

2-Bromo-*p*-terphenylSuk-Hee Moon,<sup>a</sup> Heesook Yoon<sup>b</sup> and Youngjin Kang<sup>b\*</sup>

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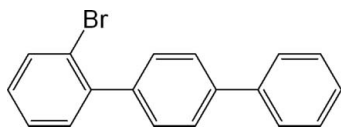
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Key indicators: single-crystal X-ray study;  $T = 293$  K; mean  $\sigma(\text{C}-\text{C}) = 0.004$  Å;  $R$  factor = 0.034;  $wR$  factor = 0.092; data-to-parameter ratio = 20.4.

In the title compound,  $\text{C}_{18}\text{H}_{13}\text{Br}$ , the dihedral angles between the mean planes of the central benzene ring and the mean planes of the outer phenyl and bromophenyl rings are  $33.47(8)$  and  $66.35(8)^\circ$ , respectively. In the crystal, weak  $\text{C}-\text{H}\cdots\pi$  and intermolecular  $\text{Br}\cdots\text{Br}$  [ $3.5503(15)$  Å] interactions contribute to the stabilization of the packing.

## Related literature

For the synthesis, see: France *et al.* (1938); Tadashi *et al.* (1962). For the Suzuki coupling reaction, see: Miyaura & Suzuki (1995). For cross-coupling reactions of *o*-halogenated arenes, see: Ishikawa & Manabe (2007). For organic light-emitting diodes, see: Kim *et al.* (2008). For related structures, see: Jones *et al.* (2005); Liang (2008); MacNeil & Decken (1999); Politzer *et al.* (2007).



## Experimental

## Crystal data

$\text{C}_{18}\text{H}_{13}\text{Br}$   $V = 2810(2)$  Å<sup>3</sup>  
 $M_r = 309.19$   $Z = 8$   
 Monoclinic,  $C2/c$  Mo  $K\alpha$  radiation  
 $a = 27.039(10)$  Å  $\mu = 2.91$  mm<sup>-1</sup>  
 $b = 7.597(3)$  Å  $T = 293$  K  
 $c = 18.907(7)$  Å  $0.30 \times 0.25 \times 0.20$  mm  
 $\beta = 133.650(5)^\circ$

## Data collection

Bruker SMART CCD area-detector 13933 measured reflections  
 diffractometer 3503 independent reflections  
 Absorption correction: multi-scan 2246 reflections with  $I > 2\sigma(I)$   
 (SADABS; Sheldrick, 1999)  $R_{\text{int}} = 0.028$   
 $T_{\text{min}} = 0.476$ ,  $T_{\text{max}} = 0.594$

## Refinement

$R[F^2 > 2\sigma(F^2)] = 0.034$  172 parameters  
 $wR(F^2) = 0.092$  H-atom parameters constrained  
 $S = 1.02$   $\Delta\rho_{\text{max}} = 0.43$  e Å<sup>-3</sup>  
 3503 reflections  $\Delta\rho_{\text{min}} = -0.65$  e Å<sup>-3</sup>

Table 1

C—H $\cdots\pi$  interactions (Å, °).

Cg2 and Cg3 are the centroids of the C7–C12 and C13–C18 rings, respectively.

D—H $\cdots$ A	D—H	H $\cdots$ A	D $\cdots$ A	D—H $\cdots$ A
C2—H2 $\cdots$ Cg3 <sup>i</sup>	0.93	2.84	3.778 (4)	148
C14—H14 $\cdots$ Cg2 <sup>ii</sup>	0.93	2.97	3.658 (5)	147

Symmetry codes: (i)  $x + \frac{1}{2}, -y + \frac{1}{2}, z + \frac{1}{2}$ ; (ii)  $-x + 1, y, -z + \frac{1}{2}$ .

Data collection: SMART (Bruker, 2000); cell refinement: SAINT-Plus (Bruker, 2000); data reduction: SAINT-Plus; program(s) used to solve structure: SHELXS97 (Sheldrick, 2008); program(s) used to refine structure: SHELXL97 (Sheldrick, 2008); molecular graphics: SHELXTL (Sheldrick, 2008); software used to prepare material for publication: SHELXTL.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: JJ2023).

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**supplementary materials**

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## 2-Bromo-*p*-terphenyl

S.-H. Moon, H. Yoon and Y. Kang

### Comment

Palladium-catalyzed cross-coupling reactions of aryl halides with arylboronic acids, often referred as Suzuki coupling reactions, are versatile synthetic methods for the preparation of unsymmetrical biaryls. The Suzuki coupling reactions have been applied extensively in the synthesis of natural products, nucleoside analogues, and pharmaceuticals (Miyaura & Suzuki, 1995). Cross-coupling reactions of *o*-halogenated arenes are very useful synthetically, if the halogen atom is converted to other functional groups, such as carbazole, anthracene and fluorene (Ishikawa & Manabe, 2007). Anthracene based terphenyl derivatives are widely used as emitting and/or host materials in organic light-emitting diodes (OLEDs) (Kim *et al.*, 2008). To be good host materials in OLEDs, the host must have larger energy gap between the HOMO (Highest Occupied Molecular Orbital) and the LUMO (Lowest Unoccupied Molecular orbital) than in a dopant, because energy transfer occurs from host to dopant.

The introduction of substituents at the *ortho*-position of biaryl and terphenyl groups is often used in the preparation of an efficient host with a wide band gap, because the substituents suppress effective  $\pi$ -conjugation throughout the whole molecule. Therefore, the structures of biaryl and terphenyl derivatives bearing a halogen atom at the *ortho*-position are attractive as good precursors to materials oriented chemists and physicists. The title compound, C<sub>18</sub>H<sub>13</sub>Br(I), was synthesized by the Pd-catalyzed cross coupling of 4-biphenylboronic acid with 1-bromo-2-iodobenzene in the presence of base (Na<sub>2</sub>CO<sub>3</sub>).

The dihedral angles between the mean planes of the central phenyl ring (C7-C12) and the mean planes of the outer phenyl (C13-C18) and the brominated phenyl (C1-C6) rings, are 33.47 (8)° and 66.35 (8)°, respectively (Fig. 1). All bond lengths and bond angles are normal and comparable to those observed in similar structures (MacNeil & Decken, 1999; Jones *et al.*, 2005).

Weak C–H...Cg  $\pi$ -ring interactions are observed [C2–H2...Cg3; H2...Cg3 =  $\text{\AA}$ ; C2–H2...Cg = 148°, C2...Cg3–H2 = 3.778 (4)  $\text{\AA}$ ; 1/2+x, 1/2-y, 1/2+z and C14–H14...Cg2; H14...Cg2 = 2.97  $\text{\AA}$ ; C14–H14...Cg2 = 147°, C14...Cg2–H14 = 3.658 (5)  $\text{\AA}$ ; 1-x, y, 1/2-z; where Cg2 and Cg3 are the centroids of C7—C12 and C13—C18, respectively] (Fig. 2). Weak Br1...Br1 interactions also exist (3.5503 (15)  $\text{\AA}$ ; Politzer *et al.*, 2007; Liang, 2008) and along with C–H...Cg  $\pi$ -ring interactions contribute to the stabilization of crystal packing.

### Experimental

A mixture of 4-biphenylboronic acid (0.1 mol), 1-bromo-2-iodobenzene (0.1 mol), Na<sub>2</sub>CO<sub>3</sub> (0.6 mol, 2M in H<sub>2</sub>O), and Pd(PPh<sub>3</sub>)<sub>4</sub> (5% mol) was refluxed for 12 h. After being cooled to room temperature, the reaction mixture was quenched by water. The aqueous layer was extracted with CH<sub>2</sub>Cl<sub>2</sub>, and the combined organic layers were sequentially washed with saturated aqueous NaCl (20 mL), dried with MgSO<sub>4</sub>, filtered, and concentrated under reduced pressure. The residue was purified by silica gel column chromatography using CH<sub>2</sub>Cl<sub>2</sub> and hexane to give the titled compound as a colorless solid.

# supplementary materials

Analytical data (France, *et al.*, 1938; Tadashi, *et al.*, 1962).  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , 300 MHz): 7.65 (m, 5H), 7.51 (m, 4H), 7.40 (m, 3H), 7.21 (m, 1H); MS(EI,  $m/z$ ): 309 [ $\text{M}^+$ ]. Slow evaporation of  $\text{CH}_2\text{Cl}_2$  gave suitable single crystals for X-ray analysis.

## Refinement

All H-atoms were positioned geometrically and refined using a riding model with  $\text{C-H} = 0.93 \text{ \AA}$ , and with  $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$ .

## Figures

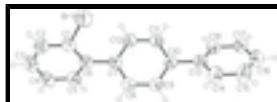


Fig. 1. Molecular structure of the title compound, showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level.



Fig. 2. Weak  $\text{Br}\cdots\text{Br}$  and  $\text{C-H}\cdots\text{Cg}$   $\pi$ -ring interactions (dashed lines) in the title compound.

## 2-Bromo-*p*-terphenyl

### Crystal data

$\text{C}_{18}\text{H}_{13}\text{Br}$

$M_r = 309.19$

Monoclinic,  $C2/c$

Hall symbol:  $-C\ 2yc$

$a = 27.039 (10) \text{ \AA}$

$b = 7.597 (3) \text{ \AA}$

$c = 18.907 (7) \text{ \AA}$

$\beta = 133.650 (5)^\circ$

$V = 2810 (2) \text{ \AA}^3$

$Z = 8$

$F(000) = 1248$

$D_x = 1.462 \text{ Mg m}^{-3}$

Mo  $K\alpha$  radiation,  $\lambda = 0.71073 \text{ \AA}$

Cell parameters from 3654 reflections

$\theta = 2.1\text{--}28.4^\circ$

$\mu = 2.91 \text{ mm}^{-1}$

$T = 293 \text{ K}$

Block, colorless

$0.30 \times 0.25 \times 0.20 \text{ mm}$

### Data collection

Bruker SMART CCD area-detector diffractometer

3503 independent reflections

Radiation source: fine-focus sealed tube graphite

2246 reflections with  $I > 2\sigma(I)$

$\varphi$  and  $\omega$  scans

$R_{\text{int}} = 0.028$

$\theta_{\text{max}} = 28.4^\circ$ ,  $\theta_{\text{min}} = 2.1^\circ$

Absorption correction: multi-scan (SADABS; Sheldrick, 1999)

$h = -34\text{--}36$

$T_{\text{min}} = 0.476$ ,  $T_{\text{max}} = 0.594$

$k = -9\text{--}10$

13933 measured reflections

$l = -25 \rightarrow 25$

*Refinement*

Refinement on  $F^2$

Primary atom site location: structure-invariant direct methods

Least-squares matrix: full

Secondary atom site location: difference Fourier map

$R[F^2 > 2\sigma(F^2)] = 0.034$

Hydrogen site location: inferred from neighbouring sites

$wR(F^2) = 0.092$

H-atom parameters constrained

$S = 1.02$

$w = 1/[\sigma^2(F_o^2) + (0.0341P)^2 + 2.6031P]$

where  $P = (F_o^2 + 2F_c^2)/3$

3503 reflections

$(\Delta/\sigma)_{\max} = 0.001$

172 parameters

$\Delta\rho_{\max} = 0.43 \text{ e } \text{\AA}^{-3}$

0 restraints

$\Delta\rho_{\min} = -0.65 \text{ e } \text{\AA}^{-3}$

*Special details*

**Geometry.** All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

**Refinement.** Refinement of  $F^2$  against ALL reflections. The weighted  $R$ -factor  $wR$  and goodness of fit  $S$  are based on  $F^2$ , conventional  $R$ -factors  $R$  are based on  $F$ , with  $F$  set to zero for negative  $F^2$ . The threshold expression of  $F^2 > \sigma(F^2)$  is used only for calculating  $R$ -factors(gt) etc. and is not relevant to the choice of reflections for refinement.  $R$ -factors based on  $F^2$  are statistically about twice as large as those based on  $F$ , and  $R$ -factors based on ALL data will be even larger.

*Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters ( $\text{\AA}^2$ )*

	$x$	$y$	$z$	$U_{\text{iso}}^*/U_{\text{eq}}$
Br1	0.721104 (15)	0.25216 (4)	0.56047 (2)	0.07170 (13)
C1	0.69010 (12)	0.4341 (3)	0.59063 (16)	0.0458 (5)
C2	0.73645 (13)	0.5631 (3)	0.65377 (18)	0.0565 (6)
H2	0.7807	0.5590	0.6797	0.068*
C3	0.71685 (15)	0.6982 (3)	0.67834 (19)	0.0613 (7)
H3	0.7478	0.7861	0.7210	0.074*
C4	0.65143 (16)	0.7030 (3)	0.6398 (2)	0.0616 (7)
H4	0.6384	0.7930	0.6575	0.074*
C5	0.60498 (13)	0.5756 (3)	0.57514 (18)	0.0552 (6)
H5	0.5606	0.5819	0.5489	0.066*
C6	0.62281 (11)	0.4369 (3)	0.54788 (15)	0.0434 (5)
C7	0.57071 (12)	0.3039 (3)	0.47552 (17)	0.0446 (5)
C8	0.51546 (12)	0.3516 (3)	0.37957 (17)	0.0519 (6)
H8	0.5104	0.4684	0.3609	0.062*
C9	0.46779 (12)	0.2289 (3)	0.31111 (18)	0.0522 (6)
H9	0.4310	0.2648	0.2472	0.063*
C10	0.47356 (11)	0.0529 (3)	0.33573 (16)	0.0441 (5)

## supplementary materials

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C11	0.52859 (12)	0.0067 (3)	0.43275 (16)	0.0520 (6)
H11	0.5334	-0.1097	0.4519	0.062*
C12	0.57609 (13)	0.1291 (3)	0.50101 (17)	0.0524 (6)
H12	0.6124	0.0940	0.5653	0.063*
C13	0.42539 (11)	-0.0832 (3)	0.26121 (16)	0.0453 (5)
C14	0.39663 (13)	-0.0664 (4)	0.16585 (18)	0.0592 (6)
H14	0.4062	0.0328	0.1483	0.071*
C15	0.35413 (16)	-0.1948 (4)	0.0972 (2)	0.0730 (8)
H15	0.3359	-0.1824	0.0340	0.088*
C16	0.33855 (14)	-0.3410 (4)	0.1214 (2)	0.0703 (8)
H16	0.3098	-0.4273	0.0749	0.084*
C17	0.36580 (13)	-0.3588 (3)	0.2151 (2)	0.0598 (7)
H17	0.3550	-0.4569	0.2316	0.072*
C18	0.40904 (13)	-0.2318 (3)	0.28455 (19)	0.0519 (6)
H18	0.4275	-0.2457	0.3477	0.062*

### Atomic displacement parameters ( $\text{\AA}^2$ )

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
Br1	0.0723 (2)	0.0729 (2)	0.0885 (2)	0.00301 (14)	0.0625 (2)	-0.01335 (15)
C1	0.0545 (14)	0.0446 (12)	0.0456 (13)	0.0024 (11)	0.0373 (12)	0.0014 (10)
C2	0.0533 (14)	0.0587 (15)	0.0542 (14)	-0.0045 (12)	0.0358 (13)	0.0008 (12)
C3	0.0735 (19)	0.0519 (14)	0.0538 (16)	-0.0128 (13)	0.0421 (15)	-0.0089 (12)
C4	0.085 (2)	0.0461 (14)	0.0686 (17)	0.0016 (13)	0.0585 (17)	-0.0044 (12)
C5	0.0604 (15)	0.0474 (14)	0.0635 (16)	0.0056 (12)	0.0449 (14)	0.0019 (12)
C6	0.0498 (13)	0.0417 (12)	0.0408 (12)	0.0028 (10)	0.0320 (11)	0.0049 (9)
C7	0.0478 (13)	0.0444 (12)	0.0457 (13)	0.0023 (10)	0.0338 (12)	0.0007 (10)
C8	0.0521 (14)	0.0397 (13)	0.0531 (15)	0.0063 (11)	0.0322 (13)	0.0065 (11)
C9	0.0461 (13)	0.0519 (15)	0.0438 (13)	0.0079 (11)	0.0254 (11)	0.0078 (11)
C10	0.0424 (12)	0.0472 (12)	0.0451 (12)	0.0016 (10)	0.0312 (11)	0.0007 (10)
C11	0.0570 (15)	0.0439 (13)	0.0462 (14)	0.0000 (11)	0.0323 (13)	0.0063 (11)
C12	0.0528 (14)	0.0498 (14)	0.0406 (12)	-0.0006 (11)	0.0270 (12)	0.0044 (11)
C13	0.0404 (12)	0.0480 (13)	0.0467 (13)	0.0030 (10)	0.0298 (11)	0.0010 (10)
C14	0.0581 (15)	0.0671 (17)	0.0520 (15)	-0.0102 (13)	0.0378 (13)	-0.0029 (13)
C15	0.0733 (19)	0.085 (2)	0.0504 (16)	-0.0171 (16)	0.0388 (16)	-0.0123 (15)
C16	0.0628 (18)	0.0634 (18)	0.0646 (19)	-0.0129 (14)	0.0363 (16)	-0.0165 (14)
C17	0.0541 (15)	0.0479 (14)	0.0654 (17)	-0.0005 (12)	0.0367 (14)	0.0014 (13)
C18	0.0493 (13)	0.0500 (14)	0.0504 (14)	0.0041 (11)	0.0322 (12)	0.0047 (11)

### Geometric parameters ( $\text{\AA}$ , $^\circ$ )

Br1—C1	1.897 (2)	C9—H9	0.9300
C1—C2	1.375 (3)	C10—C11	1.391 (3)
C1—C6	1.391 (3)	C10—C13	1.489 (3)
C2—C3	1.375 (4)	C11—C12	1.376 (3)
C2—H2	0.9300	C11—H11	0.9300
C3—C4	1.372 (4)	C12—H12	0.9300
C3—H3	0.9300	C13—C18	1.390 (3)
C4—C5	1.374 (4)	C13—C14	1.391 (3)

C4—H4	0.9300	C14—C15	1.378 (4)
C5—C6	1.397 (3)	C14—H14	0.9300
C5—H5	0.9300	C15—C16	1.374 (4)
C6—C7	1.489 (3)	C15—H15	0.9300
C7—C8	1.383 (3)	C16—C17	1.377 (4)
C7—C12	1.386 (3)	C16—H16	0.9300
C8—C9	1.379 (3)	C17—C18	1.380 (3)
C8—H8	0.9300	C17—H17	0.9300
C9—C10	1.389 (3)	C18—H18	0.9300
C2—C1—C6	122.4 (2)	C9—C10—C11	117.1 (2)
C2—C1—Br1	116.95 (18)	C9—C10—C13	121.9 (2)
C6—C1—Br1	120.61 (17)	C11—C10—C13	120.9 (2)
C3—C2—C1	119.5 (2)	C12—C11—C10	121.5 (2)
C3—C2—H2	120.2	C12—C11—H11	119.2
C1—C2—H2	120.2	C10—C11—H11	119.2
C4—C3—C2	119.8 (2)	C11—C12—C7	121.1 (2)
C4—C3—H3	120.1	C11—C12—H12	119.5
C2—C3—H3	120.1	C7—C12—H12	119.5
C3—C4—C5	120.4 (2)	C18—C13—C14	118.1 (2)
C3—C4—H4	119.8	C18—C13—C10	121.7 (2)
C5—C4—H4	119.8	C14—C13—C10	120.2 (2)
C4—C5—C6	121.5 (2)	C15—C14—C13	120.8 (3)
C4—C5—H5	119.2	C15—C14—H14	119.6
C6—C5—H5	119.2	C13—C14—H14	119.6
C1—C6—C5	116.3 (2)	C16—C15—C14	120.4 (3)
C1—C6—C7	123.5 (2)	C16—C15—H15	119.8
C5—C6—C7	120.2 (2)	C14—C15—H15	119.8
C8—C7—C12	117.8 (2)	C15—C16—C17	119.6 (3)
C8—C7—C6	120.5 (2)	C15—C16—H16	120.2
C12—C7—C6	121.7 (2)	C17—C16—H16	120.2
C9—C8—C7	121.2 (2)	C16—C17—C18	120.4 (3)
C9—C8—H8	119.4	C16—C17—H17	119.8
C7—C8—H8	119.4	C18—C17—H17	119.8
C8—C9—C10	121.3 (2)	C17—C18—C13	120.8 (2)
C8—C9—H9	119.3	C17—C18—H18	119.6
C10—C9—H9	119.3	C13—C18—H18	119.6
C6—C1—C2—C3	1.8 (4)	C8—C9—C10—C13	-175.5 (2)
Br1—C1—C2—C3	-179.94 (19)	C9—C10—C11—C12	-1.3 (3)
C1—C2—C3—C4	0.0 (4)	C13—C10—C11—C12	175.5 (2)
C2—C3—C4—C5	-1.4 (4)	C10—C11—C12—C7	0.2 (4)
C3—C4—C5—C6	1.0 (4)	C8—C7—C12—C11	1.0 (4)
C2—C1—C6—C5	-2.2 (3)	C6—C7—C12—C11	-178.2 (2)
Br1—C1—C6—C5	179.65 (16)	C9—C10—C13—C18	-149.7 (2)
C2—C1—C6—C7	176.8 (2)	C11—C10—C13—C18	33.6 (3)
Br1—C1—C6—C7	-1.4 (3)	C9—C10—C13—C14	31.9 (3)
C4—C5—C6—C1	0.8 (3)	C11—C10—C13—C14	-144.8 (2)
C4—C5—C6—C7	-178.2 (2)	C18—C13—C14—C15	-1.1 (4)
C1—C6—C7—C8	-113.1 (3)	C10—C13—C14—C15	177.4 (3)

## supplementary materials

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C5—C6—C7—C8	65.9 (3)	C13—C14—C15—C16	1.0 (5)
C1—C6—C7—C12	66.1 (3)	C14—C15—C16—C17	-0.1 (5)
C5—C6—C7—C12	-115.0 (3)	C15—C16—C17—C18	-0.7 (4)
C12—C7—C8—C9	-0.9 (4)	C16—C17—C18—C13	0.6 (4)
C6—C7—C8—C9	178.2 (2)	C14—C13—C18—C17	0.3 (3)
C7—C8—C9—C10	-0.3 (4)	C10—C13—C18—C17	-178.2 (2)
C8—C9—C10—C11	1.4 (4)		

### Hydrogen-bond geometry ( $\text{\AA}$ , $^\circ$ )

Cg2 and Cg3 are the centroids of the C7—C12 and C13—C18 rings, respectively.

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
C2—H2 $\cdots$ Cg3 <sup>i</sup>	0.93	2.84	3.778 (4)	148
C14—H14 $\cdots$ Cg2 <sup>ii</sup>	0.93	2.97	3.658 (5)	147

Symmetry codes: (i)  $x+1/2, -y+1/2, z+1/2$ ; (ii)  $-x+1, y, -z+1/2$ .



Fig. 1

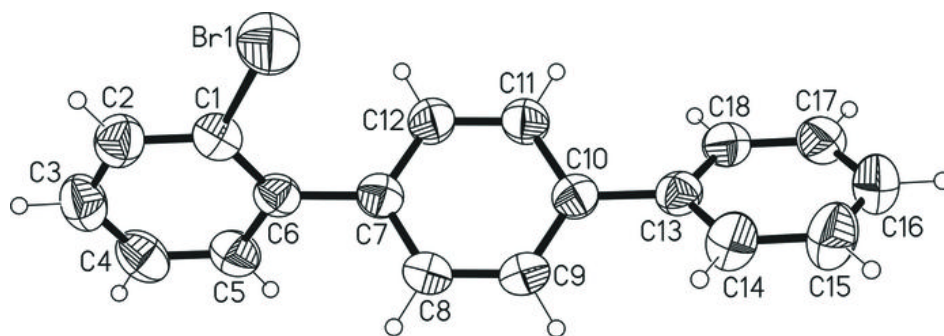


Fig. 2

