

**Rebecca J. Abergel and
 Mircea Dinca***

College of Chemistry, University of California,
 Berkeley, Berkeley, CA, 94720-1460, USA

Correspondence e-mail: mdinca@berkeley.edu

Key indicators

Single-crystal X-ray study
 T = 167 K
 Mean $\sigma(\text{C}-\text{C}) = 0.009 \text{ \AA}$
 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>.

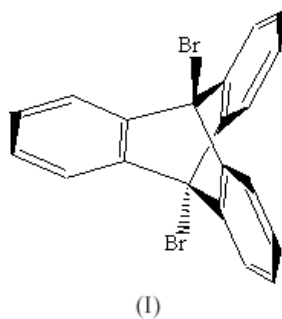
9,10-Dibromotriptycene

The molecule of the title compound, $\text{C}_{20}\text{H}_{12}\text{Br}_2$, has high rigidity and approximate threefold symmetry, but no crystallographically imposed molecular symmetry.

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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 $R\bar{3}$, 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.



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

$\text{C}_{20}\text{H}_{12}\text{Br}_2$
 $M_r = 412.12$
 Monoclinic, $P2_1/a$
 $a = 8.0753 (8) \text{ \AA}$
 $b = 13.698 (1) \text{ \AA}$
 $c = 14.054 (1) \text{ \AA}$
 $\beta = 92.639 (2)^\circ$
 $V = 1552.9 (3) \text{ \AA}^3$
 $Z = 4$

$D_x = 1.763 \text{ Mg m}^{-3}$
 Mo $K\alpha$ radiation
 Cell parameters from 1610 reflections
 $\theta = 2.9\text{--}23.1^\circ$
 $\mu = 5.23 \text{ mm}^{-1}$
 $T = 167.2 \text{ K}$
 Parallelepiped, colorless
 $0.12 \times 0.08 \times 0.03 \text{ mm}$

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 $F^2 > 3\sigma(F^2)$
 $R_{\text{int}} = 0.021$
 $\theta_{\text{max}} = 26.4^\circ$
 $h = -10 \rightarrow 6$
 $k = -17 \rightarrow 17$
 $l = -17 \rightarrow 17$

Refinement

Refinement on F
 $R = 0.042$
 $wR = 0.054$
 $S = 2.08$
2073 reflections
199 parameters

H-atom parameters constrained
 $w = 1/[\sigma^2(F_o) + 0.00022|F_o|^2]$
 $(\Delta/\sigma)_{\text{max}} = 0.006$
 $\Delta\rho_{\text{max}} = 0.74 \text{ e } \text{\AA}^{-3}$
 $\Delta\rho_{\text{min}} = -0.33 \text{ e } \text{\AA}^{-3}$

Table 1

Selected geometric parameters (\AA , $^\circ$).

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 \AA and $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$.

Data collection: *SMART* (Bruker, 2001–2003); cell refinement: *SAINTE* (Bruker, 2003); data reduction: *SAINTE*; program(s) used to solve structure: *SIR92* (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*.

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References

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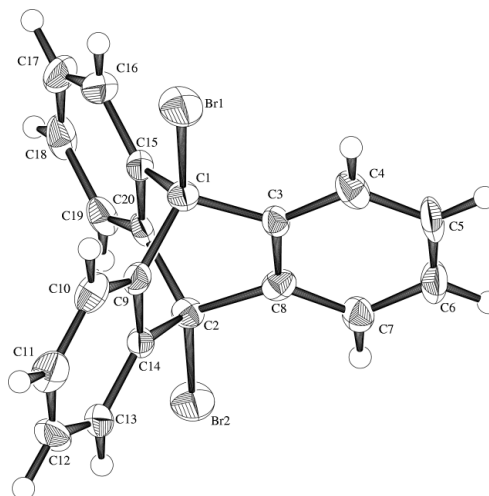


Figure 1

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

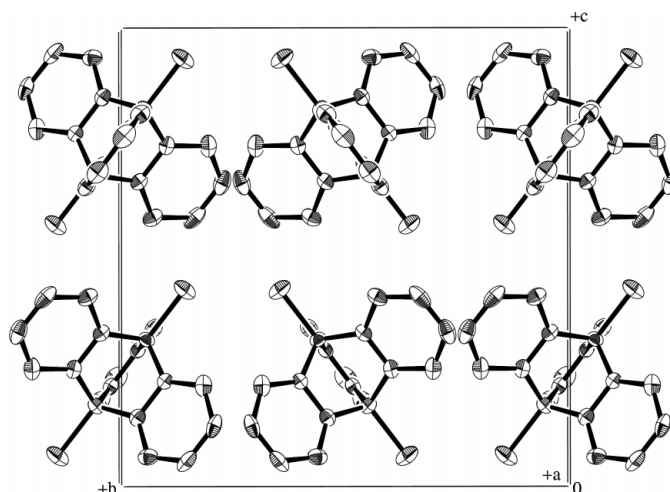


Figure 2

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

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