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1,1,1-Tris(phenylsulfonyloxymethyl)-ethane

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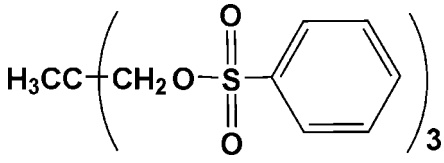
Key indicators: single-crystal X-ray study; T = 173 K; mean σ(C–C) = 0.004 Å; R factor = 0.052; wR factor = 0.126; data-to-parameter ratio = 18.2.

In the crystal structure of the title compound, $C_{23}H_{24}O_9S_3$, intermolecular C—H···O hydrogen bonds are found, which link the molecules into a three-dimensional network. Weak C—H···π interactions are also present in the structure.

Related literature

Intermolecular C—H···π interactions are also found in the crystal structure of the analogous sulfonate compound (Kakeya *et al.*, 2006). The bond lengths and angles are comparable with those found in related aromatic sulfonates (Kakeya *et al.*, 2006; Manivannan *et al.*, 2005).

For related literature, see: Allen *et al.* (1987); Fleischer *et al.* (1971); Geue & Searle (1983).



Experimental

Crystal data

$C_{23}H_{24}O_9S_3$
M_r = 540.60
Triclinic, $P\overline{1}$
a = 5.8962 (5) Å
b = 14.6650 (14) Å
c = 15.1812 (14) Å
α = 69.164 (2)°
β = 85.096 (3)°
γ = 87.685 (2)°
V = 1222.28 (19) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.36 mm^{-1}
T = 173 (2) K
0.21 × 0.12 × 0.11 mm

Data collection

Bruker SMART APEX CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.919, T_{max} = 0.962
9027 measured reflections
5782 independent reflections
4717 reflections with $I > 2\sigma(I)$
R_{int} = 0.026

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.052
$wR(F^2)$ = 0.126
S = 1.03
5782 reflections
317 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.52 e Å^{-3}
$\Delta\rho_{min}$ = −0.34 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C1—H1C···O2^{i}	0.98	2.53	3.426 (3)	152
C10—H10···O5^{ii}	0.95	2.59	3.361 (3)	138
C14—H14···O8^{iii}	0.95	2.49	3.222 (3)	134
C21—H21···$Cg1^{iv}$	0.95	2.92	3.766 (9)	149

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

Data collection: *SMART-W2K/NT* (Bruker, 2003); cell refinement: *SAINT-W2K/NT* (Bruker, 2003); data reduction: *SAINT-W2K/NT*; program(s) used to solve structure: *SHELXTL-NT* (Bruker, 2003); program(s) used to refine structure: *SHELXTL-NT*; molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *SHELXTL-NT*.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: AT2347).

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supplementary materials

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1,1,1-Tris(phenylsulfonyloxymethyl)ethane

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Comment

We report here the title compound, (I) which is the precursor compound for branched acyclic polyamine ligands of the metal cage complexes (Geue & Searle, 1983). The structure of (I), with the atom-numbering scheme, is shown in Fig. 1. The C—C distances in phenyl ring [1.372 (4) − 1.392 (3) Å] are within normal ranges for aromatic systems. The phenyl rings (C6—C11, C12—C17 and C18—C23) are planar, with a largest deviation of 0.0108 (19) Å from the plane being that of atom C12. The S-Csp^2 bond lengths, *viz*. S1—C6 [1.754 (2) Å], S2—C12 [1.757 (2) Å] and S3—C18 [1.756 (2) Å], agree with the general S—Csp^2 bond length (1.75 Å, Allen *et al.*, 1987). Other S—C, S—O, S═O bond lengths are comparable to those found in related structures in that they all contain the *p*-toluenesulfonyl groups (Kakeya *et al.*, 2006, Manivannan *et al.*, 2005). Analysis of the crystal packing of the title compound shows the existence of the hydrogen-bonding interactions (C—H···O and C—H···π, where *Cg*1 is the centroid of the ring formed by C12—C17), which connect the neighbouring molecules to form a three-dimensional network as shown in Fig. 2 and Table 1.

Experimental

The title compound (I) was synthesized according to the previously reported method of Fleischer *et al.* (1971). Crystals suitable for X-ray diffraction were obtained by slow evaporation of a solution in acetone at 298 K. ^{1}H NMR ($CDCl_3$, δ, p.p.m.): 7.54–7.7.84 (m, 15H, C_6H_5), 3.82 (s, 6H, CH_2), 0.92 (s, 3H, CH_3). Analysis calculated for $C_{23}H_{24}O_9S_3$: C 28.32, H 4.75%. Found: C 51.07, H 4.32%.

Refinement

The H atoms were placed in calculated positions, with C—H = 0.98 Å (for CH_3), 0.99 Å (for CH_2) or 0.95 Å (for phenyl ring), and refined using a riding model, with U_{iso}(H) = 1.2U_{eq} of the carrier atoms.

Figures

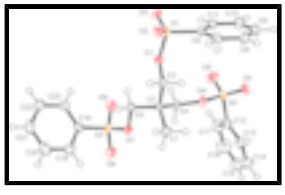

Fig. 1. A perspective view of the title compound with the atom-numbering scheme. Displacement ellipsoids are shown at the 50% probability level.

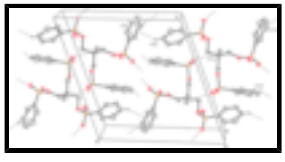

Fig. 2. A molecular packing diagram of (I).

1,1,1-Tris(phenylsulfonyloxymethyl)ethane

Crystal data

$C_{23}H_{24}O_9S_3$	$Z = 2$
$M_r = 540.60$	$F_{000} = 564$
Triclinic, $P\overline{1}$	$D_x = 1.469$ Mg m^{-3}
Hall symbol: -P 1	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
$a = 5.8962$ (5) Å	Cell parameters from 2403 reflections
$b = 14.6650$ (14) Å	$\theta = 2.4$–27.7º
$c = 15.1812$ (14) Å	$\mu = 0.36$ mm^{-1}
$\alpha = 69.164$ (2)º	$T = 173$ (2) K
$\beta = 85.096$ (3)º	Plate, colourless
$\gamma = 87.685$ (2)º	0.21 × 0.12 × 0.11 mm
$V = 1222.28$ (19) Å^3	

Data collection

Bruker SMART APEX CCD area-detector diffractometer	5782 independent reflections
Radiation source: fine-focus sealed tube	4717 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.026$
Detector resolution: 8.366 pixels mm^{-1}	$\theta_{max} = 27.9$º
$T = 173(2)$ K	$\theta_{min} = 1.4$º
φ and ω scans	$h = -7 \rightarrow 7$
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	$k = -19 \rightarrow 13$
$T_{min} = 0.919$, $T_{max} = 0.962$	$l = -19 \rightarrow 19$
9027 measured reflections	

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.052$	H-atom parameters constrained
$wR(F^2) = 0.126$	$w = 1/[\sigma^2(F_o^2) + (0.056P)^2 + 0.5823P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.03$	$(\Delta/\sigma)_{max} < 0.001$
5782 reflections	$\Delta\rho_{max} = 0.52$ e Å^{-3}
317 parameters	$\Delta\rho_{min} = -0.34$ e Å^{-3}
Primary atom site location: structure-invariant direct methods	Extinction correction: none

Special details

Geometry. Least-squares planes (*x*,*y*,*z* in crystal coordinates) and deviations from them (* indicates atom used to define plane)

− 2.4060 (0.0064) *x* + 3.1536 (0.0154) *y* + 13.2033 (0.0089) *z* = 14.2134 (0.0208)

* 0.0092 (0.0018) C18 * −0.0072 (0.0020) C19 * −0.0003 (0.0022) C20 * 0.0059 (0.0020) C21 * −0.0040 (0.0019) C22 * −0.0036 (0.0018) C23

Rms deviation of fitted atoms = 0.0058

2.1818 (0.0070) *x* + 13.2877 (0.0075) *y* + 8.9329 (0.0152) *z* = 14.2436 (0.0115)

Angle to previous plane (with approximate e.s.d.) = 73.42 (0.09)

* −0.0108 (0.0019) C12 * 0.0080 (0.0019) C13 * 0.0012 (0.0022) C14 * −0.0077 (0.0023) C15 * 0.0050 (0.0024) C16 * 0.0043 (0.0022) C17

Rms deviation of fitted atoms = 0.0069

2.2980 (0.0056) *x* − 1.4353 (0.0147) *y* + 12.8260 (0.0084) *z* = 4.7002 (0.0133)

Angle to previous plane (with approximate e.s.d.) = 73.71 (0.09)

* −0.0005 (0.0016) C6 * −0.0065 (0.0017) C7 * 0.0069 (0.0017) C8 * −0.0001 (0.0018) C9 * −0.0069 (0.0017) C10 * 0.0071 (0.0016) C11

Rms deviation of fitted atoms = 0.0056

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 $F^2 > 2\text{sigma}(F^2)$ is used only for calculating *R*-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. *R*-factors based on F^2 are statistically about twice as large as those based on F, and R– factors based on ALL data will be even larger.

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

	x	*y*	*z*	U_{iso}*/U_{eq}
C1	0.6339 (4)	0.79403 (17)	0.70459 (17)	0.0265 (5)
H1A	0.6937	0.7421	0.6823	0.040*
H1B	0.6493	0.7743	0.7726	0.040*
H1C	0.7197	0.8539	0.6711	0.040*
C2	0.3810 (4)	0.81257 (15)	0.68526 (15)	0.0191 (4)
C3	0.3718 (4)	0.85520 (16)	0.57846 (15)	0.0212 (4)
H3A	0.4453	0.9199	0.5529	0.025*
H3B	0.4542	0.8118	0.5491	0.025*
C4	0.2474 (4)	0.71808 (15)	0.72799 (16)	0.0215 (4)
H4A	0.2671	0.6880	0.7965	0.026*
H4B	0.0833	0.7311	0.7193	0.026*
C5	0.2762 (4)	0.88670 (16)	0.72637 (15)	0.0231 (5)
H5A	0.3603	0.9488	0.6995	0.028*
H5B	0.1154	0.8998	0.7113	0.028*

C6	0.1352 (4)	0.78195 (16)	0.42971 (15)	0.0216 (4)
C7	0.3463 (4)	0.76503 (17)	0.38950 (17)	0.0275 (5)
H7	0.4632	0.8122	0.3728	0.033*
C8	0.3819 (5)	0.67742 (18)	0.37438 (18)	0.0332 (6)
H8	0.5257	0.6638	0.3482	0.040*
C9	0.2103 (5)	0.61014 (18)	0.39704 (18)	0.0345 (6)
H9	0.2365	0.5508	0.3857	0.041*
C10	0.0002 (5)	0.62803 (17)	0.43616 (18)	0.0318 (6)
H10	−0.1177	0.5815	0.4509	0.038*
C11	−0.0376 (4)	0.71391 (16)	0.45363 (16)	0.0265 (5)
H11	−0.1802	0.7262	0.4817	0.032*
C12	0.2772 (4)	0.47976 (16)	0.81194 (17)	0.0278 (5)
C13	0.4939 (4)	0.43840 (18)	0.82266 (19)	0.0350 (6)
H13	0.6065	0.4559	0.7710	0.042*
C14	0.5435 (5)	0.3711 (2)	0.9099 (2)	0.0449 (7)
H14	0.6903	0.3416	0.9182	0.054*
C15	0.3801 (6)	0.3473 (2)	0.9842 (2)	0.0522 (8)
H15	0.4141	0.3007	1.0436	0.063*
C16	0.1677 (6)	0.3903 (2)	0.9735 (2)	0.0553 (9)
H16	0.0570	0.3740	1.0258	0.066*
C17	0.1142 (5)	0.4573 (2)	0.8869 (2)	0.0433 (7)
H17	−0.0324	0.4871	0.8794	0.052*
C18	0.1555 (4)	1.00176 (17)	0.86626 (16)	0.0243 (5)
C19	0.3510 (5)	1.0291 (2)	0.8941 (2)	0.0393 (6)
H19	0.4608	0.9816	0.9243	0.047*
C20	0.3843 (5)	1.1268 (2)	0.8774 (2)	0.0459 (7)
H20	0.5169	1.1467	0.8968	0.055*
C21	0.2256 (5)	1.19530 (19)	0.83256 (19)	0.0387 (6)
H21	0.2489	1.2623	0.8217	0.046*
C22	0.0341 (5)	1.16772 (19)	0.80351 (19)	0.0383 (6)
H22	−0.0734	1.2157	0.7719	0.046*
C23	−0.0027 (4)	1.07034 (18)	0.82008 (18)	0.0317 (5)
H23	−0.1349	1.0509	0.8000	0.038*
O1	0.1335 (2)	0.86482 (11)	0.55679 (10)	0.0215 (3)
O2	0.2426 (3)	0.96243 (11)	0.39114 (11)	0.0297 (4)
O3	−0.1545 (3)	0.91299 (12)	0.44856 (12)	0.0284 (4)
O4	0.3364 (3)	0.65333 (11)	0.67915 (11)	0.0245 (3)
O5	0.3164 (3)	0.51765 (13)	0.63121 (13)	0.0398 (5)
O6	−0.0313 (3)	0.57333 (13)	0.70084 (14)	0.0396 (5)
O7	0.2905 (3)	0.84512 (11)	0.82898 (11)	0.0275 (4)
O8	0.1688 (3)	0.82379 (13)	0.98686 (12)	0.0374 (4)
O9	−0.1156 (3)	0.86594 (13)	0.86820 (13)	0.0374 (4)
S1	0.08321 (9)	0.89170 (4)	0.45003 (4)	0.02113 (14)
S2	0.20808 (10)	0.55550 (4)	0.69854 (4)	0.02768 (15)
S3	0.10533 (10)	0.87705 (4)	0.89391 (4)	0.02641 (15)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0219 (11)	0.0250 (12)	0.0312 (13)	−0.0008 (9)	−0.0027 (9)	−0.0081 (10)
C2	0.0213 (10)	0.0164 (10)	0.0199 (10)	−0.0007 (8)	−0.0028 (8)	−0.0064 (8)
C3	0.0190 (10)	0.0209 (11)	0.0221 (11)	−0.0017 (8)	−0.0015 (8)	−0.0056 (9)
C4	0.0229 (11)	0.0149 (10)	0.0260 (11)	0.0009 (8)	0.0014 (9)	−0.0073 (8)
C5	0.0328 (12)	0.0173 (10)	0.0197 (11)	0.0019 (9)	−0.0041 (9)	−0.0068 (8)
C6	0.0260 (11)	0.0188 (10)	0.0208 (11)	0.0036 (8)	−0.0040 (9)	−0.0080 (8)
C7	0.0290 (12)	0.0272 (12)	0.0279 (12)	0.0002 (10)	0.0001 (10)	−0.0124 (10)
C8	0.0375 (14)	0.0298 (13)	0.0332 (14)	0.0090 (11)	−0.0020 (11)	−0.0136 (11)
C9	0.0551 (17)	0.0216 (12)	0.0292 (13)	0.0068 (11)	−0.0076 (12)	−0.0116 (10)
C10	0.0409 (14)	0.0218 (12)	0.0316 (13)	−0.0051 (10)	−0.0056 (11)	−0.0072 (10)
C11	0.0282 (12)	0.0236 (12)	0.0255 (12)	0.0001 (9)	−0.0032 (9)	−0.0058 (9)
C12	0.0329 (13)	0.0172 (11)	0.0323 (13)	−0.0037 (9)	−0.0063 (10)	−0.0063 (9)
C13	0.0337 (14)	0.0279 (13)	0.0374 (14)	−0.0028 (10)	−0.0053 (11)	−0.0036 (11)
C14	0.0437 (16)	0.0350 (15)	0.0467 (17)	0.0000 (12)	−0.0177 (13)	0.0001 (13)
C15	0.067 (2)	0.0383 (17)	0.0391 (17)	−0.0107 (15)	−0.0143 (15)	0.0047 (13)
C16	0.062 (2)	0.053 (2)	0.0383 (17)	−0.0103 (16)	0.0093 (15)	−0.0034 (14)
C17	0.0398 (16)	0.0391 (16)	0.0446 (17)	−0.0010 (12)	0.0047 (13)	−0.0086 (13)
C18	0.0292 (12)	0.0256 (11)	0.0201 (11)	0.0010 (9)	−0.0012 (9)	−0.0109 (9)
C19	0.0356 (14)	0.0334 (14)	0.0510 (17)	0.0028 (11)	−0.0141 (12)	−0.0154 (13)
C20	0.0412 (16)	0.0418 (16)	0.061 (2)	−0.0094 (13)	−0.0080 (14)	−0.0246 (15)
C21	0.0562 (18)	0.0252 (13)	0.0355 (15)	−0.0045 (12)	0.0013 (13)	−0.0122 (11)
C22	0.0503 (17)	0.0278 (13)	0.0344 (14)	0.0083 (12)	−0.0075 (12)	−0.0080 (11)
C23	0.0327 (13)	0.0328 (13)	0.0329 (13)	0.0046 (11)	−0.0086 (10)	−0.0147 (11)
O1	0.0203 (8)	0.0230 (8)	0.0207 (8)	0.0009 (6)	−0.0007 (6)	−0.0072 (6)
O2	0.0393 (10)	0.0206 (8)	0.0259 (9)	−0.0031 (7)	0.0009 (7)	−0.0046 (7)
O3	0.0272 (9)	0.0280 (9)	0.0300 (9)	0.0079 (7)	−0.0074 (7)	−0.0101 (7)
O4	0.0288 (8)	0.0147 (7)	0.0303 (9)	−0.0003 (6)	0.0009 (7)	−0.0092 (6)
O5	0.0616 (12)	0.0262 (9)	0.0383 (11)	0.0076 (9)	−0.0140 (9)	−0.0181 (8)
O6	0.0321 (10)	0.0276 (9)	0.0570 (13)	−0.0027 (8)	−0.0163 (9)	−0.0093 (9)
O7	0.0380 (9)	0.0248 (8)	0.0217 (8)	0.0081 (7)	−0.0061 (7)	−0.0105 (7)
O8	0.0578 (12)	0.0288 (9)	0.0216 (9)	0.0023 (8)	−0.0039 (8)	−0.0040 (7)
O9	0.0359 (10)	0.0357 (10)	0.0401 (11)	−0.0089 (8)	−0.0011 (8)	−0.0125 (8)
S1	0.0250 (3)	0.0169 (3)	0.0208 (3)	0.0024 (2)	−0.0028 (2)	−0.0058 (2)
S2	0.0335 (3)	0.0164 (3)	0.0345 (3)	−0.0003 (2)	−0.0101 (3)	−0.0091 (2)
S3	0.0344 (3)	0.0226 (3)	0.0220 (3)	−0.0006 (2)	−0.0021 (2)	−0.0075 (2)

Geometric parameters (Å, °)

C1—C2	1.539 (3)	C13—C14	1.388 (4)
C1—H1A	0.9800	C13—H13	0.9500
C1—H1B	0.9800	C14—C15	1.372 (4)
C1—H1C	0.9800	C14—H14	0.9500
C2—C3	1.521 (3)	C15—C16	1.375 (5)
C2—C5	1.522 (3)	C15—H15	0.9500
C2—C4	1.524 (3)	C16—C17	1.385 (4)

C3—O1	1.461 (2)	C16—H16	0.9500
C3—H3A	0.9900	C17—H17	0.9500
C3—H3B	0.9900	C18—C23	1.381 (3)
C4—O4	1.456 (3)	C18—C19	1.382 (3)
C4—H4A	0.9900	C18—S3	1.756 (2)
C4—H4B	0.9900	C19—C20	1.382 (4)
C5—O7	1.466 (3)	C19—H19	0.9500
C5—H5A	0.9900	C20—C21	1.376 (4)
C5—H5B	0.9900	C20—H20	0.9500
C6—C11	1.388 (3)	C21—C22	1.372 (4)
C6—C7	1.392 (3)	C21—H21	0.9500
C6—S1	1.754 (2)	C22—C23	1.382 (4)
C7—C8	1.388 (3)	C22—H22	0.9500
C7—H7	0.9500	C23—H23	0.9500
C8—C9	1.376 (4)	O1—S1	1.5775 (16)
C8—H8	0.9500	O2—S1	1.4263 (16)
C9—C10	1.384 (4)	O3—S1	1.4239 (16)
C9—H9	0.9500	O4—S2	1.5706 (16)
C10—C11	1.382 (3)	O5—S2	1.4228 (19)
C10—H10	0.9500	O6—S2	1.4247 (19)
C11—H11	0.9500	O7—S3	1.5765 (17)
C12—C17	1.379 (4)	O8—S3	1.4228 (18)
C12—C13	1.389 (3)	O9—S3	1.4231 (19)
C12—S2	1.757 (2)		
C2—C1—H1A	109.5	C12—C13—H13	120.5
C2—C1—H1B	109.5	C15—C14—C13	119.9 (3)
H1A—C1—H1B	109.5	C15—C14—H14	120.0
C2—C1—H1C	109.5	C13—C14—H14	120.0
H1A—C1—H1C	109.5	C14—C15—C16	120.7 (3)
H1B—C1—H1C	109.5	C14—C15—H15	119.7
C3—C2—C5	108.18 (17)	C16—C15—H15	119.7
C3—C2—C4	111.32 (17)	C15—C16—C17	120.4 (3)
C5—C2—C4	108.81 (17)	C15—C16—H16	119.8
C3—C2—C1	106.74 (17)	C17—C16—H16	119.8
C5—C2—C1	111.14 (18)	C12—C17—C16	118.9 (3)
C4—C2—C1	110.63 (18)	C12—C17—H17	120.6
O1—C3—C2	108.46 (16)	C16—C17—H17	120.6
O1—C3—H3A	110.0	C23—C18—C19	121.2 (2)
C2—C3—H3A	110.0	C23—C18—S3	119.94 (19)
O1—C3—H3B	110.0	C19—C18—S3	118.86 (19)
C2—C3—H3B	110.0	C20—C19—C18	119.0 (3)
H3A—C3—H3B	108.4	C20—C19—H19	120.5
O4—C4—C2	106.97 (16)	C18—C19—H19	120.5
O4—C4—H4A	110.3	C21—C20—C19	120.1 (3)
C2—C4—H4A	110.3	C21—C20—H20	120.0
O4—C4—H4B	110.3	C19—C20—H20	120.0
C2—C4—H4B	110.3	C22—C21—C20	120.6 (3)
H4A—C4—H4B	108.6	C22—C21—H21	119.7
O7—C5—C2	107.36 (17)	C20—C21—H21	119.7

O7—C5—H5A	110.2	C21—C22—C23	120.2 (3)
C2—C5—H5A	110.2	C21—C22—H22	119.9
O7—C5—H5B	110.2	C23—C22—H22	119.9
C2—C5—H5B	110.2	C18—C23—C22	119.0 (2)
H5A—C5—H5B	108.5	C18—C23—H23	120.5
C11—C6—C7	121.4 (2)	C22—C23—H23	120.5
C11—C6—S1	118.83 (17)	C3—O1—S1	117.30 (13)
C7—C6—S1	119.79 (17)	C4—O4—S2	118.34 (13)
C8—C7—C6	118.3 (2)	C5—O7—S3	118.26 (14)
C8—C7—H7	120.8	O3—S1—O2	120.24 (10)
C6—C7—H7	120.8	O3—S1—O1	104.44 (9)
C9—C8—C7	120.5 (2)	O2—S1—O1	109.50 (9)
C9—C8—H8	119.7	O3—S1—C6	109.04 (10)
C7—C8—H8	119.7	O2—S1—C6	108.75 (10)
C8—C9—C10	120.7 (2)	O1—S1—C6	103.57 (9)
C8—C9—H9	119.6	O5—S2—O6	120.25 (12)
C10—C9—H9	119.6	O5—S2—O4	103.92 (10)
C11—C10—C9	119.8 (2)	O6—S2—O4	109.54 (10)
C11—C10—H10	120.1	O5—S2—C12	108.62 (11)
C9—C10—H10	120.1	O6—S2—C12	108.60 (12)
C10—C11—C6	119.3 (2)	O4—S2—C12	104.83 (10)
C10—C11—H11	120.4	O8—S3—O9	120.10 (11)
C6—C11—H11	120.4	O8—S3—O7	103.38 (10)
C17—C12—C13	121.1 (2)	O9—S3—O7	109.48 (10)
C17—C12—S2	120.2 (2)	O8—S3—C18	109.52 (11)
C13—C12—S2	118.53 (19)	O9—S3—C18	108.91 (11)
C14—C13—C12	119.0 (3)	O7—S3—C18	104.22 (10)
C14—C13—H13	120.5		
C5—C2—C3—O1	−65.9 (2)	C21—C22—C23—C18	0.1 (4)
C4—C2—C3—O1	53.6 (2)	C2—C3—O1—S1	−170.43 (13)
C1—C2—C3—O1	174.42 (16)	C2—C4—O4—S2	−171.61 (14)
C3—C2—C4—O4	54.6 (2)	C2—C5—O7—S3	−151.65 (15)
C5—C2—C4—O4	173.71 (17)	C3—O1—S1—O3	−169.93 (14)
C1—C2—C4—O4	−63.9 (2)	C3—O1—S1—O2	−39.92 (17)
C3—C2—C5—O7	−178.97 (17)	C3—O1—S1—C6	75.94 (16)
C4—C2—C5—O7	60.0 (2)	C11—C6—S1—O3	−26.1 (2)
C1—C2—C5—O7	−62.1 (2)	C7—C6—S1—O3	153.34 (18)
C11—C6—C7—C8	−0.5 (4)	C11—C6—S1—O2	−158.96 (18)
S1—C6—C7—C8	179.99 (18)	C7—C6—S1—O2	20.5 (2)
C6—C7—C8—C9	1.2 (4)	C11—C6—S1—O1	84.64 (19)
C7—C8—C9—C10	−0.7 (4)	C7—C6—S1—O1	−95.88 (19)
C8—C9—C10—C11	−0.7 (4)	C4—O4—S2—O5	171.92 (16)
C9—C10—C11—C6	1.3 (4)	C4—O4—S2—O6	42.22 (18)
C7—C6—C11—C10	−0.7 (3)	C4—O4—S2—C12	−74.13 (17)
S1—C6—C11—C10	178.72 (18)	C17—C12—S2—O5	−139.7 (2)
C17—C12—C13—C14	2.0 (4)	C13—C12—S2—O5	36.1 (2)
S2—C12—C13—C14	−173.8 (2)	C17—C12—S2—O6	−7.3 (3)
C12—C13—C14—C15	−0.8 (4)	C13—C12—S2—O6	168.50 (19)
C13—C14—C15—C16	−0.7 (5)	C17—C12—S2—O4	109.7 (2)

C14—C15—C16—C17	1.1 (5)	C13—C12—S2—O4	−74.5 (2)
C13—C12—C17—C16	−1.6 (4)	C5—O7—S3—O8	179.79 (15)
S2—C12—C17—C16	174.1 (2)	C5—O7—S3—O9	50.67 (18)
C15—C16—C17—C12	0.1 (5)	C5—O7—S3—C18	−65.71 (17)
C23—C18—C19—C20	1.7 (4)	C23—C18—S3—O8	−137.7 (2)
S3—C18—C19—C20	−176.2 (2)	C19—C18—S3—O8	40.3 (2)
C18—C19—C20—C21	−0.8 (5)	C23—C18—S3—O9	−4.5 (2)
C19—C20—C21—C22	−0.4 (5)	C19—C18—S3—O9	173.4 (2)
C20—C21—C22—C23	0.8 (4)	C23—C18—S3—O7	112.2 (2)
C19—C18—C23—C22	−1.4 (4)	C19—C18—S3—O7	−69.8 (2)
S3—C18—C23—C22	176.55 (19)		

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C1—H1C···O2^{i}	0.98	2.53	3.426 (3)	152
C10—H10···O5^{ii}	0.95	2.59	3.361 (3)	138
C14—H14···O8^{iii}	0.95	2.49	3.222 (3)	134
C21—H21···Cg1^{iv}	0.95	2.92	3.766 (9)	149

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

Fig. 1

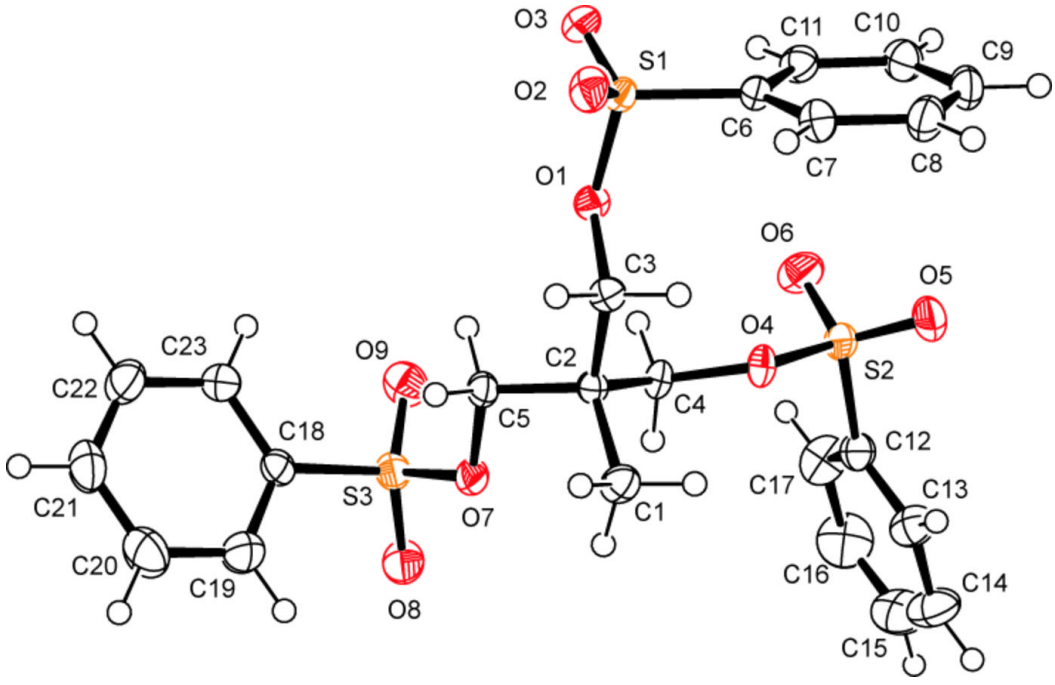
O3
S1
O2
C11
C10
C9
C6
C7
C8
O1
C3
O6
O5
O4
S2
C23
O9
C2
C22
C5
C4
C18
C12
C17
C13
S3
O7
C1
C21
C20
C19
O8
C16
C14
C15

Fig. 2