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1,2,4-Triiodobenzene

Igor Novak

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1,2,4-Triiodobenzene

Igor Novak

Charles Sturt University, POB 883, Orange NSW
2800, Australia

Correspondence e-mail: inovak@csu.edu.au

Key indicators

Single-crystal X-ray study

T = 223 K

Mean $\sigma(\text{C}-\text{C}) = 0.010 \text{ \AA}$

R factor = 0.032

wR factor = 0.062

Data-to-parameter ratio = 23.5

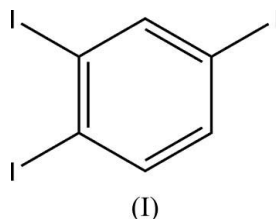
For details of how these key indicators were
automatically derived from the article, see
<http://journals.iucr.org/e>.

In the crystal structure of the title compound, $\text{C}_6\text{H}_3\text{I}_3$, the molecules are planar and the packing displays a herringbone motif. Molecules are held together by long weak non-bonding $\text{I}\cdots\text{I}$ interactions.

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Comment

Knowledge of the crystal structures of halobenzenes and halonaphthalenes is necessary for the development of force fields which can predict disorder and mixed crystal formation in haloaromatics (van Eijck *et al.*, 2002). However, such development requires the availability of a large database of appropriate crystal structures which can be used for parameterization purposes. Iodo-substituted aromatics were poorly represented in the database used to design such force fields. Only diiodo-substituted benzenes, without iodonaphthalenes, were represented in the database (van Eijck *et al.*, 2002).



The molecular structure parameters of (I), *e.g.* C—I bond lengths and endocyclic bond angles, are similar to those found in iodobenzenes reported previously (Margraf & Bats, 2006; Novak & Li, 2006; Novak & Li, 2007; Steer *et al.* 1970) (Fig. 1). The intramolecular $\text{I}\cdots\text{I}$ separation between vicinal I atoms is 3.67 (1) \AA , which is smaller than the sum of the van der Waals radii of iodine (4.3 \AA) and thus indicative of a certain amount of steric crowding. There is evidence of splaying in iodo-benzenes (Table 1), *i.e.* the decrease of CCI angles from 119 to 116°, suggesting a relief of $\text{I}\cdots\text{I}$ steric repulsion. The splaying is the greatest in the 1,2,3-triiodo isomer where steric compression of iodines is the most prominent.

The crystal packing of (I) is interesting, because it does not comprise stacking of aromatic rings as in other polyiodobenzenes, but adopts a herringbone motif (Fig. 2) which is common amongst aromatic hydrocarbons (Desiraju & Gavezzotti, 1989). The aromatic planes are slanted at 117 (1)°. Furthermore, the shortest intermolecular contact involving $\text{I}\cdots\text{I}$ separations of 3.907 (9) \AA is longer than in other iodo-benzenes (see references above). Another type of non-bonding van der Waals interaction present in (I) is expressed through an $\text{H}\cdots\text{I}$ intermolecular contact of 3.14 \AA .

The molecules of (I) are planar and belong to the low-symmetry C_s point group. We can conclude that the iodobenzene molecules of low symmetry, *e.g.* (I), have weak intermolecular contacts.

Experimental

The synthesis of 1,2,4-triiodobenzene was performed according to the procedure reported previously by Novak *et al.* (2002). Single crystals were obtained from the sublimate.

Crystal data

$C_6H_3I_3$	$V = 884.95 (18) \text{ \AA}^3$
$M_r = 455.78$	$Z = 4$
Orthorhombic, $Pba2$	Mo $K\alpha$ radiation
$a = 12.6534 (14) \text{ \AA}$	$\mu = 10.51 \text{ mm}^{-1}$
$b = 16.1729 (19) \text{ \AA}$	$T = 223 (2) \text{ K}$
$c = 4.3244 (5) \text{ \AA}$	$0.22 \times 0.08 \times 0.02 \text{ mm}$

Data collection

Bruker SMART CCD area-detector diffractometer	6090 measured reflections
Absorption correction: multi-scan (SADABS; Sheldrick, 2001)	2019 independent reflections
$T_{\min} = 0.206$, $T_{\max} = 0.817$	1889 reflections with $I > 2\sigma(I)$
	$R_{\text{int}} = 0.060$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.032$	$\Delta\rho_{\max} = 1.21 \text{ e \AA}^{-3}$
$wR(F^2) = 0.062$	$\Delta\rho_{\min} = -0.80 \text{ e \AA}^{-3}$
$S = 1.01$	Absolute structure: Flack (1983),
2019 reflections	862 Friedel pairs
86 parameters	Flack parameter: 0.13 (9)
H-atom parameters constrained	

Table 1

Molecular geometries (\AA , $^\circ$) in some iodobenzenes.

Compound	C—C—I	C—C—C	I...I
1,3,5-Triiodobenzene	119 (1)	121.7 (6)	None
1,2,4,5-Tetraiodobenzene	117 (1)	120.0 (5)	3.67 (2)
1,2,3-Triiodobenzene	116 (1)	118.0 (4)	3.60 (2)
1,2,4-Triiodobenzene	117 (1)	120.0 (5)	3.67 (2)

C—C—C corresponds to endocyclic angles at C atoms with vicinal I atoms. C—C—I corresponds to the angle involving iodine with at least one vicinal H atom.

H atoms were positioned geometrically ($C-H = 0.94 \text{ \AA}$) and refined as riding, with $U_{\text{iso}}(\text{H}) = 1.33U_{\text{eq}}(\text{C})$ for H6, $2.26U_{\text{eq}}(\text{C})$ for H5 and $2.5U_{\text{eq}}(\text{C})$ for H3. The highest peak is located 0.85 \AA from atom I3.

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

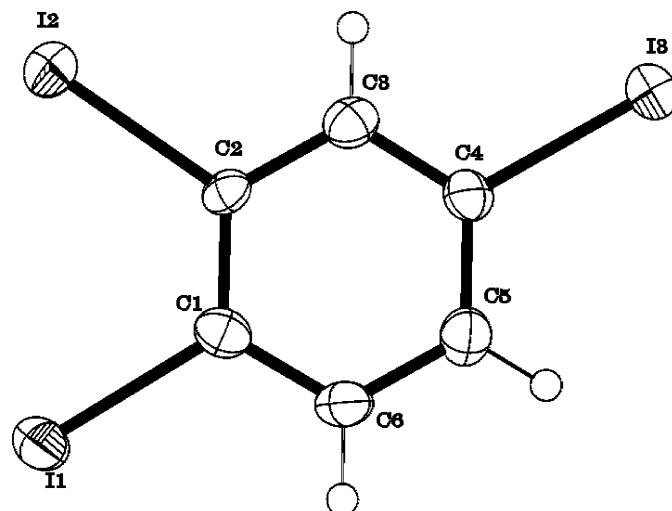


Figure 1

Molecular structure of (I), with displacement parameters drawn at the 50% probability level.

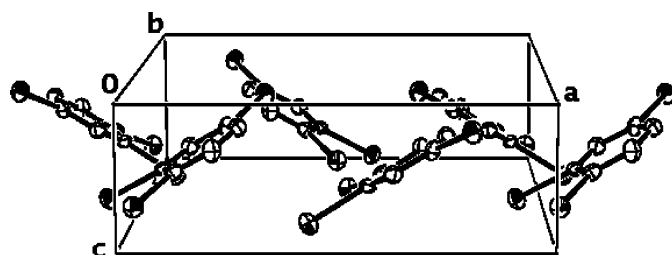


Figure 2

A packing diagram of (I), viewed down the b axis, displaying the herringbone pattern. H atoms have been omitted.

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