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Key indicators

Single-crystal X-ray study
 $T = 294$ K
Mean $\sigma(\text{C}-\text{C}) = 0.004$ Å
 R factor = 0.040
 wR factor = 0.107
Data-to-parameter ratio = 16.3For details of how these key indicators were
automatically derived from the article, see
<http://journals.iucr.org/e>.

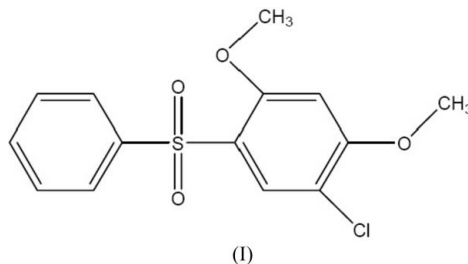
1-Benzenesulfonyl-5-chloro-2,4-dimethoxybenzene

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In the title compound, $\text{C}_{14}\text{H}_{13}\text{ClO}_4\text{S}$, the dihedral angle between the two benzene rings is $73.0(2)^\circ$. The supramolecular aggregation is completed by means of $\text{C}-\text{H}\cdots\text{O}$ hydrogen bonds involving a sulfone O atom and an aromatic CH group, forming centrosymmetric dimers.

Comment

Sulfones, based on tetrahedrally coordinated S^{VI} atoms, do not exhibit rotational disorder, which makes them an interesting building block in supramolecular chemistry (Guo & Yuan, 2005; Robinson *et al.*, 2001). The title compound, (I), was synthesized by reacting 1,3-dimethoxybenzene and benzenesulfonyl chloride (see *Experimental*) and had not been previously reported. An X-ray crystal structure determination of (I) was undertaken in order to elucidate its conformation and the results are presented here.



The molecular structure of (I) is shown in Fig. 1. For sulfone atom S1, formally S^{VI} , the $\text{S}-\text{C}$ and $\text{S}=\text{O}$ bond lengths and the $\text{O}=\text{S}=\text{O}$ and $\text{C}-\text{S}-\text{C}$ angles are all in normal ranges (Table 1), and compare well with those observed in other related compounds (*e.g.* Podlaha *et al.*, 1986; Julia *et al.*, 1986; Mo & Berg, 1982; Hauback & Mo, 1990). Least-squares plane calculations show that the dihedral angle between the phenyl (C1–C6) and benzene (C7–C12) planes is $73.0(2)^\circ$, and that atoms O3 and O4 are almost coplanar with the benzene ring.

The crystal structure of (I) is stabilized through $\text{C}-\text{H}\cdots\text{O}$ hydrogen bonds (Table 2). Aromatic group C2–H2 acts as a hydrogen-bond donor to atom O1 from an adjacent sulfone group, forming centrosymmetric dimers (Fig. 2).

Experimental

A dichloromethane solution of 1,3-dimethoxybenzene (1.0 equivalent) and benzenesulfonyl chloride (2.10 equivalents) was added dropwise to a stirred suspension of aluminium trichloride (2.10 equivalents) in dichloromethane, under nitrogen. Once addition was complete, the reaction mixture was stirred at 298 K for 72 h. The resulting solution was then poured over a mixture of crushed ice and concentrated HCl. The organic layer was separated and washed with

an aqueous 5% KOH solution. The base extracts were combined, neutralized with concentrated HCl and extracted with diethyl ether. The ether extracts were dried over MgSO₄ and the solvent was removed under reduced pressure. The resulting residue was recrystallized from methanol, affording prismatic colourless crystals.

Crystal data

C₁₄H₁₃ClO₄S
M_r = 312.75
 Orthorhombic, *Pbca*
a = 7.3423 (16) Å
b = 19.487 (4) Å
c = 20.022 (4) Å
V = 2864.7 (10) Å³

Z = 8
D_x = 1.450 Mg m⁻³
 Mo *K*α radiation
 μ = 0.42 mm⁻¹
T = 294 (2) K
 Prism, colourless
 0.26 × 0.22 × 0.20 mm

Data collection

Bruker SMART-1000 CCD area-detector diffractometer
 φ and ω scans
 Absorption correction: multi-scan (*SADABS*; Bruker, 1997)
T_{min} = 0.898, *T_{max}* = 0.921

15348 measured reflections
 2981 independent reflections
 1860 reflections with *I* > 2σ(*I*)
R_{int} = 0.054
 θ_{\max} = 26.6°

Refinement

Refinement on *F*²
R [*F*² > 2σ(*F*²)] = 0.040
wR (*F*²) = 0.107
S = 1.01
 2981 reflections
 183 parameters
 H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0452P)^2 + 0.9214P]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\max} = 0.001$
 $\Delta\rho_{\max} = 0.21 \text{ e } \text{Å}^{-3}$
 $\Delta\rho_{\min} = -0.33 \text{ e } \text{Å}^{-3}$

Table 1

Selected geometric parameters (Å, °).

S1—O2	1.4342 (19)	S1—C1	1.758 (3)
S1—O1	1.4348 (17)	S1—C7	1.764 (2)
O2—S1—O1	118.38 (11)	O2—S1—C7	109.06 (11)
O2—S1—C1	107.73 (12)	O1—S1—C7	106.18 (11)
O1—S1—C1	108.03 (11)	C1—S1—C7	106.94 (11)

Table 2

Hydrogen-bond geometry (Å, °).

<i>D</i> —H... <i>A</i>	<i>D</i> —H	H... <i>A</i>	<i>D</i> ... <i>A</i>	<i>D</i> —H... <i>A</i>
C2—H2...O1 ⁱ	0.93	2.45	3.344 (5)	162

Symmetry code: (i) $-x + 2, -y, -z + 1$.

H atoms were included in calculated positions, with aromatic C—H distances constrained to 0.93 Å and methyl C—H distances constrained to 0.96 Å. The isotropic displacement parameters for H atoms were fixed at 1.2*U*_{eq}(C) for aromatic CH and 1.5*U*_{eq}(C) for methyl H atoms.

Data collection: *SMART* (Bruker, 1997); cell refinement: *SAINT* (Bruker, 1997); 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, 1997); software used to prepare material for publication: *SHELXTL*.

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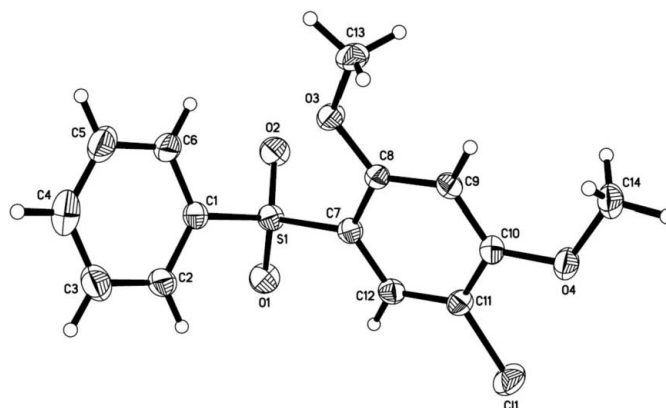


Figure 1

The molecular structure of (I), showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 30% probability level.

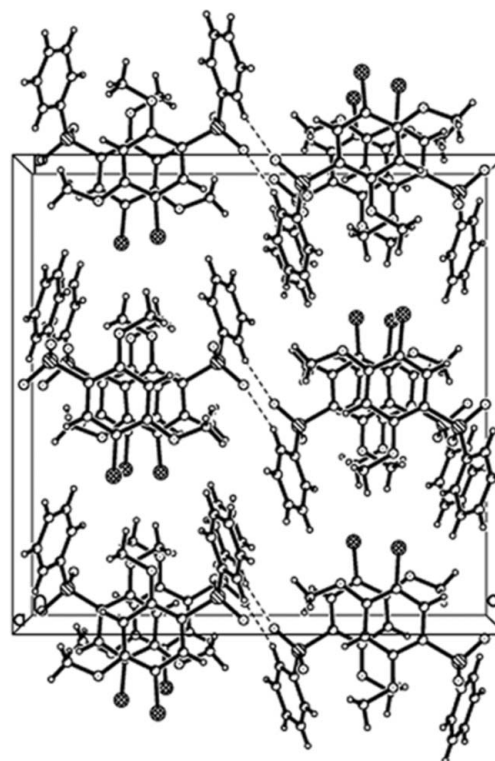


Figure 2

The packing of the molecules, viewed down the *a* axis. Hydrogen bonds are shown as dashed lines.

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