

## 4-Fluoro-3-nitrophenyl methyl sulfone

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## Key indicators

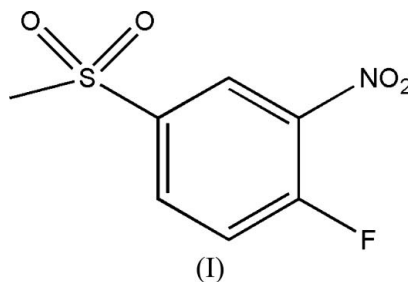
Single-crystal X-ray study  
 $T = 298$  K  
Mean  $\sigma(\text{C}-\text{C}) = 0.003$  Å  
 $R$  factor = 0.044  
 $wR$  factor = 0.115  
Data-to-parameter ratio = 12.5For details of how these key indicators were  
automatically derived from the article, see  
<http://journals.iucr.org/e>.

In the title compound,  $\text{C}_7\text{H}_6\text{FNO}_4\text{S}$ , the average  $\text{S}-\text{C}$  and  $\text{S}=\text{O}$  bond lengths are 1.762 (2) and 1.4266 (19) Å, respectively. The crystal structure is stabilized by intra- and intermolecular  $\text{C}-\text{H}\cdots\text{O}$  hydrogen bonds.

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## Comment

Phenyl methyl sulfones are a useful class of compounds showing important biological applications as drug-resistant viral variant inhibitors (Radi *et al.*, 2005). An X-ray crystallographic structure analysis of the title compound, (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. Bond lengths and angles are not unusual and compare well with those observed in other analogues (Podlaha *et al.*, 1986; Julia *et al.*, 1986; Hauback & Mo, 1990; Li *et al.*, 2003; Guo & Yuan, 2005). The  $\text{S}=\text{O}$  bond lengths within the  $\text{SO}_2$  group are almost equal, with an average value of 1.4266 (19) Å. The average bond length for the two  $\text{C}-\text{S}$  bonds is 1.762 (2) Å. The nitro group is tilted by  $16.7$  (3)° with respect to the plane of the benzene ring.

The crystal structure of (I) is stabilized by intra- and intermolecular  $\text{C}-\text{H}\cdots\text{O}$  hydrogen-bonding interactions (Table 2).

## Experimental

A mixture of anhydrous sodium sulfite (0.25 mol), sodium bicarbonate (0.30 mol) and water (100 ml) was put in a beaker provided with a mechanical stirrer and thermometer, and heated on a hot plate at 343–353 K, while 3-nitro-4-fluorobenzenesulfonyl chloride (0.1 mol) was added dropwise with stirring. The solid sodium-substituted benzene sulfinate that separated was collected by filtration and mixed with sodium bicarbonate (0.1 mol) and dimethyl sulfate (0.08 mol) in a three-necked round-bottomed flask equipped with a mechanical stirrer, a reflux condenser, and a separatory funnel. Water (10–20 ml) was added dropwise, and the solution was refluxed for 5 h. After

cooling to room temperature, the mixture was extracted with benzene (30 ml × 3) and dried with anhydrous calcium chloride. The drying agent was removed by filtration and the remaining solid was washed with benzene. Benzene was then removed from the filtrate by distillation under reduced pressure, and the solid compound (I) that separated was dried further at about 10 mmHg. The product was finally purified by recrystallization from an ethanol–water mixture (1:1 v/v). Single crystals suitable for X-ray analysis were obtained by slow evaporation of an ethyl acetate–toluene (4:1 v/v) solution (m.p. 383–384 K).

Crystal data

C<sub>7</sub>H<sub>6</sub>FNO<sub>4</sub>S  
*M<sub>r</sub>* = 219.19  
 Monoclinic, *P*2<sub>1</sub>/*c*  
*a* = 7.8514 (15) Å  
*b* = 9.7882 (18) Å  
*c* = 12.215 (2) Å  
 $\beta$  = 108.595 (3)°  
*V* = 889.8 (3) Å<sup>3</sup>  
*Z* = 4  
*D<sub>x</sub>* = 1.636 Mg m<sup>-3</sup>  
 Mo *K*α radiation  
 $\mu$  = 0.37 mm<sup>-1</sup>  
*T* = 298 (2) K  
 Block, colourless  
 0.38 × 0.31 × 0.30 mm

Data collection

Bruker APEX area-detector diffractometer  
 $\varphi$  and  $\omega$  scans  
 Absorption correction: multi-scan (*SADABS*; Bruker, 2002)  
*T<sub>min</sub>* = 0.873, *T<sub>max</sub>* = 0.898  
 4551 measured reflections  
 1603 independent reflections  
 1525 reflections with *I* > 2σ(*I*)  
*R<sub>int</sub>* = 0.015  
 $\theta_{max}$  = 25.2°

Refinement

Refinement on *F*<sup>2</sup>  
*R*[*F*<sup>2</sup> > 2σ(*F*<sup>2</sup>)] = 0.044  
*wR*(*F*<sup>2</sup>) = 0.115  
*S* = 1.13  
 1603 reflections  
 128 parameters  
 H-atom parameters constrained  
 $w = 1/[\sigma^2(F_o^2) + (0.0563P)^2 + 0.4108P]$   
 where  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta/\sigma)_{max} < 0.001$   
 $\Delta\rho_{max} = 0.26 \text{ e } \text{Å}^{-3}$   
 $\Delta\rho_{min} = -0.25 \text{ e } \text{Å}^{-3}$

Table 1 Selected geometric parameters (Å, °).

S1–O3	1.4244 (19)	S1–C4	1.774 (2)
S1–O4	1.4287 (18)	F1–C1	1.333 (3)
S1–C7	1.745 (3)		
O3–S1–O4	117.55 (12)	O2–N1–C2	117.2 (2)
O3–S1–C7	109.13 (14)	O1–N1–C2	119.2 (2)
O4–S1–C7	109.43 (14)	F1–C1–C6	118.4 (2)
O3–S1–C4	107.88 (10)	F1–C1–C2	120.9 (2)
O4–S1–C4	107.08 (10)	C3–C2–N1	117.7 (2)
C7–S1–C4	105.02 (11)	C1–C2–N1	122.2 (2)
O2–N1–O1	123.6 (2)		
F1–C1–C2–C3	178.8 (2)	O4–S1–C4–C3	144.72 (17)
F1–C1–C2–N1	–0.8 (3)	C7–S1–C4–C3	–99.0 (2)
O3–S1–C4–C3	17.3 (2)	F1–C1–C6–C5	–178.5 (2)

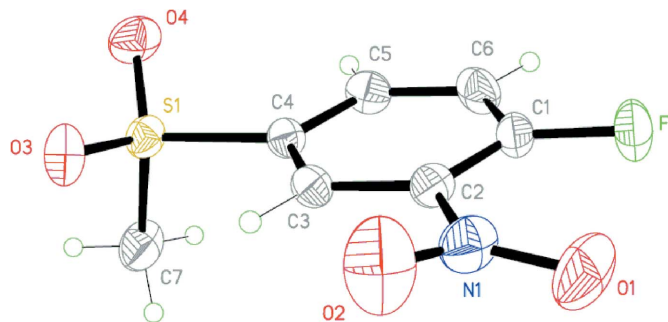


Figure 1 The molecular structure of (I), showing the atom-numbering scheme and displacement ellipsoids at the 50% probability level.

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>
C3–H3···O3	0.93	2.54	2.906 (3)	104
C5–H5···O3 <sup>i</sup>	0.93	2.55	3.379 (3)	148
C6–H6···O4 <sup>ii</sup>	0.93	2.39	3.292 (3)	162

Symmetry codes: (i) *x*,  $-y + \frac{1}{2}$ , *z* –  $\frac{1}{2}$ ; (ii)  $-x + 1$ ,  $y + \frac{1}{2}$ ,  $-z - \frac{1}{2}$ .

All H atoms were placed in geometrically idealized positions and constrained to ride on their parent atoms with C–H distances in the range 0.93–0.96 Å and *U<sub>iso</sub>*(H) = 1.2*U<sub>eq</sub>*(C), or 1.5*U<sub>eq</sub>*(C) for methyl H atoms.

Data collection: *SMART* (Bruker, 2002); cell refinement: *SAINTE* (Bruker, 2002); data reduction: *SAINTE*; 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*.

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