169 (6)	0.0228 (6)	0.0266 (7)	-0.0005 (5)	-0.0004 (5)	-0.0102 (5)
O3	0.0157 (6)	0.0193 (6)	0.0229 (6)	-0.0036 (5)	-0.0008 (5)	-0.0047 (5)
O4	0.0241 (7)	0.0420 (8)	0.0130 (6)	-0.0132 (6)	-0.0020 (5)	0.0002 (5)
O5	0.0147 (6)	0.0289 (7)	0.0246 (6)	-0.0020 (5)	-0.0027 (5)	-0.0026 (5)
O6	0.0168 (6)	0.0146 (5)	0.0276 (6)	-0.0005 (5)	0.0041 (5)	-0.0045 (5)
O7	0.0240 (7)	0.0302 (7)	0.0257 (7)	0.0022 (6)	-0.0003 (5)	-0.0131 (6)
08	0.0238 (6)	0.0235 (6)	0.0219 (6)	0.0034 (5)	-0.0048 (5)	-0.0076 (5)
09	0.0229 (6)	0.0144 (5)	0.0237 (6)	0.0017 (5)	-0.0047 (5)	-0.0030 (5)
O10	0.0185 (7)	0.0374 (8)	0.0202 (6)	-0.0108 (6)	0.0027 (5)	-0.0039 (6)
C1	0.0169 (8)	0.0196 (8)	0.0178 (7)	0.0002 (6)	-0.0029 (6)	-0.0016 (6)
C2	0.0140 (8)	0.0170 (8)	0.0196 (8)	-0.0006 (6)	-0.0017 (6)	-0.0019 (6)
C3	0.0174 (8)	0.0172 (8)	0.0176 (8)	-0.0029 (6)	0.0008 (6)	-0.0027 (6)
C4	0.0171 (8)	0.0179 (7)	0.0136 (7)	-0.0022 (6)	-0.0009 (6)	-0.0006 (6)
C5	0.0170 (8)	0.0213 (8)	0.0155 (7)	-0.0042 (6)	-0.0012 (6)	0.0003 (6)
C6	0.0177 (8)	0.0194 (8)	0.0193 (8)	-0.0012 (7)	-0.0051 (7)	-0.0008 (6)
C7	0.0162 (8)	0.0220 (9)	0.0229 (8)	0.0007 (7)	-0.0026 (7)	-0.0070 (7)
C8	0.0200 (9)	0.0303 (10)	0.0290 (10)	0.0039 (8)	-0.0069 (7)	-0.0084 (8)
C9	0.0235 (9)	0.0212 (8)	0.0406 (11)	-0.0007 (8)	-0.0030 (8)	-0.0072 (8)
C10	0.0209 (9)	0.0158 (8)	0.0219 (8)	-0.0023 (6)	0.0004 (6)	-0.0028 (6)
C11	0.0179 (8)	0.0205 (8)	0.0181 (8)	-0.0014 (7)	0.0004 (7)	-0.0032 (6)
C12	0.0176 (8)	0.0166 (7)	0.0155 (7)	0.0021 (6)	-0.0003 (6)	-0.0014 (6)
C13	0.0174 (8)	0.0125 (7)	0.0183 (8)	0.0010 (6)	0.0006 (6)	-0.0010 (6)
C14	0.0173 (8)	0.0151 (7)	0.0173 (7)	-0.0002 (6)	-0.0016 (6)	0.0009 (6)
C15	0.0199 (9)	0.0216 (8)	0.0194 (8)	-0.0043 (7)	0.0000 (7)	-0.0020 (7)
C16	0.0272 (9)	0.0192 (8)	0.0156 (8)	-0.0010 (7)	-0.0001 (7)	-0.0014 (6)
C17	0.0290 (10)	0.0252 (9)	0.0323 (10)	-0.0045 (8)	-0.0071 (8)	-0.0029 (8)
C18	0.0697 (17)	0.0351 (12)	0.0247 (10)	-0.0063 (12)	0.0037 (10)	0.0069 (9)

Geometric parameters (Å, °)

S1—C3	1.8373 (17)	С5—Н5А	0.9800
S1—S2	2.0335 (6)	С6—Н6А	0.9700
S2—C12	1.8386 (17)	С6—Н6В	0.9700
O1—C1	1.408 (2)	С7—С9	1.510(3)
O1—C4	1.4442 (19)	С7—С8	1.517 (2)
O2—C1	1.425 (2)	C8—H8A	0.9600

O2—C7	1.427 (2)	C8—H8B	0.9600
O3—C2	1.432 (2)	C8—H8C	0.9600
O3—C7	1.440 (2)	С9—Н9А	0.9600
O4—C5	1.423 (2)	С9—Н9В	0.9600
O4—H4O	0.8200	С9—Н9С	0.9600
O5—C6	1.430 (2)	C10-C11	1.533 (2)
О5—Н5О	0.8200	C10—H10A	0.9800
O6—C10	1.421 (2)	C11—C12	1.522 (2)
O6—C13	1.4446 (19)	C11—H11A	0.9800
O7—C10	1.403 (2)	C12—C13	1.528 (2)
O7—C16	1.440 (2)	C12—H12	0.9800
O8—C16	1.423 (2)	C13—C14	1.527 (2)
O8—C11	1.426 (2)	C13—H13	0.9800
O9—C14	1.434 (2)	C14—C15	1.511 (2)
О9—Н9О	0.8200	C14—H14	0.9800
O10-C15	1.427 (2)	C15—H15A	0.9700
O10—H10O	0.8200	C15—H15B	0.9700
C1—C2	1.547 (2)	C16—C18	1.506 (3)
C1—H1	0.9800	C16—C17	1.510 (3)
C2—C3	1.522 (2)	C17—H17A	0.9600
С2—Н2	0.9800	С17—Н17В	0.9600
C3—C4	1.529 (2)	С17—Н17С	0.9600
С3—Н3	0.9800	C18—H18A	0.9600
C4—C5	1.514 (2)	C18—H18B	0.9600
C4—H4	0.9800	C18—H18C	0.9600
C5—C6	1.510(2)		
C3—S1—S2	98.99 (6)	С7—С9—Н9А	109.5
C12—S2—S1	99.69 (6)	С7—С9—Н9В	109.5
C1—O1—C4	107.15 (12)	Н9А—С9—Н9В	109.5
C1—O2—C7	109.10 (13)	С7—С9—Н9С	109.5
C2—O3—C7	107.43 (13)	Н9А—С9—Н9С	109.5
С5—О4—Н4О	109.5	Н9В—С9—Н9С	109.5
С6—О5—Н5О	109.5	O7—C10—O6	112.76 (14)
C10—O6—C13	108.45 (12)	O7—C10—C11	105.18 (14)
C10—O7—C16	110.64 (13)	O6—C10—C11	107.37 (13)
C16—O8—C11	109.08 (13)	O7—C10—H10A	110.5
С14—О9—Н9О	109.5	O6—C10—H10A	110.5
С15—О10—Н10О	109.5	C11-C10-H10A	110.5
O1—C1—O2	110.35 (13)	O8—C11—C12	109.33 (14)
O1—C1—C2	107.32 (13)	O8—C11—C10	103.76 (13)
O2—C1—C2	104.33 (13)	C12-C11-C10	103.25 (13)
O1—C1—H1	111.5	O8—C11—H11A	113.2
O2—C1—H1	111.5	C12-C11-H11A	113.2
C2—C1—H1	111.5	C10-C11-H11A	113.2
O3—C2—C3	109.47 (13)	C11—C12—C13	101.52 (13)
O3—C2—C1	104.45 (13)	C11—C12—S2	108.41 (12)
C3—C2—C1	103.61 (13)	C13—C12—S2	110.74 (11)
O3—C2—H2	112.9	C11—C12—H12	111.9
C3—C2—H2	112.9	C13—C12—H12	111.9

C1—C2—H2	112.9	S2—C12—H12	111.9
C2—C3—C4	102.08 (13)	O6—C13—C14	109.48 (13)
C2—C3—S1	109.50 (12)	O6-C13-C12	103.11 (13)
C4—C3—S1	111.67 (11)	C14—C13—C12	115.88 (14)
С2—С3—Н3	111.1	O6-C13-H13	109.4
С4—С3—Н3	111.1	C14—C13—H13	109.4
S1—C3—H3	111.1	С12—С13—Н13	109.4
O1—C4—C5	111.01 (13)	O9—C14—C15	111.09 (14)
O1—C4—C3	103.07 (13)	O9—C14—C13	106.17 (13)
C5—C4—C3	116.36 (13)	C15—C14—C13	112.10 (14)
O1—C4—H4	108.7	O9—C14—H14	109.1
С5—С4—Н4	108.7	C15—C14—H14	109.1
C3—C4—H4	108.7	C13-C14-H14	109.1
O4—C5—C6	111.65 (14)	O10-C15-C14	107.40 (13)
O4—C5—C4	104.38 (13)	O10-C15-H15A	110.2
C6—C5—C4	111.21 (14)	C14—C15—H15A	110.2
O4—C5—H5A	109.8	O10-C15-H15B	110.2
С6—С5—Н5А	109.8	C14—C15—H15B	110.2
С4—С5—Н5А	109.8	H15A—C15—H15B	108.5
O5—C6—C5	107.91 (13)	O8—C16—O7	105.71 (13)
О5—С6—Н6А	110.1	O8—C16—C18	108.36 (15)
С5—С6—Н6А	110.1	O7—C16—C18	109.05 (17)
O5—C6—H6B	110.1	O8—C16—C17	111.09 (15)
С5—С6—Н6В	110.1	O7—C16—C17	108.93 (15)
H6A—C6—H6B	108.4	C18—C16—C17	113.40 (17)
O2—C7—O3	104.00 (13)	С16—С17—Н17А	109.5
O2—C7—C9	109.33 (14)	С16—С17—Н17В	109.5
O3—C7—C9	108.17 (15)	H17A—C17—H17B	109.5
O2—C7—C8	110.29 (15)	С16—С17—Н17С	109.5
O3—C7—C8	111.04 (14)	H17A—C17—H17C	109.5
С9—С7—С8	113.56 (15)	H17B—C17—H17C	109.5
С7—С8—Н8А	109.5	C16-C18-H18A	109.5
С7—С8—Н8В	109.5	C16-C18-H18B	109.5
H8A—C8—H8B	109.5	H18A—C18—H18B	109.5
С7—С8—Н8С	109.5	C16—C18—H18C	109.5
H8A—C8—H8C	109.5	H18A—C18—H18C	109.5
H8B—C8—H8C	109.5	H18B—C18—H18C	109.5
C3—S1—S2—C12	-81.01 (8)	C16—O7—C10—O6	-110.42 (15)
C4—O1—C1—O2	89.04 (15)	C16—O7—C10—C11	6.27 (18)
C4—O1—C1—C2	-24.05 (17)	C13—O6—C10—O7	101.54 (16)
C7—O2—C1—O1	-131.43 (14)	C13—O6—C10—C11	-13.84 (17)
C7—O2—C1—C2	-16.44 (17)	C16—O8—C11—C12	133.98 (14)
C7—O3—C2—C3	133.13 (14)	C16—O8—C11—C10	24.34 (17)
C7—O3—C2—C1	22.72 (16)	O7—C10—C11—O8	-18.43 (17)
O1—C1—C2—O3	113.11 (14)	O6—C10—C11—O8	101.89 (15)
O2—C1—C2—O3	-3.99 (16)	O7—C10—C11—C12	-132.51 (14)
O1—C1—C2—C3	-1.50 (17)	O6—C10—C11—C12	-12.19 (17)
O2—C1—C2—C3	-118.60 (14)	O8—C11—C12—C13	-78.46 (16)
O3—C2—C3—C4	-86.56 (15)	C10-C11-C12-C13	31.52 (16)

C1—C2—C3—C4	24.41 (16)	O8—C11—C12—S2	164.88 (11)
O3—C2—C3—S1	154.98 (11)	C10-C11-C12-S2	-85.14 (13)
C1—C2—C3—S1	-94.05 (13)	S1—S2—C12—C11	-84.82 (11)
S2—S1—C3—C2	-87.01 (11)	S1—S2—C12—C13	164.62 (10)
S2—S1—C3—C4	160.68 (10)	C10-06-C13-C14	158.11 (13)
C1—O1—C4—C5	165.20 (13)	C10-06-C13-C12	34.22 (16)
C1—O1—C4—C3	39.93 (15)	C11-C12-C13-O6	-40.33 (16)
C2—C3—C4—O1	-39.16 (15)	S2-C12-C13-O6	74.62 (14)
S1—C3—C4—O1	77.74 (13)	C11-C12-C13-C14	-159.90 (14)
C2—C3—C4—C5	-160.87 (14)	S2-C12-C13-C14	-44.95 (17)
S1—C3—C4—C5	-43.97 (17)	O6—C13—C14—O9	-174.31 (12)
O1—C4—C5—O4	177.28 (13)	C12-C13-C14-O9	-58.27 (18)
C3—C4—C5—O4	-65.29 (18)	O6-C13-C14-C15	64.22 (17)
O1—C4—C5—C6	56.74 (18)	C12-C13-C14-C15	-179.75 (14)
C3—C4—C5—C6	174.17 (14)	O9—C14—C15—O10	67.98 (18)
O4—C5—C6—O5	67.08 (17)	C13-C14-C15-O10	-173.41 (14)
C4—C5—C6—O5	-176.77 (13)	C11O8C16O7	-20.99 (18)
C1—O2—C7—O3	30.63 (17)	C11-O8-C16-C18	-137.78 (17)
C1—O2—C7—C9	145.97 (15)	C11-O8-C16-C17	97.02 (17)
C1—O2—C7—C8	-88.49 (17)	C10—O7—C16—O8	8.42 (18)
C2—O3—C7—O2	-33.02 (16)	C10-07-C16-C18	124.73 (17)
C2—O3—C7—C9	-149.18 (14)	C10-07-C16-C17	-111.03 (16)
C2—O3—C7—C8	85.58 (17)		

Hydrogen-bond geometry (Å, °)

D—H···A	<i>D</i> —Н	$H \cdots A$	$D \cdots A$	D—H··· A
O4—H4O…O10 ⁱ	0.82	1.94	2.7249 (18)	159
O5—H5O····O3 ⁱ	0.82	1.99	2.8055 (18)	176
O9—H9O…O5 ⁱⁱ	0.82	2.05	2.8338 (17)	159
O10—H10O…O9 ⁱⁱⁱ	0.82	2.04	2.8305 (18)	163
	. 1 /2			

Symmetry codes: (i) *x*-1, *y*, *z*; (ii) *x*+1, *y*, *z*; (iii) *x*+1/2, -*y*+3/2, -*z*+1.



Fig. 1



