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4-(Methylsulfonyl)benzaldehyde

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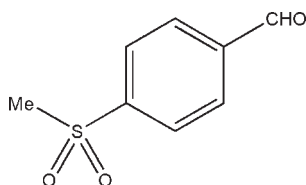
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Key indicators: single-crystal X-ray study; $T = 293$ K; mean $\sigma(\text{C}-\text{C}) = 0.003$ Å; R factor = 0.034; wR factor = 0.126; data-to-parameter ratio = 13.6.

In the crystal of the title compound, $\text{C}_8\text{H}_8\text{O}_3\text{S}$, the molecules are linked into a three-dimensional array by intermolecular $\text{C}-\text{H}\cdots\text{O}$ hydrogen bonds.

Related literature

For reference bond-length data, see: Allen *et al.* (1987). For a related structure, see: Ma (2008). For synthetic details, see: Rivett *et al.* (1979).



Experimental

Crystal data

$\text{C}_8\text{H}_8\text{O}_3\text{S}$
 $M_r = 184.20$
Monoclinic, $P2_1/c$
 $a = 6.1280$ (12) Å
 $b = 8.0400$ (16) Å
 $c = 16.734$ (3) Å
 $\beta = 90.07$ (3)°

$V = 824.5$ (3) Å³
 $Z = 4$
Mo $K\alpha$ radiation
 $\mu = 0.35$ mm⁻¹
 $T = 293$ K
 $0.30 \times 0.20 \times 0.20$ mm

Data collection

Enraf–Nonius CAD-4 diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
 $T_{\min} = 0.902$, $T_{\max} = 0.933$
1643 measured reflections

1495 independent reflections
1310 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.013$
3 standard reflections every 200 reflections
intensity decay: 1%

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.034$
 $wR(F^2) = 0.126$
 $S = 1.00$
1495 reflections

110 parameters
H-atom parameters constrained
 $\Delta\rho_{\text{max}} = 0.22$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.26$ e Å⁻³

Table 1

Hydrogen-bond geometry (Å, °).

$D-\text{H}\cdots A$	$D-\text{H}$	$\text{H}\cdots A$	$D\cdots A$	$D-\text{H}\cdots A$
$\text{C4}-\text{H4A}\cdots\text{O3}^{\text{i}}$	0.93	2.57	3.457 (3)	159
$\text{C1}-\text{H1D}\cdots\text{O1}^{\text{ii}}$	0.96	2.56	3.518 (3)	176

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

Data collection: *CAD-4 Software* (Enraf–Nonius 1989); cell refinement: *CAD-4 Software*; data reduction: *XCAD4* (Harms & Wocadlo, 1995); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: WN2364).

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supplementary materials

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4-(Methylsulfonyl)benzaldehyde

S.-S. Qian and H.-Y. Cui

Comment

The title compound has been of great of interest for many years. It acts as an important precursor for the synthesis of amino alcohols with applications to the synthesis of the antibiotics chloramphenicol, fluoramphenicol and thiamphenicol. Here we report its crystal structure.

In the title compound (Fig. 1), all bond lengths are within normal ranges (Allen *et al.*, 1987) and comparable to the values observed in a closely related compound (Ma, 2008). The C1—S—C2—C3 torsion angle is 75.07 (17)°.

In the crystal structure, molecules are linked through intermolecular C—H···O hydrogen bonds (Table 1; Fig. 2).

Experimental

The title compound was synthesized according to a literature method (Rivett *et al.*, 1979). 0.1 g of the title compound was dissolved in acetonitrile (20 ml). Single crystals suitable for X-ray diffraction were obtained by spontaneous evaporation of the solvent.

Refinement

All H atoms were placed in geometrical positions and constrained to ride on their parent atoms with C—H distances in the range 0.93–0.96 Å, They were treated as riding atoms, with $U_{\text{iso}}(\text{H}) = kU_{\text{eq}}(\text{C})$, where $k = 1.5$ for methyl and 1.2 for all other H atoms.

Figures

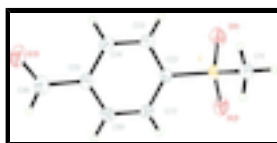


Fig. 1. The molecular structure of the title compound, showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 35% probability level. Hydrogen atoms are shown as small spheres of arbitrary radius.

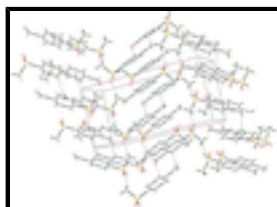


Fig. 2. The crystal packing of the title compound. Dashed lines indicate hydrogen bonds.

4-(Methylsulfonyl)benzaldehyde

Crystal data

$C_8H_8O_3S$	$F_{000} = 384$
$M_r = 184.20$	$D_x = 1.484 \text{ Mg m}^{-3}$
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation, $\lambda = 0.71073 \text{ \AA}$
$a = 6.1280 (12) \text{ \AA}$	Cell parameters from 25 reflections
$b = 8.0400 (16) \text{ \AA}$	$\theta = 9\text{--}13^\circ$
$c = 16.734 (3) \text{ \AA}$	$\mu = 0.35 \text{ mm}^{-1}$
$\beta = 90.07 (3)^\circ$	$T = 293 \text{ K}$
$V = 824.5 (3) \text{ \AA}^3$	Block, yellow
$Z = 4$	$0.30 \times 0.20 \times 0.20 \text{ mm}$

Data collection

Enraf–Nonius CAD-4 diffractometer	$R_{\text{int}} = 0.013$
Radiation source: fine-focus sealed tube	$\theta_{\text{max}} = 25.2^\circ$
Monochromator: graphite	$\theta_{\text{min}} = 2.4^\circ$
$T = 293 \text{ K}$	$h = -7 \rightarrow 0$
$\omega/2\theta$ scans	$k = -9 \rightarrow 0$
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	$l = -20 \rightarrow 20$
$T_{\text{min}} = 0.902$, $T_{\text{max}} = 0.933$	3 standard reflections
1643 measured reflections	every 200 reflections
1495 independent reflections	intensity decay: 1%
1310 reflections with $I > 2\sigma(I)$	

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)] = 0.034$	$w = 1/[\sigma^2(F_o^2) + (0.1P)^2 + 0.095P]$
$wR(F^2) = 0.126$	where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.00$	$(\Delta/\sigma)_{\text{max}} < 0.001$
1495 reflections	$\Delta\rho_{\text{max}} = 0.22 \text{ e \AA}^{-3}$
110 parameters	$\Delta\rho_{\text{min}} = -0.26 \text{ e \AA}^{-3}$
Primary atom site location: structure-invariant direct methods	Extinction correction: SHELXL97 (Sheldrick, 2008), $F_c^* = kF_c[1 + 0.001x F_c^2 \lambda^3 / \sin(2\theta)]^{-1/4}$
Secondary atom site location: difference Fourier map	Extinction coefficient: 0.028 (6)

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds 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 $F^2 > 2\sigma(F^2)$ 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 (\AA^2)

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
S	0.25890 (8)	0.43803 (6)	0.17148 (3)	0.0397 (3)
O1	0.1031 (3)	0.5283 (2)	0.21856 (10)	0.0647 (5)
O2	0.4429 (3)	0.5269 (2)	0.13956 (10)	0.0590 (5)
C1	0.3533 (4)	0.2698 (3)	0.22913 (12)	0.0479 (5)
H1B	0.4308	0.3111	0.2749	0.072*
H1C	0.4492	0.2022	0.1975	0.072*
H1D	0.2314	0.2041	0.2465	0.072*
C2	0.1206 (3)	0.3429 (2)	0.09056 (10)	0.0338 (4)
C3	-0.0839 (3)	0.2728 (3)	0.10317 (12)	0.0436 (5)
H3A	-0.1484	0.2768	0.1534	0.052*
O3	-0.3837 (3)	0.0537 (2)	-0.10080 (11)	0.0631 (5)
C4	-0.1897 (3)	0.1971 (3)	0.04005 (12)	0.0427 (5)
H4A	-0.3256	0.1482	0.0477	0.051*
C5	-0.0929 (3)	0.1941 (2)	-0.03484 (11)	0.0373 (5)
C6	0.1115 (4)	0.2644 (3)	-0.04627 (12)	0.0432 (5)
H6A	0.1757	0.2613	-0.0966	0.052*
C7	0.2200 (3)	0.3388 (2)	0.01639 (11)	0.0392 (5)
H7A	0.3575	0.3854	0.0090	0.047*
C8	-0.2049 (4)	0.1147 (3)	-0.10336 (13)	0.0504 (6)
H8A	-0.1315	0.1119	-0.1520	0.061*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S	0.0415 (4)	0.0387 (4)	0.0387 (4)	-0.00006 (19)	-0.0065 (2)	-0.00429 (18)
O1	0.0675 (11)	0.0680 (11)	0.0586 (10)	0.0206 (9)	-0.0087 (9)	-0.0250 (8)
O2	0.0628 (10)	0.0582 (9)	0.0560 (9)	-0.0261 (8)	-0.0096 (8)	0.0025 (8)
C1	0.0512 (12)	0.0505 (12)	0.0421 (11)	0.0021 (10)	-0.0120 (9)	0.0027 (9)
C2	0.0330 (9)	0.0330 (9)	0.0352 (9)	0.0010 (7)	-0.0039 (7)	0.0013 (7)
C3	0.0365 (10)	0.0567 (12)	0.0374 (10)	-0.0024 (9)	0.0051 (8)	-0.0022 (9)
O3	0.0617 (11)	0.0626 (10)	0.0649 (11)	-0.0178 (8)	-0.0167 (8)	-0.0050 (8)
C4	0.0331 (10)	0.0461 (11)	0.0488 (11)	-0.0050 (8)	-0.0015 (8)	0.0001 (8)

supplementary materials

C5	0.0398 (10)	0.0323 (9)	0.0396 (10)	0.0018 (8)	-0.0072 (8)	0.0008 (7)
C6	0.0472 (11)	0.0486 (11)	0.0338 (10)	-0.0028 (9)	0.0041 (8)	0.0009 (8)
C7	0.0352 (10)	0.0432 (10)	0.0391 (10)	-0.0045 (8)	0.0005 (8)	0.0030 (8)
C8	0.0595 (14)	0.0469 (12)	0.0448 (11)	-0.0042 (11)	-0.0090 (10)	-0.0014 (9)

Geometric parameters (\AA , $^\circ$)

S—O1	1.4355 (17)	C3—H3A	0.9300
S—O2	1.4385 (17)	O3—C8	1.201 (3)
S—C1	1.759 (2)	C4—C5	1.387 (3)
S—C2	1.7703 (18)	C4—H4A	0.9300
C1—H1B	0.9600	C5—C6	1.388 (3)
C1—H1C	0.9600	C5—C8	1.480 (3)
C1—H1D	0.9600	C6—C7	1.377 (3)
C2—C7	1.384 (3)	C6—H6A	0.9300
C2—C3	1.390 (3)	C7—H7A	0.9300
C3—C4	1.380 (3)	C8—H8A	0.9300
O1—S—O2	118.34 (12)	C2—C3—H3A	120.5
O1—S—C1	107.85 (11)	C3—C4—C5	119.86 (18)
O2—S—C1	109.17 (11)	C3—C4—H4A	120.1
O1—S—C2	108.66 (10)	C5—C4—H4A	120.1
O2—S—C2	107.77 (9)	C4—C5—C6	120.28 (18)
C1—S—C2	104.13 (9)	C4—C5—C8	120.61 (18)
S—C1—H1B	109.5	C6—C5—C8	119.11 (19)
S—C1—H1C	109.5	C7—C6—C5	120.46 (18)
H1B—C1—H1C	109.5	C7—C6—H6A	119.8
S—C1—H1D	109.5	C5—C6—H6A	119.8
H1B—C1—H1D	109.5	C6—C7—C2	118.71 (17)
H1C—C1—H1D	109.5	C6—C7—H7A	120.6
C7—C2—C3	121.62 (17)	C2—C7—H7A	120.6
C7—C2—S	119.04 (14)	O3—C8—C5	124.8 (2)
C3—C2—S	119.34 (14)	O3—C8—H8A	117.6
C4—C3—C2	119.05 (18)	C5—C8—H8A	117.6
C4—C3—H3A	120.5		
O1—S—C2—C7	140.91 (17)	C3—C4—C5—C6	1.1 (3)
O2—S—C2—C7	11.52 (19)	C3—C4—C5—C8	-179.47 (18)
C1—S—C2—C7	-104.34 (17)	C4—C5—C6—C7	-0.4 (3)
O1—S—C2—C3	-39.78 (18)	C8—C5—C6—C7	-179.85 (18)
O2—S—C2—C3	-169.16 (16)	C5—C6—C7—C2	-0.4 (3)
C1—S—C2—C3	74.97 (17)	C3—C2—C7—C6	0.6 (3)
C7—C2—C3—C4	0.1 (3)	S—C2—C7—C6	179.91 (14)
S—C2—C3—C4	-179.23 (15)	C4—C5—C8—O3	2.4 (3)
C2—C3—C4—C5	-0.9 (3)	C6—C5—C8—O3	-178.2 (2)

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

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
C4—H4A \cdots O3 ⁱ	0.93	2.57	3.457 (3)	159

C1—H1D···O1ⁱⁱ 0.96 2.56 3.518 (3) 176
 Symmetry codes: (i) $-x-1, -y, -z$; (ii) $-x, y-1/2, -z+1/2$.

Fig. 1

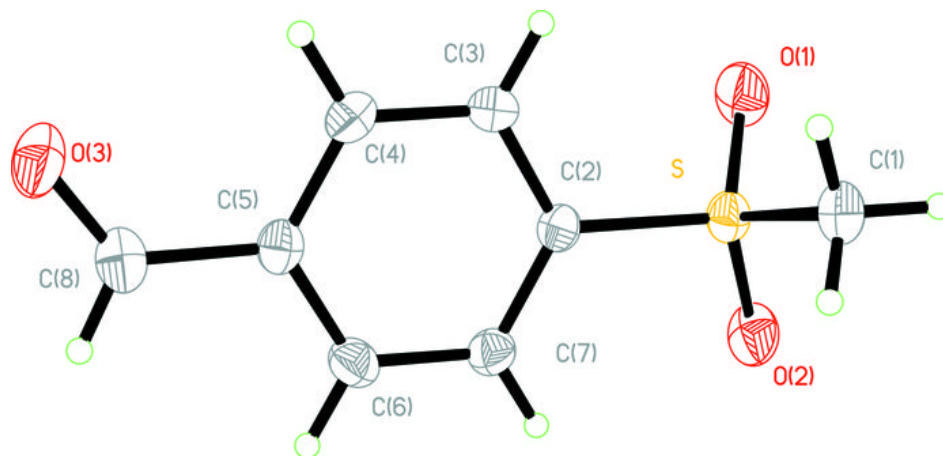


Fig. 2

