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1,2-Dibromo-4,5-bis(bromomethyl)benzene

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Key indicators

Single-crystal X-ray study
T = 292 K
Mean σ(C–C) = 0.007 Å
R factor = 0.042
wR factor = 0.106
Data-to-parameter ratio = 23.7

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

In the crystal structure of the title compound, $C_8H_6Br_4$, the packing of the molecules is mainly governed by an intermolecular π–π interaction.

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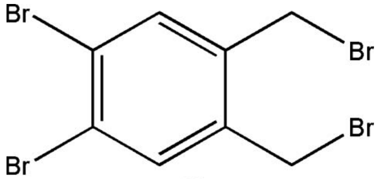
Comment

Apart from their intrinsic use as dyes and pigments, phthalocyanines show a number of special properties which account for the great research interest related to exciting future prospects (Leznoff & Lever, 1989). Furthermore, phthalocyanine compounds are of considerable interest because of their molecular stacking properties and because of their ability, when doped, to function as electronic conductors (Allcock & Neenan, 1986). The title compound, (I), is an important intermediate for preparation of phthalocyanines (Allcock & Neenan, 1986; Gürek *et al.*, 1991; Gümüs *et al.*, 1992). In this paper, we report the crystal structure of (I) (Fig. 1 and Table 1).



(I)

An intermolecular π–π interaction seems to be effective in stabilizing the crystal structure (Fig. 2). The centroid–centroid distance between adjacent benzene rings is 3.786 (3) Å and the interplanar distance is 3.546 (2) Å. There are no inter- or intramolecular hydrogen-bonding interactions.

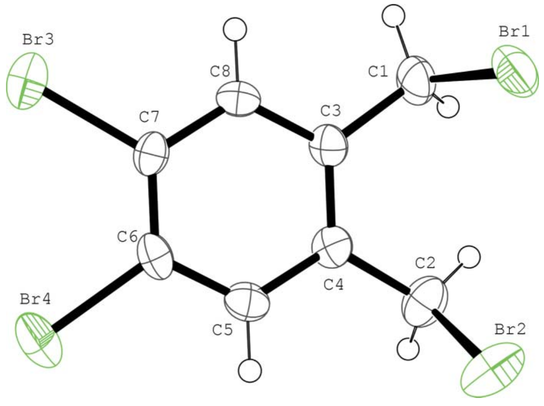


Figure 1
The molecular structure of (I), showing the atom-labeling scheme. Displacement ellipsoids are drawn at the 50% probability level.

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Experimental

The title compound was synthesized according to the procedure reported by Allcock & Neenan (1986). Crystals appropriate for X-ray diffraction were obtained by slow evaporation of a petroleum ether solution at 283 K.

Crystal data

$C_8H_6Br_4$
$M_r = 421.77$
Orthorhombic, *Pbca*
$a = 7.8798\ (10)$ Å
$b = 16.225\ (2)$ Å
$c = 16.894\ (2)$ Å
$V = 2159.8\ (5)$ Å^3
$Z = 8$
$D_x = 2.594$ Mg m^{-3}
Mo $K\alpha$ radiation
$\mu = 14.85$ mm^{-1}
$T = 292\ (2)$ K
Block, colorless
0.20 × 0.20 × 0.20 mm

Data collection

Bruker SMART 4K CCD area-detector diffractometer
φ and ω scans
Absorption correction: none
17417 measured reflections
2582 independent reflections
1619 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.081$
$\theta_{\rm max} = 28.0°$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.042$
$wR(F^2) = 0.107$
$S = 1.00$
2582 reflections
109 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0527P)^2]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\rm max} < 0.001$
$\Delta\rho_{\rm max} = 0.94$ e Å^{-3}
$\Delta\rho_{\rm min} = -1.16$ e Å^{-3}

Table 1
Selected bond lengths (Å).

Br1—C1	1.956 (6)	Br2—C2	1.954 (6)
Br3—C7	1.886 (5)	Br4—C6	1.887 (5)

H atoms were positioned geometrically [C—H = 0.93 (CH) and 0.97 Å (CH_2)] and constrained to ride on their parent atoms [$U_{\rm iso}$(H) = $1.2U_{\rm eq}$(C)]. The deepest hole is located 0.72 Å from atom Br1.

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINT* (Bruker, 2001); data reduction: *SAINT*; 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: *SHELXTL* (Sheldrick, 2001).

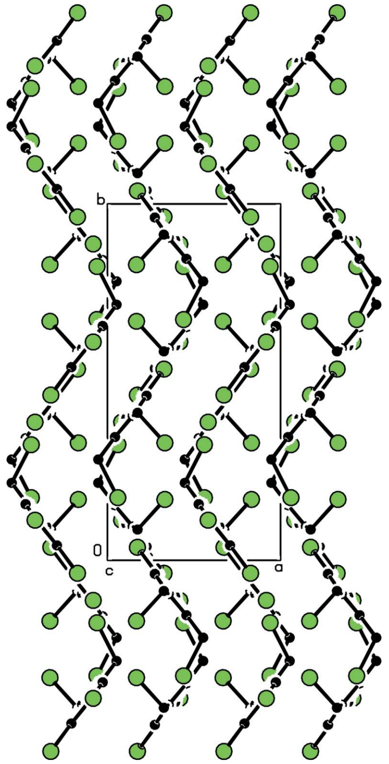

Figure 2
A packing diagram of (I), viewed along the *c* axis. H atoms have been omitted for clarity.

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