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4,4′-Diiodobiphenyl

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Key indicators

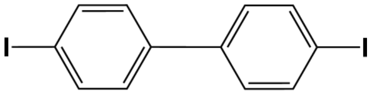
Single-crystal X-ray study
T = 174 K
Mean σ(C–C) = 0.003 Å
R factor = 0.020
wR factor = 0.042
Data-to-parameter ratio = 20.1

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

4,4′-Diiodobiphenyl, $C_{12}H_8I_2$, crystallizes as a homologous isomorph of the high-temperature form of *p*-diiodobenzene. The molecule is planar and lies on a center of symmetry. Each I atom is in contact with five others at distances between 4.0 and 4.5 Å.

Comment

A number 4,4′-disubstituted biphenyls have similar packing patterns. The dimethyl (Casalone *et al.*, 1969), dichloro (Brock *et al.*, 1978), and dibromo (Kronebusch *et al.*, 1976*b*) compounds are isomorphous, with the molecules lined up end-to-end with $X\cdots X$ contacts. The bromocyano (Kronebusch *et al.*, 1976*a*) and iodocyano (Britton & Gleason, 1991) differ only in that there are $X\cdots$N interactions; otherwise the packing is the same. In all of these structures, the torsion angles between the benzene rings are *ca* 40°. The structure of the corresponding diiodo compound, (I), was undertaken with the expectation of adding one more example to this list. Somewhat surprisingly, it has a different arrangement, with planar molecules.



(I)

Fig. 1 shows the labeling and the anisotropic displacement ellipsoids for the compound. The bond lengths and angles are normal. The molecule lies on a center of symmetry.

The molecules pack in two-dimensional puckered layers normal to the *a* axis. Fig. 2 shows shows one such layer; each I atom makes two I$\cdots$I contacts. There are also three other I$\cdots$I contacts to adjacent layers. The metric data for these interactions are given in Table 1. This structure is similar to that of the high-temperature polymorph of *p*-diiodobenzene (Alcobe *et al.*, 1994; Boese & Miebach, 1996). Both have space group *Pccn*; the cell constants for the diiodobenzene compound are a = 7.437, b = 6.155, and c = 17.047 Å. If these are compared with the values for (I), a and b are close to the same in both compounds and c is *ca* 8.6 Å longer in the biphenyl compound, which is the increase to be expected from adding the addi-

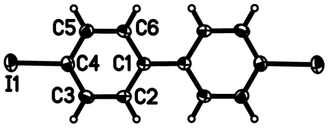


Figure 1
The molecule of (I). Displacement ellipsoids are drawn at the 50% probability level. Unlabeled atoms are related to labeled atoms by a center of symmetry at ($\frac{1}{2}$, $\frac{1}{2}$, $\frac{1}{2}$).

tional benzene ring. This is an example of what Kitaigorodsky (1961) has called 'homologous isomorphism.' Based on this, the structure of 4,4″-diiodo-*p*-terphenyl might be predicted to have space group *Pccn* with cell constants *ca* 7 × 6 × 34 Å.

Bent (1968) pointed out that the shortest $X—I\cdots I—Y$ intermolecular interactions involving small molecules usually occur with the $X—I\cdots I$ angle near linear and the $I\cdots I—Y$ angle near tetrahedral, or *vice versa*. The interpretation was that the I atom at the center of the linear interaction is a Lewis acid (electron acceptor) and the other is a Lewis base (electron donor). In centrosymmetric diiodides, each I atom often acts in both capacities, leading to a two-dimensional array. Such an array is seen here. However, the other three contacts are not much longer, and presumably not much weaker, than those in the layer, but they do not have the angular arrangement to be thought of as Lewis acid–base interactions.

Experimental

The title compound was obtained from Aldrich Chemical Co. Inc. Crystals were grown from acetone, benzene, dichloromethane, chloroform, carbon tetrachloride, and acetonitrile. Several habits were found, *viz*. prisms, clear plates, and striated plates, but all had the same unit cell. Except for the normal change with temperature, there is no difference between the unit cell at room temperature and that at 173 K. A prism grown from acetone was used for the structure determination. The crystallization from the above six solvents was a search for other polymorphs. That there are other polymorphs still seems likely, although none were found, since the 4,4′-dibromobiphenyl structure is one likely possibility, and a homologous isomorph corresponding to the low-temperature polymorph of *p*-diiodobenzene is another.

Crystal data

$C_{12}H_8I_2$
$M_r = 405.98$
Orthorhombic, *Pccn*
$a = 7.4189\ (18)$ Å
$b = 25.667\ (6)$ Å
$c = 5.9653\ (15)$ Å
$V = 1135.9\ (5)$ Å^3
$Z = 4$
$D_x = 2.374$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 3990 reflections
$\theta = 2.8–27.4°$
$\mu = 5.49$ mm^{-1}
$T = 174\ (2)$ K
Prism, colorless
0.40 × 0.25 × 0.20 mm

Data collection

Bruker SMART area-detector diffractometer
ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996; Blessing, 1995)
$T_{min} = 0.20$, $T_{max} = 0.33$
12 120 measured reflections
1306 independent reflections
1233 reflections with $I > 2\sigma(I)$
$R_{int} = 0.026$
$\theta_{max} = 27.5°$
$h = -9 \rightarrow 9$
$k = -33 \rightarrow 33$
$l = -7 \rightarrow 7$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.020$
$wR(F^2) = 0.042$
$S = 1.23$
1306 reflections
65 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.016P)^2 + 0.834P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.41$ e Å^{-3}
$\Delta\rho_{min} = -0.53$ e Å^{-3}
Extinction correction: *SHELXTL*
Extinction coefficient: 0.0076 (2)

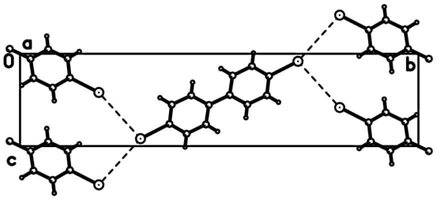


Figure 2
The unit-cell contents, viewed normal to (100). Only one layer of molecules is shown. The $I\cdots I$ intermolecular contacts are shown as dashed lines.

Table 1
Distances and angles (Å, °) in $C—I\cdots I—C$ contacts in 4,4′-diiodobiphenyl and *p*-diiodobenzene.

I'	$X—I\cdots I'$	$I\cdots I'$	$I\cdots I'—X$	Reference
I^{i}	159.0 (2)	4.015 (1)	125.7 (2)	*a*
I^{ii}	105.0 (2)	4.015 (1)	159.0 (2)	*a*
I^{iii}	125.7 (2)	4.292 (1)	125.7 (2)	*a*
I^{iv}	109.1 (2)	4.483 (1)	73.9 (2)	*a*
I^{v}	73.9 (2)	4.483 (1)	109.2 (2)	*a*
I'	164.2	4.109	98.2	*b*
I''	98.2	4.109	164.2	*b*
I'''	127.2	4.160	127.2	*b*
I''''	116.0	4.400	70.9	*b*
I'''''	70.9	4.400	116.0	*b*

References: (*a*) this work; (*b*) *p*-diiodobenzene (Boese & Miebach, 1996). Symmetry codes: (i) $x, \frac{3}{2} - y, -\frac{1}{2} + z$; (ii) $x, \frac{3}{2} - y, \frac{1}{2} + z$; (iii) $\frac{1}{2} - x, \frac{3}{2} - y, z$; (iv) $\frac{1}{2} - x, y, -\frac{1}{2} + z$; (v) $\frac{1}{2} - x, y, \frac{1}{2} + z$.

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

Data collection: *SMART* (Bruker, 2002); cell refinement: *SAINT* (Bruker, 2002); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 1997); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

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