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3-Chloro-2-methylbenzene-1-sulfonyl chloride

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3-Chloro-2-methylbenzene-1-sulfonyl chloride

Luisa Chan^a and Lee Daniels^{b*}

^aNanosyn, 3760 Haven Ave., Menlo Park, CA 94025, USA, and ^bRigaku Americas Corp., 9009 New Trails Dr., The Woodlands, TX 77381, USA
Correspondence e-mail: lee.daniels@rigaku.com

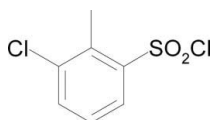
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Key indicators: single-crystal X-ray study; $T = 293$ K; mean $\sigma(\text{C}-\text{C}) = 0.004$ Å; disorder in main residue; R factor = 0.047; wR factor = 0.126; data-to-parameter ratio = 19.1.

In the structure of the title compound, $\text{C}_7\text{H}_6\text{Cl}_2\text{O}_2\text{S}$, the three methyl hydrogen atoms are disordered over two sets of positions with essentially equal occupancy.

Related literature

For related literature, see: Brennan *et al.* (2006).



Experimental

Crystal data

$\text{C}_7\text{H}_6\text{Cl}_2\text{O}_2\text{S}$
 $M_r = 225.08$
Monoclinic, $C2/c$
 $a = 11.7233$ (16) Å
 $b = 9.8849$ (13) Å
 $c = 16.216$ (2) Å
 $\beta = 100.143$ (2)°

$V = 1849.8$ (4) Å³
 $Z = 8$
Mo $K\alpha$ radiation
 $\mu = 0.88$ mm⁻¹
 $T = 293$ (2) K
 $0.50 \times 0.44 \times 0.33$ mm

Data collection

Rigaku SCXmini diffractometer
Absorption correction: multi-scan
(*ABSCOR*; Higashi, 1995)
 $T_{\min} = 0.53$, $T_{\max} = 0.76$

6310 measured reflections
2101 independent reflections
1551 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.028$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.047$
 $wR(F^2) = 0.126$
 $S = 1.04$
2101 reflections
110 parameters

H atoms treated by a mixture of independent and constrained refinement
 $\Delta\rho_{\max} = 0.49$ e Å⁻³
 $\Delta\rho_{\min} = -0.47$ e Å⁻³

Data collection: *SCXmini* (Rigaku, 2006); cell refinement: *PROCESS-AUTO* (Rigaku, 1998); data reduction: *PROCESS-AUTO*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1990); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *CrystalStructure* (Rigaku, 2005); software used to prepare material for publication: *CrystalStructure* and *publCIF* (Westrip, 2007).

The authors thank Dr David Lonergan for suggesting a list of possibly crystalline reagents.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: SG2163).

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supplementary materials

Acta Cryst. (2007). E63, o2435 [doi:10.1107/S1600536807017059]

3-Chloro-2-methylbenzene-1-sulfonyl chloride

L. Chan and L. Daniels

Comment

3-chloro-2-methylbenzenesulfonyl derivatives have shown biological activity as hydroxysteroid dehydrogenase inhibitors. These derivatives have potential as medicants to treat diseases mediated by hydroxysteroid dehydrogenase, such as type-2 diabetes (Brennan *et al.*, 2006).

Experimental

The data collection sample was selected directly from many nicely formed specimens found in the bottle from the manufacturer.

Refinement

A Fourier map around the expected positions of the methyl group H atoms clearly indicated two equivalent orientations. Both sets were included (riding model) and their occupancies refined, although the refined value is indistinguishable from 0.50. The C—H distance and C—C—H angles for the methyl H atoms were fixed, but the groups were allowed to rotate around the C—C bond.

Figures

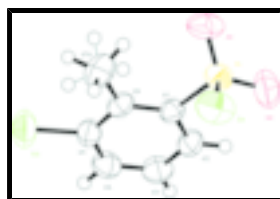


Fig. 1. View of the title molecule, with ellipsoids drawn at the 50% probability level. Bonds to the methyl H atoms are drawn with different line styles to distinguish the two alternate orientations.

3-chloro-2-methylbenzene-1-sulfonyl chloride

Crystal data

$C_7H_6Cl_2O_2S$

$M_r = 225.08$

Monoclinic, $C2/c$

$a = 11.7233$ (16) Å

$b = 9.8849$ (13) Å

$c = 16.216$ (2) Å

$\beta = 100.143$ (2)°

$F_{000} = 912$

$D_x = 1.616$ Mg m⁻³

Mo $K\alpha$ radiation

$\lambda = 0.71075$ Å

Cell parameters from 5438 reflections

$\theta = 3.1$ – 27.5 °

$\mu = 0.88$ mm⁻¹

$T = 293$ (2) K

supplementary materials

$V = 1849.8(4) \text{ \AA}^3$
 $Z = 8$

Prism, colourless
 $0.50 \times 0.44 \times 0.33 \text{ mm}$

Data collection

Rigaku SCXmini
diffractometer

1551 reflections with $I > 2\sigma(I)$

Monochromator: graphite

$R_{\text{int}} = 0.028$

$T = 293(2) \text{ K}$

$\theta_{\text{max}} = 27.5^\circ$

ω scans

$\theta_{\text{min}} = 3.5^\circ$

Absorption correction: multi-scan
(ABSCOR; Higashi, 1995)

$h = -15 \rightarrow 15$

$T_{\text{min}} = 0.53, T_{\text{max}} = 0.76$

$k = -12 \rightarrow 12$

6310 measured reflections

$l = -16 \rightarrow 20$

2101 independent reflections

Refinement

Refinement on F^2

H atoms treated by a mixture of
independent and constrained refinement

Least-squares matrix: full

$$w = 1/[\sigma^2(F_o^2) + (0.0529P)^2 + 2.2518P]$$

$R[F^2 > 2\sigma(F^2)] = 0.047$

where $P = (F_o^2 + 2F_c^2)/3$

$wR(F^2) = 0.126$

$(\Delta/\sigma)_{\text{max}} < 0.001$

$S = 1.04$

$\Delta\rho_{\text{max}} = 0.49 \text{ e \AA}^{-3}$

2101 reflections

$\Delta\rho_{\text{min}} = -0.47 \text{ e \AA}^{-3}$

110 parameters

Extinction correction: none

Primary atom site location: structure-invariant direct
methods

Secondary atom site location: difference Fourier map

Hydrogen site location: inferred from neighbouring
sites

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	$U_{\text{iso}}^*/U_{\text{eq}}$	Occ. (<1)
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Cl1	0.34739 (8)	-0.05390 (11)	0.72960 (6)	0.0881 (4)	
Cl2	0.00368 (8)	-0.33397 (9)	0.46807 (7)	0.0842 (3)	
S1	0.22728 (7)	0.07269 (8)	0.66422 (5)	0.0567 (2)	
O1	0.1375 (2)	0.0813 (3)	0.71120 (13)	0.0744 (7)	
O2	0.2877 (3)	0.1917 (3)	0.64869 (16)	0.0909 (8)	
C1	0.1833 (2)	-0.0162 (3)	0.56917 (16)	0.0440 (6)	
C2	0.2169 (3)	0.0433 (3)	0.49984 (19)	0.0553 (7)	
H1	0.2617	0.1214	0.5059	0.077*	
C3	0.1835 (3)	-0.0139 (3)	0.42236 (18)	0.0614 (8)	
H3	0.2052	0.0257	0.3755	0.086*	
C4	0.1182 (3)	-0.1296 (3)	0.41408 (18)	0.0561 (7)	
H2	0.0953	-0.1687	0.3616	0.079*	
C5	0.0868 (2)	-0.1876 (3)	0.48380 (18)	0.0496 (6)	
C6	0.1180 (2)	-0.1350 (3)	0.56484 (16)	0.0450 (6)	
C7	0.0831 (3)	-0.2042 (4)	0.6395 (2)	0.0720 (9)	
H4A	0.1392 (3)	-0.2724 (4)	0.6602 (2)	0.101*	0.51 (4)
H5A	0.0796 (3)	-0.1387 (4)	0.6827 (2)	0.101*	0.51 (4)
H6A	0.0084 (3)	-0.2454 (4)	0.6232 (2)	0.101*	0.51 (4)
H4B	0.0100 (3)	-0.1690 (4)	0.6485 (2)	0.101*	0.49 (4)
H5B	0.0763 (3)	-0.2997 (4)	0.6293 (2)	0.101*	0.49 (4)
H6B	0.1409 (3)	-0.1877 (4)	0.6883 (2)	0.101*	0.49 (4)

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl1	0.0692 (5)	0.1192 (8)	0.0678 (6)	0.0225 (5)	-0.0101 (4)	-0.0142 (5)
Cl2	0.0835 (6)	0.0593 (5)	0.1071 (7)	-0.0258 (4)	0.0097 (5)	-0.0104 (5)
S1	0.0602 (4)	0.0650 (5)	0.0453 (4)	-0.0035 (3)	0.0105 (3)	-0.0092 (3)
O1	0.0691 (14)	0.1077 (19)	0.0487 (12)	0.0131 (13)	0.0169 (10)	-0.0114 (12)
O2	0.121 (2)	0.0754 (15)	0.0774 (16)	-0.0412 (15)	0.0193 (15)	-0.0218 (13)
C1	0.0435 (13)	0.0500 (14)	0.0401 (13)	-0.0022 (11)	0.0115 (11)	0.0021 (11)
C2	0.0644 (17)	0.0526 (16)	0.0533 (16)	-0.0148 (14)	0.0224 (14)	-0.0003 (13)
C3	0.075 (2)	0.071 (2)	0.0429 (15)	-0.0047 (16)	0.0237 (15)	0.0036 (14)
C4	0.0595 (17)	0.0640 (17)	0.0445 (15)	0.0028 (14)	0.0081 (13)	-0.0060 (14)
C5	0.0428 (13)	0.0428 (13)	0.0617 (17)	-0.0012 (11)	0.0051 (12)	-0.0009 (12)
C6	0.0402 (12)	0.0478 (14)	0.0478 (14)	0.0014 (11)	0.0102 (11)	0.0106 (12)
C7	0.079 (2)	0.074 (2)	0.065 (2)	-0.0148 (17)	0.0178 (17)	0.0248 (17)

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

Cl1—S1	2.0363 (12)	C4—C5	1.374 (4)
Cl2—C5	1.738 (3)	C5—C6	1.401 (4)
S1—O1	1.406 (2)	C6—C7	1.508 (4)
S1—O2	1.419 (3)	C7—H4B	0.9600
S1—C1	1.770 (3)	C7—H6A	0.9600
C1—C2	1.386 (4)	C7—H4A	0.9600
C1—C6	1.397 (4)	C7—H5B	0.9600
C2—C3	1.371 (4)	C7—H6B	0.9600
C3—C4	1.370 (4)	C7—H5A	0.9600

supplementary materials

O1—S1—O2	119.41 (17)	C1—C6—C5	114.2 (2)
O1—S1—C1	111.75 (13)	C1—C6—C7	124.4 (3)
O2—S1—C1	109.58 (14)	C5—C6—C7	121.5 (3)
O1—S1—C11	105.65 (11)	H6A—C7—H4A	109.5
O2—S1—C11	106.32 (14)	H6A—C7—H5A	109.5
C1—S1—C11	102.52 (10)	H4A—C7—H5A	109.5
C2—C1—C6	123.2 (2)	H4B—C7—H5B	109.5
C2—C1—S1	114.5 (2)	H4B—C7—H6B	109.5
C6—C1—S1	122.28 (19)	H5B—C7—H6B	109.5
C3—C2—C1	119.5 (3)	H4A—C7—C6	109.5
C4—C3—C2	119.9 (3)	H5A—C7—C6	109.5
C3—C4—C5	119.6 (3)	H6A—C7—C6	109.5
C4—C5—C6	123.6 (3)	H4B—C7—C6	109.5
C4—C5—C12	116.8 (2)	H5B—C7—C6	109.5
C6—C5—C12	119.6 (2)	H6B—C7—C6	109.5

Fig. 1

