Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

9,10-Dibromotriptycene

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Key indicators

Single-crystal X-ray study
T = 167 K
Mean σ(C–C) = 0.009 Å
R factor = 0.042
wR factor = 0.054
Data-to-parameter ratio = 10.4

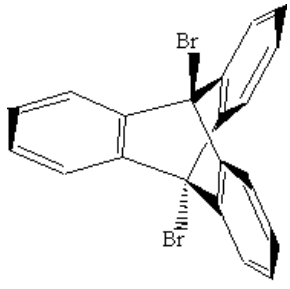
For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

Received 29 April 2004
Accepted 7 June 2004
Online 26 June 2004

The molecule of the title compound, $C_{20}H_{12}Br_2$, has high rigidity and approximate threefold symmetry, but no crystallographically imposed molecular symmetry.

Comment

9,10–Dibromotriptycene, (I), along with other dihalotriptycenes, can be used for further functionalization of triptycenes (Adcock & Iyer, 1988; Adcock *et al.*, 2001). The bond distances and angles in (I) are consistent with those reported in analogous mono- and di-substituted triptycenes. The C—Br distances, 1.933 (5) and 1.952 (5) Å, and the Br—C—C angles, ranging from 111.7 (4) to 113.3 (4)°, are similar to the corresponding values in 9-bromotriptycene (1.97 Å and 111.4°; Palmer & Templeton, 1968). The structure supports the conclusion that triptycene derivatives are highly symmetrical and rigid molecules. It is interesting to note that the molecule exhibits pseudo-threefold symmetry (as shown by the interplanar angles between the benzene rings: 123.7 (2), 121.5 (1), and 114.8 (2)°). Unlike 9-bromotriptycene, which crystallizes in $R\overline{3}$, it does not crystallize in a space group with threefold symmetry. Also, despite the largely aromatic nature of the molecule, no π-stacking is observed in the crystal structure.



(I)

Experimental

The title compound was prepared according to a previously published procedure (Bohm *et al.*, 1974). Pale yellow crystals were grown by sublimation of the crude product and characterized by mass spectrometry and NMR.

Crystal data

$C_{20}H_{12}Br_2$
M_r = 412.12
Monoclinic, $P2_1/a$
a = 8.0753 (8) Å
b = 13.698 (1) Å
c = 14.054 (1) Å
β = 92.639 (2)°
V = 1552.9 (3) Å^3
Z = 4
D_x = 1.763 Mg m^{-3}
Mo Kα radiation
Cell parameters from 1610 reflections
θ = 2.9–23.1°
μ = 5.23 mm^{-1}
T = 167.2 K
Parallelepiped, colorless
0.12 × 0.08 × 0.03 mm

 DOI: 10.1107/S1600536804013753

Data collection

Bruker SMART APEX CCD diffractometer
ω scans
Absorption correction: multi-scan (Blessing, 1995)
T_{min} = 0.683, T_{max} = 0.855
9101 measured reflections
3164 independent reflections
2073 reflections with $F^2 > 3\sigma(F^2)$
R_{int} = 0.021
θ_{max} = 26.4°
$h = -10 \rightarrow 6$
$k = -17 \rightarrow 17$
$l = -17 \rightarrow 17$

Refinement

Refinement on F
R = 0.042
wR = 0.054
S = 2.08
2073 reflections
199 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o) + 0.00022|F_o|^2]$
$(\Delta/\sigma)_{max}$ = 0.006
$\Delta\rho_{max}$ = 0.74 e Å^{-3}
$\Delta\rho_{min}$ = −0.33 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Br1—C1	1.952 (5)	C1—C15	1.519 (8)
Br2—C2	1.933 (5)	C2—C8	1.535 (8)
C1—C3	1.523 (8)	C2—C14	1.521 (7)
C1—C9	1.524 (8)	C2—C20	1.532 (7)
Br1—C1—C3	111.7 (4)	Br2—C2—C8	112.0 (4)
Br1—C1—C9	112.3 (4)	Br2—C2—C14	113.2 (4)
Br1—C1—C15	112.1 (4)	Br2—C2—C20	113.3 (4)
C3—C1—C9	106.6 (4)	C8—C2—C14	106.0 (4)
C3—C1—C15	106.8 (5)	C8—C2—C20	105.7 (4)
C9—C1—C15	107.1 (4)	C14—C2—C20	106.1 (4)

H atoms were positioned geometrically and refined as riding, with C—H = 0.95 Å and U_{iso}(H) = 1.2U_{eq}(C).

Data collection: *SMART* (Bruker, 2001–2003); cell refinement: *SAINT* (Bruker, 2003); data reduction: *SAINT*; program(s) used to solve structure: *SIR*92 (Altomare *et al.*, 1993); program(s) used to refine structure: *teXsan* (Molecular Structure Corporation & Rigaku Corporation, 1998); molecular graphics: *teXsan*; software used to prepare material for publication: *teXsan*.

The authors gratefully acknowledge Professor Kenneth N. Raymond, Dr. Frederick J. Hollander, and Dr. Allen G. Oliver for help with the crystal structure solution, and Steven S. Kaye for supplying the sample.

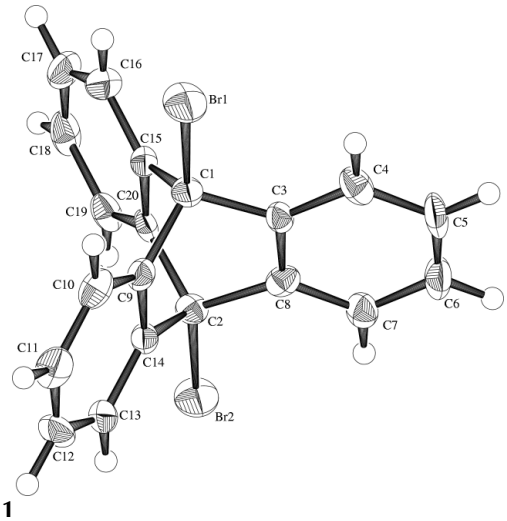


Figure 1
Molecular structure of the title compound, showing the atom-numbering scheme and 50% probability displacement ellipsoids for the non-H atoms.

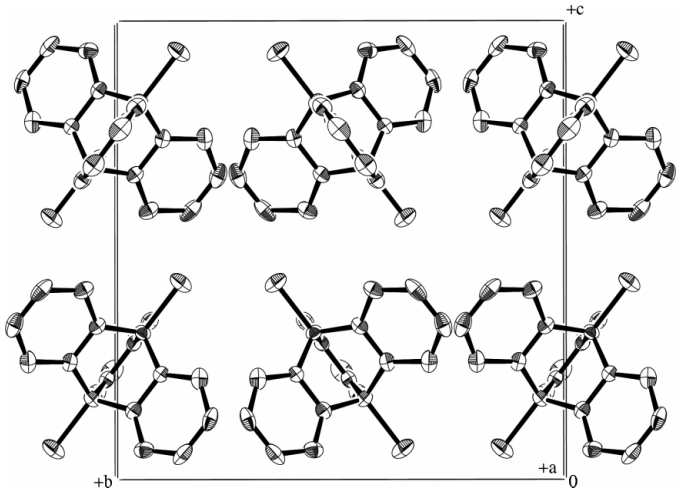


Figure 2
The unit-cell contents, projected down the *a* axis. H atoms have been omitted.

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