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2-(4-Methylphenylsulfonyl)-1,3-diphenylprop-2-en-1-one

Jian-Ming Gu, Xiu-Rong Hu* and Wei-Ming Xu

Center of Analysis and Measurement, Zhejiang University, Hangzhou, Zhejiang 310028, People's Republic of China

Correspondence e-mail:
huxiurong@yahoo.com.cn

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In the title compound, $C_{22}H_{18}O_3S$, the phenyl group and sulfonyl substituent are *trans* with respect to the olefinic bond.

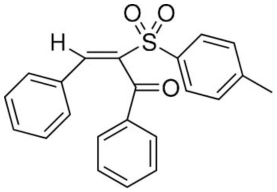
Key indicators

Single-crystal X-ray study
T = 296 K
Mean σ(C–C) = 0.003 Å
R factor = 0.045
wR factor = 0.141
Data-to-parameter ratio = 17.4

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

Comment

Vinyl sulfones have now become generally accepted useful intermediates in organic synthesis, and can serve efficiently as both Michael acceptors and π partners in cycloaddition reactions (Fuchs & Braish, 1986).



(I)

In the title compound, (I), the phenyl group and sulfonyl substituent are located *trans* with respect to to the C1═C2 olefinic bond (Fig. 1). The C2—C3 bond length is shorter than that of a typical Csp^2—Csp^2 bond (1.484 Å; Allen *et al.*, 1987), because the phenyl group (atoms C3–C8) is coplanar with the olefinic bond. The torsion angle C2—C1—C9—O1 of 94.9 (3)° shows clearly that the carbonyl group C9═O1 is non-coplanar with the C1═C2 double bond. Therefore, the bond distance C1—C9 is longer than those of C2—C3 and C9—C10. Carbonyl group C9═O1 is not coplanar with phenyl group C10–C15, probably as a result of steric effect.s Intermolecular π-π stacking is observed in the crystal structure (Fig. 2). The benzene ring (C3–C8) and its symmetry-related partner (1 −

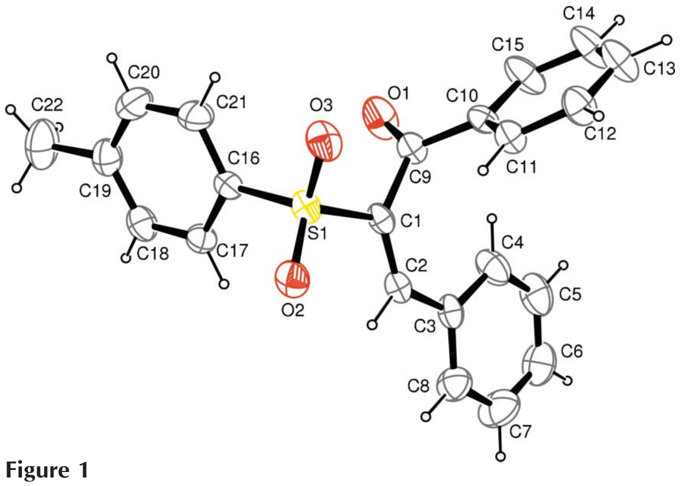


Figure 1
The molecular structure of (I), showing 30% probability displacement ellipsoids.

x, $1 - y$, $1 - z$) are parallel to one another, and the distance between the centroids of these benzene rings is 3.821 Å.

Experimental

Compound (I) was synthesized according to a literature method (Reddy *et al.*, 1990). 1-Phenyl-2-(4-methylphenylsulfonyl)ethanone (5.5 g, 20 mmol) and benzaldehyde (2.1 g, 20 mmol) were mixed in EtOH (50 ml). To the mixture, EtONa (1.7 g, 25 mmol) was added. The mixture was stirred at room temperature for 24 h. After extraction with CH_2Cl_2 and drying with anhydrous $MgSO_4$, the product (I) was obtained (5.62 g, 77.5%). Crystals of (I) were grown from an ethanol solution by slow evaporation.

Crystal data

$C_{22}H_{18}O_3S$
$M_r = 362.44$
Monoclinic, $P2_1/n$
$a = 13.6890$ (4) Å
$b = 8.2386$ (2) Å
$c = 16.7066$ (5) Å
$\beta = 92.9198$ (9)°
$V = 1881.69$ (9) Å^3
$Z = 4$
$D_x = 1.279$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 12090 reflections
$\theta = 2.5$–27.4°
$\mu = 0.19$ mm^{-1}
$T = 296$ (1) K
Block, colorless
0.60 × 0.40 × 0.20 mm

Data collection

Rigaku R-AXIS RAPID diffractometer
ω scans
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
$T_{min} = 0.827$, $T_{max} = 0.963$
18258 measured reflections
4301 independent reflections
3067 reflections with $F^2 > 2\sigma(F^2)$
$R_{int} = 0.025$
$\theta_{max} = 27.4°$
$h = -17 \rightarrow 17$
$k = -10 \rightarrow 10$
$l = -21 \rightarrow 21$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.045$
$wR(F^2) = 0.141$
$S = 1.00$
4116 reflections
236 parameters
H-atom parameters constrained
$w = 1/[0.0024F_o^2 + \sigma(F_o^2)]/(4F_o^2)$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.29$ e Å^{-3}
$\Delta\rho_{min} = -0.28$ e Å^{-3}
Extinction correction: Larson (1970)
Extinction coefficient: 124 (37)

Table 1
Selected geometric parameters (Å, °).

C1—C2	1.332 (3)	C2—C3	1.467 (2)
C1—C9	1.510 (2)		
S1—C1—C2—C3	176.5 (2)	C1—C2—C3—C4	−0.5 (4)
C2—C1—C9—O1	94.9 (3)	O1—C9—C10—C15	−24.2 (4)

The H atoms were placed in calculated positions, with C—H = 0.96–0.98 Å, and included in the refinement as riding, with $U_{iso}(H) = 1.2U_{eq}$(carrier atom). Because constraints were made in the 2θ range in the refinement, there is a large difference between the number of independent reflections and the reflections used in the refinement.

Data collection: *PROCESS-AUTO* (Rigaku, 1998); cell refinement: *PROCESS-AUTO*; data reduction: *CrystalStructure* (Rigaku/MSC, 2004); program(s) used to solve structure: *SIR97* (Altomare *et al.*, 1999); program(s) used to refine structure: *CRYSTALS* (Betteridge *et al.*, 2003); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *CrystalStructure*.

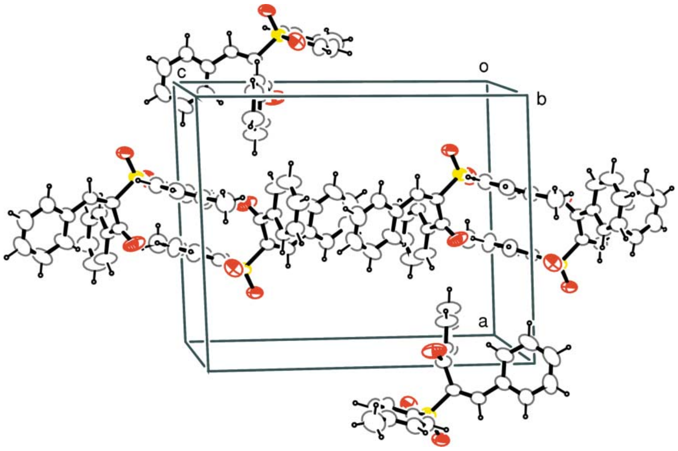


Figure 2
The crystal packing of (I).

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