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1-Bromo-2-(bromomethyl)naphthalene

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Key indicators

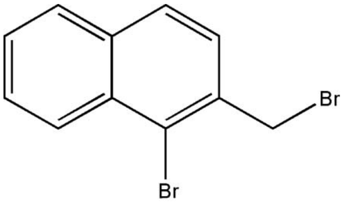
Single-crystal X-ray study
T = 93 K
Mean σ(C–C) = 0.002 Å
R factor = 0.036
wR factor = 0.087
Data-to-parameter ratio = 50.0

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

In the title compound, $C_{11}H_8Br_2$, the crystal packing is dominated by intermolecular Br$\cdots$Br and C—H$\cdots\pi$ contacts.

Comment

Although bromine-substituted derivates of naphthalene are useful tools for metal-catalysed coupling reactions (Takahashi *et al.*, 1980), crystal structures of these compounds have rarely been examined. One such case is 1-bromo-2-naphthaldehyde (Koppenhoefer & Bats, 1986) which crystallizes with stabilizing C—H$\cdots$O and C—H$\cdots$Br contacts. We describe here the crystal structure of 1-bromo-2-(bromomethyl)-naphthalene, (I), another representative example of this type of compound, which features no hydrogen-acceptor O atom but an additional Br atom, enabling Br$\cdots$Br contacts.



(I)

The bromomethyl side arm is almost perpendicular to the naphthalene ring system, with an angle of 91.85 (2)° between the Br2/C11/C2 plane and the ten atoms of the naphthalene ring system, while Br1 is coplanar [0.018 (1) Å]. The crystal structure of (I) is dominated by weak Br$\cdots$Br contacts of the so-called side-on type, resulting in chains along the crystallographic a axis. This electrophile–nucleophile pairing interaction is found in many bromine- or iodine-substituted aryl compounds, the θ_1 and θ_2 angles being 170±10 and 90±10°, respectively (Desiraju, 1989; Ramasubbu *et al.*, 1986). In the crystal structure of (I), the distance between the halogen atoms is 3.6611 (3) Å, slightly shorter than the sum of the van der Waals radii, whereas the angles θ_1 (C1—Br1$\cdots$Br2) and θ_2 (C11—Br2$\cdots$Br1) are 164.4 (1) and 95.2 (1)°, respectively. In addition, weak C—H$\cdots\pi$ contacts (C11—H11$B\cdots Cg2$ 2.89 Å and 130°; $Cg2$ is the centroid of the C5–C10 ring) and a weak intermolecular C—H$\cdots$Br contact [C11—H11$B\cdots$Br2^{i} 3.04 Å and 132°; symmetry code: (i) $-x, 1-y, 1-z$] are present in this solid-state structure.

Experimental

The title compound, (I), was synthesized in two steps as described by Weber *et al.* (1984), including reaction of 2-methylnaphthalene with bromine to give 1-bromo-2-methylnaphthalene (82%) and subse-

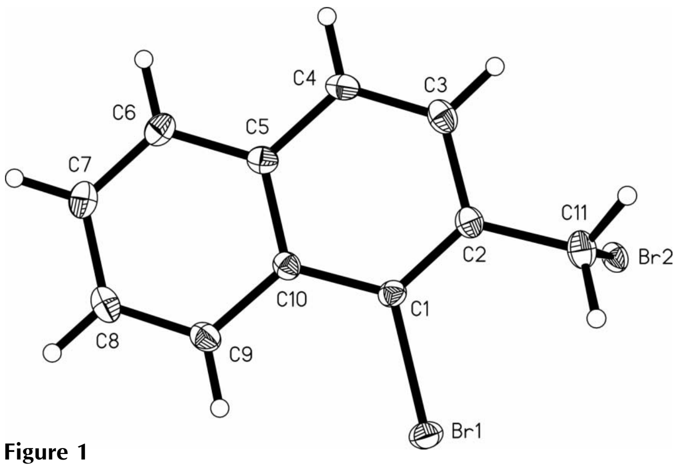


Figure 1
The molecular structure of (I), showing 50% probability displacement ellipsoids for non-H atoms.

quent bromination with *N*-bromosuccinimide. Recrystallization from hexane yielded (I) (74%) as colourless needles suitable for X-ray crystallographic analysis.

Crystal data

$C_{11}H_8Br_2$
$M_r = 299.99$
Triclinic, $P\bar{1}$
$a = 6.9074$ (4) Å
$b = 8.3754$ (4) Å
$c = 8.5433$ (4) Å
$\alpha = 92.054$ (3)°
$\beta = 101.246$ (3)°
$\gamma = 94.013$ (3)°
$V = 482.95$ (4) Å^3
$Z = 2$
Mo $K\alpha$ radiation
$\mu = 8.34$ mm^{-1}
$T = 93$ (2) K
0.25 × 0.21 × 0.20 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2000)
$T_{\min} = 0.127$, $T_{\max} = 0.286$ (expected range = 0.084–0.189)
22317 measured reflections
5954 independent reflections
4333 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.050$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.036$
$wR(F^2) = 0.087$
$S = 1.01$
5954 reflections
119 parameters
H-atom parameters constrained
$\Delta\rho_{\max} = 1.67$ e Å^{-3}
$\Delta\rho_{\min} = -2.09$ e Å^{-3}

The H atoms were positioned geometrically and allowed to ride on their parent atoms, with C—H = 0.95 Å and $U_{\rm iso}(H) = 1.2–1.5U_{\rm eq}(C)$. The highest residual electron density peak is located 0.70 Å from atom Br2 and the deepest hole is located 0.68 Å from atom Br1.

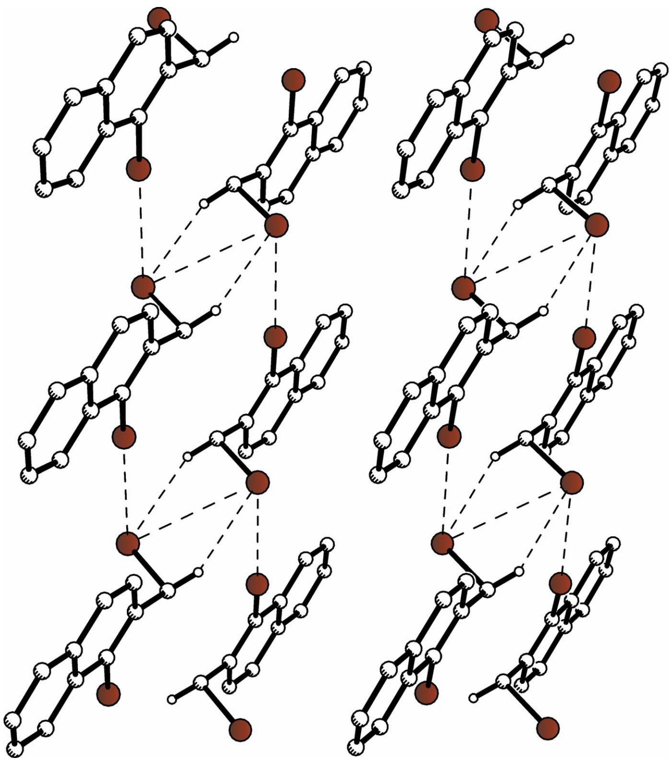


Figure 2
Packing diagram of (I), viewed down the *c* axis. All H atoms except H11*B* have been omitted for clarity. Dashed lines indicate either Br1···Br2 or C11—H11*B*···Br2 contacts.

Data collection: *SMART* (Bruker, 2004); cell refinement: *SAINT* (Bruker, 2004); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *PLATON* (Spek, 2003).

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