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1,4-Bis(bromomethyl)benzene

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Key indicators

Single-crystal X-ray study
T = 297 K
Mean σ(C–C) = 0.007 Å
R factor = 0.047
wR factor = 0.149
Data-to-parameter ratio = 18.4

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

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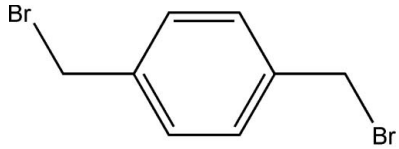
In the title compound, $C_8H_8Br_2$, the molecules are located on inversion centres and are connected through weak intermolecular Br···Br interactions into layers parallel to the (102) plane.

Comment

1,4-Bis(halomethyl)benzene compounds have played a very important role in the preparation of bridging ligands used in supramolecular chemistry (Hoskins *et al.*, 1997*a*,*b*; Wen *et al.*, 2005; Zhang *et al.*, 2005). However, to date only 1,4-bis(chloromethyl)benzene has been crystallographically characterized (Basaran *et al.*, 1992). In this paper, we report the crystal structure of an isomorphous compound, 1,4-bis(bromomethyl)benzene, (I).



(I)

The asymmetric unit of (I) contains one half-molecule; the molecule is located on an inversion centre (Fig. 1). No unexpected bond lengths or angles are observed.

In the packing of (I), neither hydrogen bonds nor significant π–π or C—H···π interactions exist. An analysis of the crystal structure (Spek, 2003) shows that the only possible direction-specific interactions arise from intermolecular Br···Br contacts. In detail, atom Br1 at (*x*, *y*, *z*) interacts with symmetry-related Br1 atoms at $(-x, \frac{1}{2}+y, \frac{1}{2}-z)$ and $(-x, -\frac{1}{2}+y, \frac{1}{2}-z)$, with Br···Br separations of 3.73 (1) Å, slightly

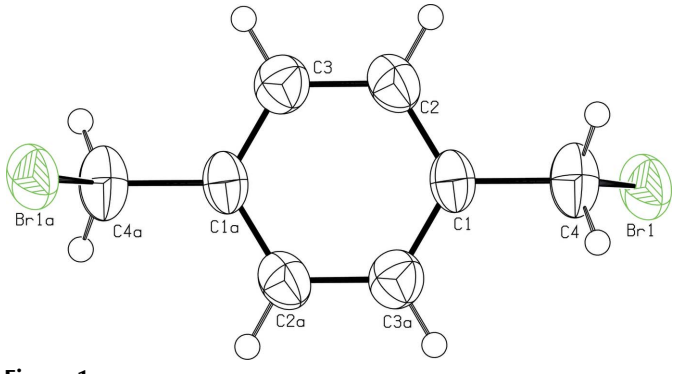


Figure 1
The molecular structure of (I), showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level. Atoms labelled with the suffix a are generated by the symmetry operator $(1-x, -y, -z)$.

longer than the sum of the van der Waals radii of Br (3.70 Å; Bondi, 1964). As a result, the crystal structure is two-dimensional, parallel to the (102) crystal plane (Fig. 2). No direction-specific interactions are observed between adjacent layers.

Experimental

The title compound was synthesized according to a reported procedure (Hoskins *et al.*, 1997*a*). Crystals suitable for X-ray analysis were formed within 2 d from a methanol solution (0.50 g in 20 ml) at 293 K.

Crystal data

$C_8H_8Br_2$
M_r = 263.96
Monoclinic, $P2_1/c$
a = 8.7424 (7) Å
b = 4.6275 (4) Å
c = 10.8189 (9) Å
β = 98.885 (1)°
V = 432.43 (6) Å^3
Z = 2
D_x = 2.027 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 9.30 mm^{-1}
T = 297 (2) K
Block, colourless
0.30 × 0.30 × 0.20 mm

Data collection

Bruker SMART APEX CCD area-detector diffractometer
0.3° wide ω exposures scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.082, T_{max} = 0.157
3213 measured reflections
848 independent reflections
712 reflections with $I > 2\sigma(I)$
R_{int} = 0.043
θ_{max} = 26.0°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.048
$wR(F^2)$ = 0.149
S = 1.06
848 reflections
46 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.1099P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.77 e Å^{-3}
$\Delta\rho_{min}$ = −0.85 e Å^{-3}

All H atoms were placed in geometrically idealized positions, with C—H = 0.93 (aromatic CH) or 0.97 Å (methylene CH_2). They were included in the refinement in the riding-model approximation, with $U_{iso}(H) = 1.2U_{eq}(C)$.

Data collection: *SMART* (Bruker, 2001); cell refinement: *SMART*; data reduction: *SAINT-Plus* (Bruker, 2001); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *PLATON* (Spek, 2003); software used to prepare material for publication: *PLATON*.

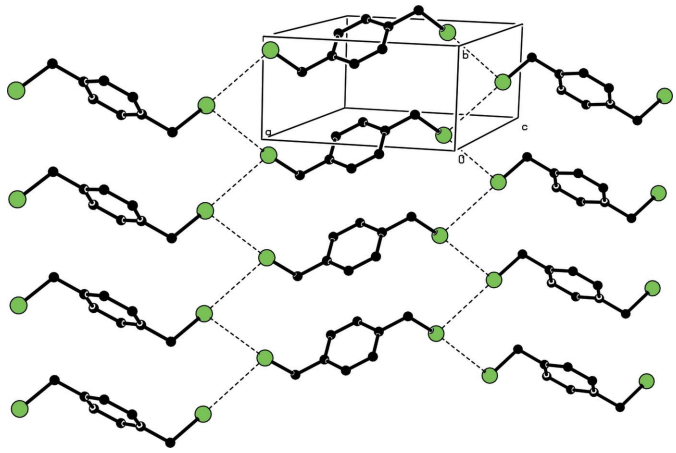


Figure 2
Part of the crystal structure of (I), showing the formation of a layer parallel to (102) through the Br···Br interactions (dashed lines). For the sake of clarity, H atoms have been omitted.

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