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# 4,4′-[4,4′-Sulfonylbis(*p*-phenyleneoxy)]-dibutanoic acid

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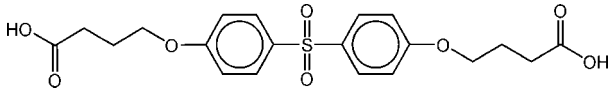
Key indicators: single-crystal X-ray study; $T$ = 296 K; mean $\sigma$(C–C) = 0.003 Å; disorder in main residue; $R$ factor = 0.045; $wR$ factor = 0.139; data-to-parameter ratio = 13.3.

In the title compound, $C_{20}H_{22}O_8S$, the dihedral angle between the two benzene rings is 81.6 (3)°. The benzene-connected portions of the alkoxy substituents are almost coplanar with their respective rings [C—C—O—C torsion angles of 174.77 (17) and −178.5 (4)°]. One of the butanoic acid groups is disordered over two conformations with a site-occupancy ratio 0.719 (6):0.281 (6). In the crystal, pairs of O—H···O hydrogen bonds link the molecules into infinite zigzag chains along [130].

## Related literature

For bisphenol S (systematic name 4,4′-sulfonyldiphenol) as a reactant in epoxy reactions and its use in fast-curing epoxy resin glues, see: Askarinejad & Morsali (2006); Danzl *et al.* (2009); Bashiri *et al.* (2009). For its use in the manufacture of pharmaceuticals, adhesives, biocides and agricultural products, see: Howard & David (2002); Howard *et al.* (2005); Yasue *et al.* (2009). For synthesis details and a related structure, see: Zheng *et al.* (2007).



## Experimental

### *Crystal data*

$C_{20}H_{22}O_8S$ $M_r$ = 422.45
Monoclinic, $C2/c$
$a$ = 30.945 (7) Å
$b$ = 8.0964 (18) Å
$c$ = 16.032 (3) Å
$\beta$ = 94.711 (5)°
$V$ = 4003.1 (15) Å$^3$
$Z$ = 8
Mo $K\alpha$ radiation
$\mu$ = 0.21 mm$^{-1}$
$T$ = 296 K
0.20 × 0.18 × 0.12 mm

### *Data collection*

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min}$ = 0.959, $T_{max}$ = 0.975
12299 measured reflections
4362 independent reflections
2927 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.041

### *Refinement*

$R[F^2 > 2\sigma(F^2)]$ = 0.045
$wR(F^2)$ = 0.139
$S$ = 1.00
4362 reflections
327 parameters
19 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.30 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.21 e Å$^{-3}$

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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| O8$B$—H8$B$···O2$^{i}$ | 0.82 | 2.07 | 2.890 (11) | 180 |
| O8—H8$A$···O2$^{i}$ | 0.82 | 1.77 | 2.587 (4) | 178 |
| O3—H3···O7$B^{ii}$ | 0.82 | 1.84 | 2.623 (13) | 159 |
| O3—H3···O7$^{ii}$ | 0.82 | 1.85 | 2.668 (5) | 177 |

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

Data collection: *SMART* (Bruker, 2007); cell refinement: *SAINT* (Bruker, 2007); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: PK2315).

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# supplementary materials

*Acta Cryst.* (2011). E**67**, o1048 [ **doi:10.1107/S1600536811011871** ]

# 4,4'-[4,4'-Sulfonylbis(*p*-phenyleneoxy)]dibutanoic acid

**C.-Y. Fu, Y.-H. Liu, Z.-L. Zhou and H. Tang**

## Comment

Bisphenol S (BPS) is an organic compound with the formula $(C_6H_4OH)_2SO_2$. It has two phenol functional groups on either side of a sulfonyl group. It is commonly used as a reactant in epoxy reactions, and is used in fast-curing epoxy resin glues (Askarinejad & Morsali, 2006; Bashiri *et al.*, 2009; Danzl *et al.*, 2009; Yasue *et al.*, 2009). Bisphenol S is also used in organic synthesis as an organosulfur source in the manufacture of pharmaceuticals, adhesives, biocides and agricultural products (Howard & David, 2002; Howard *et al.*, 2005). In this article, we present the synthesis and crystal structure of a new potential ligand derived from bisphenol S, which contains multiple oxygen donors and flexible aliphatic spacers.

As shown in Figure 1, the benzene-connected portions of the alkoxy substituents lie almost coplanar with the ring [C–C–O–C torsion angle = 174.77 (17) and -178.5 (4)°, respectively]. The two benzene rings make a dihedral angle of 81.6 (3)°. It is noteworthy that one of the butanoic acid groups is disordered over two components with site occupancy ratio 0.719 (6):0.281 (6). In the crystal, O—H···O hydrogen bonds link the molecules into a zigzag 1-D infinite chain that propagates along the [1 3 0] direction. These chains are further interwoven by C—H···O and C—H···π contacts that stabilize the packing.

## Experimental

Reagents and solvents were of commercially available quality. The title complex was synthesized according to the method of Zheng *et al.*, 2007. To a solution of bisphenol S (0.01 mol) in acetonitrile (50 ml), anhydrous potassium carbonate (0.02 mol) and ethyl 4-bromobutanoate (0.01 mol) were mixed. The mixture solution was refluxed for 6 h and filtered. The filtrate was evaporated under reduced pressure and the solid product was dissolved in water/ethanol (1:2 *v*/*v*), then sodium hydroxide (0.02 mol) was added. The solution was refluxed for another 24 h, then acidified with dilute HCl. The crude product was separated by filtration and crystals of the title compound were prepared by recrystallization from a mixture of water and ethanol (1:1).

## Refinement

All H atoms were placed in idealized positions (C—H = 0.93–0.97 Å, O—H = 0.82 Å and refined as riding atoms with $U_{iso}$(H) = 1.2$U_{eq}$(C) and with $U_{iso}$(H) = 1.5$U_{eq}$(O). One of the butanoic acid groups is disordered over two conformations with site occupancy ratio 0.719 (6):0.281 (6). All distances in the minor component were restrained to within 0.01 Å of their equivalents in the major component.

## Figures

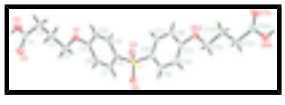


Fig. 1. The molecular structure of the title compound, with displacement ellipsoids at the 30% probability level. The disorder in the minor component has been omitted to enhance clarity.

### 4,4'-[4,4'-Sulfonylbis(*p*-phenyleneoxy)]dibutanoic acid

*Crystal data*

| | |
|---|---|
| $C_{20}H_{22}O_8S$ | $F(000) = 1776$ |
| $M_r = 422.45$ | $D_x = 1.402$ Mg m$^{-3}$ |
| Monoclinic, $C2/c$ | Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å |
| Hall symbol: -C 2yc | Cell parameters from 2472 reflections |
| $a = 30.945$ (7) Å | $\theta = 2.6$–$23.6°$ |
| $b = 8.0964$ (18) Å | $\mu = 0.21$ mm$^{-1}$ |
| $c = 16.032$ (3) Å | $T = 296$ K |
| $\beta = 94.711$ (5)° | Block, colorless |
| $V = 4003.1$ (15) Å$^3$ | 0.20 × 0.18 × 0.12 mm |
| $Z = 8$ | |

*Data collection*

| | |
|---|---|
| Bruker SMART CCD area-detector diffractometer | 4362 independent reflections |
| Radiation source: fine-focus sealed tube | 2927 reflections with $I > 2\sigma(I)$ |
| graphite | $R_{int} = 0.041$ |
| φ and ω scans | $\theta_{max} = 27.1°$, $\theta_{min} = 2.6°$ |
| Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996) | $h = -39\rightarrow35$ |
| $T_{min} = 0.959$, $T_{max} = 0.975$ | $k = -10\rightarrow8$ |
| 12299 measured reflections | $l = -20\rightarrow20$ |

*Refinement*

| | |
|---|---|
| Refinement on $F^2$ | Primary atom site location: structure-invariant direct methods |
| Least-squares matrix: full | Secondary atom site location: difference Fourier map |
| $R[F^2 > 2\sigma(F^2)] = 0.045$ | Hydrogen site location: inferred from neighbouring sites |
| $wR(F^2) = 0.139$ | H-atom parameters constrained |
| $S = 1.00$ | $w = 1/[\sigma^2(F_o^2) + (0.076P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$ |
| 4362 reflections | $(\Delta/\sigma)_{max} < 0.001$ |
| 327 parameters | $\Delta\rho_{max} = 0.30$ e Å$^{-3}$ |
| 19 restraints | $\Delta\rho_{min} = -0.21$ 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**. Refinement of $F^2$ against ALL reflections. The weighted R-factor wR and goodness of fit S are based on $F^2$, conventional R-factors R are based on F, with F set to zero for negative $F^2$. The threshold expression of $F^2 > 2\sigma(F^2)$ is used only for calculating R-factors(gt) etc. and is not relevant to the choice of reflections for refinement. R-factors based on $F^2$ are statistically about twice as large as those based on F, and R- factors based on ALL data will be even larger.

*Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters ($Å^2$)*

| | *x* | *y* | *z* | $U_{iso}$*/$U_{eq}$ | Occ. (<1) |
|---|---|---|---|---|---|
| S1 | 0.340925 (17) | 0.09320 (6) | 0.19395 (3) | 0.04130 (18) | |
| O1 | 0.21477 (5) | 0.09741 (18) | 0.44895 (9) | 0.0480 (4) | |
| O2 | 0.13002 (5) | −0.23795 (19) | 0.54170 (11) | 0.0623 (5) | |
| O3 | 0.08084 (6) | −0.0961 (2) | 0.46295 (12) | 0.0643 (5) | |
| H3 | 0.0708 | −0.1887 | 0.4537 | 0.096* | |
| O4 | 0.31868 (5) | 0.1453 (2) | 0.11609 (9) | 0.0593 (5) | |
| O5 | 0.36503 (5) | −0.05895 (19) | 0.19703 (11) | 0.0557 (4) | |
| C1 | 0.21744 (7) | −0.0104 (3) | 0.52061 (13) | 0.0467 (5) | |
| H1A | 0.2459 | −0.0025 | 0.5507 | 0.056* | |
| H1B | 0.2126 | −0.1240 | 0.5031 | 0.056* | |
| C2 | 0.18298 (7) | 0.0436 (3) | 0.57577 (14) | 0.0512 (6) | |
| H2A | 0.1909 | 0.1511 | 0.5990 | 0.061* | |
| H2B | 0.1826 | −0.0333 | 0.6221 | 0.061* | |
| C3 | 0.13776 (7) | 0.0545 (3) | 0.53276 (15) | 0.0462 (5) | |
| H3A | 0.1198 | 0.1173 | 0.5682 | 0.055* | |
| H3B | 0.1391 | 0.1158 | 0.4811 | 0.055* | |
| C4 | 0.11608 (7) | −0.1071 (3) | 0.51281 (13) | 0.0425 (5) | |
| C5 | 0.24467 (6) | 0.0837 (2) | 0.39240 (13) | 0.0374 (5) | |
| C6 | 0.28269 (6) | −0.0081 (2) | 0.40364 (13) | 0.0404 (5) | |
| H6 | 0.2888 | −0.0694 | 0.4522 | 0.049* | |
| C7 | 0.31147 (6) | −0.0073 (2) | 0.34153 (13) | 0.0401 (5) | |
| H7 | 0.3369 | −0.0687 | 0.3486 | 0.048* | |
| C8 | 0.30262 (6) | 0.0842 (2) | 0.26918 (12) | 0.0354 (4) | |
| C9 | 0.26422 (6) | 0.1752 (3) | 0.25765 (13) | 0.0419 (5) | |
| H9 | 0.2581 | 0.2361 | 0.2089 | 0.050* | |
| C10 | 0.23556 (7) | 0.1743 (3) | 0.31866 (13) | 0.0431 (5) | |
| H10 | 0.2099 | 0.2342 | 0.3109 | 0.052* | |
| O6 | 0.45017 (16) | 0.6539 (4) | 0.3091 (3) | 0.0555 (9) | 0.719 (6) |
| O7 | 0.54917 (16) | 1.1033 (5) | 0.4276 (4) | 0.0632 (11) | 0.719 (6) |
| O8 | 0.59897 (13) | 0.9699 (5) | 0.5104 (3) | 0.0758 (11) | 0.719 (6) |
| H8A | 0.6081 | 1.0636 | 0.5201 | 0.114* | 0.719 (6) |
| C11 | 0.48910 (17) | 0.6369 (5) | 0.3610 (3) | 0.0527 (11) | 0.719 (6) |
| H11A | 0.5100 | 0.5720 | 0.3332 | 0.063* | 0.719 (6) |
| H11B | 0.4836 | 0.5824 | 0.4130 | 0.063* | 0.719 (6) |
| C12 | 0.50608 (12) | 0.8096 (5) | 0.3780 (2) | 0.0552 (11) | 0.719 (6) |
| H12A | 0.5116 | 0.8619 | 0.3255 | 0.066* | 0.719 (6) |
| H12B | 0.4843 | 0.8742 | 0.4035 | 0.066* | 0.719 (6) |
| C13 | 0.54702 (12) | 0.8074 (4) | 0.4348 (3) | 0.0611 (12) | 0.719 (6) |

| | | | | | |
|---|---|---|---|---|---|
| H13A | 0.5415 | 0.7517 | 0.4864 | 0.073* | 0.719 (6) |
| H13B | 0.5688 | 0.7442 | 0.4084 | 0.073* | 0.719 (6) |
| C14 | 0.5647 (2) | 0.9760 (8) | 0.4554 (5) | 0.0500 (13) | 0.719 (6) |
| O6B | 0.4601 (3) | 0.6099 (11) | 0.3342 (8) | 0.056 (3) | 0.281 (6) |
| O7B | 0.5371 (4) | 1.1472 (15) | 0.4022 (10) | 0.079 (3) | 0.281 (6) |
| O8B | 0.5816 (5) | 0.9780 (14) | 0.4772 (8) | 0.077 (5) | 0.281 (6) |
| H8B | 0.5954 | 1.0583 | 0.4958 | 0.115* | 0.281 (6) |
| C11B | 0.4986 (3) | 0.5743 (13) | 0.3876 (7) | 0.052 (3) | 0.281 (6) |
| H11C | 0.5204 | 0.5281 | 0.3544 | 0.063* | 0.281 (6) |
| H11D | 0.4919 | 0.4925 | 0.4289 | 0.063* | 0.281 (6) |
| C12B | 0.5164 (3) | 0.7285 (11) | 0.4321 (6) | 0.064 (3) | 0.281 (6) |
| H12C | 0.4938 | 0.7772 | 0.4627 | 0.076* | 0.281 (6) |
| H12D | 0.5400 | 0.6969 | 0.4725 | 0.076* | 0.281 (6) |
| C13B | 0.5326 (5) | 0.8560 (13) | 0.3745 (7) | 0.086 (4) | 0.281 (6) |
| H13C | 0.5088 | 0.8878 | 0.3345 | 0.103* | 0.281 (6) |
| H13D | 0.5548 | 0.8061 | 0.3434 | 0.103* | 0.281 (6) |
| C14B | 0.5511 (5) | 1.0101 (16) | 0.4168 (9) | 0.070 (5) | 0.281 (6) |
| C15 | 0.42950 (8) | 0.5072 (3) | 0.28884 (15) | 0.0543 (6) | |
| C16 | 0.39020 (8) | 0.5418 (3) | 0.24433 (16) | 0.0583 (7) | |
| H16 | 0.3818 | 0.6508 | 0.2345 | 0.070* | |
| C17 | 0.36394 (7) | 0.4158 (3) | 0.21499 (14) | 0.0481 (5) | |
| H17 | 0.3376 | 0.4389 | 0.1850 | 0.058* | |
| C18 | 0.37640 (6) | 0.2527 (2) | 0.22985 (12) | 0.0373 (4) | |
| C19 | 0.41573 (7) | 0.2172 (3) | 0.27360 (13) | 0.0452 (5) | |
| H19 | 0.4241 | 0.1080 | 0.2831 | 0.054* | |
| C20 | 0.44257 (7) | 0.3452 (3) | 0.30315 (14) | 0.0530 (6) | |
| H20 | 0.4691 | 0.3225 | 0.3323 | 0.064* | |

*Atomic displacement parameters (Å$^2$)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| S1 | 0.0421 (3) | 0.0388 (3) | 0.0425 (3) | −0.0041 (2) | 0.0004 (2) | −0.0036 (2) |
| O1 | 0.0396 (8) | 0.0491 (9) | 0.0560 (9) | 0.0045 (7) | 0.0085 (7) | 0.0140 (7) |
| O2 | 0.0677 (11) | 0.0382 (9) | 0.0787 (12) | 0.0006 (8) | −0.0076 (9) | 0.0096 (8) |
| O3 | 0.0564 (10) | 0.0474 (10) | 0.0850 (12) | −0.0063 (8) | −0.0190 (9) | 0.0033 (9) |
| O4 | 0.0603 (10) | 0.0783 (12) | 0.0377 (8) | −0.0082 (9) | −0.0060 (7) | 0.0012 (8) |
| O5 | 0.0559 (10) | 0.0374 (9) | 0.0750 (11) | 0.0022 (7) | 0.0126 (8) | −0.0089 (8) |
| C1 | 0.0389 (11) | 0.0539 (14) | 0.0462 (12) | −0.0021 (10) | −0.0034 (9) | 0.0087 (10) |
| C2 | 0.0507 (13) | 0.0572 (14) | 0.0459 (12) | −0.0099 (11) | 0.0050 (10) | −0.0076 (11) |
| C3 | 0.0445 (12) | 0.0394 (12) | 0.0558 (13) | −0.0019 (9) | 0.0106 (10) | −0.0012 (10) |
| C4 | 0.0415 (12) | 0.0422 (12) | 0.0444 (12) | −0.0025 (10) | 0.0066 (9) | −0.0025 (10) |
| C5 | 0.0324 (10) | 0.0319 (11) | 0.0474 (11) | −0.0065 (8) | −0.0010 (9) | 0.0031 (9) |
| C6 | 0.0397 (11) | 0.0354 (11) | 0.0447 (11) | −0.0013 (9) | −0.0058 (9) | 0.0095 (9) |
| C7 | 0.0332 (10) | 0.0347 (11) | 0.0508 (12) | 0.0021 (9) | −0.0057 (9) | 0.0044 (9) |
| C8 | 0.0331 (10) | 0.0315 (10) | 0.0405 (10) | −0.0057 (8) | −0.0032 (8) | −0.0007 (8) |
| C9 | 0.0394 (11) | 0.0386 (11) | 0.0457 (12) | −0.0025 (9) | −0.0084 (9) | 0.0092 (9) |
| C10 | 0.0334 (11) | 0.0372 (11) | 0.0571 (13) | 0.0022 (9) | −0.0050 (9) | 0.0101 (10) |
| O6 | 0.051 (2) | 0.0397 (19) | 0.073 (3) | −0.0119 (16) | −0.0064 (15) | 0.0036 (16) |

| | | | | | | |
|---|---|---|---|---|---|---|
| O7 | 0.056 (3) | 0.048 (3) | 0.081 (3) | −0.006 (2) | −0.0220 (18) | 0.000 (2) |
| O8 | 0.082 (3) | 0.0502 (15) | 0.087 (3) | −0.0161 (15) | −0.0477 (19) | 0.0065 (18) |
| C11 | 0.057 (3) | 0.053 (3) | 0.049 (3) | −0.012 (2) | 0.008 (2) | −0.001 (2) |
| C12 | 0.052 (2) | 0.053 (2) | 0.059 (2) | −0.0150 (18) | −0.0059 (18) | 0.0000 (19) |
| C13 | 0.061 (3) | 0.044 (2) | 0.075 (3) | −0.0112 (18) | −0.0126 (19) | 0.0000 (19) |
| C14 | 0.058 (4) | 0.048 (2) | 0.042 (4) | −0.011 (3) | −0.009 (3) | −0.004 (3) |
| O6B | 0.054 (6) | 0.028 (4) | 0.084 (8) | −0.009 (4) | −0.009 (5) | 0.004 (4) |
| O7B | 0.069 (8) | 0.061 (7) | 0.105 (10) | −0.006 (5) | −0.011 (6) | −0.003 (6) |
| O8B | 0.107 (14) | 0.047 (5) | 0.069 (9) | −0.023 (8) | −0.042 (6) | −0.001 (5) |
| C11B | 0.049 (6) | 0.044 (6) | 0.061 (7) | −0.022 (5) | −0.013 (5) | −0.001 (5) |
| C12B | 0.048 (6) | 0.073 (7) | 0.070 (7) | −0.009 (5) | 0.005 (5) | −0.007 (6) |
| C13B | 0.100 (11) | 0.084 (8) | 0.074 (8) | −0.035 (8) | 0.015 (8) | −0.011 (7) |
| C14B | 0.079 (10) | 0.092 (13) | 0.036 (7) | −0.024 (10) | −0.005 (6) | 0.002 (8) |
| C15 | 0.0582 (14) | 0.0433 (14) | 0.0644 (15) | −0.0223 (12) | 0.0231 (12) | −0.0135 (11) |
| C16 | 0.0601 (16) | 0.0348 (12) | 0.0825 (18) | −0.0020 (11) | 0.0216 (14) | 0.0016 (12) |
| C17 | 0.0453 (12) | 0.0410 (12) | 0.0583 (14) | 0.0002 (10) | 0.0056 (11) | 0.0098 (10) |
| C18 | 0.0347 (10) | 0.0362 (11) | 0.0413 (11) | −0.0035 (9) | 0.0058 (8) | 0.0018 (9) |
| C19 | 0.0405 (12) | 0.0384 (12) | 0.0557 (13) | −0.0010 (9) | −0.0008 (10) | 0.0024 (10) |
| C20 | 0.0394 (12) | 0.0610 (15) | 0.0581 (14) | −0.0110 (11) | 0.0003 (10) | −0.0038 (12) |

*Geometric parameters (Å, °)*

| | | | |
|---|---|---|---|
| S1—O4 | 1.4383 (15) | C11—H11A | 0.9700 |
| S1—O5 | 1.4389 (17) | C11—H11B | 0.9700 |
| S1—C8 | 1.761 (2) | C12—C13 | 1.498 (4) |
| S1—C18 | 1.761 (2) | C12—H12A | 0.9700 |
| O1—C5 | 1.352 (2) | C12—H12B | 0.9700 |
| O1—C1 | 1.440 (2) | C13—C14 | 1.497 (6) |
| O2—C4 | 1.221 (3) | C13—H13A | 0.9700 |
| O3—C4 | 1.301 (3) | C13—H13B | 0.9700 |
| O3—H3 | 0.8200 | C14—H8B | 1.2897 |
| C1—C2 | 1.505 (3) | O6B—C15 | 1.416 (7) |
| C1—H1A | 0.9700 | O6B—C11B | 1.436 (8) |
| C1—H1B | 0.9700 | O7B—C14B | 1.208 (12) |
| C2—C3 | 1.511 (3) | O8B—C14B | 1.321 (11) |
| C2—H2A | 0.9700 | O8B—H8A | 1.2384 |
| C2—H2B | 0.9700 | O8B—H8B | 0.8200 |
| C3—C4 | 1.493 (3) | C11B—C12B | 1.519 (7) |
| C3—H3A | 0.9700 | C11B—H11C | 0.9700 |
| C3—H3B | 0.9700 | C11B—H11D | 0.9700 |
| C5—C6 | 1.391 (3) | C12B—C13B | 1.498 (7) |
| C5—C10 | 1.400 (3) | C12B—H12C | 0.9700 |
| C6—C7 | 1.390 (3) | C12B—H12D | 0.9700 |
| C6—H6 | 0.9300 | C13B—C14B | 1.510 (8) |
| C7—C8 | 1.384 (3) | C13B—H13C | 0.9700 |
| C7—H7 | 0.9300 | C13B—H13D | 0.9700 |
| C8—C9 | 1.398 (3) | C15—C20 | 1.386 (4) |
| C9—C10 | 1.373 (3) | C15—C16 | 1.387 (4) |
| C9—H9 | 0.9300 | C16—C17 | 1.364 (3) |

| | | | |
|---|---|---|---|
| C10—H10 | 0.9300 | C16—H16 | 0.9300 |
| O6—C15 | 1.375 (4) | C17—C18 | 1.390 (3) |
| O6—C11 | 1.413 (5) | C17—H17 | 0.9300 |
| O7—C14 | 1.207 (8) | C18—C19 | 1.384 (3) |
| O8—C14 | 1.323 (7) | C19—C20 | 1.387 (3) |
| O8—H8A | 0.8199 | C19—H19 | 0.9300 |
| O8—H8B | 0.7586 | C20—H20 | 0.9300 |
| C11—C12 | 1.510 (5) | | |
| O4—S1—O5 | 119.39 (10) | C13—C12—H12B | 109.4 |
| O4—S1—C8 | 107.79 (9) | C11—C12—H12B | 109.4 |
| O5—S1—C8 | 108.49 (10) | H12A—C12—H12B | 108.0 |
| O4—S1—C18 | 108.03 (10) | C14—C13—C12 | 113.5 (4) |
| O5—S1—C18 | 108.01 (10) | C14—C13—H13A | 108.9 |
| C8—S1—C18 | 104.08 (9) | C12—C13—H13A | 108.9 |
| C5—O1—C1 | 119.19 (15) | C14—C13—H13B | 108.9 |
| C4—O3—H3 | 109.5 | C12—C13—H13B | 108.9 |
| O1—C1—C2 | 107.20 (18) | H13A—C13—H13B | 107.7 |
| O1—C1—H1A | 110.3 | O7—C14—O8 | 123.4 (5) |
| C2—C1—H1A | 110.3 | O7—C14—C13 | 124.7 (6) |
| O1—C1—H1B | 110.3 | O8—C14—C13 | 111.8 (6) |
| C2—C1—H1B | 110.3 | O7—C14—H8B | 89.9 |
| H1A—C1—H1B | 108.5 | C13—C14—H8B | 145.3 |
| C1—C2—C3 | 115.04 (18) | C15—O6B—C11B | 132.5 (7) |
| C1—C2—H2A | 108.5 | C14B—O8B—H8A | 134.2 |
| C3—C2—H2A | 108.5 | C14B—O8B—H8B | 115.4 |
| C1—C2—H2B | 108.5 | O6B—C11B—C12B | 111.5 (8) |
| C3—C2—H2B | 108.5 | O6B—C11B—H11C | 109.3 |
| H2A—C2—H2B | 107.5 | C12B—C11B—H11C | 109.3 |
| C4—C3—C2 | 115.44 (19) | O6B—C11B—H11D | 109.3 |
| C4—C3—H3A | 108.4 | C12B—C11B—H11D | 109.3 |
| C2—C3—H3A | 108.4 | H11C—C11B—H11D | 108.0 |
| C4—C3—H3B | 108.4 | C13B—C12B—C11B | 113.9 (8) |
| C2—C3—H3B | 108.4 | C13B—C12B—H12C | 108.8 |
| H3A—C3—H3B | 107.5 | C11B—C12B—H12C | 108.8 |
| O2—C4—O3 | 123.0 (2) | C13B—C12B—H12D | 108.8 |
| O2—C4—C3 | 122.7 (2) | C11B—C12B—H12D | 108.8 |
| O3—C4—C3 | 114.26 (19) | H12C—C12B—H12D | 107.7 |
| O1—C5—C6 | 125.11 (18) | C12B—C13B—C14B | 115.3 (10) |
| O1—C5—C10 | 114.95 (17) | C12B—C13B—H13C | 108.5 |
| C6—C5—C10 | 119.93 (19) | C14B—C13B—H13C | 108.5 |
| C7—C6—C5 | 119.33 (18) | C12B—C13B—H13D | 108.5 |
| C7—C6—H6 | 120.3 | C14B—C13B—H13D | 108.5 |
| C5—C6—H6 | 120.3 | H13C—C13B—H13D | 107.5 |
| C8—C7—C6 | 120.56 (18) | O7B—C14B—O8B | 123.1 (12) |
| C8—C7—H7 | 119.7 | O7B—C14B—C13B | 123.7 (13) |
| C6—C7—H7 | 119.7 | O8B—C14B—C13B | 112.9 (13) |
| C7—C8—C9 | 120.04 (19) | O6—C15—C20 | 130.9 (3) |
| C7—C8—S1 | 119.87 (15) | O6—C15—C16 | 108.6 (3) |
| C9—C8—S1 | 120.02 (15) | C20—C15—C16 | 120.5 (2) |

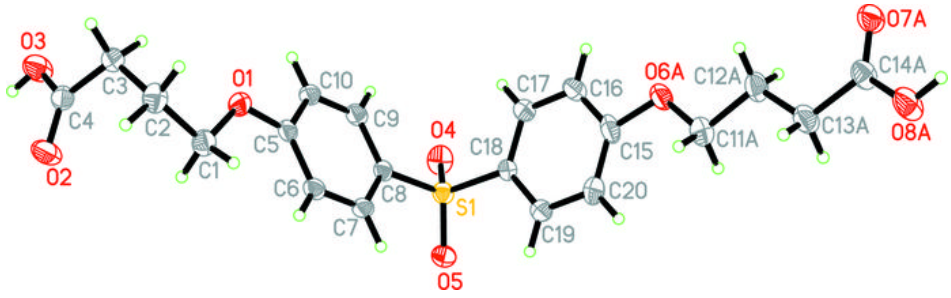
| | | | |
|---|---|---|---|
| C10—C9—C8 | 119.64 (18) | C20—C15—O6B | 107.2 (4) |
| C10—C9—H9 | 120.2 | C16—C15—O6B | 131.9 (5) |
| C8—C9—H9 | 120.2 | C17—C16—C15 | 119.9 (2) |
| C9—C10—C5 | 120.49 (19) | C17—C16—H16 | 120.0 |
| C9—C10—H10 | 119.8 | C15—C16—H16 | 120.0 |
| C5—C10—H10 | 119.8 | C16—C17—C18 | 120.2 (2) |
| C15—O6—C11 | 114.4 (3) | C16—C17—H17 | 119.9 |
| C14—O8—H8A | 109.7 | C18—C17—H17 | 119.9 |
| C14—O8—H8B | 70.7 | C19—C18—C17 | 120.29 (19) |
| O6—C11—C12 | 106.4 (4) | C19—C18—S1 | 120.77 (16) |
| O6—C11—H11A | 110.4 | C17—C18—S1 | 118.93 (16) |
| C12—C11—H11A | 110.4 | C18—C19—C20 | 119.6 (2) |
| O6—C11—H11B | 110.4 | C18—C19—H19 | 120.2 |
| C12—C11—H11B | 110.4 | C20—C19—H19 | 120.2 |
| H11A—C11—H11B | 108.6 | C15—C20—C19 | 119.5 (2) |
| C13—C12—C11 | 111.3 (4) | C15—C20—H20 | 120.3 |
| C13—C12—H12A | 109.4 | C19—C20—H20 | 120.3 |
| C11—C12—H12A | 109.4 | | |
| C5—O1—C1—C2 | 174.77 (17) | O6B—C11B—C12B—C13B | −65.6 (15) |
| O1—C1—C2—C3 | 53.5 (3) | C11B—C12B—C13B—C14B | −179.2 (11) |
| C1—C2—C3—C4 | 73.3 (3) | C12B—C13B—C14B—O7B | −120.5 (19) |
| C2—C3—C4—O2 | 12.6 (3) | C12B—C13B—C14B—O8B | 53.2 (19) |
| C2—C3—C4—O3 | −168.2 (2) | C11—O6—C15—C20 | −7.8 (7) |
| C1—O1—C5—C6 | −11.3 (3) | C11—O6—C15—C16 | 174.8 (4) |
| C1—O1—C5—C10 | 170.19 (18) | C11—O6—C15—O6B | 13.3 (16) |
| O1—C5—C6—C7 | −177.81 (18) | C11B—O6B—C15—O6 | −164 (3) |
| C10—C5—C6—C7 | 0.6 (3) | C11B—O6B—C15—C20 | −0.3 (17) |
| C5—C6—C7—C8 | 0.2 (3) | C11B—O6B—C15—C16 | 172.4 (11) |
| C6—C7—C8—C9 | −0.8 (3) | O6—C15—C16—C17 | 178.3 (3) |
| C6—C7—C8—S1 | 176.31 (15) | C20—C15—C16—C17 | 0.6 (4) |
| O4—S1—C8—C7 | 160.76 (16) | O6B—C15—C16—C17 | −171.4 (8) |
| O5—S1—C8—C7 | 30.16 (18) | C15—C16—C17—C18 | 0.2 (4) |
| C18—S1—C8—C7 | −84.68 (17) | C16—C17—C18—C19 | −0.8 (3) |
| O4—S1—C8—C9 | −22.18 (19) | C16—C17—C18—S1 | 177.98 (17) |
| O5—S1—C8—C9 | −152.77 (16) | O4—S1—C18—C19 | −146.43 (17) |
| C18—S1—C8—C9 | 92.39 (17) | O5—S1—C18—C19 | −16.0 (2) |
| C7—C8—C9—C10 | 0.4 (3) | C8—S1—C18—C19 | 99.18 (18) |
| S1—C8—C9—C10 | −176.62 (15) | O4—S1—C18—C17 | 34.8 (2) |
| C8—C9—C10—C5 | 0.4 (3) | O5—S1—C18—C17 | 165.25 (17) |
| O1—C5—C10—C9 | 177.64 (18) | C8—S1—C18—C17 | −79.57 (19) |
| C6—C5—C10—C9 | −1.0 (3) | C17—C18—C19—C20 | 0.5 (3) |
| C15—O6—C11—C12 | −178.5 (4) | S1—C18—C19—C20 | −178.27 (16) |
| O6—C11—C12—C13 | 178.5 (4) | O6—C15—C20—C19 | −178.0 (4) |
| C11—C12—C13—C14 | −178.6 (4) | C16—C15—C20—C19 | −0.9 (4) |
| C12—C13—C14—O7 | −2.6 (9) | O6B—C15—C20—C19 | 172.8 (6) |
| C12—C13—C14—O8 | 175.4 (5) | C18—C19—C20—C15 | 0.4 (3) |
| C15—O6B—C11B—C12B | −171.3 (12) | | |

*Hydrogen-bond geometry (Å, °)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| O8B—H8B···O2$^{i}$ | 0.82 | 2.07 | 2.890 (11) | 180 |
| O8—H8A···O2$^{i}$ | 0.82 | 1.77 | 2.587 (4) | 178 |
| O3—H3···O7B$^{ii}$ | 0.82 | 1.84 | 2.623 (13) | 159 |
| O3—H3···O7$^{ii}$ | 0.82 | 1.85 | 2.668 (5) | 177 |

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

**Fig. 1**


O3
C3
C4
O2
C2
C1
O1
C5
C10
C9
C6
C8
C7
O4
S1
O5
C18
C17
C16
C15
C20
C19
O6A
C12A
C11A
C13A
C14A
O7A
O8A