Acta Crystallographica Section E
Structure Reports
Online

ISSN 1600-5368

1,5-Dibromo-2,4-bis[(2-bromophenyl)ethynyl]benzene

Ian Westmoreland,* Lowell Miyagi and Emily L. Que

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

Correspondence e-mail:
westmoreland@berkeley.edu

Key indicators

Single-crystal X-ray study
T = 158 K
Mean σ(C–C) = 0.006 Å
R factor = 0.034
wR factor = 0.042
Data-to-parameter ratio = 11.8

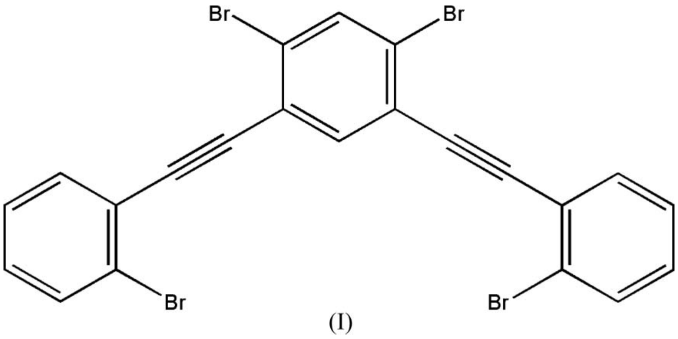
For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

In the title compound, $C_{22}H_{10}Br_4$, the two outer aromatic rings are offset from the plane occupied by the central ring.

Received 29 July 2005
Accepted 8 August 2005
Online 12 August 2005

Comment

The title compound, (I), is a synthetic precursor employed in the preparation of *syn*- and *anti* double-bent [5]phenylenes (Bong *et al.*, 2004). The latter compounds have unusual electronic properties which offer potential use as electroactive materials (Morikita *et al.*, 2001). As part of these synthetic studies, single crystals of (I) were isolated and an X-ray diffraction study undertaken to elucidate the molecular structure.



(I)

The three aromatic rings in (I) (Fig. 1) are not coplanar. The dihedral angle between ring 1 (atoms C1–C6) and the central ring 2 (C9–C15) is 28.10 (1)°, while that between ring 2 and ring 3 (C18–C23) is significantly greater, being 41.60 (2)° in the opposite direction. The dihedral angle between rings 1 and 3 is 64.81 (4)°.

The C—Br bond distances (Table 1) are all very similar, and fall within the range 1.88–1.89 Å expected for such linkages

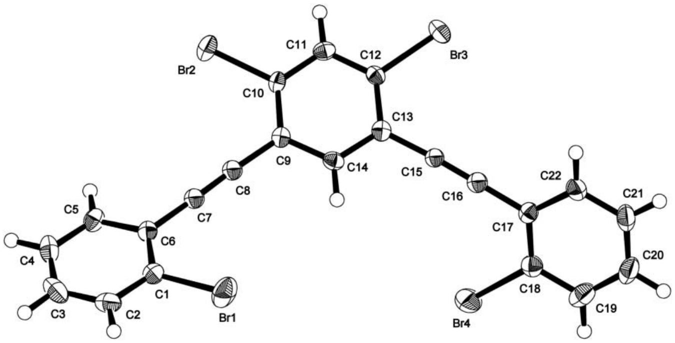


Figure 1
The structure of (I), with displacement ellipsoids drawn at the 50% probability level.

(Allen *et al.*, 1987). The C$\equiv$C triple bonds are both approximately 1.19 Å, while the connections between the Csp^2 atoms and their aromatic neighbors are between 1.43 and 1.45 Å. All these dimensions are in excellent agreement with previously reported examples (Allen *et al.*, 1987).

Experimental

Compound (I) was prepared as previously described (Bong *et al.*, 2004). Single crystals were obtained by slow evaporation of a saturated chloroform solution of (I) at room temperature.

Crystal data

$C_{22}H_{10}Br_4$
$M_r = 593.94$
Monoclinic, $P2_1/n$
$a = 10.0580$ (7) Å
$b = 8.8663$ (6) Å
$c = 21.870$ (2) Å
$\beta = 96.481$ (1)°
$V = 1937.8$ (3) Å^3
$Z = 4$

$D_x = 2.036$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 2451 reflections
$\theta = 2.3$–24.6°
$\mu = 8.34$ mm^{-1}
$T = 158$ K
Tablet, colorless
0.21 × 0.19 × 0.10 mm

Data collection

Bruker SMART 1000 diffractometer
ω scans
Absorption correction: multi-scan (Blessing, 1995)
$T_{\min} = 0.189$, $T_{\max} = 0.435$
8588 measured reflections

3198 independent reflections
2541 reflections with $F^2 > 3\sigma(F^2)$
$R_{\rm int} = 0.038$
$\theta_{\max} = 24.7°$
$h = -11 \rightarrow 11$
$k = -10 \rightarrow 10$
$l = -22 \rightarrow 25$

Refinement

Refinement on F
$R[F^2 > 2\sigma(F^2)] = 0.034$
$wR(F^2) = 0.042$
$S = 1.48$
2541 reflections
215 parameters

H-atom parameters constrained
$w = 1/[\sigma^2(F_o) + 0.00022|F_o|^2]$
$(\Delta/\sigma)_{\max} < 0.001$
$\Delta\rho_{\max} = 0.36$ e Å^{-3}
$\Delta\rho_{\min} = -0.64$ e Å^{-3}

Table 1
Selected bond lengths (Å).

Br1—C1	1.885 (5)	C7—C8	1.189 (6)
Br2—C10	1.887 (4)	C8—C9	1.449 (6)
Br3—C12	1.895 (4)	C13—C15	1.437 (6)
Br4—C18	1.882 (5)	C15—C16	1.193 (6)
C6—C7	1.438 (6)	C16—C17	1.433 (6)

H atoms were included in the riding-model approximation, with C—H = 0.97 Å and $U_{\rm iso}$(H) = 1.2$U_{\rm eq}$(C).

Data collection: *SMART* (Bruker, 1999); cell refinement: *SAINT* (Bruker, 2002); data reduction: *SAINT*; program(s) used to solve structure: *SIR92* (Altomare *et al.*, 1993); program(s) used to refine structure: *TEXSAN* (Molecular Structure Corporation and Rigaku, 1998); molecular graphics: *ORTEP3* (Farrugia, 1997); software used to prepare material for publication: *TEXSAN*.

The authors thank Dr Frederick J. Hollander and Dr Allen G. Oliver for their invaluable assistance, Professor Kenneth N. Raymond for theoretical instruction, and Ognjen Miljanic for providing crystals of the title compound.

References

Allen, F. H., Kennard, O., Watson, D. G., Brammer, L., Orpen, A. G. & Taylor, R. (1987). *J. Chem. Soc. Perkin Trans. 2*, pp. S1–19.

Altomare, A., Cascarano, G., Giacovazzo, C. & Guagliardi, A. (1993). *J. Appl. Cryst.* **26**, 343–350.

Blessing, R. H. (1995). *Acta Cryst.* A**51**, 33–38.

Bong, D. T.-Y., Chan, E. W. L., Diercks, R., Dosa, P. I., Haley, M. M., Matzger, A. J., Miljani, O., Vollhardt, K. P. C., Bond, A. D., Teat, S. J. & Stanger, A. (2004). *Org. Lett.* **6**, 2249–2252.

Bruker (1999). *SMART*. Version 5.054. Bruker AXS Inc., Madison, Wisconsin, USA.

Bruker (2002). *SAINT*. Version 6.40. Bruker AXS Inc., Madison, Wisconsin, USA.

Farrugia, L. J. (1997). *J. Appl. Cryst.* **30**, 565.

Molecular Structure Corporation & Rigaku. (1998). *TEXSAN*. MSC, 3200 Research Forest Drive, The Woodlands, TX 77381, USA, and Rigaku Corporation, 3-9-12 Akishima, Tokyo, Japan.

Morikita, T., Yamagudu, I. & Yamamoto, T. (2001). *Adv. Mater.* **13**, 1862–1864.

Acta Cryst. (2005). E**61**, o2894–o2895 Westmoreland *et al.* • $C_{22}H_{10}Br_4$ **o2895**