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# 4-(Methylsulfonyl)benzaldehyde

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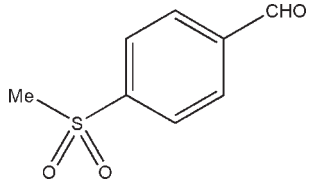
Key indicators: single-crystal X-ray study; $T$ = 293 K; mean $\sigma$(C–C) = 0.003 Å; $R$ factor = 0.034; $wR$ factor = 0.126; data-to-parameter ratio = 13.6.

In the crystal of the title compound, $C_8H_8O_3S$, the molecules are linked into a three-dimensional array by intermolecular C—H···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

$C_8H_8O_3S$
$M_r$ = 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) Å$^3$
$Z$ = 4
Mo $K\alpha$ radiation
$\mu$ = 0.35 mm$^{-1}$
$T$ = 293 K
0.30 × 0.20 × 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 $I > 2\sigma(I)$
$R_{int}$ = 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
$\Delta\rho_{max}$ = 0.22 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.26 e Å$^{-3}$

**Table 1**
Hydrogen-bond geometry (Å, °).

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| C4—H4$A$···O3$^{i}$ | 0.93 | 2.57 | 3.457 (3) | 159 |
| C1—H1$D$···O1$^{ii}$ | 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).

## References

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# supporting information

*Acta Cryst.* (2009). E**65**, o3029 [doi:10.1107/S1600536809046406]

## 4-(Methylsulfonyl)benzaldehyde

**Shao-Song Qian and Hong-You Cui**

### S1. 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).

### S2. 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.

### S3. 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 $U_{iso}$(H) = k$U_{eq}$(C), where k = 1.5 for methyl and 1.2 for all other H atoms.

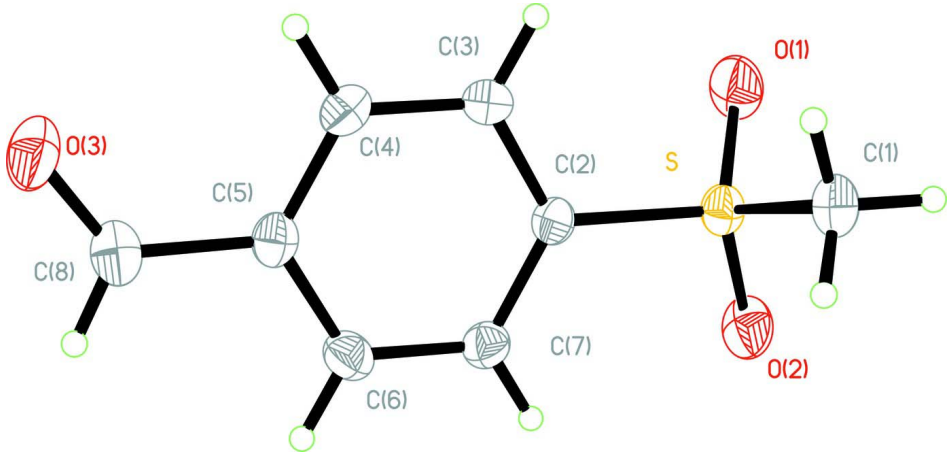


**Figure 1**

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.

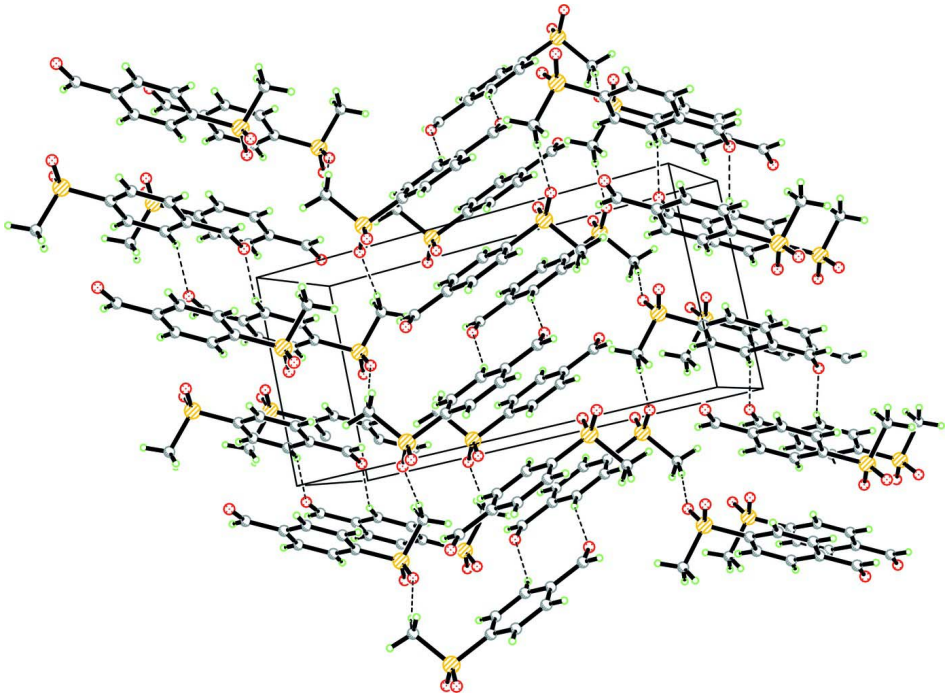

**Figure 2**

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

### 4-(Methylsulfonyl)benzaldehyde

*Crystal data*

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

*Data collection*

Enraf–Nonius CAD-4 diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
$\omega/2\theta$ scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.902$, $T_{max} = 0.933$
1643 measured reflections
1495 independent reflections
1310 reflections with $I > 2\sigma(I)$
$R_{int} = 0.013$
$\theta_{max} = 25.2°$, $\theta_{min} = 2.4°$
$h = -7\rightarrow0$
$k = -9\rightarrow0$
$l = -20\rightarrow20$
3 standard reflections every 200 reflections
intensity decay: 1%

*Refinement*

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

| | *x* | *y* | *z* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| 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 (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| 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) |
| 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 (Å, º)*

| | | | |
|---|---|---|---|
| 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 (Å, º)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| C4—H4*A*···O3$^{i}$ | 0.93 | 2.57 | 3.457 (3) | 159 |
| C1—H1*D*···O1$^{ii}$ | 0.96 | 2.56 | 3.518 (3) | 176 |

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