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Hexaiodobenzene: a redetermination at 100 K

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The X-ray crystal structure of hexaiodobenzene, C_6I_6, is reported with greatly improved precision after redetermination at 100 K. The compound is isostructural with hexachlorobenzene and hexabromobenzene. The molecule lies on an inversion centre.

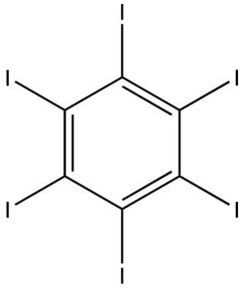
Key indicators

Single-crystal X-ray study
T = 100 K
Mean σ(C–C) = 0.007 Å
R factor = 0.022
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.

Comment

In the context of our research on halogen–halogen interactions in hexahalogenated benzenes (Reddy *et al.*, 2006), the crystal structure of hexaiodobenzene, (I) (Fig. 1), has been redetermined. This structure has been reported previously (Steer *et al.*, 1970; Khotsyanova & Smirnova, 1968), but with very limited precision. Hexahalogenated benzenes generally occur in two broad structural groups. The more common one is a monoclinic packing which is isostructural with C_6Cl_6. The less common one is a layered triclinic packing that is limited to compounds in which different halogen atoms occupy the 1,3,5- and 2,4,6-positions (Reddy *et al.*, 2006).



(I)

Hexaiodobenzene, (I), crystallizes in space group $P2_1/n$, and is isostructural with C_6Cl_6 and C_6Br_6 (Reddy *et al.*, 2006). The molecule lies on an inversion centre so that the asymmetric unit consists of a half-molecule. The planar molecules form π–π stacks, within which the molecules are 3.804 Å apart (perpendicular distance) and tilted (51.6°) to the stack direction so that π–π interactions are optimized (Fig. 2). The rest of the structure is close-packed with several short I$\cdots$I contacts [$\mathrm{I1}\cdots\mathrm{I2}^{\mathrm{i}}$ = 3.7045 (7) Å, $\mathrm{I2}\cdots\mathrm{I3}^{\mathrm{ii}}$ = 3.9485 (7) Å, $\mathrm{I3}\cdots\mathrm{I1}^{\mathrm{iii}}$ = 3.7125 (7) Å; symmetry codes: (i) $\frac{3}{2} - x, -\frac{1}{2} + y, \frac{3}{2} - z$; (ii) $1 - x, 1 - y, 2 - z$; (iii) $-\frac{1}{2} + x, \frac{1}{2} - y, \frac{1}{2} + z$].

Experimental

Synthesis of hexaiodobenzene was carried out according to the procedure reported by Mattern (1984). Single crystals were obtained by sublimation.

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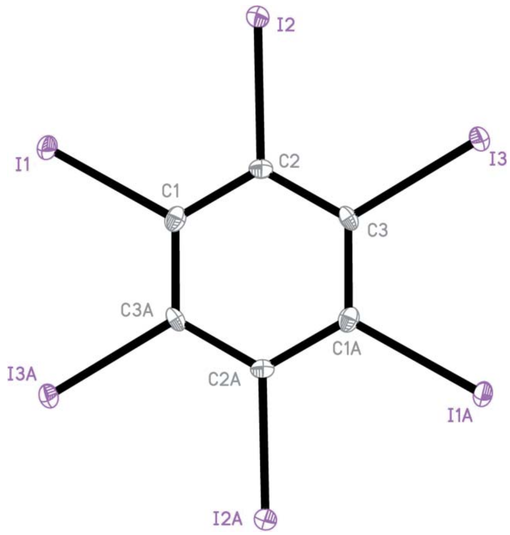

Figure 1
The molecular structure of (I) with displacement ellipsoids drawn at the 50% probability level. Atoms labelled with the suffix *A* are generated by the symmetry operator ($2 - x$, $-y$, $2 - z$).

Crystal data

C_6I_6
$M_r = 833.46$
Monoclinic, $P2_1/n$
$a = 8.8100\ (12)$ Å
$b = 4.2247\ (6)$ Å
$c = 16.191\ (2)$ Å
$\beta = 93.235\ (2)^\circ$
$V = 601.67\ (14)$ Å^3

$Z = 2$
$D_x = 4.600$ Mg m^{-3}
Mo *Kα* radiation
$\mu = 15.44$ mm^{-1}
$T = 100\ (2)$ K
Needle, yellow
0.56 × 0.15 × 0.13 mm

Data collection

Bruker SMART CCD diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.057$, $T_{max} = 0.134$

3375 measured reflections
1163 independent reflections
1148 reflections with $I > 2\sigma(I)$
$R_{int} = 0.023$
$\theta_{max} = 26.0^\circ$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.022$
$wR(F^2) = 0.052$
$S = 1.24$
1163 reflections
56 parameters

$w = 1/[\sigma^2(F_o^2) + (0.023P)^2 + 1.6335P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.003$
$\Delta\rho_{max} = 1.05$ e Å^{-3}
$\Delta\rho_{min} = -1.26$ e Å^{-3}
Extinction correction: *SHELXL97*
Extinction coefficient: 0.00171 (15)

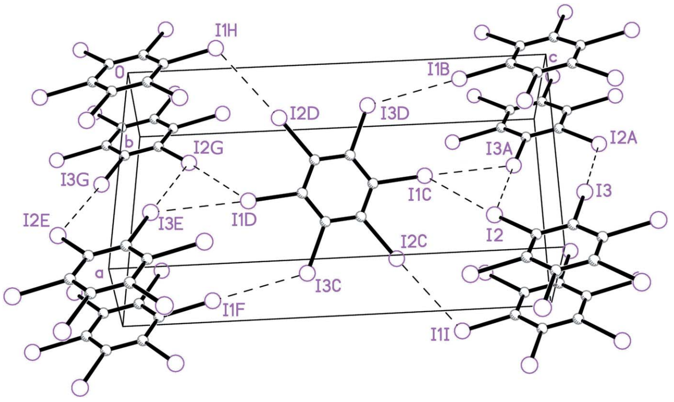

Figure 2
View of the unit-cell contents of (I), showing I···I contacts as dashed lines. [Symmetry codes: (A) $1 - x, 1 - y, 2 - z$; (B) $1 - x, -y, 2 - z$; (C) $\frac{3}{2} - x, \frac{1}{2} + y, \frac{3}{2} - z$; (D) $-\frac{1}{2} + x, \frac{1}{2} - y, -\frac{1}{2} + z$; (E) $x, y, -1 + z$; (F) $2 - x, 1 - y, 1 - z$; (G) $1 - x, 1 - y, 1 - z$; (H) $1 - x, -y, 1 - z$; (I): $x, 1 + y, z$.]

The highest peak and deepest hole in the difference density are located 0.98 Å from I2 and 0.96 Å from I1, respectively.

Data collection: *SMART* (Bruker, 2000); cell refinement: *SAINT* (Bruker, 2000); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 2000); software used to prepare material for publication: *SHELXTL*.

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