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5-Chloro-2-methyl-3-methylsulfinyl-1-benzofuran

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Key indicators

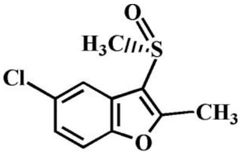
Single-crystal X-ray study
T = 173 K
Mean σ(C–C) = 0.004 Å
R factor = 0.053
wR factor = 0.112
Data-to-parameter ratio = 17.7

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

The title compound, $C_{10}H_9ClO_2S$, was prepared by the oxidation of 5-chloro-2-methyl-3-methylsulfanyl-1-benzofuran using 3-chloroperbenzoic acid. The benzofuran ring system is almost planar. No π–π or $-CH_2-H\cdots\pi$ interactions were observed.

Comment

The title compound, (I), was obtained by the oxidation of 5-chloro-3-methanesulfanyl-2-methylbenzofuran with 3-chloroperbenzoic acid. This is a related study to the previous communication of the isomeric bromo analogue (Choi *et al.*, 2007). The purpose of this work is to determine how the molecular conformation in the crystal structure is affected by the chloro substituent. The X-ray analysis of the chloro isomer has therefore been carried out and the results are presented here.



(I)

The bond lengths and angles in (I) are as expected for this type of compound (Choi *et al.*, 2007). The benzofuran unit is again almost planar, with a mean deviation of 0.012 Å from the least-squares plane defined by the nine constituent atoms.

In the crystal structure, molecules are arranged in stacks with the planes of adjacent benzofuran groups parallel (Fig. 2), and with a separation of 3.786 (8) Å between these planes. The shortest distance between ring centroids, *Cg*(furan ring)$\cdots$*Cg*(benzene ring)^{i} is 4.348 (5) Å (symmetry code as in Fig. 2). A shorter π–π stacking distance is prevented by the steric influence of the methylsulfinyl group.

Experimental

3-Chloroperbenzoic acid (77%, 471 mg, 2.10 mmol) was added in small portions to a stirred solution of 5-chloro-2-methyl-3-methylsulfanyl-1-benzofuran (425 mg, 2.0 mmol) in dichloromethane (20 ml) at 273 K. After stirring at room temperature for 1 h, the mixture was washed with saturated sodium bicarbonate solution and the organic layer separated, dried over magnesium sulfate, filtered and concentrated *in vacuo*. The residue was purified by column chromatography (ethyl acetate) to afford (I) as a colorless solid. Crystals suitable for X-ray analysis were grown by slow evaporation of an acetone solution [yield 82%, m.p. 397–398 K; R_f = 0.35 (ethyl acetate)].

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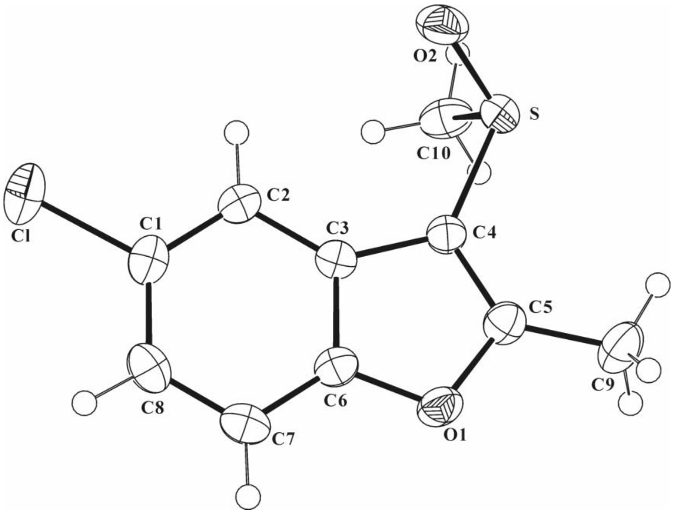

Figure 1
The molecular structure of (I), with displacement ellipsoids drawn at the 50% probability level for non–H atoms.

Crystal data

$C_{10}H_9ClO_2S$
$M_r = 228.68$
Monoclinic, $P2_1/n$
$a = 5.1413$ (3) Å
$b = 16.589$ (1) Å
$c = 12.2756$ (7) Å
$\beta = 94.689$ (1)°
$V = 1043.47$ (11) Å^3
$Z = 4$
$D_x = 1.456$ Mg m^{-3}
Mo $K\alpha$ radiation
$\mu = 0.54$ mm^{-1}
$T = 173$ (2) K
Block, colorless
0.52 × 0.43 × 0.12 mm

Data collection

Bruker SMART CCD diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1999)
$T_{\min} = 0.762$, $T_{\max} = 0.945$
6206 measured reflections
2269 independent reflections
1999 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.020$
$\theta_{\max} = 27.0°$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.053$
$wR(F^2) = 0.112$
$S = 1.20$
2269 reflections
128 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0334P)^2 + 1.1659P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} < 0.001$
$\Delta\rho_{\max} = 0.34$ e Å^{-3}
$\Delta\rho_{\min} = -0.35$ e Å^{-3}

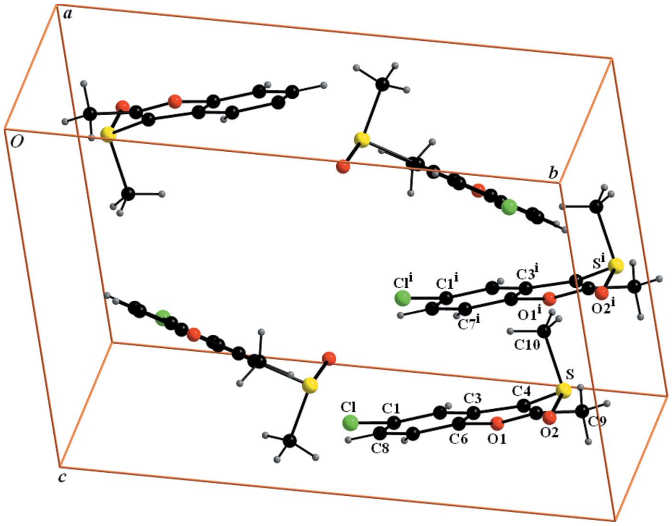

Figure 2
The packing of (I). [Symmetry code: (i) 1 + x, y, z.]

All H atoms were positioned geometrically and refined using a riding model, with C—H = 0.93 Å for aromatic H atoms and 0.96 Å for methyl H atoms, and with $U_{\rm iso}({\rm H}) = 1.2U_{\rm eq}({\rm C})$ for aromatic H atoms, and $U_{\rm iso}({\rm H}) = 1.5U_{\rm eq}({\rm C})$ for methyl H atoms.

Data collection: *SMART* (Bruker, 1997); cell refinement: *SAINT* (Bruker, 1997); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3* (Farrugia, 1997) and *DIAMOND* (Brandenburg, 1998); software used to prepare material for publication: *SHELXL97*.

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