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2,3-Diiodonaphthalene

Igor Novak

Charles Sturt University, POB 883, Orange, New South Wales 2800, Australia

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

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In the crystal structure of the title compound, $C_{10}H_6I_2$, the molecules are planar and packed in a herring-bone motif. The molecules are held together by weak I···I intermolecular interactions.

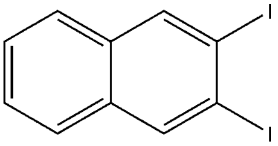
Key indicators

Single-crystal X-ray study
T = 295 K
Mean σ(C–C) = 0.011 Å
R factor = 0.060
wR factor = 0.147
Data-to-parameter ratio = 21.3

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

Comment

The analysis of the electronic structure of some iodonaphthalene molecules revealed intramolecular steric repulsions and through-space interactions between vicinal iodines (Novak *et al.* 2003). Pronounced steric repulsion between iodine substituents was also observed in the molecular structure of 1,8-diiodonaphthalene where the I atoms are twisted out of the aromatic ring plane by 5–17° (Bock *et al.* 1998). The C—I bond lengths in the title molecule (I) are slightly shorter [2.087 (7)–2.107 (7) Å than the bond lengths in its 1,8-diiodonaphthalene isomer [2.11 (1)–2.13 (1) Å] which can be attributed to strain relief in the latter. .



(I)

The geometry of the naphthalene skeleton (Cruickshank, 1957) is little changed in 1,8-diiodonaphthalene and in (I), which attests to the robustness of the aromatic core. Nonetheless, some trends in the aromatic system geometry can be observed along the sequence: the parent naphthalene, weakly sterically congested (I), and highly sterically congested 1,8-diiodonaphthalene. The most prominent trend is the lengthening of the C5—C10 bond (Fig. 1) in the two isomers which increases from 1.41 (1) Å in the parent naphthalene to 1.46 (1) Å in the 1,8-diiodo derivative. The intramolecular

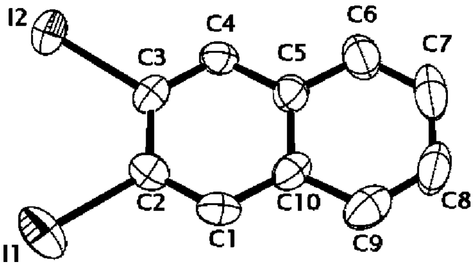


Figure 1
Molecular structure of (I) with displacement parameters drawn at the 50% probability level. H atoms have been omitted.

I···I separation in the 1,8-diiodo isomer [3.51–3.54 (1) Å] is significantly smaller than in (I) where it is 3.641 (6) Å, because the former molecule experiences much greater steric repulsion than the latter. Both values are smaller than the sum of van der Waals radii for iodine (4.3 Å). The large difference in I···I separation between 1,8-diiodonaphthalene and its isomer (I) demonstrates how prominent the strain in the former molecule is, despite the iodine out-of-plane distortion. Twisting of iodine substituents has a dramatic effect on the crystal packing. Compound (I) has one molecule in the asymmetric unit, whereas 1,8-diiodonaphthalene has six. It is not surprising, therefore, that the crystal packing of (I) (Fig. 2) is simple, comprising strands which are arranged in a herringbone motif. The molecules in the strand are packed in alternating orientations and the aromatic planes are slanted towards each other at 122 (1)°. In contrast, the molecules of 1,8-diiodonaphthalene form stacks and layers.

In (I) the short intermolecular separation distance I···I between molecules of different strands of 3.854 (9) Å is significantly shorter than the sum of van der Waals radii. These contacts reflect van der Waals interactions which hold the crystal structure together.

Experimental

The synthesis of 2,3-diiodonaphthalene was carried out according to the procedure reported previously by Novak *et al.* (2003). Single crystals of (I) were obtained from the sublimate.

Crystal data

$C_{10}H_6I_2$
$M_r = 379.95$
Orthorhombic, *Pbca*
$a = 11.9420$ (9) Å
$b = 8.0583$ (6) Å
$c = 21.0592$ (16) Å
$V = 2026.6$ (3) Å^3

$Z = 8$
$D_x = 2.491$ Mg m^{-3}
Mo *Kα* radiation
$\mu = 6.15$ mm^{-1}
$T = 295$ (2) K
Thin plate, red
0.34 × 0.20 × 0.04 mm

Data collection

Bruker SMART CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2001)
$T_{min} = 0.229$, $T_{max} = 0.791$

13214 measured reflections
2327 independent reflections
1864 reflections with $I > 2\sigma(I)$
$R_{int} = 0.047$
$\theta_{max} = 27.5°$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.060$
$wR(F^2) = 0.147$
$S = 1.13$
2327 reflections
109 parameters
H-atom parameters comstrained

$w = 1/[\sigma^2(F_o^2) + (0.0619P)^2 + 7.1027P]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 2.02$ e Å^{-3}
$\Delta\rho_{min} = -1.02$ e Å^{-3}

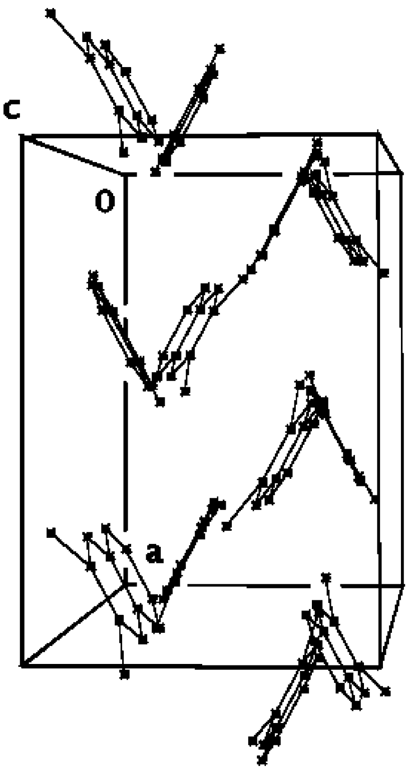


Figure 2
Crystal packing of (I), displaying the herringbone pattern. H atoms have been omitted.

H atoms were positioned geometrically (C—H = 0.93 Å) and refined as riding, with $U_{iso}(H) = 1.2U_{eq}(C)$. The highest peak is located 0.83 Å from atom I2 and the deepest hole is located 1.44 Å from atom I2.

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