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2,2″-Bis(bromomethyl)-*p*-terphenyl

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Key indicators

Single-crystal X-ray study
T = 133 K
Mean σ(C–C) = 0.002 Å
R factor = 0.025
wR factor = 0.057
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.

The molecule of the title compound, $C_{20}H_{16}Br_2$, displays crystallographic inversion symmetry. Two C—H···Br interactions link the molecules into layers parallel to ($\bar{1}$11). The shortest Br···Br contact is 4.1599 (4) Å.

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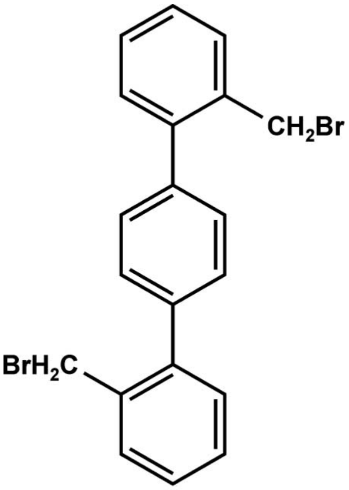
Secondary interactions in bromomethyl derivatives, Part 2. Part 1: Kuś & Jones (2003)

Comment

In order to explore the relationship between bromine–bromine interactions and the structure of poly(bromomethyl)aryl derivatives,we have synthesized a series of bromomethylarenes. Previously, we described the structure of 1,6,7-tris(bromomethyl)naphthalene (Kuś & Jones, 2003). The crystal packing of this compound shows two types of interaction: weak C—H···Br hydrogen bonds and Br···Br interactions. We describe here the crystal structure of 2,2″-bis(bromomethyl)-*para*-terphenyl, (I), which was obtained by bromination of 2,2″-dimethyl-*p*-terphenyl using *N*-bromosuccinimide in boiling tetrachloromethane.



(I)

The molecule, which displays crystallographic inversion symmetry, is shown in Fig. 1. Bond lengths and angles may be considered normal, *e.g.* the single-bond length between the rings is 1.492 (2) Å, *cf.* 1.490 (2) Å in 2,5,2″,5″-tetramethyl-*p*-terphenyl (Jones *et al.*, 2005). The angle between the central and the outer planes is 54.13 (6)°.

The molecules are linked to form layers parallel to ($\bar{1}$11) by the long and presumably very weak interactions H6···Br and H7···Br (Fig. 2 and Table 1). The shortest Br···Br contact is 4.1599 (4) Å *via* the symmetry operator $(-x, 1-y, -z)$, which is considerably longer than the double van der Waals radius and is therefore not drawn explicitly in Fig. 2. The layers are in turn linked by the short C—H···π contact C10—H10*A*···*Cg*(C4–C9), with C—H normalized to 1.08 Å, H···*Cg* = 2.71 Å and C—H···*Cg* = 121° [*Cg* is at ($x - 1, y, z$)]. The contact is very asymmetric; the H atom is much closer to atoms C4–C7 than to the other two atoms.

Experimental

Compound (I) was synthesized from 2,2″-dimethyl-*p*-terphenyl according to the method of Boeckmann & Vögtle (1981). The analytical and spectroscopic data are consistent with the literature. Single crystals were grown by slow evaporation of a chloroform solution. ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.56–7.59 (*m*, 2H), 7.55 (*s*, 4H), 7.38–7.41 (*m*, 4H), 7.32–7.35 (*m*, 2H), 4.54 (*s*, 4H). ^{13}C NMR (100 MHz): 32.42, 128.27, 128.77, 129.11, 130.64, 131.23, 135.39, 139.53, 141.75.

Crystal data

$C_{20}H_{16}Br_2$
$M_r = 416.15$
Triclinic, $P\overline{1}$
$a = 4.4286$ (4) Å
$b = 7.4756$ (6) Å
$c = 12.4664$ (12) Å
$\alpha = 96.032$ (4)°
$\beta = 98.347$ (4)°
$\gamma = 96.155$ (4)°
$V = 402.93$ (6) Å^3
$Z = 1$
$D_x = 1.715$ Mg m^{-3}
Mo *Kα* radiation
Cell parameters from 4465 reflections
$\theta = 2.7$–30.4°
$\mu = 5.02$ mm^{-1}
$T = 133$ (2) K
Rectangular prism, colourless
0.25 × 0.10 × 0.07 mm

Data collection

Bruker SMART 1000 CCD diffractometer
ω and φ scans
Absorption correction: multi-scan (*SADABS*; Bruker, 1998)
$T_{\min} = 0.488$, $T_{\max} = 0.704$
8315 measured reflections
2348 independent reflections
2056 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.026$
$\theta_{\max} = 30.0°$
$h = -6 \rightarrow 6$
$k = -10 \rightarrow 10$
$l = -17 \rightarrow 17$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.025$
$wR(F^2) = 0.057$
$S = 1.02$
2348 reflections
100 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.032P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} < 0.001$
$\Delta\rho_{\max} = 0.63$ e Å^{-3}
$\Delta\rho_{\min} = -0.33$ e Å^{-3}

Table 1
Hydrogen-bond geometry (Å, °).

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C6—H6···Br$^{\rm i}$	0.95	3.13	4.0272 (18)	158
C7—H7···Br$^{\rm ii}$	0.95	3.16	3.8764 (18)	134

Symmetry codes: (i) $-x, -y + 1, -z$; (ii) $x + 1, y + 1, z$.

H atoms were included using a riding model, with C—H = 0.95 (aromatic) and 0.99 Å (methylene). $U_{\rm iso}$(H) values were fixed at $1.2U_{\rm eq}$(C).

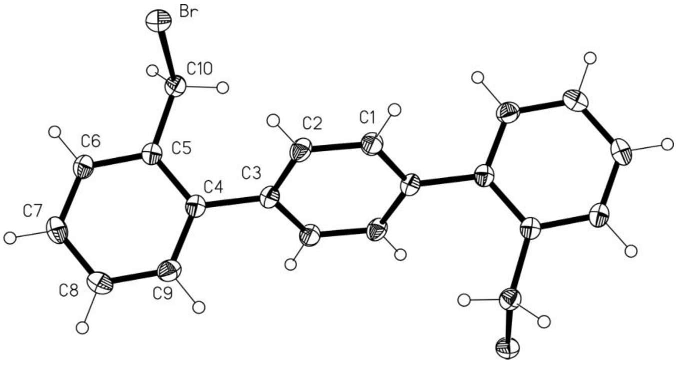


Figure 1
The molecule of the title compound in the crystal structure. Displacement ellipsoids are drawn at the 50% probability level.

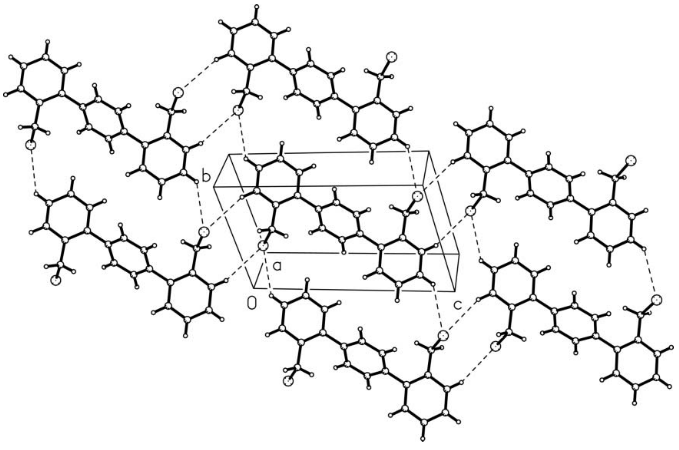


Figure 2
Packing of the title compound, viewed perpendicular to ($\overline{1}$11). Dotted lines indicate C—H···Br contacts (see Comment).

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT* (Bruker, 1998); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1990); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *XP* (Siemens, 1994); software used to prepare material for publication: *SHELXL97*.

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