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Key indicators

Single-crystal X-ray study

$T = 298\text{ K}$

Mean $\sigma(\text{C}-\text{C}) = 0.003\text{ \AA}$

R factor = 0.033

wR factor = 0.086

Data-to-parameter ratio = 14.4

For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>.

4-Methylphenyl benzyl sulfone

In the title compound, $\text{C}_{14}\text{H}_{14}\text{O}_2\text{S}$, the dihedral angle between the two benzene rings is $15.5(1)^\circ$. In the crystal structure, an intermolecular $\text{C}-\text{H}\cdots\text{O}$ interaction links the molecules into zigzag chains along the a axis.

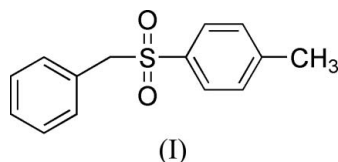
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Comment

Readily available sulfones have become useful building blocks in the preparation and functionalization of a wide variety of products (Alonso *et al.*, 2002). In the study of sulfones, some unconventional methods of synthesis have been adopted. The preparation of ethyl phenylsulfonylacetate is an example of microwave-assisted synthesis (Kingston & Haswell, 1997). The title compound, (I), can also be synthesized under microwave irradiation. The crystal structure of phenyl benzyl sulfone, (II), which is a similar compound to (I), has been reported previously (Liu *et al.*, 2005).



The dihedral angle between the planes of the benzene rings is $15.5(1)^\circ$. In the crystal structure, an intermolecular $\text{C}-\text{H}\cdots\text{O}$ hydrogen bond (Table 2) links the molecules (Fig. 1) into zigzag chains along the a axis (Fig. 2). It is interesting that the crystal structure of (I) is chiral, although the molecule has no chiral atom. In contrast, the crystal structure of (II) is achiral (space group $Pna2_1$; $Z = 4$; Liu *et al.*, 2005).

Experimental

Compound (I) was synthesized in 70% yield by the hydrocarbylation of sodium 4-methylphenylsulfinate dihydrate (2.13 g, 10 mmol) and benzyl bromide (1.2 ml, 11 mmol) in the presence of cetyl trimethylammonium bromide catalyst (1.8 g, 5 mmol). The reaction

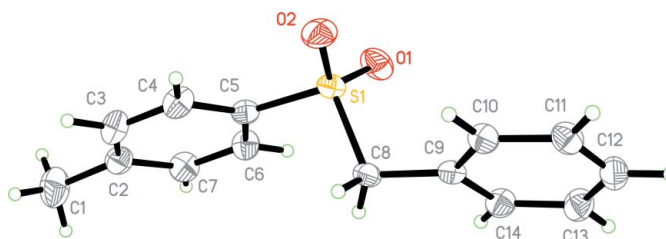


Figure 1

The molecular structure of (I) with the atom-numbering scheme, showing displacement ellipsoids at the 50% probability level.

mixture was irradiated in a 630 W microwave oven for 1 min. Crystals of (I) suitable for X-ray data collection were obtained from an ethanol solution by slow evaporation.

Crystal data

$C_{14}H_{14}O_2S$
 $M_r = 246.31$
 Orthorhombic, $P2_12_12_1$
 $a = 5.7135$ (5) Å
 $b = 12.6191$ (10) Å
 $c = 17.1549$ (14) Å
 $V = 1236.85$ (18) Å³
 $Z = 4$
 $D_x = 1.323$ Mg m⁻³

Mo $K\alpha$ radiation
 Cell parameters from 3217 reflections
 $\theta = 2.4$ – 25.0°
 $\mu = 0.25$ mm⁻¹
 $T = 298$ (2) K
 Block, colorless
 $0.26 \times 0.24 \times 0.16$ mm

Data collection

Bruker SMART APEX area-detector diffractometer
 φ and ω scans
 Absorption correction: multi-scan (SADABS; Bruker, 2002)
 $T_{\min} = 0.938$, $T_{\max} = 0.953$
 6597 measured reflections

2225 independent reflections
 2140 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.021$
 $\theta_{\text{max}} = 25.2^\circ$
 $h = -6 \rightarrow 4$
 $k = -14 \rightarrow 15$
 $l = -20 \rightarrow 20$

Refinement

Refinement on F^2
 $R[F^2 > 2\sigma(F^2)] = 0.033$
 $wR(F^2) = 0.086$
 $S = 1.06$
 2225 reflections
 155 parameters
 H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.047P)^2 + 0.2051P]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\text{max}} = 0.016$
 $\Delta\rho_{\text{max}} = 0.21$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.15$ e Å⁻³
 Absolute structure: Flack (1983),
 903 Friedel pairs
 Flack parameter: 0.08 (8)

Table 1

Selected geometric parameters (Å, °).

S1–O1	1.4252 (16)	S1–C5	1.765 (2)
S1–O2	1.4370 (17)	S1–C8	1.788 (2)
O1–S1–O2	118.45 (11)		
O1–S1–C8–C9	52.69 (18)	C5–S1–C8–C9	167.69 (15)
O2–S1–C8–C9	–77.32 (17)		

Table 2

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
C8–H8B ⁱ ···O2 ⁱ	0.97	2.49	3.447 (3)	168

Symmetry code: (i) $x + 1, y, z$.

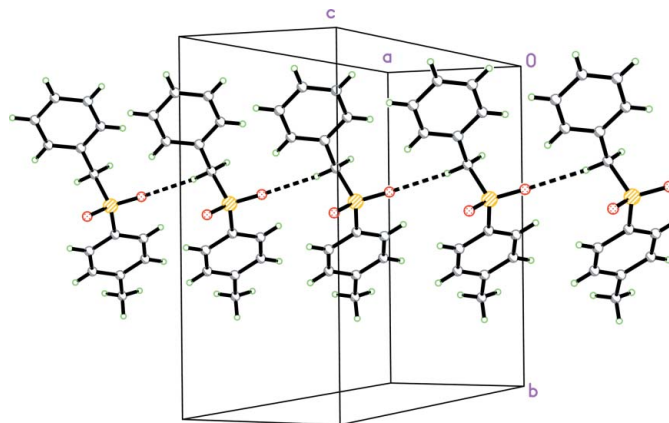


Figure 2

Illustration of a linear chain. Broken lines indicate C–H···O interactions.

H atoms bonded to C atoms were positioned geometrically and allowed to ride on their parent atoms at distances of $Csp^2-H = 0.93$ Å and $Csp^3-H = 0.97$ Å with $U_{\text{iso}}(H) = 1.2U_{\text{eq}}(Csp^2, Csp^3)$, while for methyl groups $C-H = 0.96$ Å with $U_{\text{iso}}(H) = 1.5U_{\text{eq}}(C)$.

Data collection: SMART (Bruker, 2002); cell refinement: SAINT (Bruker, 2002); data reduction: SAINT; program(s) used to solve structure: SHELXS97 (Sheldrick, 1997); program(s) used to refine structure: SHELXL97 (Sheldrick, 1997); molecular graphics: SHELXTL (Bruker, 2002); software used to prepare material for publication: SHELXL97.

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