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1,3,5-Tris(*p*-bromophenyl)benzene

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Key indicators

Single-crystal X-ray study
T = 136 K
Mean σ(C–C) = 0.011 Å
R factor = 0.035
wR factor = 0.070
Data-to-parameter ratio = 13.3

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

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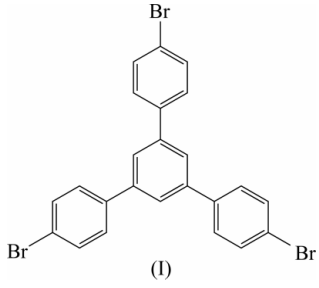
The title compound, $C_{24}H_{15}Br_3$, crystallizes in the orthorhombic space group $P2_12_12_1$ with three molecules in the asymmetric unit. The crystal was found to be inversion twinned and the appropriate twin law was applied, resulting in R_1 = 0.035 for the experimental data measured at T = 136 K.

Comment

Three molecules were found in the asymmetric unit of the title compound, (I). The three molecules are arranged in a slipped π-stacked fashion, with the central benzene ring of each molecule stacking over one of the outer phenyl rings of a neighboring molecule (see Fig. 2). The distances between the planes of the central benzene rings are approximately 3.53, 3.59 and 3.70 Å. Interplanar angles are given in Table 1 for the planes of the outer phenyl rings and the central benzene ring, for each molecule in the asymmetric unit. The most acute angle of each molecule is found with the terminal phenyl ring that is slipped π-stacked with respect to the central ring of a neighboring molecule.



(I)

There are close electrostatic interactions on the order of 2.9 Å between the Br and H atoms on neighboring molecules. The C_{Ph}—Br bond distances are consistent with those found in previously reported structures (average reported C—Br bond distance 1.94 Å). The C_{Ph}—C_{Ph} bond lengths are consistent with standard aromatic C—C distances.

Experimental

The title compound was prepared by addition of $SiCl_4$ to a solution of *p*-bromoacetophenone in absolute ethanol. Crystallization was achieved *via* slow evaporation of chloroform in a thin-walled Pyrex NMR tube.

Crystal data

$C_{24}H_{15}Br_3$
M_r = 543.09
Orthorhombic, $P2_12_12_1$
a = 14.4165 (3) Å
b = 18.9655 (4) Å
c = 21.9088 (2) Å
V = 5990.22 (19) Å^3
Z = 12
D_x = 1.807 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 6200 reflections
θ = 1.8–24.8°
μ = 6.07 mm^{-1}
T = 136 (2) K
Parallelepiped, colorless
0.37 × 0.17 × 0.07 mm

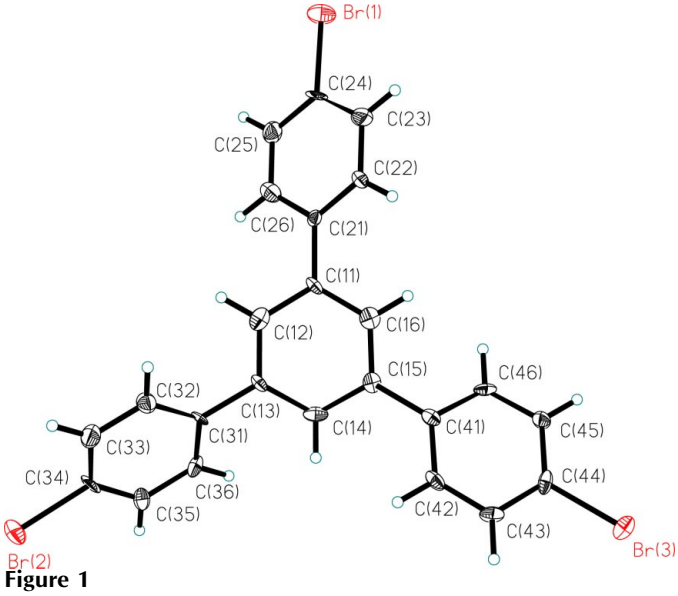


Figure 1
The molecular structure and atom-numbering scheme of the title compound. Displacement ellipsoids are shown at the 50% probability level.

Data collection

Siemens SMART CCD diffractometer
ω scans
Absorption correction: analytical (*XPREP*; Bruker, 2001)
T_{min} = 0.212, T_{max} = 0.669
26 670 measured reflections
9744 independent reflections
6390 reflections with $I > 2\sigma(I)$
R_{int} = 0.090
θ_{max} = 24.7°
$h = -10 \rightarrow 16$
$k = -20 \rightarrow 22$
$l = -25 \rightarrow 25$

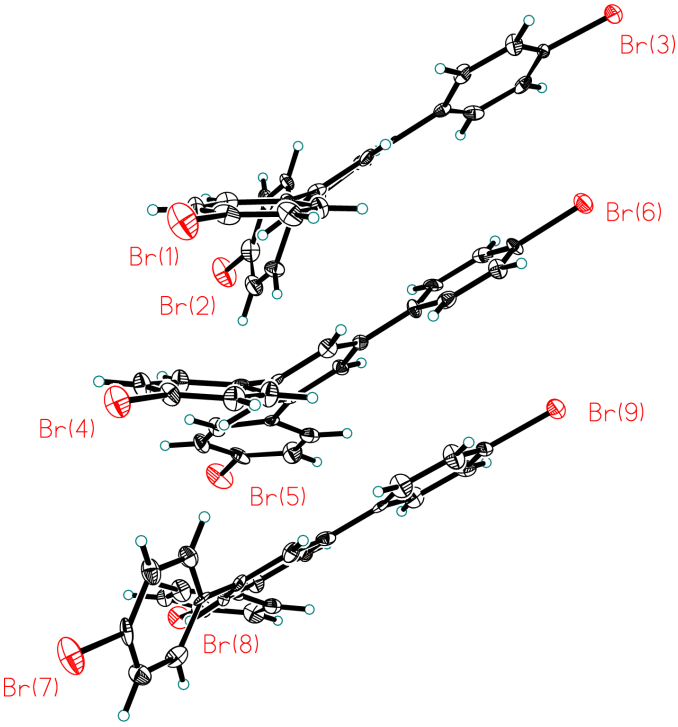


Figure 2
Elevation view of the asymmetric unit, demonstrating slipped π-stacking within the structure.

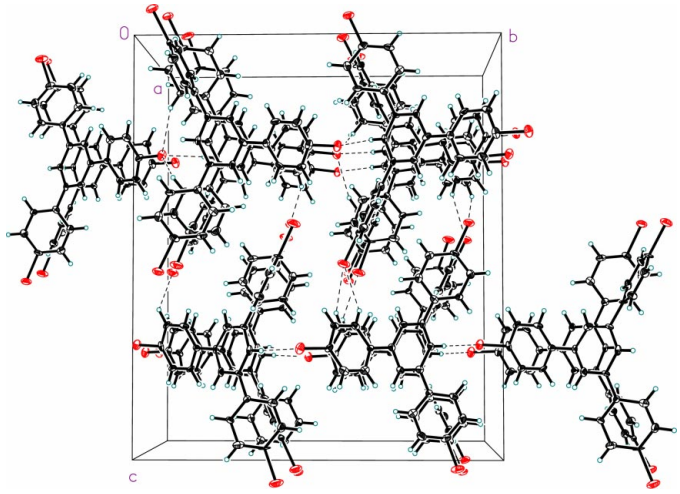


Figure 3
Packing diagram of the unit cell, showing the hydrogen-bond contacts.

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.035
$wR(F^2)$ = 0.070
S = 0.74
9744 reflections
731 parameters
H-atom parameters not refined
$w = 1/[\sigma^2(F_o^2) + (0.02P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.029
$\Delta\rho_{max}$ = 0.42 e Å^{-3}
$\Delta\rho_{min}$ = −0.56 e Å^{-3}
Absolute structure: Flack (1983), **4135 Friedel pairs [Please check]**
Flack parameter = **0.0 (3) [Please check]**

Table 1
Angles (°) between central and terminal phenyl rings in the three independent molecules of (I) **[Please supply s.u.'s for angles]**.

Molecule 1	Molecule 2	Molecule 3
35.77	40.11	45.92
42.86	30.52	36.35
21.30	24.08	4.74

A 52% inversion twin law [$\bar{1}00,0\bar{1}0,00\bar{1}$] was applied to the refinement in *SHELXTL* (Bruker, 2001). In addition, analytical face-indexed absorption corrections were applied to the reflection data. H atoms were included but not refined.

Data collection: *SMART* (Bruker, 1999); cell refinement: *SAINT* (Siemens, 1995); data reduction: *SAINT*; program(s) used to solve structure: *XS* in *SHELXTL* (Bruker, 2001); program(s) used to refine structure: *XL* in *SHELXTL*; molecular graphics: *SHELXTL*.

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