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## Structure Reports

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## 2-(2-Nitrophenylsulfinyl)acetonitrile

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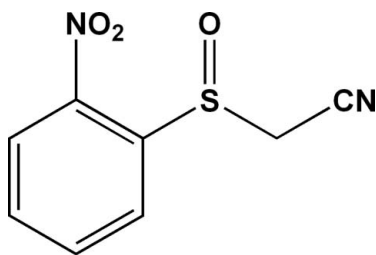
Received 18 February 2013; accepted 19 February 2013

Key indicators: single-crystal X-ray study;  $T = 295$  K; mean  $\sigma(\text{C}-\text{C}) = 0.002$  Å;  $R$  factor = 0.027;  $wR$  factor = 0.070; data-to-parameter ratio = 18.3.

In the title compound,  $\text{C}_8\text{H}_6\text{N}_2\text{O}_3\text{S}$ , the dihedral angle between the nitro group and the benzene ring is  $6.76$  ( $9^\circ$ ). The bond-angle sum at the S atom is  $308.1^\circ$ . In the crystal, molecules are linked by  $\text{C}-\text{H}\cdots\text{O}$  hydrogen bonds to generate (010) sheets. The crystal studied was found to be a racemic twin.

## Related literature

For a related structure and background to sulfoxides, see: Benmebarek *et al.* (2012). For related structures see: Yan (2010); Kobayashi *et al.* (2003).



## Experimental

## Crystal data

 $\text{C}_8\text{H}_6\text{N}_2\text{O}_3\text{S}$  $M_r = 210.21$ Orthorhombic,  $P2_12_12_1$  $a = 5.4114$  (2) Å $b = 10.7602$  (4) Å $c = 15.1837$  (5) Å $V = 884.11$  (5) Å<sup>3</sup> $Z = 4$ Mo  $K\alpha$  radiation $\mu = 0.35$  mm<sup>-1</sup> $T = 295$  K $0.26 \times 0.2 \times 0.15$  mm

## Data collection

Bruker APEXII CCD  
diffractometer  
8401 measured reflections

2348 independent reflections  
2222 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.016$

## Refinement

 $R[F^2 > 2\sigma(F^2)] = 0.027$  $wR(F^2) = 0.070$  $S = 1.05$ 

2348 reflections

128 parameters

H-atom parameters constrained

 $\Delta\rho_{\text{max}} = 0.21$  e Å<sup>-3</sup> $\Delta\rho_{\text{min}} = -0.18$  e Å<sup>-3</sup>

Absolute structure: Flack (1983),

1379 Friedel pairs

Flack parameter: 0.53 (1)

Table 1

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$\text{C6}-\text{H6}\cdots\text{O2}^{\text{i}}$	0.93	2.41	3.3198 (18)	165
$\text{C7}-\text{H7A}\cdots\text{O2}^{\text{ii}}$	0.97	2.50	3.1190 (19)	122

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

Data collection: *APEX2* (Bruker, 2011); cell refinement: *APEX2*; data reduction: *APEX2*; program(s) used to solve structure: *SIR2002* (Burla *et al.*, 2005); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3* (Farrugia, 2012) and *DIAMOND* (Brandenburg & Berndt, 2001); software used to prepare material for publication: *WinGX* (Farrugia, 2012).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB7044).

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## supporting information

*Acta Cryst.* (2013). E69, o432 [doi:10.1107/S1600536813004832]

## 2-(2-Nitrophenylsulfinyl)acetonitrile

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### S1. Comment

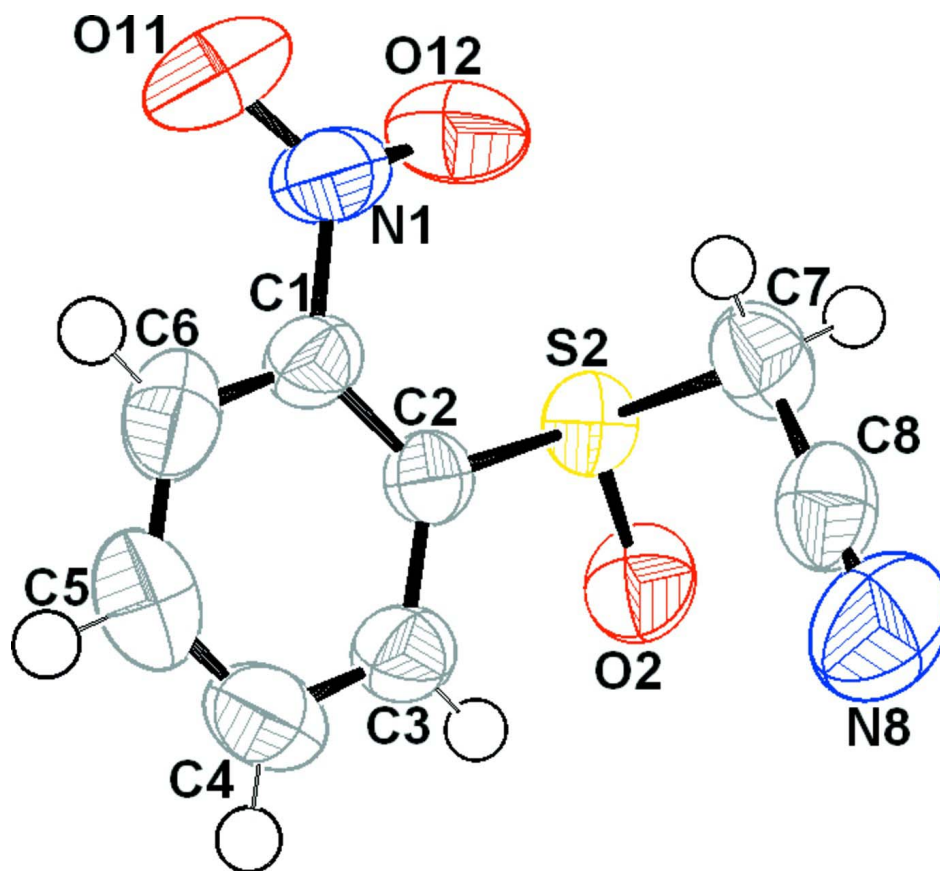
As part of our ongoing studies on the synthesis, structures and biological activity of organometallic sulfanilamide complexes (Benmebarek *et al.* 2012), we have synthesized and determined the crystal structure of the title compound, (I). The molecular geometry and the atom-numbering scheme are shown in Fig 1. The bond angle sum at the S atom is 308.1°. The nitro group forms a dihedral angle of 6.76 (9)° with the benzene ring, which is very different to that found in 2-(methylsulfinyl)benzamide (25.6°) (Yan, 2010) and in benzamide (26.3°) (Kobayashi *et al.*, 2003), and similar to chloromethylsulfinyl-2-nitrobenzene (2.7°) (Benmebarek *et al.*, 2012). The crystal structure features C—H···O hydrogen bonds (Fig. 2) forming (010) sheets.

### S2. Experimental

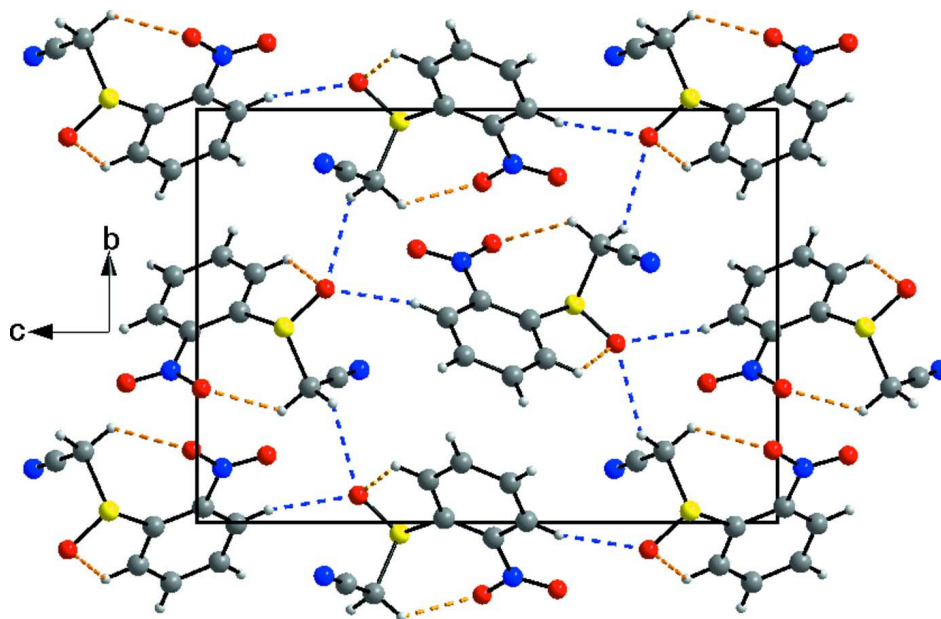
Chloromethylsulfinyl-2-nitrobenzene (2.196 g, 10 mmol) obtained according to established procedures (Benmebarek *et al.*, 2012) and potassium cyanide (0.65 g, 10 mmol) were dissolved in 75 ml aqua ethanol solution (25 ml water + 50 ml ethanol) and refluxed for 3 h under continuous stirring. Then the obtained product was evaporated at room temperature to dryness. The residue was diluted in 50 ml pure ethanol. After a few days, colourless blocks were recovered, as the solvent slowly evaporated.

### S3. Refinement

All non-H atoms were refined with anisotropic atomic displacement parameters. Approximate positions for all H atoms were first obtained from the difference electron density map. However, the H atoms were situated into idealized positions and the H-atoms have been refined within the riding atom approximation. The applied constraints were as follow:  $C_{\text{aryl}}-H_{\text{aryl}} = 0.93 \text{ \AA}$  and  $C_{\text{methylene}}-H_{\text{methylene}} = 0.97 \text{ \AA}$ .  $U_{\text{iso}}(H_{\text{aryl/methylene}}) = 1.2U_{\text{eq}}(C_{\text{aryl/methylene}})$ .

**Figure 1**

View of the asymmetric unit of, (I), with displacement ellipsoids drawn at the 50% probability level.



**Figure 2**

Packing diagram of (I) viewed down [100] showing the hydrogen bonding in alternating layers parallel to (010) planes.

**2-(2-Nitrophenylsulfinyl)acetonitrile***Crystal data*C<sub>8</sub>H<sub>6</sub>N<sub>2</sub>O<sub>3</sub>S $M_r = 210.21$ Orthorhombic,  $P2_12_12_1$ 

Hall symbol: P 2ac 2ab

 $a = 5.4114 (2) \text{ \AA}$  $b = 10.7602 (4) \text{ \AA}$  $c = 15.1837 (5) \text{ \AA}$  $V = 884.11 (5) \text{ \AA}^3$  $Z = 4$  $F(000) = 432$  $D_x = 1.579 \text{ Mg m}^{-3}$ Mo  $K\alpha$  radiation,  $\lambda = 0.71073 \text{ \AA}$ 

Cell parameters from 6191 reflections

 $\theta = 2.7\text{--}29.1^\circ$  $\mu = 0.35 \text{ mm}^{-1}$  $T = 295 \text{ K}$ 

Block, colourless

 $0.26 \times 0.2 \times 0.15 \text{ mm}$ *Data collection*Bruker APEXII CCD  
diffractometer

Radiation source: sealed tube

Graphite monochromator

 $\varphi$  and  $\omega$  scans

8401 measured reflections

2348 independent reflections

2222 reflections with  $I > 2\sigma(I)$  $R_{\text{int}} = 0.016$  $\theta_{\text{max}} = 29.1^\circ$ ,  $\theta_{\text{min}} = 4.0^\circ$  $h = -6 \rightarrow 7$  $k = -14 \rightarrow 14$  $l = -20 \rightarrow 20$ *Refinement*Refinement on  $F^2$ 

Least-squares matrix: full

 $R[F^2 > 2\sigma(F^2)] = 0.027$  $wR(F^2) = 0.070$  $S = 1.05$ 

2348 reflections

128 parameters

0 restraints

Primary atom site location: structure-invariant  
direct methodsSecondary atom site location: difference Fourier  
mapHydrogen site location: inferred from  
neighbouring sites

H-atom parameters constrained

 $w = 1/[\sigma^2(F_o^2) + (0.0327P)^2 + 0.2515P]$ where  $P = (F_o^2 + 2F_c^2)/3$  $(\Delta/\sigma)_{\text{max}} = 0.001$  $\Delta\rho_{\text{max}} = 0.21 \text{ e \AA}^{-3}$  $\Delta\rho_{\text{min}} = -0.18 \text{ e \AA}^{-3}$ Absolute structure: Flack (1983), 1379 Friedel  
pairs

Absolute structure parameter: 0.53 (1)

*Special details*

**Geometry.** All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

**Refinement.** Refinement of  $F^2$  against ALL reflections. The weighted  $R$ -factor  $wR$  and goodness of fit  $S$  are based on  $F^2$ , conventional  $R$ -factors  $R$  are based on  $F$ , with  $F$  set to zero for negative  $F^2$ . The threshold expression of  $F^2 > \sigma(F^2)$  is used only for calculating  $R$ -factors(gt) etc. and is not relevant to the choice of reflections for refinement.  $R$ -factors based on  $F^2$  are statistically about twice as large as those based on  $F$ , and  $R$ -factors based on ALL data will be even larger.

*Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters ( $\text{\AA}^2$ )*

	$x$	$y$	$z$	$U_{\text{iso}}^*/U_{\text{eq}}$
S2	0.53769 (6)	0.02767 (3)	0.15053 (2)	0.02770 (9)

O2	0.5137 (2)	-0.06613 (11)	0.22173 (7)	0.0395 (3)
O11	0.4219 (4)	0.16230 (15)	-0.12118 (8)	0.0678 (5)
O12	0.5834 (2)	0.17541 (11)	0.00821 (9)	0.0453 (3)
N1	0.4351 (3)	0.13166 (12)	-0.04412 (9)	0.0352 (3)
N8	-0.0001 (3)	0.12996 (17)	0.28063 (10)	0.0515 (4)
C1	0.2643 (3)	0.03718 (13)	-0.01153 (9)	0.0263 (3)
C2	0.2906 (2)	-0.01016 (12)	0.07377 (8)	0.0235 (2)
C3	0.1293 (3)	-0.10289 (13)	0.10054 (10)	0.0294 (3)
H3	0.1443	-0.137	0.1566	0.035*
C4	-0.0546 (3)	-0.14513 (14)	0.04407 (11)	0.0357 (3)
H4	-0.1622	-0.2071	0.0628	0.043*
C5	-0.0795 (3)	-0.09610 (15)	-0.03950 (11)	0.0376 (3)
H5	-0.2034	-0.125	-0.0767	0.045*
C6	0.0809 (3)	-0.00355 (14)	-0.06796 (9)	0.0343 (3)
H6	0.0651	0.0304	-0.124	0.041*
C7	0.4040 (3)	0.17220 (14)	0.19493 (11)	0.0341 (3)
H7A	0.5225	0.2113	0.234	0.041*
H7B	0.3711	0.2292	0.1468	0.041*
C8	0.1763 (3)	0.14879 (15)	0.24274 (10)	0.0330 (3)

*Atomic displacement parameters (Å<sup>2</sup>)*

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
S2	0.02549 (15)	0.02869 (16)	0.02891 (16)	0.00442 (13)	-0.00081 (13)	-0.00137 (13)
C1	0.0308 (6)	0.0236 (6)	0.0246 (6)	0.0010 (5)	0.0058 (5)	0.0006 (5)
O2	0.0509 (7)	0.0360 (5)	0.0316 (5)	0.0073 (5)	-0.0070 (5)	0.0061 (4)
C3	0.0344 (7)	0.0242 (6)	0.0296 (7)	-0.0001 (5)	0.0047 (6)	0.0007 (5)
O12	0.0399 (7)	0.0423 (6)	0.0537 (7)	-0.0116 (5)	0.0041 (6)	0.0087 (5)
C5	0.0359 (8)	0.0373 (8)	0.0395 (8)	0.0008 (7)	-0.0071 (7)	-0.0108 (6)
N1	0.0417 (7)	0.0303 (6)	0.0336 (6)	-0.0008 (6)	0.0104 (6)	0.0055 (5)
N8	0.0469 (10)	0.0585 (9)	0.0492 (8)	0.0082 (8)	0.0136 (8)	-0.0025 (7)
C2	0.0249 (6)	0.0216 (6)	0.0241 (6)	0.0019 (5)	0.0024 (5)	-0.0019 (5)
C4	0.0326 (7)	0.0291 (6)	0.0453 (8)	-0.0061 (6)	0.0045 (7)	-0.0038 (6)
C6	0.0440 (8)	0.0347 (7)	0.0244 (6)	0.0065 (6)	-0.0034 (6)	-0.0033 (5)
O11	0.0987 (13)	0.0692 (10)	0.0354 (6)	-0.0252 (9)	0.0125 (8)	0.0169 (6)
C8	0.0360 (8)	0.0329 (7)	0.0299 (7)	0.0085 (6)	-0.0016 (6)	-0.0045 (6)
C7	0.0337 (8)	0.0286 (7)	0.0401 (8)	0.0006 (6)	0.0013 (6)	-0.0080 (6)

*Geometric parameters (Å, °)*

S2—O2	1.4846 (11)	C5—C4	1.381 (2)
S2—C2	1.8197 (13)	C5—C6	1.390 (2)
S2—C7	1.8429 (15)	C5—H5	0.93
C1—C6	1.382 (2)	N1—O11	1.2177 (17)
C1—C2	1.3989 (18)	N8—C8	1.133 (2)
C1—N1	1.4606 (18)	C4—H4	0.93
C3—C2	1.3867 (19)	C6—H6	0.93
C3—C4	1.390 (2)	C8—C7	1.452 (2)

C3—H3	0.93	C7—H7A	0.97
O12—N1	1.2235 (19)	C7—H7B	0.97
O2—S2—C2	104.49 (6)	C3—C2—S2	115.83 (10)
O2—S2—C7	105.84 (7)	C1—C2—S2	125.91 (10)
C2—S2—C7	97.74 (7)	C5—C4—C3	120.78 (15)
C6—C1—C2	122.12 (13)	C5—C4—H4	119.6
C6—C1—N1	117.72 (12)	C3—C4—H4	119.6
C2—C1—N1	120.16 (12)	C1—C6—C5	118.86 (13)
C2—C3—C4	120.35 (13)	C1—C6—H6	120.6
C2—C3—H3	119.8	C5—C6—H6	120.6
C4—C3—H3	119.8	N8—C8—C7	179.36 (19)
C4—C5—C6	119.90 (15)	C8—C7—S2	111.69 (11)
C4—C5—H5	120	C8—C7—H7A	109.3
C6—C5—H5	120	S2—C7—H7A	109.3
O11—N1—O12	123.94 (15)	C8—C7—H7B	109.3
O11—N1—C1	118.48 (15)	S2—C7—H7B	109.3
O12—N1—C1	117.58 (12)	H7A—C7—H7B	107.9
C3—C2—C1	117.97 (13)		
C6—C1—N1—O11	-6.2 (2)	C7—S2—C2—C3	-102.58 (11)
C2—C1—N1—O11	173.11 (15)	O2—S2—C2—C1	-167.63 (11)
C6—C1—N1—O12	173.76 (14)	C7—S2—C2—C1	83.73 (12)
C2—C1—N1—O12	-7.0 (2)	C6—C5—C4—C3	0.1 (2)
C4—C3—C2—C1	-1.0 (2)	C2—C3—C4—C5	0.2 (2)
C4—C3—C2—S2	-175.24 (11)	C2—C1—C6—C5	-1.2 (2)
C6—C1—C2—C3	1.5 (2)	N1—C1—C6—C5	178.08 (13)
N1—C1—C2—C3	-177.73 (12)	C4—C5—C6—C1	0.3 (2)
C6—C1—C2—S2	175.08 (11)	O2—S2—C7—C8	-42.69 (13)
N1—C1—C2—S2	-4.16 (18)	C2—S2—C7—C8	64.82 (12)
O2—S2—C2—C3	6.06 (12)		

Hydrogen-bond geometry ( $\text{\AA}$ ,  $^\circ$ )

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
C6—H6 $\cdots$ O2 <sup>i</sup>	0.93	2.41	3.3198 (18)	165
C7—H7A $\cdots$ O2 <sup>ii</sup>	0.97	2.50	3.1190 (19)	122

Symmetry codes: (i)  $-x+1/2, -y, z-1/2$ ; (ii)  $-x+1, y+1/2, -z+1/2$ .