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2,4,6-Trichloroiodobenzene

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Key indicators

Single-crystal X-ray study
T = 90 K
Mean σ(C–C) = 0.004 Å
R factor = 0.021
wR factor = 0.052
Data-to-parameter ratio = 20.8

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

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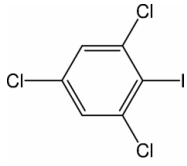
The crystal structure of 2,4,6-trichloroiodobenzene, $C_6H_2Cl_3I$, a precursor of polychlorinated biphenyls (PCBs), is described.

Comment

Chlorinated iodo- and bromobenzenes, such as 2,4,6-trichloroiodobenzene, are precursors of polychlorinated biphenyls (PCBs), a group of important and widespread environmental pollutants (Lehmler *et al.*, 2001). During attempts to develop a novel synthesis of tetra-*ortho*-substituted PCBs, we obtained crystals of the title compound, (I). In spite of its relative simplicity, the crystal structure has not been reported in the literature, but that of an isomer, 2,4,5-trichloroiodobenzene, was recently published (Kania-Korwel *et al.*, 2003). Notwithstanding the outward similarity of the two isomers, their crystal structures show dramatic differences. While the 2,4,5-trichloroiodobenzene isomer was extensively disordered in the crystalline state, the title compound is well ordered.



(I)

Experimental

The 2,4,6-trichloroiodobenzene crystals were obtained while attempting to synthesize 2,2′,4,4′,6,6′-hexachlorobiphenyl using a Suzuki coupling reaction (Lehmler & Robertson, 2001). White needles formed upon recrystallization from methanol.

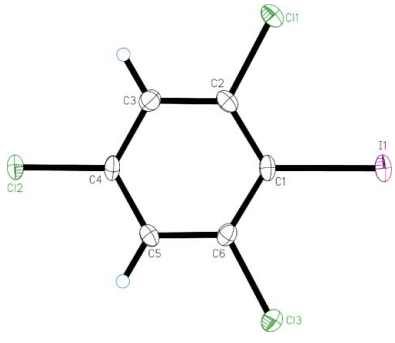


Figure 1
An ellipsoid plot of 2,4,6-trichloro-1-iodobenzene, with non-H atoms drawn at the 50% probability level.

Crystal data

$C_6H_2Cl_3I$	D_x = 2.472 Mg m^{-3}
M_r = 307.33	Mo $K\alpha$ radiation
Monoclinic, $P2_1/c$	Cell parameters from 1946 reflections
a = 3.9970 (1) Å	θ = 1.0–27.5°
b = 21.5840 (4) Å	μ = 4.76 mm^{-1}
c = 9.7510 (2) Å	T = 90.0 (2) K
β = 100.994 (1)°	Block, colourless
V = 825.79 (3) Å^3	0.15 × 0.10 × 0.10 mm
Z = 4	

Data collection

Nonius KappaCCD diffractometer	1891 independent reflections
ω scans at fixed χ = 55°	1689 reflections with $I > 2\sigma(I)$
Absorption correction: multi-scan (*SCALEPACK*; Otwinowski & Minor, 1997)	R_{int} = 0.019
	θ_{max} = 27.5°
T_{min} = 0.514, T_{max} = 0.621	$h = -5 \rightarrow 5$
3722 measured reflections	$k = -27 \rightarrow 27$
	$l = -12 \rightarrow 12$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0246P)^2 + 0.3565P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)]$ = 0.021	
$wR(F^2)$ = 0.052	
S = 1.10	$(\Delta/\sigma)_{max}$ = 0.001
1891 reflections	$\Delta\rho_{max}$ = 0.88 e Å^{-3}
91 parameters	$\Delta\rho_{min}$ = −0.84 e Å^{-3}
H-atom parameters constrained	

Data collection: *COLLECT* (Nonius, 1998); cell refinement: *SCALEPACK* (Otwinowski & Minor, 1997); data reduction: *DENZO–SMN* (Otwinowski & Minor, 1997); program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *XP* in *SHELXTL/PC* (Sheldrick, 1994); software used to prepare material for publication: *SHELX*97-2 (Sheldrick, 1997) and local programs.

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