

Acta Crystallographica Section E Structure Reports Online

ISSN 1600-5368

(*E*)-1-(2,5-Dimethyl-3-thienyl)-3-(2hydroxyphenyl)prop-2-en-1-one

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Received 4 August 2010; accepted 4 August 2010

Key indicators: single-crystal X-ray study; T = 296 K; mean σ (C–C) = 0.002 Å; R factor = 0.038; wR factor = 0.112; data-to-parameter ratio = 19.1.

In the title compound, $C_{15}H_{14}O_2S$, the dihedral angle between the aromatic rings is 8.46 –(8)°. The central enone group is planar (r.m.s. deviation = 0.0267 Å) and is oriented at a dihedral angle of 1.20 (9)° with respect to the benzene ring and at 8.27 (9)° with respect to the thiophene group. In the crystal, the molecules are linked into polymeric chains extending along the *b* axis due to intermolecular O–H···O hydrogen bonding. An *S*(6) ring motif is formed due to a short intramolecular C–H···O contact. C–H··· π interactions involving a methyl group of the 2,5-dimethylthienyl group and the benzene ring are present. π – π interactions between the centroids of the benzene and heterocyclic rings [3.7691 (9) Å] also occur.

Related literature

For background to chalcones and their biological activity, see: Bandgar & Gawande (2010); Domínguez *et al.* (2001); Hans *et al.* (2010); Kayser & Kiderlen (2001); Mojzis *et al.* (2008); Vogel *et al.* (2010). For related structures, see: Asiri *et al.* (2010*a,b*); For graph-set notation, see: Bernstein *et al.* (1995).



Experimental

Crystal data $C_{15}H_{14}O_2S$ $M_r = 258.32$

Triclinic, $P\overline{1}$ a = 7.6095 (3) Å

b = 7.7900 (3) A	
c = 12.3109 (7) Å	
$\alpha = 98.527 \ (2)^{\circ}$	
$\beta = 91.943 \ (2)^{\circ}$	
$\gamma = 115.551 \ (1)^{\circ}$	
$V = 647.19 (5) \text{ Å}^3$	

Data collection

Bruker Kappa APEXII CCD	11156 measured reflections
diffractometer	3174 independent reflections
Absorption correction: multi-scan	2720 reflections with $I > 2\sigma(I)$
(SADABS; Bruker, 2005)	$R_{\rm int} = 0.022$
$T_{\min} = 0.968, \ T_{\max} = 0.985$	

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.038$	166 parameters
$wR(F^2) = 0.112$	H-atom parameters constrained
S = 1.05	$\Delta \rho_{\rm max} = 0.30 \ {\rm e} \ {\rm \AA}^{-3}$
3174 reflections	$\Delta \rho_{\rm min} = -0.23 \text{ e } \text{\AA}^{-3}$

Table 1

Hydrogen-bond geometry (Å, °).

Cg2 is the centroid of the C1-C6 benzene ring.

$D - H \cdots A$	D-H	$H \cdot \cdot \cdot A$	$D \cdots A$	$D - \mathbf{H} \cdot \cdot \cdot A$
$D1 - H1 \cdots O2^{i}$ $C8 - H8 \cdots O1$ $C15 - H15A \cdots Cg2^{ii}$	0.82	1.8900	2.7067 (14)	174
	0.93	2.2400	2.8416 (17)	122
	0.96	2.79	3.652 (2)	150

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

Data collection: *APEX2* (Bruker, 2009); cell refinement: *SAINT* (Bruker, 2009); 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 for Windows* (Farrugia, 1997) and *PLATON* (Spek, 2009); software used to prepare material for publication: *WinGX* (Farrugia, 1999) and *PLATON*.

The authors would like to thank the Chemistry Department, King Abdul Aziz University, Jeddah, Saudi Arabia, for providing the research facilities and for the financial support of this work *via* grant No. (3–045/430).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BQ2228).

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Z = 2

Mo $K\alpha$ radiation

 $0.30 \times 0.24 \times 0.22 \text{ mm}$

 $\mu = 0.24 \text{ mm}^{-1}$

T = 296 K

Mojzis, J., Varinska, L., Mojzisova, G., Kostova, I. & Mirossay, L. (2008). *Pharmacol. Res.* 57, 259–265.
Sheldrick, G. M. (2008). *Acta Cryst.* A64, 112–122.
Spek, A. L. (2009). *Acta Cryst.* D65, 148–155. Vogel, S., Barbic, M., Jürgenliemk, G. & Heilmann, J. (2010). Eur. J. Med. Chem. 45, 2206–2213.

Acta Cryst. (2010). E66, o2259–o2260 [https://doi.org/10.1107/S1600536810031284] (E)-1-(2,5-Dimethyl-3-thienyl)-3-(2-hydroxyphenyl)prop-2-en-1-one Abdullah M. Asiri, Salman A. Khan and M. Nawaz Tahir

S1. Comment

An enone system between two aromatic rings is generally known as a chalcones. It is an important class of natural products which serve as precursors for the preparation of various flavonoids and exhibit interesting pharmacological activities (Mojzis *et al.*, 2008). Natural and synthetic chalcones have shown broad spectrum of biological activities such as anti-inflammatory (Vogel *et al.*, 2010), antituberculosis (Hans *et al.*, 2010), antifungal (Bandgar & Gawande, 2010), antimalarial (Domínguez *et al.*, 2001) and antileish-manicidal (Kayser & Kiderlen 2001). Due to wide application of chalcons in the present communication, we report the synthesis and crystal structure of title compound I (Fig. 1).

Recently we have reported the crystal structures of (II) *i.e.* (*E*)-1-(2,5-dimethyl-3-thienyl)-3-(2,4,5-trimethoxyphenyl)prop-2-en-1-one (Asiri *et al.*, 2010*a*) and (III) *i.e.* (2*E*)-3-(3,4-dimethoxyphenyl)-1-(2,5-dimethylthiophen-3-yl)prop-2en-1-one (Asiri *et al.*, 2010*b*) which are related to the title compound and differ from (I) due to substitutions at the phenyl ring.

In (I), the group A (C1—C6/O1) of salicylaldehyde, the central group B (C7—C9/O2) and group C (C10—C15/S1) of 2,5-dimethylthiophen-3-yl moiety are planar with r. m. s. deviation of 0.0063, 0.0267 and 0.0100 Å, respectively. The dihedral angles between A/B, A/C and B/C are 1.20 (9), 8.46 (8) and 8.27 (9)°, respectively. In the title compound, an S(6) ring motif (Bernstein *et al.*, 1995) is formed due to intramolecular H-bonding of C—H…O type (Table 1, Fig. 2). The title compound is stabilized in the form of polymeric chains extending along the *b* axis due to O—H…O type of intermolecular H-bonding (Table 1, Fig. 2). The C—H… π (Table 1) and π - π interactions between the centroids of phenyl and heterocyclic rings at a distance of 3.7691 (9) Å [symmetry code: 1 - *x*, 1 - *y*, - *z*] also play important role in stabilizing the molecules.

S2. Experimental

A solution of 3-acetyl-2,5-dimethylthiophene (0.38 g, 2.5 mmol) and salicylaldehyde (0.30 g, 2.5 mmol) in an ethanolic solution of NaOH (3.0 g in 10 ml of ethanol) was stirred for 16 h at room temperature. The solution was poured into ice-cold water of pH = 2 (pH adjusted by HCl). The solid was separated and dissolved in CH₂Cl₂, this solution was washed with a saturated solution of NaHCO₃ and then evaporated to dryness. The residue was recrystallized from methanol/chloroform.Yellow solid: Yield: 78%; m.p. 418–419 K.

S3. Refinement

The H-atoms were positioned geometrically (O—H = 0.86, C–H = 0.93–0.96 Å) and refined as riding with $U_{iso}(H) = xU_{eq}(C, O)$, where x = 1.5 for hydroxy & methyl and x = 1.2 for aryl H-atoms.



Figure 1

View of the title compound with the atom numbering scheme. The thermal displacements are drawn at the 50% probability level.



Figure 2

The partial packing (*PLATON*; Spek, 2009) which shows that molecules form polymeric chains extending along the *b* axis.

(E)-1-(2,5-Dimethyl-3-thienyl)-3-(2-hydroxyphenyl)prop-2-en-1-one

Crystal data

 $C_{15}H_{14}O_2S$ $M_r = 258.32$ Triclinic, *P*1 Hall symbol: -P 1 a = 7.6095 (3) Å b = 7.7900 (3) Å c = 12.3109 (7) Å a = 98.527 (2)° $\beta = 91.943$ (2)° $\gamma = 115.551$ (1)° V = 647.19 (5) Å³

Data collection

Bruker Kappa APEXII CCD diffractometer Radiation source: fine-focus sealed tube Graphite monochromator Detector resolution: 8.10 pixels mm⁻¹ ω scans Absorption correction: multi-scan (*SADABS*; Bruker, 2005) $T_{\min} = 0.968, T_{\max} = 0.985$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier
Least-squares matrix: full	map
$R[F^2 > 2\sigma(F^2)] = 0.038$	Hydrogen site location: inferred from
$wR(F^2) = 0.112$	neighbouring sites
<i>S</i> = 1.05	H-atom parameters constrained
3174 reflections	$w = 1/[\sigma^2(F_o^2) + (0.0593P)^2 + 0.1362P]$
166 parameters	where $P = (F_o^2 + 2F_c^2)/3$
0 restraints	$(\Delta/\sigma)_{\rm max} = 0.001$
Primary atom site location: structure-invariant	$\Delta \rho_{\rm max} = 0.30 \text{ e } \text{\AA}^{-3}$
direct methods	$\Delta \rho_{\rm min} = -0.23 \text{ e} \text{ Å}^{-3}$

Z = 2

F(000) = 272

 $\theta = 2.5 - 25.3^{\circ}$

 $\mu = 0.24 \text{ mm}^{-1}$

Prism, yellow

 $0.30 \times 0.24 \times 0.22$ mm

11156 measured reflections

 $\theta_{\text{max}} = 28.6^{\circ}, \ \theta_{\text{min}} = 3.0^{\circ}$

3174 independent reflections

2720 reflections with $I > 2\sigma(I)$

T = 296 K

 $R_{\rm int} = 0.022$

 $h = -10 \rightarrow 11$

 $k = -9 \rightarrow 10$

 $l = -16 \rightarrow 16$

 $D_{\rm x} = 1.326 {\rm Mg} {\rm m}^{-3}$

Mo *K* α radiation, $\lambda = 0.71073$ Å

Cell parameters from 2182 reflections

Special details

Geometry. Bond distances, angles *etc*. have been calculated using the rounded fractional coordinates. All su's are estimated from the variances of the (full) variance-covariance matrix. The cell e.s.d.'s are taken into account in the estimation of distances, angles and torsion angles

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.

F 1		1	1	• • •		• • •	• , •	1. 1	,	18	21
Fractional	atomic	coordinates	and	isofronic	or e	auivalent	isofronic	displacement	narameters	IA^4	۰,
1 / 401101141	aronne	coordinates		isonopie	01 0	quiraction	isonopie	anspracement	parameters	(**	/

	x	У	Ζ	$U_{ m iso}$ */ $U_{ m eq}$	
S 1	0.67628 (6)	1.06807 (5)	0.38493 (3)	0.0475 (1)	
01	0.75707 (17)	0.38399 (14)	-0.02745 (8)	0.0464 (3)	
O2	0.73309 (16)	1.04466 (13)	0.01642 (8)	0.0461 (3)	
C1	0.79715 (18)	0.57560 (16)	-0.16540 (10)	0.0329 (3)	

C2	0.78885 (19)	0.40687 (17)	-0.13253 (10)	0.0343 (3)
C3	0.8126 (2)	0.26851 (19)	-0.20796 (12)	0.0434 (4)
C4	0.8396 (3)	0.2929 (2)	-0.31564 (12)	0.0504 (5)
C5	0.8450 (3)	0.4557 (2)	-0.35080 (12)	0.0507 (5)
C6	0.8256 (2)	0.5950 (2)	-0.27561 (11)	0.0427 (4)
C7	0.77922 (19)	0.73111 (17)	-0.09244 (10)	0.0343 (3)
C8	0.7412 (2)	0.74553 (17)	0.01224 (11)	0.0370 (3)
C9	0.72983 (18)	0.92090 (16)	0.06888 (10)	0.0334 (3)
C10	0.71496 (18)	0.94215 (17)	0.18852 (10)	0.0337 (3)
C11	0.7304 (2)	0.81420 (19)	0.25716 (11)	0.0429 (4)
C12	0.7131 (2)	0.8629 (2)	0.36472 (12)	0.0478 (4)
C13	0.7182 (3)	0.7610(3)	0.45856 (15)	0.0714 (7)
C14	0.68407 (19)	1.08881 (17)	0.24864 (10)	0.0360 (4)
C15	0.6562 (3)	1.2516 (2)	0.21248 (12)	0.0484 (5)
H1	0.75495	0.28106	-0.01816	0.0696*
Н3	0.81024	0.15882	-0.18542	0.0520*
H4	0.85434	0.19895	-0.36531	0.0605*
Н5	0.86144	0.47102	-0.42384	0.0609*
H6	0.83168	0.70550	-0.29889	0.0513*
H7	0.79737	0.83780	-0.12429	0.0411*
H8	0.72160	0.64484	0.04996	0.0445*
H11	0.75059	0.70703	0.22980	0.0515*
H13A	0.73513	0.64780	0.43117	0.1070*
H13B	0.59731	0.72392	0.49126	0.1070*
H13C	0.82534	0.84640	0.51317	0.1070*
H15A	0.77811	1.34346	0.19316	0.0725*
H15B	0.61341	1.31403	0.27168	0.0725*
H15C	0.55936	1.20163	0.14942	0.0725*

Atomic displacement parameters $(Å^2)$

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S 1	0.0656 (3)	0.0486 (2)	0.0318 (2)	0.0290 (2)	0.0077 (2)	0.0051 (1)
O1	0.0804 (7)	0.0384 (5)	0.0371 (5)	0.0376 (5)	0.0187 (5)	0.0171 (4)
O2	0.0761 (7)	0.0373 (5)	0.0389 (5)	0.0353 (5)	0.0124 (5)	0.0139 (4)
C1	0.0395 (6)	0.0311 (5)	0.0311 (6)	0.0176 (5)	0.0049 (5)	0.0075 (4)
C2	0.0425 (7)	0.0312 (5)	0.0321 (6)	0.0183 (5)	0.0060 (5)	0.0075 (4)
C3	0.0581 (8)	0.0336 (6)	0.0423 (7)	0.0244 (6)	0.0073 (6)	0.0047 (5)
C4	0.0663 (10)	0.0471 (8)	0.0384 (7)	0.0292 (7)	0.0063 (7)	-0.0037 (6)
C5	0.0690 (10)	0.0560 (8)	0.0285 (6)	0.0291 (7)	0.0091 (6)	0.0061 (6)
C6	0.0581 (8)	0.0422 (7)	0.0332 (7)	0.0250 (6)	0.0081 (6)	0.0126 (5)
C7	0.0435 (7)	0.0298 (5)	0.0353 (6)	0.0201 (5)	0.0061 (5)	0.0101 (4)
C8	0.0528 (7)	0.0299 (5)	0.0358 (6)	0.0238 (5)	0.0077 (5)	0.0094 (5)
C9	0.0413 (6)	0.0285 (5)	0.0343 (6)	0.0185 (5)	0.0044 (5)	0.0075 (4)
C10	0.0399 (6)	0.0301 (5)	0.0335 (6)	0.0174 (5)	0.0046 (5)	0.0065 (4)
C11	0.0595 (8)	0.0399 (6)	0.0379 (7)	0.0280 (6)	0.0075 (6)	0.0124 (5)
C12	0.0636 (9)	0.0472 (7)	0.0384 (7)	0.0276 (7)	0.0067 (6)	0.0145 (6)
C13	0.1111 (16)	0.0748 (12)	0.0457 (9)	0.0510(11)	0.0156 (10)	0.0288 (8)

C14	0.0428 (7)	0.0336 (6)	0.0329 (6)	0.0186 (5)	0.0030 (5)	0.0044 (5)
C15	0.0726 (10)	0.0449 (7)	0.0412 (7)	0.0395 (7)	0.0063 (7)	0.0046 (6)

Geometric parameters (Å, °)

$\begin{array}{c ccccccccccccccccccccccccccccccccccc$				
S1C14 1.7099 (13) C12C13 1.504 (2) 01C2 1.3476 (16) C14C15 1.498 (2) 02C9 1.2298 (15) C3H3 0.9300 01H1 0.8200 C4H4 0.9300 C1C6 1.4011 (18) C5H5 0.9300 C1C7 1.4564 (18) C6H6 0.9300 C2C3 1.393 (2) C8H8 0.9300 C3C4 1.377 (2) C11H11 0.9300 C4C5 1.384 (2) C13H13A 0.9600 C5C6 1.381 (2) C13-H13B 0.9600 C7C8 1.3295 (18) C15H15A 0.9600 C8C9 1.4777 (18) C15H15A 0.9600 C10C11 1.4372 (19) C15H15C 0.9600 C10C14 1.3788 (19) 1 1 S1C4 ⁱ 3.686 (2) C8H11 2.7400 S1H4 ⁱ 3.1500 C9H1 ⁱⁿ 3.0800 O1C2 ⁱⁱ 2.7067 (14) C9H1 ⁱⁿ 3.0800 O1C5 ⁱⁱⁱ 3.9386 (19) H1O2 ⁱⁱⁱⁱ 3.9800 </td <td>S1—C12</td> <td>1.7228 (16)</td> <td>C11—C12</td> <td>1.349 (2)</td>	S1—C12	1.7228 (16)	C11—C12	1.349 (2)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	S1—C14	1.7099 (13)	C12—C13	1.504 (2)
$02-C9$ 1.2298 (15) C3-H3 0.9300 $01-H1$ 0.8200 C4-H4 0.9300 $C1-C6$ 1.4011 (18) C5-H5 0.9300 $C1-C7$ 1.4564 (18) C6-H6 0.9300 $C1-C2$ 1.4083 (17) C7-H7 0.9300 $C2-C3$ 1.339 (2) C8-H8 0.9300 $C2-C3$ 1.339 (2) C1-H11 0.9300 $C4-C5$ 1.384 (2) C13-H13A 0.9600 $C5-C6$ 1.381 (2) C13-H13B 0.9600 $C7-C8$ 1.3295 (18) C13-H13C 0.9600 $C9-C10$ 1.4717 (18) C15-H15C 0.9600 $C10-C11$ 1.4372 (19) C15-H15C 0.9600 $C10-C14$ 1.3788 (19) U U $S1-C4^{4}$ 3.686 (2) C8-H11 2.7400 $S1-H4^{4}$ 3.1500 C9-H116' 3.0600 $O1-C2^{10}$ 2.3986 (19) H1-C15''' 2.9800 $O1-C5^{1}$ 3.9806 (19) H1-H15''' 2.98	O1—C2	1.3476 (16)	C14—C15	1.498 (2)
$\begin{array}{ccccccc} 0.1-H1 & 0.8200 & C4-H4 & 0.9300 \\ C1-C6 & 1.4011 (18) & C5-H5 & 0.9300 \\ C1-C7 & 1.4564 (18) & C6-H6 & 0.9300 \\ C1-C2 & 1.4083 (17) & C7-H7 & 0.9300 \\ C2-C3 & 1.393 (2) & C8-H8 & 0.9300 \\ C3-C4 & 1.377 (2) & C11-H11 & 0.9300 \\ C4-C5 & 1.384 (2) & C13-H13A & 0.9600 \\ C5-C6 & 1.381 (2) & C13-H13B & 0.9600 \\ C7-C8 & 1.3295 (18) & C13-H13C & 0.9600 \\ C8-C9 & 1.4777 (18) & C15-H15A & 0.9600 \\ C9-C10 & 1.4713 (17) & C15-H15B & 0.9600 \\ C10-C11 & 1.4782 (19) & C15-H15C & 0.9600 \\ C10-C14 & 1.3788 (19) & & & & & & & & \\ S1-C4' & 3.686 (2) & C8-H11 & 2.7400 \\ S1-H4^{2} & 3.1500 & C9-H15C & 3.0600 \\ O1-O2^{26} & 2.7067 (14) & C9-H15C & 3.0600 \\ O1-C2^{26} & 3.2790 (18) & C15-H15A & 2.9800 \\ O1-C5^{9} & 3.3986 (19) & H1-O2^{26} & 1.8900 \\ O2-C15 & 2.919 (2) & H1-H18 & 2.6800 \\ O1-C9' & 3.3986 (19) & H1-O2^{26} & 1.8900 \\ O2-C15 & 2.919 (2) & H1-H18 & 2.2700 \\ O2-C15 & 2.919 (2) & H1-H18 & 2.2700 \\ O2-C7' & 3.3745 (19) & H1-H15A^{26} & 2.5800 \\ O1-H15A^{26} & 2.2800 & H3-O2^{26} & 2.7600 \\ O1-H15A^{26} & 2.8300 & H3-O2^{26} & 2.7600 \\ O1-H15A^{26} & 2.8300 & H3-O2^{26} & 2.7600 \\ O1-H15A^{26} & 2.8300 & H3-O2^{26} & 2.7600 \\ O1-H15A^{27} & 2.7600 & H6-H7 & 2.3200 \\ O2-H1^{18} & 2.2400 & H3-H1 & 2.2700 \\ O2-H1^{18} & 2.2400 & H3-H1 & 2.2700 \\ O2-H1^{18} & 2.6000 & H7-H16 & 2.3200 \\ O2-H1^{18} & 2.6000 & H7-H16 & 2.3200 \\ O2-H1^{18} & 2.6000 & H7-H16 & 2.3200 \\ O2-H15C & 2.6200 & H7-H6 & 2.3200 \\ O2-H15C & 2.6200 & H7-H16 & 2.4000 \\ C2-C14' & 3.583 (2) & H8-C11 & 2.6800 \\ C3-C14' & 3.599 (2) & H8-H11 & 2.1800 \\ C4-C14' & 3.590 \\ H1-H13A & 2.5900 \\ H1-H$	O2—C9	1.2298 (15)	С3—Н3	0.9300
C1C6 1.4011 (18) C5H5 0.9300 C1C7 1.4564 (18) C6H6 0.9300 C1C2 1.4083 (17) C7H7 0.9300 C2C3 1.393 (2) C8H8 0.9300 C3C4 1.377 (2) C11H11 0.9300 C4C5 1.384 (2) C13H13A 0.9600 C5C6 1.381 (2) C13H13B 0.9600 C5C6 1.381 (2) C15H15A 0.9600 C9C10 1.4717 (18) C15H15A 0.9600 C10C11 1.4372 (19) C15H15C 0.9600 C10C14 1.3788 (19) U U S1C4' 3.686 (2) C8H1 2.7400 S1H4 [#] 3.1500 C9H15C 3.0600 O1C14 1.3788 (19) H102 ^m 3.0800 O1C15 ^m 3.2790 (18) C15H1 ¹⁷ 2.9800 O1C15 ^m 3.2790 (18) C15H1 ¹⁷ 2.9800 O1C15 ^m 3.3986 (19) H102 ^m	O1—H1	0.8200	C4—H4	0.9300
C1C7 1.4564 (18) C6H6 0.9300 C1C2 1.4083 (17) C7-H7 0.9300 C2C3 1.393 (2) C8H8 0.9300 C3C4 1.377 (2) C11H11 0.9300 C4C5 1.384 (2) C13H13A 0.9600 C5C6 1.381 (2) C13H13B 0.9600 C7C8 1.3295 (18) C13H13C 0.9600 C7C8 1.3295 (18) C15H15A 0.9600 C10C11 1.4372 (19) C15H15C 0.9600 C10C14 1.3788 (19) S1C4 ⁱ 3.686 (2) C8H1 3.0600 C1C14 1.3788 (19) 3.0800 S1C4 ⁱ 3.686 (2) C8H1 ⁱ 3.0800 <	C1—C6	1.4011 (18)	С5—Н5	0.9300
C1-C21.4083 (17)C7-H70.9300C2-C31.393 (2)C8-H80.9300C3-C41.377 (2)C11-H110.9300C4-C51.384 (2)C13-H13A0.9600C5-C61.381 (2)C13-H13B0.9600C7-C81.3295 (18)C13-H13C0.9600C8-C91.4717 (18)C15-H15A0.9600C9-C101.4713 (17)C15-H15A0.9600C10-C111.4372 (19)C15-H15C0.9600C10-C141.3788 (19)TTS1-C4 ⁴ 3.686 (2)C8-H112.7400S1-H4 ⁱⁱ 3.1500C9-H1 ^{ix} 3.0600O1-C2 ⁱⁱⁱ 2.7067 (14)C9-H1 ^{ix} 3.0800O1-C2 ⁱⁱⁱ 2.7067 (14)C15-H17*2.9800O1-C2 ⁱⁱⁱ 3.2790 (18)C15-H1 ^{ix} 2.9800O1-C2 ⁱⁱⁱ 3.2790 (18)C15-H1 ^{ix} 2.9800O2-C152.919 (2)H1-H15A ⁱⁱⁱ 2.9800O2-C152.919 (2)H1-H15A ⁱⁱⁱ 2.5600O1-H15A ⁱⁱⁱ 2.7000H1-H15C ⁱⁱⁱ 2.5800O1-H15A ⁱⁱⁱ 2.7000H1-H15C ⁱⁱⁱ 2.5800O1-H15A ⁱⁱⁱ 2.7000H1-H15C ⁱⁱⁱ 2.3200O2-C1 ⁱⁱ 3.8300H2-C22.4000O2-H3 ^{ix} 2.7600H6-H72.3200O2-H3 ^{ix} 2.7600H6-H72.3200O2-H15C2.6200H7-H62.3200O2-H15C2.6200H7-H15C ⁱⁱ 2.6000O2-H15C ⁱⁱⁱ 2.7700H8-C112.6800 <tr<< td=""><td>C1—C7</td><td>1.4564 (18)</td><td>С6—Н6</td><td>0.9300</td></tr<<>	C1—C7	1.4564 (18)	С6—Н6	0.9300
C2-C31.393 (2)C8-H80.9300C3-C41.377 (2)C11-H110.9300C4-C51.384 (2)C13-H13A0.9600C5-C61.381 (2)C13-H13B0.9600C7-C81.3295 (18)C13-H13C0.9600C8-C91.4777 (18)C15-H15A0.9600C9-C101.4713 (17)C15-H15B0.9600C10-C111.4372 (19)C15-H15C0.9600C10-C141.3788 (19)VVS1-C4 ¹ 3.686 (2)C8-H112.7400S1-H4 ²ⁱ 3.1500C9-H15C3.0600O1-O2 ²ⁱⁱ 2.7067 (14)C9-H1 ¹ 82.8600O1-C5 ⁴ⁱ 3.2790 (18)C15-H172.9800O1-C5 ⁴ⁱ 3.2790 (18)C15-H11 ¹⁸ 2.9800O2-C152.919 (2)H1···H32.2700O2-C162.3916 (17)H1···C5 ¹⁶ⁱ 2.9800O2-C17 ¹⁴ 3.3460 (17)H1···C5 ¹⁶ⁱ 2.9800O2-C182.919 (2)H1···H32.2700O2-C7 ³ 3.3745 (19)H1···H15A ¹¹ 2.5600O1-··H182.2400H3···H12.2700O2-··C7 ¹⁴ 2.8800H3···O2 ¹⁶ 3.1500O2-··H15A ¹¹ 2.8800H3···H12.2800O2-··H15A ¹¹ 2.6000H1····H15C ¹¹ 2.6000O1-··H182.2400H3···H12.2200O2-··C7 ¹⁵ 3.830 (17)H1····H15C ¹¹ 2.6000O2-··H16A2.3200C2-··C102.6000O2-··H172.6000H1····H15C ¹¹ </td <td>C1—C2</td> <td>1.4083 (17)</td> <td>С7—Н7</td> <td>0.9300</td>	C1—C2	1.4083 (17)	С7—Н7	0.9300
C3-C41.377 (2)C11-H110.9300C4-C51.384 (2)C13-H13A0.9600C5-C61.381 (2)C13-H13B0.9600C7-C81.3295 (18)C13-H13C0.9600C8-C91.4777 (18)C15-H15A0.9600C9-C101.4713 (17)C15-H15B0.9600C10-C111.4372 (19)C15-H15C0.9600C10-C141.3788 (19)	C2—C3	1.393 (2)	C8—H8	0.9300
C4—C51.384 (2)C13—H13A0.9600C5—C61.381 (2)C13—H13C0.9600C7—C81.3295 (18)C13—H13C0.9600C8—C91.4777 (18)C15—H15A0.9600C9—C101.4713 (17)C15—H15B0.9600C10—C111.4372 (19)C15—H15C0.9600C10—C141.4372 (19)C15—H15C3.0600C10—C14	C3—C4	1.377 (2)	C11—H11	0.9300
C5-C61.381 (2)C13-H13B0.9600C7-C81.3295 (18)C13-H13C0.9600C8-C91.4777 (18)C15-H15A0.9600C9-C101.4713 (17)C15-H15A0.9600C10-C111.4372 (19)C15-H15C0.9600C10-C141.3788 (19)	C4—C5	1.384 (2)	C13—H13A	0.9600
$C7-C8$ $1.3295 (18)$ $C13-H13C$ 0.9600 $C8-C9$ $1.4777 (18)$ $C15-H15A$ 0.9600 $C9-C10$ $1.4713 (17)$ $C15-H15B$ 0.9600 $C10-C11$ $1.4372 (19)$ $C15-H15C$ 0.9600 $C10-C14$ $1.3788 (19)$ V V $S1\cdots C4^i$ $3.686 (2)$ $C8\cdots H11$ 2.7400 $S1\cdots H4^{ii}$ 3.1500 $C9\cdots H15C$ 3.0600 $O1\cdots O2^{in}$ $2.7067 (14)$ $C9\cdots H1^v$ 3.0800 $O1\cdots C4^i$ $3.2790 (18)$ $C15\cdots H1^v$ 2.9800 $O1\cdots C4^{ji}$ $3.2790 (18)$ $C15\cdots H1^v$ 2.9800 $O1\cdots C9^{ii}$ $3.2986 (19)$ $H1\cdots C9^{ii}$ 1.8900 $O2\cdots C1^v$ $3.4160 (17)$ $H1\cdots C15^{iii}$ 2.9800 $O2\cdots C7^v$ $3.4160 (17)$ $H1\cdots H13$ 2.2700 $O2\cdots C7^v$ $3.745 (19)$ $H1\cdots H15C^{iii}$ 2.5800 $O1\cdots H15A^{iii}$ 2.7900 $H1\cdots H15C^{iii}$ 2.5800 $O1\cdots H15A^{iii}$ 2.8800 $H3\cdots O2^{2ii}$ 2.7600 $O1\cdots H15A^{iii}$ 2.8800 $H3\cdots O2^{2ii}$ 2.700 $O2\cdots C7^v$ $3.745 (19)$ $H1\cdots H15C^{iii}$ 2.3200 $O2\cdots H1^v$ 2.8800 $H3\cdots O2^{2ii}$ 2.700 $O1\cdots H15A^{iii}$ 2.800 $H3\cdots O2^{2ii}$ 2.700 $O2\cdots H1^v$ 2.6000 $H3\cdots O$	C5—C6	1.381 (2)	C13—H13B	0.9600
C8—C91.4777 (18)C15—H15A0.9600C9—C101.4713 (17)C15—H15B0.9600C10—C111.4372 (19)C15—H15C0.9600C10—C141.3788 (19)	С7—С8	1.3295 (18)	C13—H13C	0.9600
C9-C101.4713 (17)C15-H15B0.9600C10-C111.4372 (19)C15-H15C0.9600C10-C141.3788 (19)C15-H15C0.9600S1-··C4i3.686 (2)C8···H112.7400S1···C4i3.1500C9···H15C3.0600O1···C2 ⁱⁱⁱ 2.7067 (14)C9···H1 ^{iv} 3.0800O1···C32.8416 (17)C11···H82.6800O1···C4i3.2790 (18)C15···H1 ^{iv} 2.9800O1···C9i3.3986 (19)H1···C2 ⁱⁱⁱ 1.8900O2···O1 ^{iv} 2.7067 (14)H1···C9 ⁱⁱⁱ 2.9800O2···C152.919 (2)H1···H32.2700O2···C152.919 (2)H1···H32.5600O1···H15A ⁱⁱⁱ 2.5800H3···O2 ⁱⁱⁱ 2.5800O1···H15A ⁱⁱⁱ 2.7000H1···H15A ⁱⁱⁱ 2.5800O1···H15C ⁱⁱⁱ 2.8800H3···O2 ⁱⁱⁱ 3.1500O2···C173.3745 (19)H1···H15A ⁱⁱⁱ 3.1500O2···C152.919 (2)H1···H32.2700O2···C152.919 (2)H1···H32.3200O2···C152.9000H4··S1 ⁱⁱⁱ 3.1500O2···C152.8800H3···O22.4000O2···H1 ⁱ N1.8900H4··S1 ⁱⁱⁱ 3.1500O2···H1 ⁱ S2.6200H7···H62.3200O2···H15C2.6200H7···H15C ⁱⁱⁱ 2.6000O2···H15C ⁱⁱ 2.7700H8···C12.6800C3···O2 ⁱⁱ 3.4160 (17)H8···C12.6800C3···O2 ⁱⁱ 3.4160 (17)H8···C12.6800 </td <td>C8—C9</td> <td>1.4777 (18)</td> <td>C15—H15A</td> <td>0.9600</td>	C8—C9	1.4777 (18)	C15—H15A	0.9600
$\begin{array}{ccccc} C10-C11 & 1.4372 (19) & C15-H15C & 0.9600 \\ C10-C14 & 1.3788 (19) & & & & & & & & & & & & & & & & & & &$	C9—C10	1.4713 (17)	C15—H15B	0.9600
C10—C141.3788 (19) $S1\cdots C4^i$ $3.686 (2)$ $C8\cdots H11$ 2.7400 $S1\cdots H4^{ii}$ 3.1500 $C9\cdots H15C$ 3.0600 $O1\cdots O2^{iii}$ $2.7067 (14)$ $C9\cdots H1^{iv}$ 3.0800 $O1\cdots C5^{iii}$ $3.2790 (18)$ $C15\cdots H1^{iv}$ 2.9800 $O1\cdots C9^j$ $3.3986 (19)$ $H1\cdots C9^{iii}$ 1.8900 $O2\cdots C1^{iv}$ $2.7067 (14)$ $H1\cdots C9^{iii}$ 3.0800 $O2\cdots C1^{iv}$ $2.7067 (14)$ $H1\cdots C9^{iii}$ 2.9800 $O2\cdots C1^{iv}$ $2.7067 (14)$ $H1\cdots C15^{iii}$ 2.9800 $O2\cdots C1^{iv}$ $2.7067 (14)$ $H1\cdots C15^{iii}$ 2.9800 $O2\cdots C1^{iv}$ $3.3745 (19)$ $H1\cdots H15A^{iii}$ 2.5600 $O2\cdots C7^{v}$ $3.3745 (19)$ $H1\cdots H15C^{iii}$ 2.5800 $O1\cdots H15A^{iii}$ 2.7000 $H1\cdots H15C^{iii}$ 2.5800 $O1\cdots H15C^{iii}$ 2.8800 $H3\cdots H1$ 2.2700 $O2\cdots H1^{iv}$ 1.8900 $H4\cdots S1^{viii}$ 3.1500 $O2\cdots H1^{iv}$ 1.8900 $H4\cdots S1^{viii}$ 3.1500 $O2\cdots H1^{iv}$ 2.8300 $H7\cdots O2$ 2.4000 $O2\cdots H15C$ 2.6200 $H7\cdots H15C^{ii}$ 2.6000 $O2\cdots H15C^{ii}$ 2.4000 $H7\cdots H15C^{ii}$ 2.6000 $O2\cdots H15C^{ii}$ $3.583 (2)$ $H8\cdots C1$ 2.6800 $O2\cdots H15C^{ii}$ $3.583 (2)$ $H8\cdots C1$ 2.6800 $O2\cdots H15C^{ii}$ $3.686 (2)$ $H1\cdots H15C^{ii}$ 2.6800 $O2\cdots H15C^{ii}$ $3.583 (2)$ $H8\cdots C1$ 2.6800 $O2\cdots H1$	C10—C11	1.4372 (19)	C15—H15C	0.9600
S1C4'3.686 (2)C8H112.7400S1H4'''3.1500C9H1SC3.0600O1O2''''2.7067 (14)C9H1''3.0800O1C2'''2.8416 (17)C11H82.6800O1C15'''3.2790 (18)C15H1''2.9800O1C9'3.3986 (19)H1C9'''3.0800O2O1''2.7067 (14)H1C9'''3.0800O2C152.919 (2)H1H132.9800O2C7'3.3745 (19)H1H15A'''2.9800O1H15A'''2.7000H1H15A'''2.5600O1H15C'''2.8800H3O2'''2.5800O1H15C'''2.8800H3O2'''3.1500O2G7'3.3745 (19)H1H15C'''3.1500O1H15C'''2.8800H3O2'''3.1500O2H1''1.8900H4S1'''3.1500O2H1''1.8900H4S1'''3.2200O2H1''2.6200H7H62.3200O2H15C2.6200H7H62.3200O2H15C2.6200H7H15C''2.6000O2H15C2.6200H7H162.3200O2H1''3.583 (2)H8C22.9000C3Q2'''3.583 (2)H8C12.6800C3C14'3.559 (2)H8H112.1800C4S1'3.686 (2)H1K82.7400C6C14'3.642 (2)H1H82.1800C7C9'3.5138 (19)H1H13A2.5900	C10—C14	1.3788 (19)		
S1···C4i $3.686 (2)$ C8···H11 2.7400 S1···H4ii 3.1500 C9···H15C 3.0600 O1···C2iii $2.7067 (14)$ C9···H1iv 3.0800 O1···C8 $2.8416 (17)$ C11···H8 2.6800 O1···C15 ⁱⁱⁱ $3.2790 (18)$ C15···H1iv 2.9800 O1···C9i $3.3986 (19)$ H1···C9 ⁱⁱⁱ 3.0800 O2···C15 $2.7067 (14)$ H1···C9 ⁱⁱⁱ 3.0800 O2···C15 $2.919 (2)$ H1···H3 2.2700 O2···C7v $3.3745 (19)$ H1···H15A ⁱⁱⁱ 2.5600 O1···H15A ⁱⁱⁱ 2.7000 H1···H15C ⁱⁱⁱ 2.5800 O1···H15C ⁱⁱⁱ 2.8800 H3···O2 ⁱⁱⁱ 3.1500 O2···11v 2.8800 H3···O2 ⁱⁱⁱ 3.1500 O2···11sA 2.7600 H4···S1 ^{vii} 3.1500 O2···11sA 2.6000 H4···S1 ^{vii} 3.1500 O2···H1v 1.8900 H4···S1 ^{vii} 3.1500 O2···H1v 2.6000 H7···O2 2.4000 O2···H1sA 2.8300 H7···O2 2.4000 O2···H1SC 2.6200 H7···H6 2.3200 O2···H7 2.4000 H7···H15C ^{vi} 2.6000 O2···H7 2.7700 H8···O1 2.2400 C2···C10 ⁱ $3.583 (2)$ H8···C11 2.6800 C3···C14 ⁱ $3.559 (2)$ H8···H11 2.1800 C3···C14 ⁱ $3.559 (2)$ H8···H11 2.1800 C4···S1 ⁱ $3.686 (2)$ H11···H3A 2.5900				
S1···H4ii 3.1500 C9···H15C 3.0600 O1···O2 ⁱⁱⁱ 2.7067 (14)C9···H1 ^{iv} 3.0800 O1···C8 2.8416 (17)C11···H8 2.6800 O1···C15 ⁱⁱⁱ 3.2790 (18)C15···H1 ^{iv} 2.9800 O1···C9 ⁱⁱ 3.3986 (19)H1···O2 ⁱⁱⁱ 1.8900 O2···O1 ^{iv} 2.7067 (14)H1···C9 ⁱⁱⁱ 3.0800 O2···C15 2.919 (2)H1···H3 2.2700 O2···C7 ^v 3.3745 (19)H1···H15A ⁱⁱⁱ 2.5600 O1···H15A ⁱⁱⁱ 2.7900 H1···H15A ⁱⁱⁱ 2.5800 O1···H15C ⁱⁱⁱ 2.8800 H3···O2 ⁱⁱⁱ 2.700 O2···H1 ^{iv} 1.8900 H4···S1 ^{vii} 3.1500 O2···H1 ^{iv} 1.8900 H4···S1 ^{viii} 3.1500 O2···H1 ^{iv} 2.7600 H6···H7 2.3200 O2···H1 ^{iv} 2.6200 H7···H6 2.3200 O2···H15A 2.6200 H7···H6 2.3200 O2···H15C 2.6200 H7···H15C ^{vi} 2.6000 O2···H15C 2.6200 H7···H6 2.3200 O2···H15C 2.6200 H7···H15C ^{vi} 2.6000 O2···H15C ^{vi} 2.7700 H8···O1 2.2400 C2···C10 ⁱ 3.583 (2)H8···C2 2.9000 C3···C14 ⁱ 3.686 (2)H11····R8 2.1800 C3···C14 ⁱ 3.686 (2)H11····R8 2.1800 C4···S1 ⁱ 3.686 (2)H11····R9 2.7400 C6···C14 ^v 3.5138 (19)H11···H13A 2.5900	S1····C4 ⁱ	3.686 (2)	C8…H11	2.7400
$O1 \cdots O2^{iii}$ $2.7067 (14)$ $C9 \cdots H1^{iv}$ 3.0800 $O1 \cdots C8$ $2.8416 (17)$ $C11 \cdots H8$ 2.6800 $O1 \cdots C15^{iii}$ $3.2790 (18)$ $C15 \cdots H1^{iv}$ 2.9800 $O1 \cdots C9^i$ $3.3986 (19)$ $H1 \cdots C2^{iii}$ 1.8900 $O2 \cdots O1^{iv}$ $2.7067 (14)$ $H1 \cdots C9^{iii}$ 3.0800 $O2 \cdots C3^{iv}$ $3.4160 (17)$ $H1 \cdots C15^{iii}$ 2.9800 $O2 \cdots C3^{iv}$ $3.4160 (17)$ $H1 \cdots H153$ 2.9800 $O2 \cdots C15$ $2.919 (2)$ $H1 \cdots H153$ 2.5600 $O2 \cdots C7^{v}$ $3.3745 (19)$ $H1 \cdots H15C^{iii}$ 2.5800 $O1 \cdots H15A^{iii}$ 2.7900 $H1 \cdots H15C^{iii}$ 2.5800 $O1 \cdots H15A^{iii}$ 2.7900 $H3 \cdots O2^{iii}$ 2.7600 $O1 \cdots H15C^{iii}$ 2.8800 $H3 \cdots O2^{iii}$ 2.7600 $O1 \cdots H15C^{iii}$ 2.8800 $H3 \cdots O1$ 2.2700 $O2 \cdots H1^{iv}$ 1.8900 $H4 \cdots S1^{vii}$ 3.1500 $O2 \cdots H1^{iv}$ 2.8300 $H7 \cdots O2$ 2.4000 $O2 \cdots H1^{iv}$ 2.8300 $H7 \cdots H1$ 2.3200 $O2 \cdots H1^{iv}$ 2.6200 $H7 \cdots H1$ 2.2400 $O2 \cdots H1^{iv}$ 2.4000 $H7 \cdots H1$ 2.2400 $O2 \cdots H1^{iv}$ 2.7700 $H8 \cdots O1$ 2.2400 $O2 \cdots H1^{iv}$ $3.4160 (17)$ $H8 \cdots C11$ 2.6800 $O2 \cdots H1^{iv}$ $3.583 (2)$ $H8 \cdots C11$ 2.6800 $O2 \cdots H1^{iv}$ $3.559 (2)$ $H8 \cdots H11$ 2.1800 $C3 \cdots C14^{ii}$ $3.559 (2)$ $H8 \cdots H11$	S1…H4 ⁱⁱ	3.1500	C9…H15C	3.0600
$O1 \cdots C8$ $2.8416 (17)$ $C11 \cdots H8$ 2.6800 $O1 \cdots C15^{iii}$ $3.2790 (18)$ $C15 \cdots H1^{iv}$ 2.9800 $O1 \cdots C9^i$ $3.3986 (19)$ $H1 \cdots O2^{iii}$ 1.8900 $O2 \cdots C1^{iv}$ $2.7067 (14)$ $H1 \cdots C9^{iii}$ 3.0800 $O2 \cdots C3^{iv}$ $3.4160 (17)$ $H1 \cdots C15^{iii}$ 2.9800 $O2 \cdots C15$ $2.919 (2)$ $H1 \cdots H3$ 2.2700 $O2 \cdots C7^v$ $3.3745 (19)$ $H1 \cdots H15A^{iii}$ 2.5600 $O1 \cdots H15A^{iii}$ 2.7900 $H1 \cdots H15C^{iii}$ 2.5800 $O1 \cdots H15A^{iii}$ 2.7900 $H3 \cdots O2^{iii}$ 2.7600 $O1 \cdots H15C^{iii}$ 2.8800 $H3 \cdots O2^{iii}$ 2.7600 $O1 \cdots H15C^{iii}$ 2.800 $H3 \cdots H1$ 2.2700 $O2 \cdots H1^{iv}$ 1.8900 $H4 \cdots S1^{vii}$ 3.1500 $O2 \cdots H1^{iv}$ 1.8900 $H6 \cdots H7$ 2.3200 $O2 \cdots H1^{iv}$ 2.6200 $H7 \cdots H6$ 2.3200 $O2 \cdots H1^{iv}$ 2.6200 $H7 \cdots H6$ 2.3200 $O2 \cdots H1^{iv}$ 2.4000 $H7 \cdots H15C^{vi}$ 2.6000 $O2 \cdots H1^{iv}$ 2.4000 $H7 \cdots H15C^{vi}$ 2.6000 $O2 \cdots H1^{iv}$ 2.4000 $H7 \cdots H15C^{vi}$ 2.6000 $O2 \cdots H1^{iv}$ $3.513 (2)$ $H8 \cdots C11$ 2.6800 $O2 \cdots H1^{iv}$ $3.4160 (17)$ $H8 \cdots C11$ 2.6800 $O2 \cdots H1^{ii}$ $3.559 (2)$ $H8 \cdots H11$ 2.1800 $O3 \cdots O2^{iii}$ $3.4160 (17)$ $H8 \cdots C11$ 2.6800 $O3 \cdots O2^{iv}$ $3.548 (2)$ $H11 $	O1…O2 ⁱⁱⁱ	2.7067 (14)	C9…H1 ^{iv}	3.0800
$O1\cdots C15^{iii}$ $3.2790 (18)$ $C15\cdots H1^{iv}$ 2.9800 $O1\cdots C9^i$ $3.3986 (19)$ $H1\cdots O2^{iii}$ 1.8900 $O2\cdots O1^{iv}$ $2.7067 (14)$ $H1\cdots C9^{iii}$ 3.0800 $O2\cdots C3^{iv}$ $3.4160 (17)$ $H1\cdots C15^{iii}$ 2.9800 $O2\cdots C15$ $2.919 (2)$ $H1\cdots H3$ 2.2700 $O2\cdots C7^v$ $3.3745 (19)$ $H1\cdots H15A^{iii}$ 2.5600 $O1\cdots H15A^{iii}$ 2.7900 $H1\cdots H15C^{iii}$ 2.5800 $O1\cdots H15C^{iii}$ 2.8800 $H3\cdots O2^{iii}$ 2.7600 $O1\cdots H15C^{iii}$ 2.8800 $H3\cdots H1$ 2.2700 $O2\cdots H1^v$ 1.8900 $H4\cdots S1^{vii}$ 3.1500 $O2\cdots H1^{iv}$ 1.8900 $H4\cdots S1^{vii}$ 3.1500 $O2\cdots H1^{iv}$ 2.7600 $H6\cdots H7$ 2.3200 $O2\cdots H1^{iv}$ 2.6200 $H7\cdots H6$ 2.3200 $O2\cdots H1^{iv}$ 2.6200 $H7\cdots H15C^{vi}$ 2.6000 $O2\cdots H1^{it}$ 2.7700 $H8\cdots O1$ 2.2400 $O2\cdots H1^{it}$ $3.583 (2)$ $H8\cdots C2$ 2.9000 $O2\cdots H1^{it}$ $3.583 (2)$ $H8\cdots C11$ 2.6800 $O2\cdots H1^{it}$ $3.583 (2)$ $H8\cdots C11$ 2.6800 $O2\cdots C1^{it}$ $3.686 (2)$ $H1\cdots H8$ 2.1800 $C4\cdots S1^{i}$ $3.686 (2)$ $H1\cdots H8$ 2.1800 $C4\cdots C1^{it}$ $3.5138 (19)$ $H1\cdots H13A$ 2.5900	O1…C8	2.8416 (17)	С11…Н8	2.6800
$O1\cdots C9^i$ $3.3986(19)$ $H1\cdots O2^{iii}$ 1.8900 $O2\cdots O1^{iv}$ $2.7067(14)$ $H1\cdots C9^{iii}$ 3.0800 $O2\cdots C3^{iv}$ $3.4160(17)$ $H1\cdots C15^{iii}$ 2.9800 $O2\cdots C15$ $2.919(2)$ $H1\cdots H3$ 2.2700 $O2\cdots C7^v$ $3.3745(19)$ $H1\cdots H15A^{iii}$ 2.5600 $O1\cdots H15A^{iii}$ 2.7900 $H1\cdots H15C^{iii}$ 2.5800 $O1\cdots H15C^{iii}$ 2.8800 $H3\cdots O2^{iii}$ 2.7600 $O1\cdots H15C^{iii}$ 2.8800 $H3\cdots O2^{iii}$ 2.7600 $O1\cdots H8$ 2.2400 $H3\cdots H1$ 2.2700 $O2\cdots H1^{iv}$ 1.8900 $H4\cdots S1^{vii}$ 3.1500 $O2\cdots H3^{iv}$ 2.7600 $H6\cdots H7$ 2.3200 $O2\cdots H15A$ 2.8300 $H7\cdots O2$ 2.4000 $O2\cdots H15A$ 2.6200 $H7\cdots H15C^{vi}$ 2.3200 $O2\cdots H15C$ 2.6200 $H7\cdots H15C^{vi}$ 2.6000 $O2\cdots H15C$ 2.6200 $H7\cdots H15C^{vi}$ 2.9000 $O2\cdots H15C^{vi}$ 2.7700 $H8\cdots O1$ 2.2400 $O2\cdots H15C^{vi}$ $3.583(2)$ $H8\cdots C11$ 2.6800 $O2\cdots H15C^{vi}$ $3.583(2)$ $H8\cdots C11$ 2.8800 $O2\cdots H15C^{vi}$ $3.686(2)$ $H1\cdots C8$ 2.7400 $C4\cdots S1^{i}$ $3.686(2)$ $H1\cdots H8$ 2.1800 $C4\cdots S1^{i}$ $3.642(2)$ $H1\cdots H8$ 2.5900	O1…C15 ⁱⁱⁱ	3.2790 (18)	C15···H1 ^{iv}	2.9800
0201^{iv} $2.7067 (14)$ $H1C9^{iii}$ 3.0800 $02C3^{iv}$ $3.4160 (17)$ $H1C15^{iii}$ 2.9800 $02C15$ $2.919 (2)$ $H1H3$ 2.2700 $02C7^{\gamma}$ $3.3745 (19)$ $H1H15A^{iii}$ 2.5600 $01H15A^{iii}$ 2.7900 $H1H15C^{iii}$ 2.5800 $01H15C^{iii}$ 2.8800 $H3O2^{iii}$ 2.7600 $01H15C^{iii}$ 2.8800 $H3O2^{iii}$ 2.7600 $01H18$ 2.2400 $H3H1$ 2.2700 $02H1^{iv}$ 1.8900 $H4S1^{vii}$ 3.1500 $02H1^{iv}$ 2.7600 $H6H7$ 2.3200 $02H15A$ 2.8300 $H7O2$ 2.4000 $02H15A$ 2.6200 $H7H6$ 2.3200 $02H15C$ 2.6200 $H7H6$ 2.3200 $02H7$ 2.4000 $H7H15C^{vi}$ 2.6000 $02H7$ 2.4000 $H7H15C^{vi}$ 2.6000 $02H7$ $3.583 (2)$ $H8O1$ 2.2400 $02H7$ $3.4160 (17)$ $H8O1$ 2.6800 $03O2^{iii}$ $3.4160 (17)$ $H8C11$ 2.6800 $03O2^{iii}$ $3.686 (2)$ $H1C8$ 2.7400 $C4S1^{1}$ $3.686 (2)$ $H1H8$ 2.1800 $C7C9^{v}$ $3.5138 (19)$ $H1H13A$ 2.5900	O1…C9 ⁱ	3.3986 (19)	H1···O2 ⁱⁱⁱ	1.8900
$O2\cdots C3^{iv}$ $3.4160 (17)$ $H1\cdots C15^{iii}$ 2.9800 $O2\cdots C15$ $2.919 (2)$ $H1\cdots H3$ 2.2700 $O2\cdots C7^{v}$ $3.3745 (19)$ $H1\cdots H15A^{iii}$ 2.5600 $O1\cdots H15A^{iii}$ 2.7900 $H1\cdots H15C^{iii}$ 2.5800 $O1\cdots H15C^{iii}$ 2.8800 $H3\cdots O2^{iii}$ 2.7600 $O1\cdots H8$ 2.2400 $H3\cdots H1$ 2.2700 $O2\cdots H1^{iv}$ 1.8900 $H4\cdots S1^{vii}$ 3.1500 $O2\cdots H3^{iv}$ 2.7600 $H6\cdots H7$ 2.3200 $O2\cdots H15A$ 2.8300 $H7\cdots O2$ 2.4000 $O2\cdots H15A$ 2.6200 $H7\cdots H6$ 2.3200 $O2\cdots H15C$ 2.6200 $H7\cdots H6$ 2.3200 $O2\cdots H7$ 2.4000 $H7\cdots H15C^{vi}$ 2.6000 $O2\cdots H7$ $3.583 (2)$ $H8\cdots C1$ 2.6800 $C2\cdots C10^{i}$ $3.583 (2)$ $H8\cdots C1$ 2.6800 $C3\cdots O2^{iii}$ $3.4160 (17)$ $H8\cdots H11$ 2.1800 $C4\cdots S1^{i}$ $3.686 (2)$ $H1\cdots H8$ 2.7400 $C4\cdots S1^{i}$ $3.638 (19)$ $H1\cdots H13A$ 2.5900	O2…O1 ^{iv}	2.7067 (14)	H1···C9 ⁱⁱⁱ	3.0800
$O2\cdots C15$ 2.919 (2) $H1\cdots H3$ 2.2700 $O2\cdots C7^{v}$ 3.3745 (19) $H1\cdots H15A^{iii}$ 2.5600 $O1\cdots H15A^{iii}$ 2.7900 $H1\cdots H15C^{iii}$ 2.5800 $O1\cdots H15C^{iii}$ 2.8800 $H3\cdots O2^{iii}$ 2.7600 $O1\cdots H8$ 2.2400 $H3\cdots H1$ 2.2700 $O2\cdots H1^{iv}$ 1.8900 $H4\cdots S1^{vii}$ 3.1500 $O2\cdots H1^{iv}$ 2.7600 $H6\cdots H7$ 2.3200 $O2\cdots H15A$ 2.8300 $H7\cdots O2$ 2.4000 $O2\cdots H15C$ 2.6200 $H7\cdots H6$ 2.3200 $O2\cdots H15C$ 2.6200 $H7\cdots H15C^{vi}$ 2.6000 $O2\cdots H7$ 2.4000 $H7\cdots H15C^{vi}$ 2.6000 $O2\cdots H15C^{vi}$ 2.7700 $H8\cdots O1$ 2.2400 $C2\cdots C10^{i}$ 3.583 (2) $H8\cdots C2$ 2.9000 $C3\cdots O2^{iii}$ 3.4160 (17) $H8\cdots C11$ 2.6800 $C3\cdots C14^{i}$ 3.559 (2) $H8\cdots H11$ 2.1800 $C4\cdots S1^{i}$ 3.686 (2) $H1\cdots H8$ 2.7400 $C6\cdots C14^{v}$ 3.442 (2) $H11\cdots H8$ 2.1800 $C7\cdots C9^{v}$ 3.5138 (19) $H11\cdots H13A$ 2.5900	O2···C3 ^{iv}	3.4160 (17)	H1…C15 ⁱⁱⁱ	2.9800
$O2\cdots C7^v$ $3.3745 (19)$ $H1\cdots H15A^{iii}$ 2.5600 $O1\cdots H15A^{iii}$ 2.7900 $H1\cdots H15C^{iii}$ 2.5800 $O1\cdots H15C^{iii}$ 2.8800 $H3\cdots O2^{iii}$ 2.7600 $O1\cdots H8$ 2.2400 $H3\cdots H1$ 2.2700 $O2\cdots H1^{iv}$ 1.8900 $H4\cdots S1^{vii}$ 3.1500 $O2\cdots H3^{iv}$ 2.7600 $H6\cdots H7$ 2.3200 $O2\cdots H15A$ 2.8300 $H7\cdots O2$ 2.4000 $O2\cdots H15C$ 2.6200 $H7\cdots H6$ 2.3200 $O2\cdots H15C$ 2.6200 $H7\cdots H15C^{vi}$ 2.6000 $O2\cdots H15C^{vi}$ 2.7700 $H8\cdots O1$ 2.2400 $C2\cdots C10^i$ $3.583 (2)$ $H8\cdots C2$ 2.9000 $C3\cdots O2^{iii}$ $3.4160 (17)$ $H8\cdots C11$ 2.6800 $C3\cdots C14^i$ $3.559 (2)$ $H8\cdots H11$ 2.1800 $C4\cdots S1^i$ $3.686 (2)$ $H1\cdots C8$ 2.7400 $C6\cdots C14^v$ $3.442 (2)$ $H1\cdots H13A$ 2.5900	O2…C15	2.919 (2)	H1…H3	2.2700
$O1\cdotsH15A^{iii}$ 2.7900 $H1\cdotsH15C^{iii}$ 2.5800 $O1\cdotsH15C^{iii}$ 2.8800 $H3\cdotsO2^{iii}$ 2.7600 $O1\cdotsH8$ 2.2400 $H3\cdotsH1$ 2.2700 $O2\cdotsH1^{iv}$ 1.8900 $H4\cdotsS1^{vii}$ 3.1500 $O2\cdotsH3^{iv}$ 2.7600 $H6\cdotsH7$ 2.3200 $O2\cdotsH15A$ 2.8300 $H7\cdotsO2$ 2.4000 $O2\cdotsH15C$ 2.6200 $H7\cdotsH6$ 2.3200 $O2\cdotsH15C$ 2.6200 $H7\cdotsH15C^{vi}$ 2.6000 $O2\cdotsH15C^{vi}$ 2.7700 $H8\cdotsO1$ 2.2400 $O2\cdotsH15C^{vi}$ 3.583 (2) $H8\cdotsC2$ 2.9000 $C2\cdotsC10^{i}$ 3.583 (2) $H8\cdotsC11$ 2.6800 $C3\cdotsO2^{iii}$ 3.4160 (17) $H8\cdotsH11$ 2.1800 $C4\cdotsS1^{i}$ 3.686 (2) $H11\cdotsH8$ 2.1800 $C4\cdotsC14^{v}$ 3.442 (2) $H11\cdotsH3A$ 2.5900	O2…C7 ^v	3.3745 (19)	H1…H15A ⁱⁱⁱ	2.5600
$O1\cdots H15C^{iii}$ 2.8800 $H3\cdots O2^{iii}$ 2.7600 $O1\cdots H8$ 2.2400 $H3\cdots H1$ 2.2700 $O2\cdots H1^{iv}$ 1.8900 $H4\cdots S1^{vii}$ 3.1500 $O2\cdots H3^{iv}$ 2.7600 $H6\cdots H7$ 2.3200 $O2\cdots H15A$ 2.8300 $H7\cdots O2$ 2.4000 $O2\cdots H15C$ 2.6200 $H7\cdots H6$ 2.3200 $O2\cdots H15C$ 2.6200 $H7\cdots H5C^{vi}$ 2.6000 $O2\cdots H15C^{vi}$ 2.700 $H8\cdots O1$ 2.2400 $O2\cdots H15C^{vi}$ 2.7700 $H8\cdots C1$ 2.6800 $C2\cdots C10^i$ 3.583 (2) $H8\cdots C1$ 2.6800 $C3\cdots O2^{iii}$ 3.4160 (17) $H8\cdots C11$ 2.6800 $C3\cdots C14^i$ 3.559 (2) $H8\cdots H11$ 2.1800 $C4\cdots S1^i$ 3.686 (2) $H1\cdots H8$ 2.1800 $C6\cdots C14^v$ 3.442 (2) $H1\cdots H13A$ 2.5900	O1…H15A ⁱⁱⁱ	2.7900	H1···H15C ⁱⁱⁱ	2.5800
$O1\cdots H8$ 2.2400 $H3\cdots H1$ 2.2700 $O2\cdots H1^{iv}$ 1.8900 $H4\cdots S1^{vii}$ 3.1500 $O2\cdots H3^{iv}$ 2.7600 $H6\cdots H7$ 2.3200 $O2\cdots H15A$ 2.8300 $H7\cdots O2$ 2.4000 $O2\cdots H15C$ 2.6200 $H7\cdots H6$ 2.3200 $O2\cdots H7$ 2.4000 $H7\cdots H15C^{vi}$ 2.6000 $O2\cdots H15C^{vi}$ 2.7700 $H8\cdots O1$ 2.2400 $C2\cdots C10^i$ 3.583 (2) $H8\cdots C2$ 2.9000 $C3\cdots O2^{iii}$ 3.4160 (17) $H8\cdots C11$ 2.6800 $C3\cdots C14^i$ 3.559 (2) $H8\cdots H11$ 2.1800 $C4\cdots S1^i$ 3.686 (2) $H11\cdots R8$ 2.7400 $C6\cdots C14^v$ 3.442 (2) $H11\cdots H13A$ 2.5900	O1…H15C ⁱⁱⁱ	2.8800	H3····O2 ⁱⁱⁱ	2.7600
$O2\cdots H1^{iv}$ 1.8900 $H4\cdots S1^{vii}$ 3.1500 $O2\cdots H3^{iv}$ 2.7600 $H6\cdots H7$ 2.3200 $O2\cdots H15A$ 2.8300 $H7\cdots O2$ 2.4000 $O2\cdots H15C$ 2.6200 $H7\cdots H6$ 2.3200 $O2\cdots H7$ 2.4000 $H7\cdots H15C^{vi}$ 2.6000 $O2\cdots H15C^{vi}$ 2.7700 $H8\cdots O1$ 2.2400 $C2\cdots C10^i$ $3.583 (2)$ $H8\cdots C2$ 2.9000 $C3\cdots O2^{iii}$ $3.4160 (17)$ $H8\cdots C11$ 2.6800 $C3\cdots C14^i$ $3.559 (2)$ $H8\cdots H11$ 2.1800 $C4\cdots S1^i$ $3.686 (2)$ $H11\cdots R8$ 2.7400 $C6\cdots C14^v$ $3.442 (2)$ $H11\cdots H3A$ 2.5900	O1…H8	2.2400	H3…H1	2.2700
$O2\cdots H3^{iv}$ 2.7600 $H6\cdots H7$ 2.3200 $O2\cdots H15A$ 2.8300 $H7\cdots O2$ 2.4000 $O2\cdots H15C$ 2.6200 $H7\cdots H6$ 2.3200 $O2\cdots H7$ 2.4000 $H7\cdots H15C^{vi}$ 2.6000 $O2\cdots H15C^{vi}$ 2.7700 $H8\cdots O1$ 2.2400 $C2\cdots C10^i$ 3.583 (2) $H8\cdots C2$ 2.9000 $C3\cdots O2^{iii}$ 3.4160 (17) $H8\cdots C11$ 2.6800 $C3\cdots C14^i$ 3.559 (2) $H8\cdots H11$ 2.1800 $C4\cdots S1^i$ 3.686 (2) $H11\cdots H8$ 2.1800 $C6\cdots C14^v$ 3.442 (2) $H11\cdots H8$ 2.1800 $C7\cdots C9^v$ 3.5138 (19) $H11\cdots H13A$ 2.5900	O2…H1 ^{iv}	1.8900	H4…S1 ^{vii}	3.1500
$O2\cdots H15A$ 2.8300 $H7\cdots O2$ 2.4000 $O2\cdots H15C$ 2.6200 $H7\cdots H6$ 2.3200 $O2\cdots H7$ 2.4000 $H7\cdots H15C^{vi}$ 2.6000 $O2\cdots H15C^{vi}$ 2.7700 $H8\cdots O1$ 2.2400 $C2\cdots C10^i$ 3.583 (2) $H8\cdots C2$ 2.9000 $C3\cdots O2^{iii}$ 3.4160 (17) $H8\cdots C11$ 2.6800 $C3\cdots C14^i$ 3.559 (2) $H8\cdots H11$ 2.1800 $C4\cdots S1^i$ 3.686 (2) $H11\cdots H8$ 2.7400 $C6\cdots C14^v$ 3.442 (2) $H11\cdots H3$ 2.5900	O2···H3 ^{iv}	2.7600	H6…H7	2.3200
$O2\cdots H15C$ 2.6200 $H7\cdots H6$ 2.3200 $O2\cdots H7$ 2.4000 $H7\cdots H15C^{vi}$ 2.6000 $O2\cdots H15C^{vi}$ 2.7700 $H8\cdots O1$ 2.2400 $C2\cdots C10^i$ 3.583 (2) $H8\cdots C2$ 2.9000 $C3\cdots O2^{iii}$ 3.4160 (17) $H8\cdots C11$ 2.6800 $C3\cdots C14^i$ 3.559 (2) $H8\cdots H11$ 2.1800 $C4\cdots S1^i$ 3.686 (2) $H11\cdots C8$ 2.7400 $C6\cdots C14^v$ 3.442 (2) $H11\cdots H8$ 2.1800 $C7\cdots C9^v$ 3.5138 (19) $H11\cdots H13A$ 2.5900	O2…H15A	2.8300	Н7…О2	2.4000
$O2\cdots H7$ 2.4000 $H7\cdots H15C^{vi}$ 2.6000 $O2\cdots H15C^{vi}$ 2.7700 $H8\cdots O1$ 2.2400 $C2\cdots C10^i$ 3.583 (2) $H8\cdots C2$ 2.9000 $C3\cdots O2^{iii}$ 3.4160 (17) $H8\cdots C11$ 2.6800 $C3\cdots C14^i$ 3.559 (2) $H8\cdots H11$ 2.1800 $C4\cdots S1^i$ 3.686 (2) $H11\cdots C8$ 2.7400 $C6\cdots C14^v$ 3.442 (2) $H11\cdots H8$ 2.1800 $C7\cdots C9^v$ 3.5138 (19) $H11\cdots H13A$ 2.5900	O2…H15C	2.6200	Н7…Н6	2.3200
$\begin{array}{ccccc} O2 \cdots H15 C^{vi} & 2.7700 & H8 \cdots O1 & 2.2400 \\ C2 \cdots C10^{i} & 3.583 (2) & H8 \cdots C2 & 2.9000 \\ C3 \cdots O2^{iii} & 3.4160 (17) & H8 \cdots C11 & 2.6800 \\ C3 \cdots C14^{i} & 3.559 (2) & H8 \cdots H11 & 2.1800 \\ C4 \cdots S1^{i} & 3.686 (2) & H11 \cdots C8 & 2.7400 \\ C6 \cdots C14^{v} & 3.442 (2) & H11 \cdots H8 & 2.1800 \\ C7 \cdots C9^{v} & 3.5138 (19) & H11 \cdots H13A & 2.5900 \end{array}$	O2…H7	2.4000	H7…H15C ^{vi}	2.6000
$\begin{array}{ccccc} C2 \cdots C10^{i} & 3.583 \ (2) & H8 \cdots C2 & 2.9000 \\ C3 \cdots O2^{iii} & 3.4160 \ (17) & H8 \cdots C11 & 2.6800 \\ C3 \cdots C14^{i} & 3.559 \ (2) & H8 \cdots H11 & 2.1800 \\ C4 \cdots S1^{i} & 3.686 \ (2) & H11 \cdots C8 & 2.7400 \\ C6 \cdots C14^{v} & 3.442 \ (2) & H11 \cdots H8 & 2.1800 \\ C7 \cdots C9^{v} & 3.5138 \ (19) & H11 \cdots H13A & 2.5900 \end{array}$	O2…H15C ^{vi}	2.7700	H8…O1	2.2400
$C3\cdots O2^{iii}$ $3.4160(17)$ $H8\cdots C11$ 2.6800 $C3\cdots C14^i$ $3.559(2)$ $H8\cdots H11$ 2.1800 $C4\cdots S1^i$ $3.686(2)$ $H11\cdots C8$ 2.7400 $C6\cdots C14^v$ $3.442(2)$ $H11\cdots H8$ 2.1800 $C7\cdots C9^v$ $3.5138(19)$ $H11\cdots H13A$ 2.5900	C2…C10 ⁱ	3.583 (2)	H8…C2	2.9000
$C3\cdots C14^i$ $3.559(2)$ $H8\cdots H11$ 2.1800 $C4\cdots S1^i$ $3.686(2)$ $H11\cdots C8$ 2.7400 $C6\cdots C14^v$ $3.442(2)$ $H11\cdots H8$ 2.1800 $C7\cdots C9^v$ $3.5138(19)$ $H11\cdots H13A$ 2.5900	C3···O2 ⁱⁱⁱ	3.4160 (17)	H8…C11	2.6800
C4…S1i3.686 (2)H11…C82.7400C6…C14v3.442 (2)H11…H82.1800C7…C9v3.5138 (19)H11…H13A2.5900	C3…C14 ⁱ	3.559 (2)	H8…H11	2.1800
C6…C14 ^v 3.442 (2)H11…H82.1800C7…C9 ^v 3.5138 (19)H11…H13A2.5900	$C4 \cdots S1^i$	3.686 (2)	H11…C8	2.7400
C7···C9 ^v 3.5138 (19) H11···H13A 2.5900	C6…C14 ^v	3.442 (2)	H11…H8	2.1800
	C7···C9 ^v	3.5138 (19)	H11…H13A	2.5900

C7···O2 ^v	3.3745 (19)	H13A…H11	2.5900
C8…O1	2.8416 (17)	H15A…O1 ^{iv}	2.7900
C9…O1 ⁱ	3.3986 (19)	H15A…O2	2.8300
C9…C7 ^v	3.5138 (19)	H15A…H1 ^{iv}	2.5600
C10…C2 ⁱ	3.583 (2)	H15A…C1 ^v	3.0600
C14…C3 ⁱ	3.559 (2)	H15A…C5 ^v	3.0500
C14…C6 ^v	3.442 (2)	H15A…C6 ^v	2.9600
C15…O2	2.919 (2)	H15C…O1 ^{iv}	2.8800
C15····O1 ^{iv}	3.2790 (18)	H15C…O2	2.6200
C1H12A ^v	3.0600	H15C…C9	3.0600
С2…Н8	2.9000	H15C···H1 ^{iv}	2.5800
C5H15A ^v	3 0500	H15C····O2 ^{vi}	2,7700
C6···H15A ^v	2 9600	H15C····C7 ^{vi}	2 9200
C7···H15C ^{vi}	2 9200	H15C···H7 ^{vi}	2.5200
	2.9200		2.0000
C12—S1—C14	93.47 (7)	С2—С3—Н3	120.00
C2-01-H1	109.00	C4—C3—H3	120.00
$C^2 - C^1 - C^7$	124 39 (11)	C3-C4-H4	120.00
$C_{6} - C_{1} - C_{7}$	118 02 (11)	C5-C4-H4	120.00
C_{2} C_{1} C_{6}	117.59(12)	C4—C5—H5	121.00
$01 - C^2 - C^3$	121 65 (12)	С4 С5 Н5	121.00
C1 - C2 - C3	121.03(12) 120.04(12)	C1-C6-H6	119.00
$C_1 = C_2 = C_3$	120.04(12) 118 31 (12)	C_{1} C_{0} H_{6}	119.00
$C_{1} = C_{2} = C_{1}$	110.31(12) 120.50(13)	C_{1} C_{7} H_{7}	115.00
$C_2 = C_3 = C_4$	120.30(13) 120.72(15)	C^{2} C^{7} H^{7}	115.00
$C_{3} - C_{4} - C_{5}$	120.75(13)	C_{0}	113.00
C4 - C5 - C0	110.00(14) 100.02(12)	$C = C = H \delta$	120.00
C1 = C0 = C3	122.23(13) 120.57(12)	C_{9} C_{8} H_{8}	120.00
$C1 - C^{2} - C^{2}$	130.57(12)		123.00
C/-C8-C9	120.25 (11)		123.00
02 - C9 - C10	121.58 (12)	C12—C13—H13A	109.00
C8—C9—C10	118.20 (11)	С12—С13—Н13В	109.00
02	120.22 (11)	С12—С13—Н13С	109.00
C9—C10—C14	123.69 (11)	H13A—C13—H13B	109.00
C11—C10—C14	111.61 (11)	H13A—C13—H13C	110.00
C9—C10—C11	124.70 (12)	H13B—C13—H13C	109.00
C10—C11—C12	114.24 (13)	C14—C15—H15A	109.00
S1—C12—C13	121.37 (12)	C14—C15—H15B	109.00
C11—C12—C13	128.61 (15)	C14—C15—H15C	109.00
S1—C12—C11	110.00 (11)	H15A—C15—H15B	109.00
S1—C14—C15	118.86 (10)	H15A—C15—H15C	109.00
C10—C14—C15	130.46 (12)	H15B—C15—H15C	110.00
S1—C14—C10	110.68 (10)		
C14 S1 C12 C11	0.02(10)	C4 C5 C(C1	1.2 (2)
C14 = S1 = C12 = C12	0.02(10)	$C_{4} = C_{2} = C_{0} = C_{1}$	-1.2(3)
$C_{14} = S_{14} = C_{14} = C_{15}$	-1/8./3(15)	$C_1 - C_2 - C_3 - C_2$	-1/9.80(15)
C12 - S1 - C14 - C10	-0.21(12)	$C_{1} = C_{2} = C_{2} = C_{2}$	8.5 (2)
C12— $S1$ — $C14$ — $C15$	1/9.18 (14)	$C_{1} = C_{8} = C_{9} = C_{10}$	-1/1.60 (14)
C6—C1—C2—O1	-178.51 (14)	O2—C9—C10—C11	-173.33(14)

C6—C1—C2—C3	1.3 (2)	O2—C9—C10—C14	6.7 (2)
C7—C1—C2—O1	1.8 (2)	C8—C9—C10—C11	6.6 (2)
C7—C1—C2—C3	-178.36 (14)	C8—C9—C10—C14	-173.36 (14)
C2-C1-C6-C5	0.1 (2)	C9—C10—C11—C12	179.67 (14)
C7—C1—C6—C5	179.74 (16)	C14-C10-C11-C12	-0.37 (19)
C2-C1-C7-C8	-4.6 (3)	C9—C10—C14—S1	-179.69 (11)
C6—C1—C7—C8	175.77 (16)	C9—C10—C14—C15	1.0 (3)
O1—C2—C3—C4	178.23 (16)	C11—C10—C14—S1	0.36 (16)
C1—C2—C3—C4	-1.6 (2)	C11—C10—C14—C15	-178.95 (16)
C2—C3—C4—C5	0.4 (3)	C10-C11-C12-S1	0.21 (18)
C3—C4—C5—C6	0.9 (3)	C10-C11-C12-C13	178.83 (17)

Symmetry codes: (i) -*x*+1, -*y*+1, -*z*; (ii) *x*, *y*+1, *z*+1; (iii) *x*, *y*-1, *z*; (iv) *x*, *y*+1, *z*; (v) -*x*+2, -*y*+2, -*z*; (vi) -*x*+1, -*y*+2, -*z*; (vii) *x*, *y*-1, *z*-1.

Hydrogen-bond geometry (Å, °)

Cg2 is the centroid of the C1–C6 phenyl ring.

D—H···A	<i>D</i> —Н	H···A	$D \cdots A$	<i>D</i> —H··· <i>A</i>
01—H1…O2 ⁱⁱⁱ	0.82	1.8900	2.7067 (14)	174
С8—Н8…О1	0.93	2.2400	2.8416 (17)	122
C15—H15 A ···Cg2 ^v	0.96	2.79	3.652 (2)	150

Symmetry codes: (iii) *x*, *y*–1, *z*; (v) –*x*+2, –*y*+2, –*z*.