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Phenylmethanesulfonyl fluoride

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Key indicators

Single-crystal X-ray study
T = 294 K
Mean σ(C–C) = 0.007 Å
R factor = 0.043
wR factor = 0.115
Data-to-parameter ratio = 7.8

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

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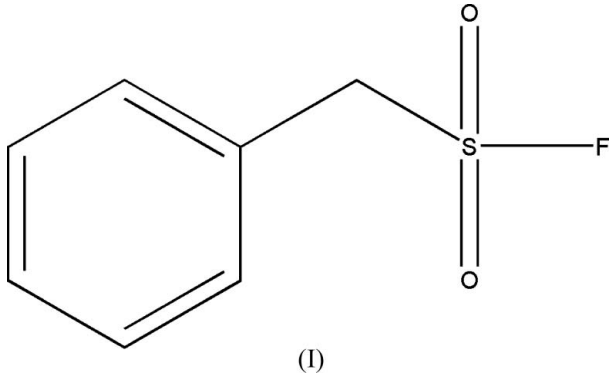
The asymmetric unit of the title compound, $C_7H_6FO_2S$, contains only one half-molecule; a mirror plane passes through F, S, and the methylene C atom, and bisects the benzene ring. The S atom is sp^3 hybridized.

Comment

Phenylmethanesulfonyl fluoride, (I), is an inhibitor of serine proteases and widely used in the extraction of active protein from cells and tissues (Koffman *et al.*, 1991).



(I)

The asymmetric unit of (I) (Fig. 1) contains only one half-molecule. The bond lengths and angles are within normal ranges (Allen *et al.*, 1987). Atoms H1, C1, C4, C5, S1 and F1 lie

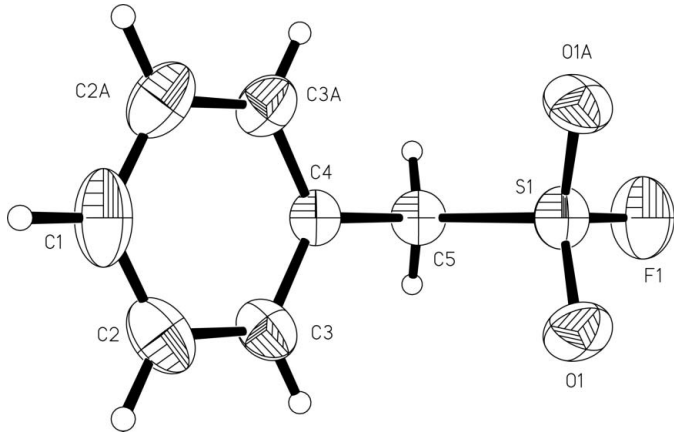


Figure 1
The molecular structure of (I), showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 35% probability level. [Symmetry code: (A) $-x, y, z$.]

on a mirror plane. The angles around atom S1 range from 106.0 (3) to 111.8 (3)°, which indicates the sp^3 hybridization of S1. The phenyl ring is, of course, planar and atoms C5 and S1 are displaced by 0.013 (3) and 1.675 (2) Å, respectively, from that plane.

Experimental

The title compound was obtained by recrystallization of its impure industrial product. The crystal used for data collection was obtained by slow evaporation of a methanol solution, at 298 K, over a period of 10 d.

Crystal data

$C_7H_6FO_2S$
M_r = 173.18
Orthorhombic, $Pmn2_1$
a = 9.2880 (19) Å
b = 8.8160 (18) Å
c = 4.812 (1) Å
V = 394.02 (14) Å^3
Z = 2
D_x = 1.460 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 0.37 mm^{-1}
T = 294 (2) K
Block, colorless
0.30 × 0.20 × 0.10 mm

Data collection

Bruker SMART CCD diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2001)
T_{min} = 0.897, T_{max} = 0.964
867 measured reflections
461 independent reflections
383 reflections with $I > 2\sigma(I)$
R_{int} = 0.025
θ_{max} = 26.0°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.043
$wR(F^2)$ = 0.115
S = 1.10
461 reflections
59 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0555P)^2 + 0.106P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.29 e Å^{-3}
$\Delta\rho_{min}$ = −0.21 e Å^{-3}
Extinction correction: *SHELXL97*
Extinction coefficient: 0.103 (17)

H atoms were positioned geometrically, with C—H = 0.93 and 0.96 Å for aromatic and methylene H atoms, respectively, and constrained to ride on their parent atoms, with U_{iso}(H) = 1.2U_{eq}(C).

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINT* (Bruker, 2001); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXL97*; software used to prepare material for publication: *SHELXL97*.

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