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1,5-Diiodonaphthalene

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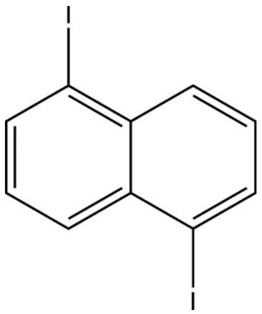
Key indicators: single-crystal X-ray study; T = 223 K; mean σ(C–C) = 0.006 Å; R factor = 0.033; wR factor = 0.077; data-to-parameter ratio = 25.5.

In the crystal structure of the title compound, $C_{10}H_6I_2$, the molecules are planar and packed in T-shaped edge-to-face mode. They are held together by weak I$\cdots\pi$ and I$\cdots$I non-bonding intermolecular interactions.

Related literature

The analysis of the electronic structure of 1,8-diiodonaphthalene has revealed the existence of intramolecular steric repulsions and through-space interactions between vicinal iodines (Novak *et al.*, 2003). Pronounced steric repulsion between iodine substituents was also observed in its structure in which the I atoms are twisted out of the aromatic ring plane by 5–17° (Bock *et al.*, 1998).

For related literature, see: Cruickshank (1957); Nguyen *et al.* (1999); Novak (2007).



Experimental

Crystal data

$C_{10}H_6I_2$
M_r = 379.95
Orthorhombic, $P2_12_12_1$
a = 7.0211 (5) Å
b = 11.5366 (8) Å
c = 12.1874 (8) Å
V = 987.17 (12) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 6.31 mm^{-1}
T = 223 (2) K
0.40 × 0.30 × 0.22 mm

Data collection

Bruker SMART CCD area-detector Diffractometer
Absorption correction: multi-scan *SADABS* (Sheldrick, 2001) T_{min} = 0.121, T_{max} = 0.249
8070 measured reflections
2783 independent reflections
2640 reflections with $I > 2\sigma(I)$
R_{int} = 0.024

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.033
$wR(F^2)$ = 0.077
S = 1.09
2783 reflections
109 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.74 e Å^{-3}
$\Delta\rho_{min}$ = −0.91 e Å^{-3}
Absolute structure: Flack (1983), 1116 Friedel pairs
Flack parameter: 0.001 (4)

Table 1
Parameters for weak intermolecular interactions (Å).

I$\cdots$I		I$\cdots\pi$	
I1$\cdots$I2	3.291 (8)	I2$\cdots$C6	3.508 (9)

Data collection: *SMART* (Bruker, 1997); cell refinement: *SMART* (Bruker, 1997); data reduction: *SAINT* (Bruker, 1997); 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*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: KP2102).

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supplementary materials

Acta Cryst. (2007). E**63**, o2726 [**doi:10.1107/S1600536807020508**]

1,5-Diiodonaphthalene

I. Novak

Comment

The structure of isomer (I) has C—I bond lengths (2.090–2.103 Å) which are slightly shorter than the bond lengths in 1,8-diiodonaphthalene (2.11–2.13 Å). This can be attributed to the requirement for strain relief in the latter. The geometry of the naphthalene skeleton in (I) is similar to the parent naphthalene (Cruickshank, 1957) except for the C5—C10 bond which at 1.431 (4) Å is longer in (I) compared to 1.410 Å in the parent naphthalene. The molecules of (I) are planar (Figure 1).

The most interesting feature of the title compound (I) is its crystal packing (Figure 2) which is different from the packings in 1,8-diiodonaphthalene (Bock *et al.* 1998) or 2,3-diiodonaphthalene (Novak 2007). In the last two compounds crystal packing comprises π -π stacking and herringbone motif, respectively with individual molecules being held together by I···I non-bonding, van der Waals forces. In (I) on the other hand the molecules are packed in a way which facilitates T-shaped edge-face mode of intermolecular interaction (Nguyen *et al.* 1999). The separations pertaining to the shortest intermolecular contacts, which hold the structure together are given in Table 1.

Experimental

The synthesis of 1,5-diiodonaphthalene was carried out according to the procedure reported previously by Novak *et al.* (2003). Single crystals of (I) were obtained from the sublimate.

Refinement

H atoms were positioned geometrically (C—H = 0.94 Å) and refined as riding with U_{iso} (H) = 1.2 U_{eq} (C). The highest peak is located 0.74 Å from atom I1 and the deepest hole is located -0.908 Å from atom I1. This is a chiral space group. The Friedel equivalents were not merged. The Flack value indicates the correct absolute structure. However, the molecule is not chiral, it is the packing that results in the chiral space group.

Figures

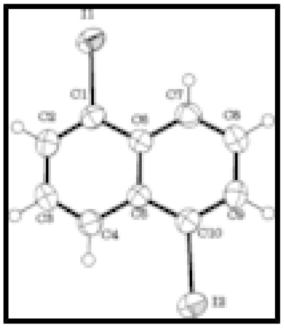

Fig. 1. Molecular structure of (I) with displacement parameters drawn at the 50% probability level.

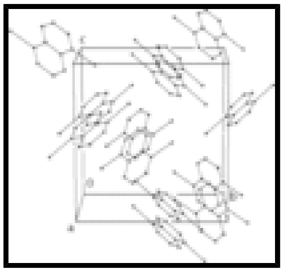

Fig. 2. Crystal packing of (I) viewed along *a* axis. H atoms have been omitted.

1,5-Diiodonaphthalene

Crystal data

$C_{10}H_6I_2$

$M_r = 379.95$

Orthorhombic, $P2_12_12_1$

Hall symbol: P 2ac 2ab

$a = 7.0211$ (5) Å

$b = 11.5366$ (8) Å

$c = 12.1874$ (8) Å

$V = 987.17$ (12) Å^3

$Z = 4$

$F_{000} = 688$

$D_x = 2.556$ Mg m^{-3}

Mo *K*α radiation
λ = 0.71073 Å

Cell parameters from 4117 reflections

θ = 2.9–29.4°

μ = 6.31 mm^{-1}

$T = 223$ (2) K

RECTANGULAR ROD, red

0.40 × 0.30 × 0.22 mm

Data collection

Bruker SMART CCD area-detector Diffractometer

Radiation source: fine-focus sealed tube

Monochromator: graphite

$T = 223(2)$ K

ω scans

Absorption correction: multi-scan
SADABS (Sheldrick, 2001)

$T_{\min} = 0.121$, $T_{\max} = 0.249$

8070 measured reflections

2783 independent reflections

2640 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.024$

$\theta_{\max} = 30.0°$

$\theta_{\min} = 2.4°$

$h = -9 \rightarrow 9$

$k = -14 \rightarrow 15$

$l = -16 \rightarrow 13$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.033$

$wR(F^2) = 0.077$

$S = 1.09$

2783 reflections

109 parameters

Hydrogen site location: inferred from neighbouring sites

H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.039P)^2 + 0.3767P]$
where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{\max} = 0.002$

$\Delta\rho_{\max} = 0.74$ e Å^{-3}

$\Delta\rho_{\min} = -0.91$ e Å^{-3}

Extinction correction: none

Primary atom site location: structure-invariant direct methods	Absolute structure: Flack (1983), 1116 Friedel pairs
Secondary atom site location: difference Fourier map	Flack parameter: 0.001 (4)

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted R-factor wR and goodness of fit S are based on F^2, conventional R-factors R are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > 2\text{sigma}(F^2)$ is used only for calculating R-factors(gt) etc. and is not relevant to the choice of reflections for refinement. R-factors based on F^2 are statistically about twice as large as those based on F, and R- factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	*y*	*z*	$U_{\rm iso}$*/$U_{\rm eq}$
I1	0.49839 (5)	0.36624 (3)	1.00766 (3)	0.05194 (10)
I2	1.04897 (4)	0.85089 (3)	0.75365 (3)	0.05002 (10)
C1	0.5745 (6)	0.5033 (4)	0.9044 (3)	0.0392 (8)
C2	0.4501 (6)	0.5338 (4)	0.8239 (4)	0.0455 (10)
H2	0.3342	0.4939	0.8161	0.055*
C3	0.4960 (8)	0.6258 (4)	0.7519 (4)	0.0454 (8)
H3	0.4093	0.6462	0.6964	0.054*
C4	0.6596 (6)	0.6846 (4)	0.7609 (3)	0.0411 (8)
H4	0.6860	0.7454	0.7119	0.049*
C5	0.7929 (5)	0.6560 (3)	0.8436 (3)	0.0339 (7)
C6	0.7516 (6)	0.5630 (4)	0.9176 (3)	0.0349 (8)
C7	0.8822 (6)	0.5353 (4)	1.0011 (4)	0.0431 (9)
H7	0.8525	0.4754	1.0504	0.052*
C8	1.0531 (7)	0.5938 (5)	1.0127 (4)	0.0455 (10)
H8	1.1402	0.5728	1.0678	0.055*
C9	1.0939 (6)	0.6865 (4)	0.9391 (4)	0.0438 (10)
H9	1.2078	0.7286	0.9465	0.053*
C10	0.9689 (5)	0.7142 (4)	0.8581 (3)	0.0373 (8)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
I1	0.0586 (2)	0.04360 (17)	0.05359 (17)	−0.01052 (14)	0.00536 (16)	0.00267 (12)
I2	0.05333 (18)	0.04250 (17)	0.05423 (17)	−0.00836 (11)	0.00393 (14)	0.00466 (14)
C1	0.043 (2)	0.036 (2)	0.0386 (19)	−0.0013 (17)	0.0048 (17)	−0.0050 (15)
C2	0.038 (2)	0.050 (3)	0.049 (2)	−0.0025 (19)	−0.0029 (18)	−0.0041 (19)
C3	0.0436 (18)	0.052 (2)	0.040 (2)	0.003 (2)	−0.0097 (17)	0.002 (2)
C4	0.0428 (19)	0.043 (2)	0.038 (2)	0.0001 (16)	−0.0003 (18)	−0.0015 (19)
C5	0.0344 (17)	0.0306 (19)	0.0366 (17)	0.0019 (15)	0.0025 (14)	−0.0043 (15)
C6	0.0388 (19)	0.036 (2)	0.0303 (17)	0.0038 (16)	0.0028 (14)	−0.0033 (15)

C7	0.049 (2)	0.041 (2)	0.040 (2)	0.0015 (17)	−0.0015 (19)	0.0000 (18)
C8	0.043 (2)	0.053 (3)	0.041 (2)	0.004 (2)	−0.006 (2)	0.0018 (19)
C9	0.040 (2)	0.045 (2)	0.047 (2)	−0.0025 (18)	−0.0044 (18)	−0.0083 (19)
C10	0.037 (2)	0.036 (2)	0.0393 (19)	−0.0002 (17)	0.0024 (16)	−0.0047 (15)

Geometric parameters (Å, °)

I1—C1	2.090 (4)	C5—C10	1.417 (5)
I2—C10	2.103 (4)	C5—C6	1.432 (6)
C1—C2	1.360 (6)	C6—C7	1.406 (6)
C1—C6	1.431 (6)	C7—C8	1.384 (7)
C2—C3	1.414 (7)	C7—H7	0.9400
C2—H2	0.9400	C8—C9	1.425 (7)
C3—C4	1.339 (7)	C8—H8	0.9400
C3—H3	0.9400	C9—C10	1.358 (6)
C4—C5	1.415 (5)	C9—H9	0.9400
C4—H4	0.9400		

C2—C1—C6	121.0 (4)	C7—C6—C1	122.6 (4)
C2—C1—I1	117.8 (3)	C7—C6—C5	119.6 (4)
C6—C1—I1	121.2 (3)	C1—C6—C5	117.8 (4)
C1—C2—C3	119.7 (4)	C8—C7—C6	121.9 (4)
C1—C2—H2	120.1	C8—C7—H7	119.0
C3—C2—H2	120.1	C6—C7—H7	119.0
C4—C3—C2	121.7 (4)	C7—C8—C9	118.4 (4)
C4—C3—H3	119.2	C7—C8—H8	120.8
C2—C3—H3	119.2	C9—C8—H8	120.8
C3—C4—C5	120.5 (4)	C10—C9—C8	120.2 (4)
C3—C4—H4	119.7	C10—C9—H9	119.9
C5—C4—H4	119.7	C8—C9—H9	119.9
C4—C5—C10	123.7 (4)	C9—C10—C5	122.9 (4)
C4—C5—C6	119.3 (4)	C9—C10—I2	116.3 (3)
C10—C5—C6	116.9 (3)	C5—C10—I2	120.8 (3)

Parameters for weak intermolecular interactions (Å)

I···I		I···π	
I1···I2	3.291 (8)	I2···C6	3.508 (9)

Fig. 1

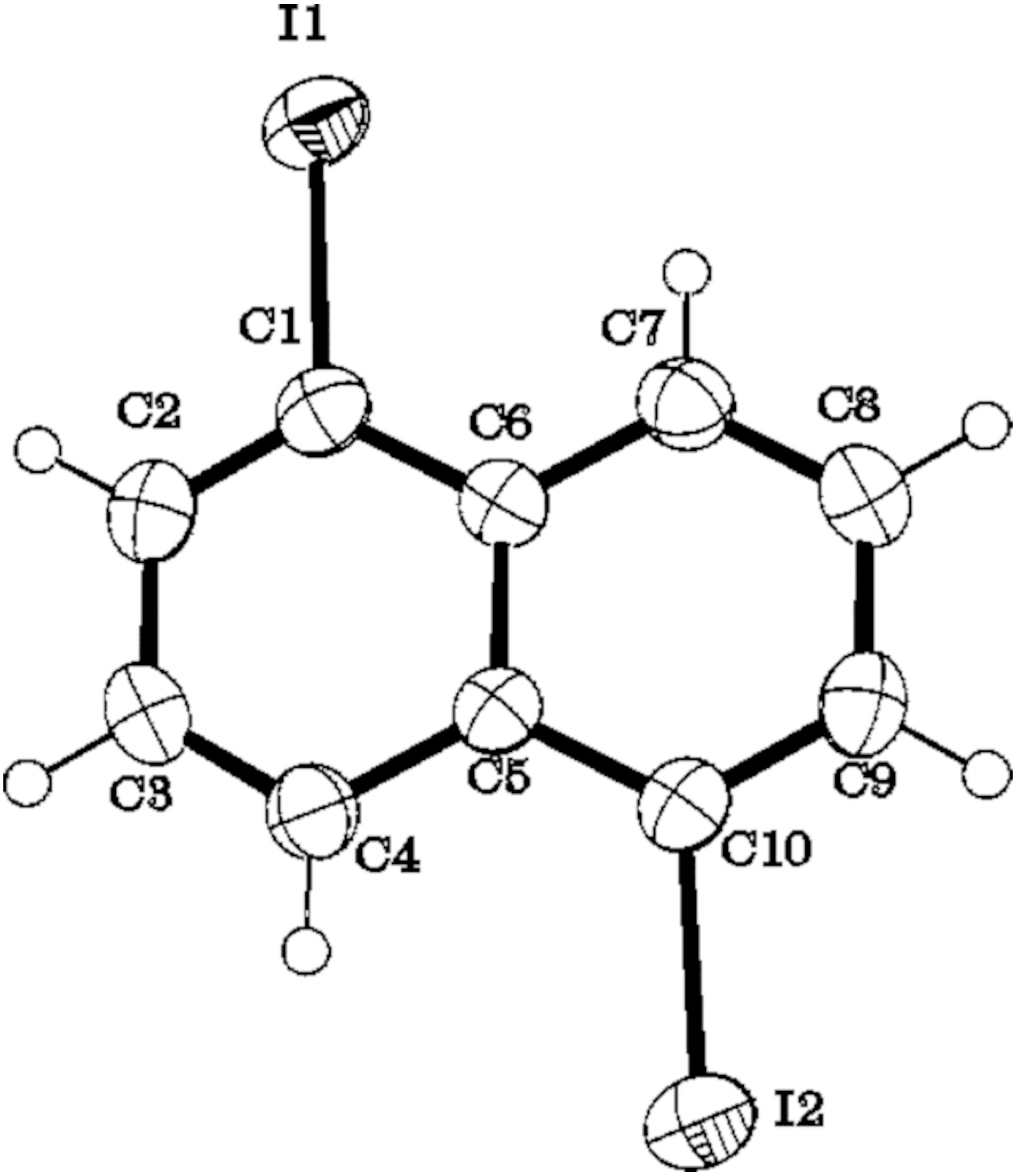

Fig. 2