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2-Iodobenzenesulfonyl chloride

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Key indicators

Single-crystal X-ray study
T = 93 K
Mean σ(C–C) = 0.004 Å
R factor = 0.016
wR factor = 0.033
Data-to-parameter ratio = 14.8

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

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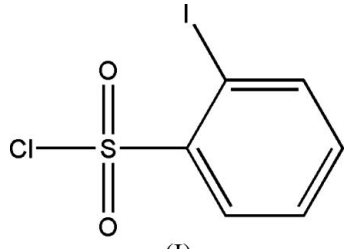
In the molecule of 2-iodobenzenesulfonyl chloride, $C_6H_4IO_2S^+\cdot Cl^-$, the *ortho* substitution by large atoms causes angular distortions at the ring C atoms rather than significant displacement of the substituents out of the ring plane.

Comment

The title compound, (I) (Fig. 1), was prepared as an intermediate in the synthesis of dibenzo[*ce*][1,2]dithiine and its related oxides (Aucott *et al.*, 2004; Aucott *et al.*, 2004*a*,*b*; Aucott, Kilian *et al.*, 2005; Aucott, Milton *et al.*, 2005) as part of a study of conformationally restricted molecules.



(I)

Compound (I) crystallizes in the monoclinic space group $P2_1/n$. The aromatic ring is essentially planar, with atom S1 0.14 (1) Å and I1 −0.08 (1) Å from this plane. The SO_2Cl group is oriented with O2 close to the aromatic plane [0.16 (1) Å] and O1 and Cl1 lying 1.13 (1) and −1.165 (1) Å above and below this plane, respectively. The *ortho* substitution of two heavy atoms results in enlargement of angles at carbon of the aromatic ring; C2—C1—I1 = 125.00 (18)° and S1—C2—C1 = 123.23 (19)°.

Experimental

2-Iodobenzenesulfonyl chloride was prepared as previously described (Chau & Kice, 1977) and was crystallized from chloroform/hexane (1:1 *v*/*v*) to give well formed colourless blocks.

Crystal data

$C_6H_4IO_2S^+\cdot Cl^-$
M_r = 302.50
Monoclinic, $P2_1/n$
a = 8.338 (3) Å
b = 12.741 (3) Å
c = 8.517 (2) Å
β = 109.797 (7)°
V = 851.3 (4) Å^3
Z = 4
D_x = 2.360 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 3111 reflections
θ = 2.5–25.4°
μ = 4.26 mm^{-1}
T = 93 (2) K
Block, colourless
0.10 × 0.10 × 0.08 mm

Data collection

Rigaku MM007/Mercury CCD diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2001)
T_{min} = 0.600, T_{max} = 0.710
4840 measured reflections
1496 independent reflections
1457 reflections with $I > 2\sigma(I)$
R_{int} = 0.013
θ_{max} = 25.4°
$h = -10 \rightarrow 9$
$k = -15 \rightarrow 12$
$l = -8 \rightarrow 10$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.016
$wR(F^2)$ = 0.033
S = 1.13
1496 reflections
101 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0044P)^2 + 1.4521P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.47 e Å^{-3}
$\Delta\rho_{min}$ = −0.46 e Å^{-3}

All H atoms were included in calculated positions (C—H = 0.95 Å) and were refined as riding atoms, with $U_{iso}(H) = 1.2U_{eq}(C)$.

Data collection: *CrystalClear* (Rigaku/MSC, 2004); cell refinement: *CrystalClear*; data reduction: *CrystalClear*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997*a*); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997*a*); molecular graphics: *SHELXTL* (Sheldrick, 1997*b*); software used to prepare material for publication: *SHELXTL*.

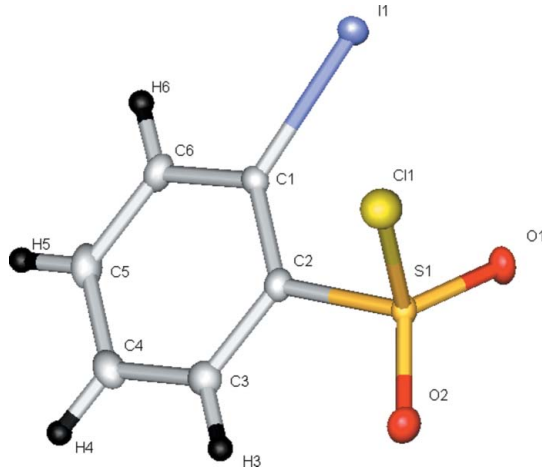


Figure 1
The structure of (I), with displacement ellipsoids drawn at the 50% probability level.

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