

$S = 0.972$
 1874 reflections
 145 parameters
 H atoms not refined
 $w = 1/[\sigma^2(F_o^2) + (0.0407P)^2]$
 where $P = (F_o^2 + 2F_c^2)/3$

Extinction correction: none
 Scattering factors from
*International Tables for
 Crystallography* (Vol. C)

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4-Chlorophenyl 2,6-Dimethylphenyl Sulfone

JEYAKANTHAN JEYARAMAN AND D. VELMURUGAN

Department of Crystallography and Biophysics, University of Madras, Guindy Campus, Madras 600 025, India. E-mail: crystal@giasmd01.vsnl.net.in

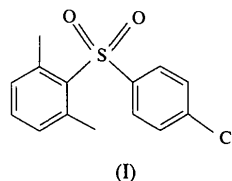
(Received 18 December 1996; accepted 14 April 1997)

Abstract

The phenyl rings in molecules of the title compound, C₁₄H₁₃ClO₂S, are perpendicular to one another. The crystal is stabilized by weak C—H···O intermolecular hydrogen bonding.

Comment

Like many sulfonamides and sulfones, the title compound, (I), has medicinal value (Krishnaiah, Narayana Raju, Lu, Chen & Narasinga Rao, 1995). It displays bond lengths which agree well with accepted values [*International Tables for Crystallography* (1992, Vol. C, Table 9.5.1.1)]. The C1—S1—C1' angle of 103.2(1)° is markedly less than the tetrahedral angle, 109.5°. This may be due to the short O2···C7 contact of 2.730(4) Å. The phenyl rings are perpendicular [dihedral angle 91.2(1)°] to one another.



The title structure was solved by direct methods using *SHELXS86* (Sheldrick, 1985). All non-H atoms were refined with anisotropic displacement parameters. All H atoms were located from difference Fourier maps and were included in the structure-factor calculations with isotropic displacement parameters equal to 1.1 U_{eq} of the respective carrier atom, but the parameters were not refined (*SHELXL93*; Sheldrick, 1993). The geometrical calculations were performed using *PARST* (Nardelli, 1983).

Data collection: *TEXSAN* (Molecular Structure Corporation, 1989). Cell refinement: *TEXSAN*. Data reduction: *TEXSAN*. Molecular graphics: *ORTEPII* (Johnson, 1976). Software used to prepare material for publication: *SHELXL93*.

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Supplementary data for this paper are available from the IUCr electronic archives (Reference: DE1054). Services for accessing these data are described at the back of the journal.

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The crystal packing is stabilized by a weak intermolecular hydrogen bond [C2'—H2' 0.94(2), C2'···O2' 3.452(4), H2'···O2' 2.72(3) Å and C2'—H2'···O2' 136(2)°; symmetry code: (i) $-x + \frac{1}{2}, y - \frac{1}{2}, z + \frac{3}{2}$].

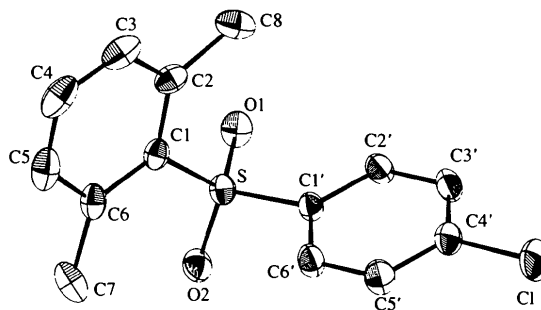


Fig. 1. The 50% probability displacement ellipsoid plot of the title molecule with the atom-numbering scheme. H atoms have been omitted.

Experimental

The title compound was prepared by oxidation of the corresponding sulfide or sulfoxide with excess hydrogen peroxide in acetic acid. Single crystals were obtained by slow evaporation of an ethanol solution (Chandrasekaran, 1991).

Crystal data

$C_{14}H_{13}ClO_2S$

$M_r = 280.75$

Monoclinic

$C2/c$

$a = 20.239 (5) \text{ \AA}$

$b = 10.911 (2) \text{ \AA}$

$c = 15.197 (6) \text{ \AA}$

$\beta = 126.580 (11)^\circ$

$V = 2694.8 (14) \text{ \AA}^3$

$Z = 8$

$D_x = 1.384 \text{ Mg m}^{-3}$

D_m not measured

Mo $K\alpha$ radiation

$\lambda = 0.71069 \text{ \AA}$

Cell parameters from 25 reflections

$\theta = 14\text{--}18^\circ$

$\mu = 0.429 \text{ mm}^{-1}$

$T = 293 (2) \text{ K}$

Rectangular block

$0.20 \times 0.15 \times 0.15 \text{ mm}$

Transparent

Data collection

Rigaku AFC-7S diffractometer

$\omega/2\theta$ scans

Absorption correction: none

2934 measured reflections

2367 independent reflections

1744 reflections with

$I > 2\sigma(I)$

$R_{int} = 0.033$

$\theta_{max} = 25.02^\circ$

$h = 0 \rightarrow 24$

$k = 0 \rightarrow 12$

$l = -18 \rightarrow 14$

3 standard reflections

every 100 reflections

frequency: 60 min

intensity decay: $< 1\%$

Refinement

Refinement on F^2

$R[F^2 > 2\sigma(F^2)] = 0.051$

$wR(F^2) = 0.153$

$S = 1.056$

2367 reflections

215 parameters

H atoms refined

$w = 1/[\sigma^2(F_o^2) + (0.0666P)^2 + 4.2184P]$

where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{max} = 0.067$

$\Delta\rho_{max} = 0.29 \text{ e \AA}^{-3}$

$\Delta\rho_{min} = -0.32 \text{ e \AA}^{-3}$

Extinction correction: none

Scattering factors from

International Tables for Crystallography (Vol. C)

Table 1. Selected geometric parameters (\AA , $^\circ$)

S1—O1	1.431 (2)	S1—C1	1.779 (3)
S1—O2	1.437 (2)	Cl—C4'	1.734 (3)
S1—C1'	1.775 (2)		
O1—S1—O2	116.76 (12)	C6—C1—S1	120.6 (2)
O1—S1—C1'	108.61 (11)	C2—C1—S1	117.6 (2)
O2—S1—C1'	106.69 (11)	C6'—C1'—S1	119.2 (2)
O1—S1—C1	110.04 (11)	C2'—C1'—S1	120.2 (2)
O2—S1—C1	110.56 (12)	C3'—C4'—C1	120.1 (2)
C1'—S1—C1	103.24 (12)	C5'—C4'—C1	118.6 (2)

Data collection: *MSCIAFC Diffractometer Control Software* (Molecular Structure Corporation, 1988). Cell refinement: *MSCIAFC Diffractometer Control Software*. Data reduction: *MSCIAFC Diffractometer Control Software*. Program(s) used to solve structure: *SHELXS86* (Sheldrick, 1985). Program(s) used to refine structure: *SHELXL93* (Sheldrick, 1993). Molecular graphics: *ORTEP92* (Vicković, 1994). Software used to prepare material for publication: *PARST* (Nardelli, 1983).

Supplementary data for this paper are available from the IUCr electronic archives (Reference: MU1313). Services for accessing these data are described at the back of the journal.

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3-Benzoyl-2-methylindole

M. PAZ MARTINEZ-ALCAZAR,^a ISABEL FONSECA,^b FELIX H. CANO,^b J. GONZALO RODRIGUEZ^c AND ANAHI URRUTIA^c

^aFacultad de Ciencias Experimentales y Tecnicas, Departamento de Ciencias Basicas, Universidad San Pablo, CEU, 28668-Boadilla del Monte, Madrid, Spain, ^bInstituto de Quimica-Fisica Rocasolano-CSIC, Departamento de Cristalografía, Serrano 119, E-28006 Madrid, Spain, and ^cFacultad de Ciencias, Departamento de Quimica Organica, Universidad Autonoma, Cantoblanco, 28049-Madrid, Spain. E-mail: xisabel@roca.csic.es

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Abstract

The crystal and molecular structure of $C_{16}H_{13}NO$ has been determined. Bond lengths and angles are within normal ranges and molecules are held together in the crystal by intermolecular N—H \cdots O hydrogen bonding.

Comment

The specific alkylation or acylation of the indole ring is an important question for the preparation of derivatives on position 3 or 1 and the appropriate alkyl or acyl derivatives serve for the preparation of aspidosperm alkaloids in which we are interested (Rodriguez & Urrutia, 1996). Reactions of methylindolylmagnesium salts with benzoyl chloride give 3-benzoyl-2-methylindole, (I), in all cases; this product claimed our attention because of the orange colour of the crystals and