Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

4-Acetylphenyl phenyl sulfone

Sheng-Rong Guo* and Yan-Qin Yuan

Department of Chemistry, Lishui College, 323000 Lishui Zhejiang, People's Republic of China

Correspondence e-mail: guosr9608@sina.com

Received 7 September 2005
Accepted 21 October 2005
Online 10 November 2005

Key indicators

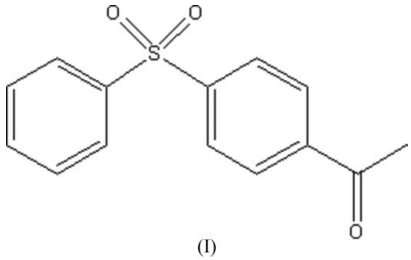
Single-crystal X-ray study
T = 298 K
Mean σ(C–C) = 0.003 Å
R factor = 0.045
wR factor = 0.119
Data-to-parameter ratio = 14.0

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

The title compound, $C_{14}H_{12}O_3S$, is an important synthetic intermediate in organic synthesis whose derivatives show favourable antiviral activity [Tetsushi, Yuji, Hirotaka, Masaki, Katsunori & Shozo (2003). *Green Chem.* **6**, 690–692]. The average S—C and S═O bond lengths are1.781 (3) and 1.436 (2) Å, respectively, and the two benzene planes are almost perpendicular to one another, forming a dihedral angle of 103.79 (9)°.

Comment

Diphenyl sulfones are an important class of compounds showing biological activity as fungicides and antipsychogtic agents (Wolf, 1999). The title compound, (I), was prepared by a microwave-assisted solvent-free synthesis. The molecular structure of (I) (Fig. 1 and Table 1) was also confirmed by physical and spectroscopic data.



(I)

The molecular structure of (I) is shown in Fig. 1. The skeleton displays no crystallographic symmetry. The two benzene planes are almost perpendicular to one another, forming a dihedral angle of 103.79 (9)°. The S═O bond lengths within the SO_2 group are almost equal, with an average value of 1.432 (17) Å. The average bond length for the four C–S bonds is 1.768 (2) Å. The O–S–O bond angle is 119.79 (11)°. These bond lengths and angles are all in normal ranges and compare well those observed in other analogues (Podlaha *et al.*, 1986; Julia *et al.*, 1986; Hauback & Mo, 1990; Li

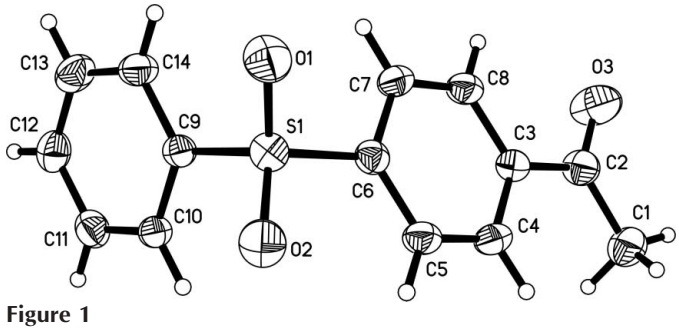


Figure 1
The structure (I) showing the atomic numbering scheme and displacement ellipsoids at the 50% probability level.

et al., 2003). The molecular structure of title compound was also affirmed by physical and spectral data.

Experimental

Solvent-free reaction of benzenesulfonyl chloride with 2-methyl-2-phenyl-1,3-dithiolane (Kazuhiko & Hitomi, 1992) followed by microwave irradiation for 20 min (Boyapati *et al.*, 2000) and hydrolysis with dilute HCl gave compound (I). Single crystals suitable for X-ray data collection were obtained on slow evaporation of an ethyl acetate/petroleum ether (4:1 *v*/*v*) solution (m.p. 363–364 K). IR (KBr, ν cm^{-1}): 2908, 1690, 1080, 817; ^{1}H NMR ($CDCl_3$): δ 8.06 (*m*, 4H), 7.97 (*d*, 2H), 7.59 (*m*, 3H), 2.62 (*s*, 3H).

Crystal data

$C_{14}H_{12}O_3S$
M_r = 260.31
Orthorhombic, *Pbcn*
a = 21.300 (8) Å
b = 7.756 (3) Å
c = 15.227 (6) Å
V = 2515.5 (17) Å^3
Z = 8
D_x = 1.375 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 5196 reflections
θ = 2.4–26.3°
μ = 0.25 mm^{-1}
T = 298 (2) K
Block, colourless
0.32 × 0.24 × 0.20 mm

Data collection

Bruker SMART CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2002)
T_{min} = 0.923, T_{max} = 0.951
12493 measured reflections
2297 independent reflections
2096 reflections with $I > 2\sigma(I)$
R_{int} = 0.023
θ_{max} = 25.3°
$h = -25 \rightarrow 22$
$k = -9 \rightarrow 9$
$l = -18 \rightarrow 12$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.045
$wR(F^2)$ = 0.119
S = 1.08
2297 reflections
164 parameters
$w = 1/[\sigma^2(F_o^2) + (0.0616P)^2 + 1.0763P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.30 e Å^{-3}
$\Delta\rho_{min}$ = −0.25 e Å^{-3}

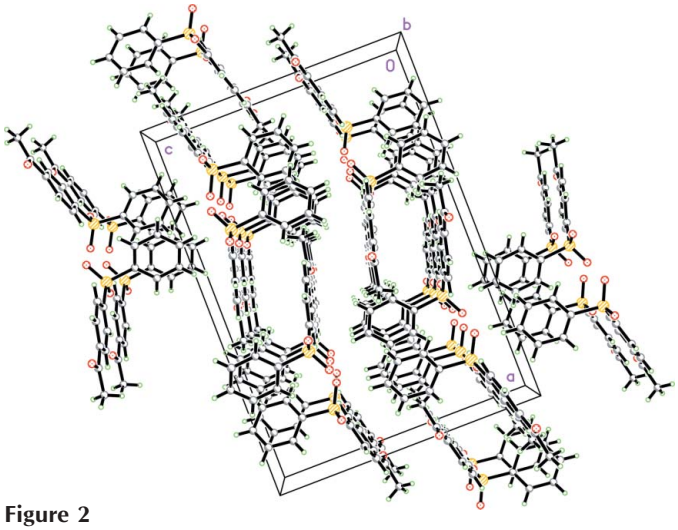


Figure 2
Packing diagram viewed down the *c* axis.

Table 1
Selected geometric parameters (Å, °).

S1—O2	1.4308 (17)	C2—C3	1.498 (3)
S1—O1	1.4321 (17)	C3—C4	1.384 (3)
S1—C9	1.761 (2)	C3—C8	1.392 (3)
S1—C6	1.774 (2)	C4—C5	1.377 (3)
O3—C2	1.207 (3)	C5—C6	1.376 (3)
C1—C2	1.486 (3)		
O2—S1—O1	119.79 (11)	C4—C3—C8	118.67 (19)
O2—S1—C9	107.85 (10)	C4—C3—C2	122.30 (19)
O1—S1—C9	108.14 (10)	C8—C3—C2	119.03 (19)
O2—S1—C6	107.46 (10)	C5—C4—C3	121.18 (19)
O1—S1—C6	108.67 (10)	C5—C6—S1	119.72 (16)
C9—S1—C6	103.79 (9)	C7—C6—S1	119.14 (15)
O3—C2—C1	120.3 (2)	C14—C9—S1	119.97 (16)
O3—C2—C3	119.5 (2)	C10—C9—S1	119.02 (15)
C1—C2—C3	120.2 (2)		
O3—C2—C3—C4	−176.0 (3)	S1—C6—C7—C8	−176.98 (16)
C4—C5—C6—C7	−0.7 (3)	O2—S1—C9—C14	145.65 (17)
C4—C5—C6—S1	178.11 (17)	O1—S1—C9—C14	14.74 (19)
O2—S1—C6—C5	6.7 (2)	C6—S1—C9—C14	−100.55 (17)
O1—S1—C6—C5	137.74 (18)	O2—S1—C9—C10	−34.17 (18)
C9—S1—C6—C5	−107.34 (18)	O1—S1—C9—C10	−165.07 (15)
O2—S1—C6—C7	−174.38 (16)	C6—S1—C9—C10	79.63 (17)
O1—S1—C6—C7	−43.38 (19)	S1—C9—C10—C11	−179.81 (16)
C9—S1—C6—C7	71.54 (18)	S1—C9—C14—C13	−179.78 (17)

All H atoms were initially located in a difference Fourier map and were placed in geometrically idealized positions and constrained to ride on their parent atoms, with C—H distances in the range 0.95–1.00 Å and with U_{iso}(H) = 1.2U_{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: *XP* (Bruker, 2002); software used to prepare material for publication: *SHELXL97*.

This work was supported by the Youth Foundation of Lishui College, China (No. QN05003).

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