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Crystal structure of 2-isopropyl-4-methoxy-5-methylphenyl 4-methylbenzenesulfonate

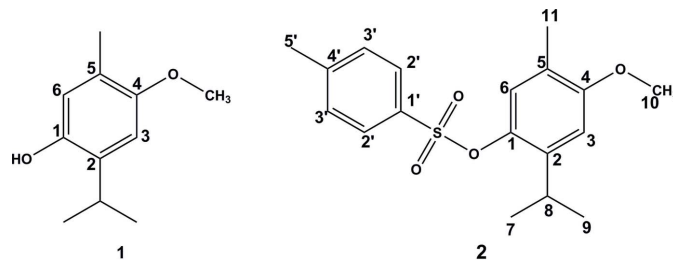
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The title compound, C₁₈H₂₂O₄S, an hemisynthetic product, was obtained by the tosylation reaction of the naturally occurring meroterpene *p*-methoxythymol. The molecule comprises a tetrasubstituted phenyl ring linked to a toluene-sulfonate through one of its O atoms. In the crystal, C—H···O and C—H···π interactions link the molecules, forming a three-dimensional network.

1. Chemical context

Tosylation of alcohols is an important transformation in organic synthesis. This transformation is usually achieved with *p*-toluene sulfonyl chloride, which is very reactive (Greene & Wuts, 1999; Yoshida *et al.*, 1999). Tosylate is an important functional group in organic synthesis as it makes a good leaving group (Wagner & Zokk, 1955; Sandler & Karo, 1983). Indeed, tosylates are used as intermediates in the synthesis of several drugs (Kim *et al.*, 1995; Morgan *et al.*, 1997). Furthermore, they have also been found to possess important biological activities (Kacem *et al.*, 2002; Kaleemullah *et al.*, 2012).



The hemisynthesis of 2-isopropyl-4-methoxy-5-methylphenyl 4-methylbenzenesulfonate **2** from naturally occurring *p*-methoxythymol **1** was undertaken with the aim of preparing meroterpenic tosylate. X-ray single-crystal structure analysis allowed its full structure to be confirmed unambiguously.

2. Structural commentary

Compound **2** is built up from a tetrasubstituted phenyl ring linked to a toluenesulfonate unit through one of its oxygen atoms (Fig. 1). The two phenyl rings form a dihedral angle of 60.03 (9)°. Atoms S1 and C5' are coplanar with the C1'–C6' phenyl ring, their distances from the plane being 0.057 (3) and 0.031 (3) Å, respectively. Considering the connected atoms of

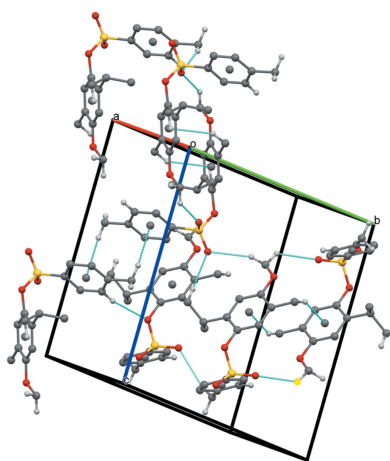


Table 1

Hydrogen-bond geometry (Å, °).

Cg1 and Cg2 are the centroids of the phenyl rings C1–C6 and C1'–C6', respectively.

D–H...A	D–H	H...A	D...A	D–H...A
C3'–H3'...O1 ⁱ	0.95	2.67	3.610 (2)	169
C5'–H5'3...O3 ⁱⁱ	0.98	2.66	3.589 (3)	159
C7–H7A...O4 ⁱⁱⁱ	0.98	2.72	3.693 (3)	175
C10–H10B...O3 ^{iv}	0.98	2.61	3.317 (3)	130
C10–H10A...O4 ⁱⁱⁱ	0.98	2.70	3.521 (3)	142
C5'–H5'2...Cg2 ^v	0.98	2.84	3.706	148
C11–H11B...Cg1 ^{iv}	0.98	2.75	3.635	150
C9–H9A...Cg2	0.98	2.70	3.5373	144

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

the four substituents on the C1–C6 phenyl ring, three of them O2, C8 and C11 are roughly in the plane of the phenyl ring, deviating by only 0.011 (3), 0.014 (3) and 0.012 (3) Å, respectively, from the mean plane, whereas atom O1 is displaced slightly out of the plane by 0.101 (3) Å. This slight distortion might be related to the occurrence of a weak C–H... π interaction between the C9 atom and the centroid Cg2 of the C1'–C6' phenyl ring (Table 1).

3. Supramolecular features

In the crystal, pairs of molecules are linked through C–H...O interactions (Table 1), forming pseudo-dimer arranged around inversion centers (Fig. 2). Further C–H...O hydrogen bonds and C–H... π interactions (Table 1, Fig. 2) lead to the formation of a three-dimensional network.

4. Database survey

A search of the Cambridge Structural Database (CSD, version 5.38, last update May 2017; Groom *et al.*, 2016) for a tosylate fragment bearing an organic substituent on one of its oxygen atoms revealed only three hits. Two of these compounds are

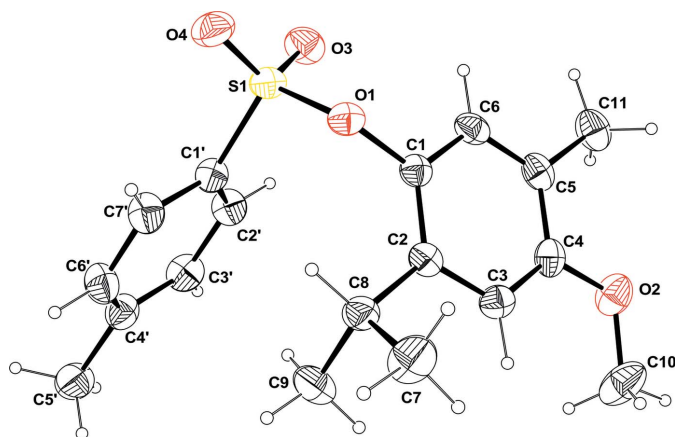


Figure 1

Molecular view of compound **2** with the atom-labelling scheme. Displacement ellipsoids are drawn at the 50% probability level.

Table 2

Selected structural parameters of compound **2** compared with closely related structures.

	2	KAWDAN ^a	TMPDTS ^b
C1'–S1	1.749 (2)	1.748	1.732
S1–O1	1.597 (1)	1.598	1.599
O1–C1	1.428 (2)	1.425	1.428
C1'–S1–O1	104.76 (8)	98.83	102.37
S1–O1–C1	120.71 (11)	116.07	119.84
Dihedral angle	60.03 (9)	15.32	43.02

References: *a* Niestroj *et al.* (1998); *b* Wiczorek *et al.* (1975).

closely related to compound **2**. The first, 5-bromo-2,3-dimethylphenol-1-(4-methylphenylsulfonyloxy)benzene (KAWDAN; Niestroj *et al.*, 1998), is built up from a tosylate attached to a phenyl ring substituted by two methyl groups and one bromine atom whereas the second, tetramethyl-*p*-phenylene *p*-ditoluenesulfonate (TMPDTS; Wiczorek *et al.*, 1975), is built up from a tetramethyl-substituted phenyl ring attached to two tosylate units. A comparison of selected distances in compound **2** with those of two structures reveals that the geometries are very similar for all three compounds (Table 2). The most marked difference is the dihedral angle between the phenyl rings, 60.03 (9)° in **2** and 15.32 and 43.02° in KAWDAN and TMPDTS, respectively. The large dihedral angle in TMPDTS might be related to the occurrence of two bulky substituents on the central phenyl ring.

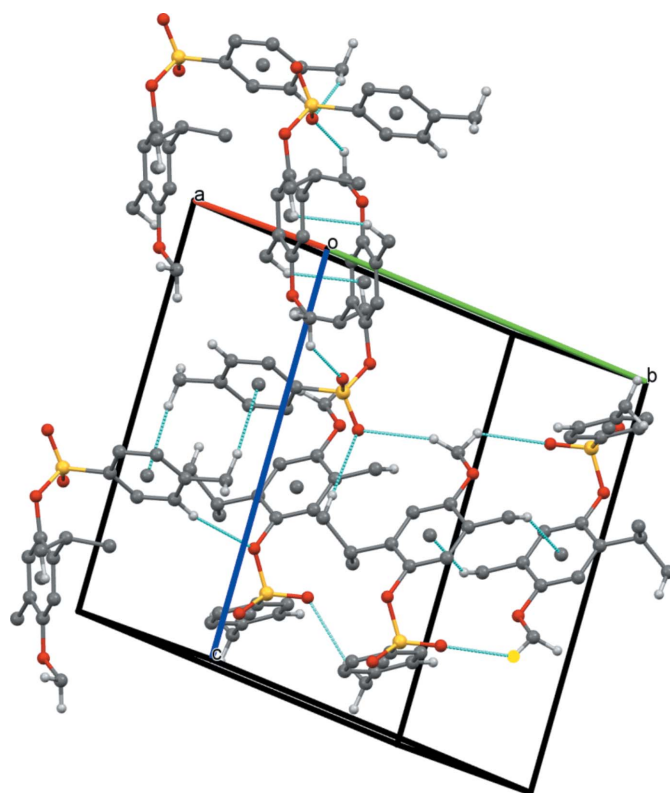


Figure 2

Partial packing view showing the C–H...O and C–H... π interactions (dotted lines). Only H atoms involved in hydrogen bonding are shown.

5. Synthesis and crystallization

In a 100 mL flask, 430 mg (2.33 mmol) of *p*-methoxythymol **1** were dissolved in 15 mL of pyridine and then 908 mg (4.66 mmol) of *para*-toluenesulfonyl chloride were added. The reaction mixture was heated to reflux for two h. The end of the reaction was controlled by TLC. The reaction mixture was washed with a hydrochloric acid solution (0.1 M) to neutral pH, extracted three times with ethyl ether (3 × 20 mL), dried over anhydrous Na₂SO₄ and concentrated under reduced pressure. The crude product was purified by silica gel column chromatography using hexane/ethyl acetate (94:6) as eluent to give 360 mg (1.07 mmol, 46% yield) of 2-isopropyl-4-methoxy-5-methylphenyl 4-methylbenzenesulfonate **2**. X-ray quality colourless crystals were obtained by slow evaporation of a petroleum ether solution of the title compound.

NMR data for compound 2: ¹H NMR (300 MHz, CDCl₃): 6.66 (s, H-6), 6.84 (s, H-3), 3.45 (sept, H-8), 1.09 (d, H-9, H-10), 2.13 (s, H-7), 3.72 (s, H-10), 7.33 (d, H-3'), 7.75 (d, H-2'), 2.43 (s, H-5') ppm. ¹³C NMR (75 MHz, CDCl₃): 156.4 (C-1), 124.0 (C-2), 107.5 (C-3), 145.2 (C-4), 139.8 (C-5), 124.1 (C-6), 15.7 (C-7), 26.8 (C-8), 23.1 (C-9, C-10), 55.4 (OCH₃), 145.2 (C-1'), 129.7 (C-2'), 128.4 (C-3'), 139.7 (C-4'), 21.5 (C-5') ppm.

6. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 3. All H atoms were fixed geometrically and treated as riding with C–H = 1.0 (methine), 0.98 (methyl) or 0.95 Å (aromatic) with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{CH and CH}_2)$ or $U_{\text{iso}}(\text{H}) = 1.5U_{\text{eq}}(\text{CH}_3)$.

Acknowledgements

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Table 3

Experimental details.

Crystal data	
Chemical formula	C ₁₈ H ₂₂ O ₄ S
<i>M_r</i>	334.41
Crystal system, space group	Monoclinic, <i>P2₁/n</i>
Temperature (K)	173
<i>a</i> , <i>b</i> , <i>c</i> (Å)	8.2226 (6), 14.5382 (9), 14.7230 (8)
β (°)	100.020 (6)
<i>V</i> (Å ³)	1733.17 (19)
<i>Z</i>	4
Radiation type	Mo <i>K</i> α
μ (mm ⁻¹)	0.20
Crystal size (mm)	0.35 × 0.25 × 0.10
Data collection	
Diffractometer	Rigaku Oxford Diffraction Xcalibur Eos Gemini ultra
Absorption correction	Multi-scan (<i>CrysAlis PRO</i> ; Rigaku OD, 2015)
<i>T_{min}</i> , <i>T_{max}</i>	0.791, 1.000
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	18172, 3532, 2777
<i>R_{int}</i>	0.044
($\sin \theta/\lambda$) _{max} (Å ⁻¹)	0.625
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, <i>S</i>	0.042, 0.110, 1.06
No. of reflections	3532
No. of parameters	213
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{\text{max}}$, $\Delta\rho_{\text{min}}$ (e Å ⁻³)	0.34, -0.34

Computer programs: *CrysAlis PRO* (Rigaku OD, 2015), *SIR97* (Altomare *et al.*, 1999), *SHELXL2014* (Sheldrick, 2015), *ORTEP-3 for Windows* (Farrugia, 1997) and *Mercury* (Macrae *et al.*, 2008).

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Crystal structure of 2-isopropyl-4-methoxy-5-methylphenyl 4-methylbenzenesulfonate

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Computing details

Data collection: *CrysAlis PRO* (Rigaku OD, 2015); cell refinement: *CrysAlis PRO* (Rigaku OD, 2015); data reduction: *CrysAlis PRO* (Rigaku OD, 2015); program(s) used to solve structure: *SIR97* (Altomare *et al.*, 1999); program(s) used to refine structure: *SHELXL2014* (Sheldrick, 2015); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997) and *Mercury* (Macrae *et al.*, 2008); software used to prepare material for publication: *SHELXL2014* (Sheldrick, 2015).

2-Isopropyl-4-methoxy-5-methylphenyl 4-methylbenzenesulfonate

Crystal data

$C_{18}H_{22}O_4S$

$M_r = 334.41$

Monoclinic, $P2_1/n$

$a = 8.2226$ (6) Å

$b = 14.5382$ (9) Å

$c = 14.7230$ (8) Å

$\beta = 100.020$ (6)°

$V = 1733.17$ (19) Å³

$Z = 4$

$F(000) = 712$

$D_x = 1.282$ Mg m⁻³

Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å

Cell parameters from 4433 reflections

$\theta = 3.8$ – 28.5 °

$\mu = 0.20$ mm⁻¹

$T = 173$ K

Box, colourless

$0.35 \times 0.25 \times 0.10$ mm

Data collection

Rigaku Oxford Diffraction Xcalibur Eos Gemini ultra

diffractometer

Radiation source: Enhance (Mo) X-ray Source

Graphite monochromator

Detector resolution: 16.1978 pixels mm⁻¹

ω scans

Absorption correction: multi-scan

(*CrysAlis PRO*; Rigaku OD, 2015)

$T_{\min} = 0.791$, $T_{\max} = 1.000$

18172 measured reflections

3532 independent reflections

2777 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.044$

$\theta_{\max} = 26.4$ °, $\theta_{\min} = 3.1$ °

$h = -10 \rightarrow 10$

$k = -18 \rightarrow 16$

$l = -18 \rightarrow 18$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.042$

$wR(F^2) = 0.110$

$S = 1.06$

3532 reflections

213 parameters

0 restraints

Hydrogen site location: inferred from neighbouring sites

H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0459P)^2 + 0.814P]$

where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{\max} < 0.001$

$\Delta\rho_{\max} = 0.34$ e Å⁻³

$\Delta\rho_{\min} = -0.34$ e Å⁻³

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. All H atoms attached to C atoms were fixed geometrically and treated as riding with C—H = 0.95 Å (aromatic), 0.98 Å (methyl), 1.0 Å (methine) with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{CH and C=CH})$ or $U_{\text{iso}}(\text{H}) = 1.5U_{\text{eq}}(\text{CH}_3)$.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
C1	0.0729 (2)	0.19454 (12)	0.12387 (12)	0.0244 (4)
C1'	0.2295 (2)	0.11565 (13)	0.32646 (12)	0.0273 (4)
C2'	0.2423 (2)	0.02563 (13)	0.29895 (13)	0.0319 (4)
H2'	0.150817	−0.004394	0.262620	0.038*
C2	0.2184 (2)	0.20290 (12)	0.08959 (12)	0.0253 (4)
C3'	0.3907 (3)	−0.02031 (14)	0.32514 (13)	0.0351 (5)
H3'	0.400221	−0.082269	0.306238	0.042*
C3	0.2171 (2)	0.16786 (13)	0.00089 (12)	0.0281 (4)
H3	0.314049	0.172671	−0.025740	0.034*
C4	0.0786 (2)	0.12650 (13)	−0.04881 (12)	0.0283 (4)
C4'	0.5259 (2)	0.02225 (14)	0.37844 (12)	0.0323 (4)
C5	−0.0681 (2)	0.11891 (13)	−0.01288 (13)	0.0293 (4)
C5'	0.6862 (3)	−0.02793 (16)	0.40828 (15)	0.0414 (5)
H5'1	0.674385	−0.091812	0.386905	0.062*
H5'2	0.714962	−0.026864	0.475724	0.062*
H5'3	0.773618	0.002185	0.381667	0.062*
C6	−0.0682 (2)	0.15452 (13)	0.07405 (13)	0.0284 (4)
H6	−0.166024	0.151593	0.100070	0.034*
C6'	0.5098 (2)	0.11365 (15)	0.40381 (13)	0.0356 (5)
H6'	0.601735	0.144317	0.439007	0.043*
C7	0.4269 (3)	0.32911 (16)	0.09104 (15)	0.0451 (6)
H7A	0.459446	0.308452	0.033416	0.068*
H7B	0.520807	0.359505	0.129571	0.068*
H7C	0.334786	0.372516	0.077095	0.068*
C7'	0.3633 (2)	0.16037 (14)	0.37888 (13)	0.0325 (4)
H7'	0.353664	0.222483	0.397271	0.039*
C8	0.3736 (2)	0.24634 (14)	0.14252 (13)	0.0310 (4)
H8	0.349050	0.268405	0.203020	0.037*
C9	0.5123 (3)	0.17540 (18)	0.16200 (16)	0.0483 (6)
H9A	0.474804	0.122497	0.194085	0.072*
H9B	0.608770	0.203173	0.200759	0.072*
H9C	0.542309	0.155001	0.103658	0.072*
C10	0.2226 (3)	0.08648 (18)	−0.17038 (15)	0.0526 (7)
H10A	0.261778	0.149089	−0.178548	0.079*
H10B	0.203927	0.054579	−0.229920	0.079*
H10C	0.305633	0.053107	−0.126849	0.079*
C11	−0.2193 (3)	0.07531 (15)	−0.06830 (14)	0.0388 (5)

H11A	-0.307373	0.073020	-0.031237	0.058*
H11B	-0.192880	0.012726	-0.085726	0.058*
H11C	-0.256290	0.111763	-0.124059	0.058*
O1	0.06333 (15)	0.23611 (8)	0.21065 (8)	0.0269 (3)
O2	0.07192 (18)	0.09037 (10)	-0.13523 (9)	0.0391 (4)
O3	-0.08697 (16)	0.10974 (10)	0.27106 (10)	0.0378 (3)
O4	0.02806 (17)	0.24132 (10)	0.36634 (9)	0.0386 (4)
S1	0.04212 (6)	0.17449 (3)	0.29760 (3)	0.02896 (14)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0260 (9)	0.0203 (9)	0.0269 (9)	0.0030 (7)	0.0041 (7)	0.0025 (7)
C1'	0.0316 (9)	0.0231 (10)	0.0270 (9)	0.0023 (8)	0.0049 (7)	0.0001 (7)
C2'	0.0354 (10)	0.0247 (10)	0.0349 (10)	-0.0030 (8)	0.0038 (8)	-0.0036 (8)
C2	0.0248 (9)	0.0208 (9)	0.0298 (9)	-0.0004 (7)	0.0029 (7)	0.0022 (7)
C3'	0.0445 (12)	0.0226 (10)	0.0392 (11)	0.0032 (9)	0.0098 (9)	-0.0032 (8)
C3	0.0297 (9)	0.0242 (10)	0.0313 (9)	-0.0007 (8)	0.0084 (7)	0.0022 (8)
C4	0.0363 (10)	0.0210 (10)	0.0262 (9)	0.0000 (8)	0.0016 (7)	0.0025 (7)
C4'	0.0379 (11)	0.0306 (11)	0.0287 (9)	0.0052 (9)	0.0067 (8)	0.0033 (8)
C5	0.0301 (9)	0.0206 (10)	0.0349 (10)	-0.0003 (8)	-0.0013 (8)	0.0063 (8)
C5'	0.0415 (12)	0.0441 (13)	0.0398 (11)	0.0126 (10)	0.0103 (9)	0.0081 (10)
C6	0.0230 (9)	0.0255 (10)	0.0366 (10)	0.0030 (8)	0.0045 (7)	0.0067 (8)
C6'	0.0355 (11)	0.0355 (12)	0.0331 (10)	0.0002 (9)	-0.0019 (8)	-0.0039 (9)
C7	0.0464 (13)	0.0481 (14)	0.0418 (12)	-0.0235 (11)	0.0107 (10)	-0.0079 (10)
C7'	0.0395 (11)	0.0236 (10)	0.0327 (10)	0.0021 (8)	0.0017 (8)	-0.0047 (8)
C8	0.0251 (9)	0.0385 (12)	0.0297 (9)	-0.0050 (8)	0.0057 (7)	-0.0050 (8)
C9	0.0276 (10)	0.0672 (17)	0.0477 (13)	0.0069 (11)	0.0003 (9)	-0.0045 (12)
C10	0.0641 (16)	0.0617 (16)	0.0368 (12)	-0.0238 (13)	0.0219 (11)	-0.0168 (11)
C11	0.0359 (11)	0.0347 (12)	0.0416 (11)	-0.0050 (9)	-0.0046 (9)	0.0020 (9)
O1	0.0272 (6)	0.0225 (7)	0.0322 (7)	0.0011 (5)	0.0083 (5)	0.0012 (5)
O2	0.0473 (9)	0.0394 (9)	0.0305 (7)	-0.0112 (7)	0.0062 (6)	-0.0057 (6)
O3	0.0309 (7)	0.0380 (8)	0.0450 (8)	-0.0052 (6)	0.0079 (6)	0.0068 (6)
O4	0.0411 (8)	0.0403 (8)	0.0376 (8)	0.0094 (7)	0.0153 (6)	-0.0038 (6)
S1	0.0277 (2)	0.0285 (3)	0.0323 (3)	0.0020 (2)	0.00963 (18)	0.00179 (19)

Geometric parameters (Å, °)

C1—C2	1.382 (2)	C6—H6	0.9500
C1—C6	1.388 (2)	C6'—C7'	1.376 (3)
C1—O1	1.428 (2)	C6'—H6'	0.9500
C1'—C2'	1.379 (3)	C7—C8	1.526 (3)
C1'—C7'	1.390 (3)	C7—H7A	0.9800
C1'—S1	1.7486 (19)	C7—H7B	0.9800
C2'—C3'	1.386 (3)	C7—H7C	0.9800
C2'—H2'	0.9500	C7'—H7'	0.9500
C2—C3	1.400 (2)	C8—C9	1.527 (3)
C2—C8	1.513 (2)	C8—H8	1.0000

C3'—C4'	1.389 (3)	C9—H9A	0.9800
C3'—H3'	0.9500	C9—H9B	0.9800
C3—C4	1.380 (3)	C9—H9C	0.9800
C3—H3	0.9500	C10—O2	1.424 (3)
C4—O2	1.369 (2)	C10—H10A	0.9800
C4—C5	1.403 (3)	C10—H10B	0.9800
C4'—C6'	1.393 (3)	C10—H10C	0.9800
C4'—C5'	1.504 (3)	C11—H11A	0.9800
C5—C6	1.381 (3)	C11—H11B	0.9800
C5—C11	1.503 (3)	C11—H11C	0.9800
C5'—H5'1	0.9800	O1—S1	1.5967 (12)
C5'—H5'2	0.9800	O3—S1	1.4216 (14)
C5'—H5'3	0.9800	O4—S1	1.4221 (14)
C2—C1—C6	122.74 (16)	C8—C7—H7B	109.5
C2—C1—O1	118.38 (15)	H7A—C7—H7B	109.5
C6—C1—O1	118.64 (15)	C8—C7—H7C	109.5
C2'—C1'—C7'	120.86 (18)	H7A—C7—H7C	109.5
C2'—C1'—S1	120.13 (15)	H7B—C7—H7C	109.5
C7'—C1'—S1	119.00 (14)	C6'—C7'—C1'	119.26 (18)
C1'—C2'—C3'	118.97 (18)	C6'—C7'—H7'	120.4
C1'—C2'—H2'	120.5	C1'—C7'—H7'	120.4
C3'—C2'—H2'	120.5	C2—C8—C7	111.27 (16)
C1—C2—C3	116.24 (16)	C2—C8—C9	110.51 (17)
C1—C2—C8	123.71 (16)	C7—C8—C9	110.87 (17)
C3—C2—C8	120.05 (16)	C2—C8—H8	108.0
C2'—C3'—C4'	121.44 (18)	C7—C8—H8	108.0
C2'—C3'—H3'	119.3	C9—C8—H8	108.0
C4'—C3'—H3'	119.3	C8—C9—H9A	109.5
C4—C3—C2	121.63 (17)	C8—C9—H9B	109.5
C4—C3—H3	119.2	H9A—C9—H9B	109.5
C2—C3—H3	119.2	C8—C9—H9C	109.5
O2—C4—C3	123.76 (17)	H9A—C9—H9C	109.5
O2—C4—C5	114.99 (16)	H9B—C9—H9C	109.5
C3—C4—C5	121.26 (17)	O2—C10—H10A	109.5
C3'—C4'—C6'	118.20 (18)	O2—C10—H10B	109.5
C3'—C4'—C5'	121.55 (18)	H10A—C10—H10B	109.5
C6'—C4'—C5'	120.25 (18)	O2—C10—H10C	109.5
C6—C5—C4	117.33 (16)	H10A—C10—H10C	109.5
C6—C5—C11	121.84 (18)	H10B—C10—H10C	109.5
C4—C5—C11	120.83 (18)	C5—C11—H11A	109.5
C4'—C5'—H5'1	109.5	C5—C11—H11B	109.5
C4'—C5'—H5'2	109.5	H11A—C11—H11B	109.5
H5'1—C5'—H5'2	109.5	C5—C11—H11C	109.5
C4'—C5'—H5'3	109.5	H11A—C11—H11C	109.5
H5'1—C5'—H5'3	109.5	H11B—C11—H11C	109.5
H5'2—C5'—H5'3	109.5	C1—O1—S1	120.71 (11)
C5—C6—C1	120.79 (17)	C4—O2—C10	117.16 (15)

C5—C6—H6	119.6	O3—S1—O4	119.91 (9)
C1—C6—H6	119.6	O3—S1—O1	109.37 (8)
C7'—C6'—C4'	121.25 (18)	O4—S1—O1	102.77 (8)
C7'—C6'—H6'	119.4	O3—S1—C1'	109.08 (9)
C4'—C6'—H6'	119.4	O4—S1—C1'	109.79 (9)
C8—C7—H7A	109.5	O1—S1—C1'	104.76 (8)

Hydrogen-bond geometry (\AA , $^\circ$)

Cg1 and Cg2 are the centroids of the phenyl rings C1–C6 and C1'–C6', respectively.

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
C3'—H3'...O1 ⁱ	0.95	2.67	3.610 (2)	169
C5'—H5'3...O3 ⁱⁱ	0.98	2.66	3.589 (3)	159
C7—H7A...O4 ⁱⁱⁱ	0.98	2.72	3.693 (3)	175
C10—H10B...O3 ^{iv}	0.98	2.61	3.317 (3)	130
C10—H10A...O4 ⁱⁱⁱ	0.98	2.70	3.521 (3)	142
C5'—H5'2...Cg2 ^v	0.98	2.84	3.706	148
C11—H11B...Cg1 ^{iv}	0.98	2.75	3.635	150
C9—H9A...Cg2	0.98	2.70	3.5373	144

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