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1,1-Bis(bromomethyl)benzene

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Key indicators

Single-crystal X-ray study
T = 298 K
Mean σ(C–C) = 0.007 Å
R factor = 0.050
wR factor = 0.135
Data-to-parameter ratio = 21.2

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

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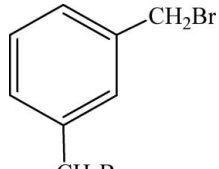
In the crystal structure of the title molecule, $C_8H_8Br_2$, there is a single C—H$\cdots\pi$(arene) interaction.

Comment

The title compound, (I), is used as an organic intermediate in the synthesis of cyclic amines (Chadim *et al.*, 2003) and as a bridging reagent to link two cyclic amine rings (Graham *et al.*, 2005). Its crystal structure is reported here.



(I)

The molecular structure of (I) is shown in Fig. 1. The bond lengths and angles are within normal ranges (Allen *et al.*, 1987). Atoms C7 and C8 are almost coplanar with the aryl ring, as reflected in the C7—C1—C2—C3 and C8—C3—C4—C5 torsion angles of −179.1 (4) and −179.5 (5)°, respectively. Atoms Br1 and Br2 are displaced, on opposite sides, by 1.829 (2) and 1.790 (1) Å, respectively, from the least-squares plane defined by atoms C1–C8.

In the crystal structure, there is a weak C—H$\cdots\pi$(arene) interaction [H8$\cdots Cg^{i}$ 2.98, C8$\cdots Cg^{i}$ 3.550 (6) Å, C8—H8$\cdots Cg^{i}$ 119 Å; Cg is the centroid of the C1–C6 ring; symmetry code: (i) x, $-1+y$, z], forming chains propagating along [010] (Fig. 2).

Experimental

The title compound was synthesized by a reported method (Stephenson *et al.*, 1963). Crystals suitable for X-ray analysis were obtained by the slow evaporation of a CH_3CN solution.

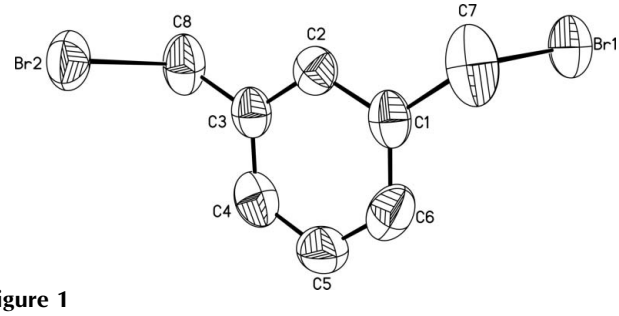


Figure 1
The molecular structure of (I), showing displacement ellipsoids drawn at the 50% probability level. H atoms have been omitted.

Crystal data

$C_8H_8Br_2$
M_r = 263.96
Monoclinic, $P2_1/n$
a = 13.084 (2) Å
b = 4.5374 (8) Å
c = 15.075 (3) Å
β = 93.846 (3)°
V = 893.0 (3) Å^3
Z = 4
D_x = 1.963 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 9.00 mm^{-1}
T = 298 (2) K
Thick plate, colorless
0.30 × 0.20 × 0.10 mm

Data collection

Bruker SMART CCD diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2000)
T_{min} = 0.151, T_{max} = 0.406
6118 measured reflections
1933 independent reflections
1221 reflections with $I > 2\sigma(I)$
R_{int} = 0.059
θ_{max} = 27.0°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.050
$wR(F^2)$ = 0.135
S = 1.00
1933 reflections
91 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0726P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.75 e Å^{-3}
$\Delta\rho_{min}$ = −0.52 e Å^{-3}

All H atoms were placed in calculated positions (C—H = 0.93–0.97 Å) and included in the riding-model approximation, with U_{iso}(H) = 1.2U_{eq}(C).

Data collection: *SMART* (Bruker, 2000); cell refinement: *SAINT* (Bruker, 2000); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 2000); software used to prepare material for publication: *SHELXTL*.

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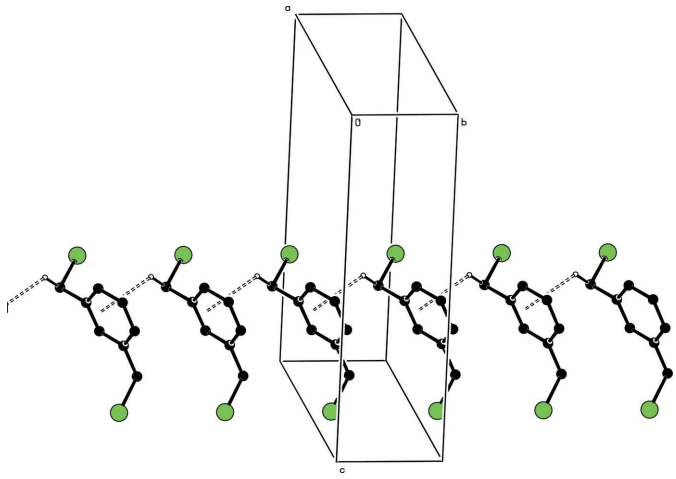

Figure 2
Part of the crystal structure of (I), showing C—H···π(arene) interactions as dashed lines. For clarity, H atoms not in the motif shown have been omitted.

References

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