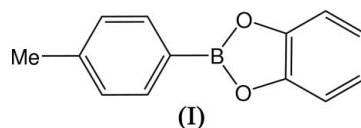


2-(*p*-Tolyl)-1,3,2-benzodioxaboroleGeorge Bramham,<sup>a</sup> Andrei S. Batsanov,<sup>b\*</sup> Todd B. Marder<sup>b</sup> and Nicholas C. Norman<sup>a</sup><sup>a</sup>School of Chemistry, University of Bristol, Bristol BS8 1TS, England, and <sup>b</sup>Department of Chemistry, University of Durham, South Road, Durham DH1 3LE, EnglandCorrespondence e-mail:  
a.s.batsanov@durham.ac.ukThe title molecule, C<sub>13</sub>H<sub>11</sub>BO<sub>2</sub>, adopts a planar conformation and a stack/herringbone packing motif in the solid state.Received 31 January 2006  
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## Comment

Compound (I) was obtained *via* cobalt-mediated borylation of 4-iodotoluene, observed during our studies of the synthesis and reactivity of cobalt boryl complexes (Dai *et al.*, 1996; Adams *et al.*, 2006).

The asymmetric unit comprises one molecule (Fig. 1), which is nearly planar (r.m.s. deviation for all non-H atoms 0.057 Å), like its prototype 2-phenyl-1,3,2-benzodioxaborole (Zettler *et al.*, 1974). The B atom is trigonal-planar; its coordination plane is inclined by 2.9 (1)° to the catechol arene ring (i) and by 3.7 (1)° to the tolyl arene ring (ii). Molecules related *via* the *b* translation form a stack with a mean interplanar separation of 3.52 (5) Å. Stacks are packed in a herringbone motif, in which planes of adjacent molecules are nearly perpendicular [dihedral angle 89.7 (1)°].

## Key indicators

Single-crystal X-ray study  
T = 120 K  
Mean  $\sigma$ (C–C) = 0.002 Å  
R factor = 0.040  
wR factor = 0.128  
Data-to-parameter ratio = 13.2For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>.

## Experimental

To a stirred light-yellow solution of [Co(PMe<sub>3</sub>)<sub>3</sub>(BO<sub>2</sub>C<sub>6</sub>H<sub>4</sub>)<sub>2</sub>] (Dai *et al.*, 1996) (0.110 g, 0.21 mmol) in hexane (2.0 ml), 4-iodotoluene (0.054 g, 0.25 mmol) was added at room temperature, resulting in a brown solution. After heating at 343 K overnight, the mixture became pink in colour. The solvent was then removed *in vacuo* and the residues were redissolved in THF (10 ml) to which was added excess CoCl<sub>2</sub>. The mixture was stirred for a further 15 min before being reduced to dryness *in vacuo*. The residues were then extracted with hexane and the resulting solution was concentrated *in vacuo*, during which a colourless solid appeared. This was redissolved by gentle heating, after which the solution was cooled slowly to give colourless crystals of (I) (0.015 g). <sup>11</sup>B NMR:  $\delta$  31.9. EI-MS *m/z* 210 (*M*<sup>+</sup>).

## Crystal data

C<sub>13</sub>H<sub>11</sub>BO<sub>2</sub>  
*M<sub>r</sub>* = 210.03  
Monoclinic, *P*2<sub>1</sub>/*c*  
*a* = 17.7405 (10) Å  
*b* = 4.9935 (4) Å  
*c* = 12.3989 (16) Å  
 $\beta$  = 100.80 (1)°  
*V* = 1078.93 (17) Å<sup>3</sup>  
*Z* = 4*D<sub>x</sub>* = 1.293 Mg m<sup>-3</sup>  
Mo *K*α radiation  
Cell parameters from 687 reflections  
 $\theta$  = 10.3–24.0°  
 $\mu$  = 0.09 mm<sup>-1</sup>  
*T* = 120 (2) K  
Plate, colourless  
0.22 × 0.15 × 0.05 mm

*Data collection*

Bruker SMART 6000 CCD area-  
detector diffractometer  
 $\omega$  scans  
Absorption correction: none  
9171 measured reflections  
2486 independent reflections

1654 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.071$   
 $\theta_{\text{max}} = 27.5^\circ$   
 $h = -23 \rightarrow 17$   
 $k = -6 \rightarrow 6$   
 $l = -16 \rightarrow 16$

*Refinement*

Refinement on  $F^2$   
 $R[F^2 > 2\sigma(F^2)] = 0.040$   
 $wR(F^2) = 0.128$   
 $S = 1.02$   
2486 reflections  
189 parameters

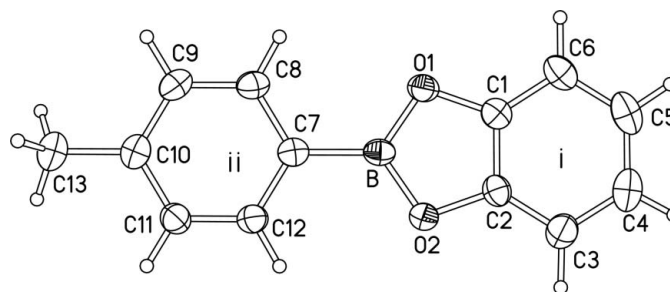
All H-atom parameters refined  
 $w = 1/[\sigma^2(F_o^2) + (0.0681P)^2]$   
where  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta/\sigma)_{\text{max}} < 0.001$   
 $\Delta\rho_{\text{max}} = 0.25 \text{ e } \text{\AA}^{-3}$   
 $\Delta\rho_{\text{min}} = -0.19 \text{ e } \text{\AA}^{-3}$

**Table 1**Selected geometric parameters ( $\text{\AA}$ ,  $^\circ$ ).

O1–C1	1.384 (2)	O2–B	1.393 (2)
O1–B	1.389 (2)	C7–B	1.533 (2)
O2–C2	1.384 (2)		
O1–B–O2	111.00 (14)	O2–B–C7	124.66 (13)
O1–B–C7	124.33 (14)		
O1–B–C7–C8	–3.0 (2)	O2–B–C7–C12	–3.4 (2)

All H atoms were refined isotropically, yielding the following distances:  $Csp^3-H = 0.98$  (2) to  $1.01$  (2)  $\text{\AA}$  and  $Csp^2-H = 0.95$  (2) to  $1.00$  (2)  $\text{\AA}$ .

Data collection: *SMART* (Bruker, 2001); cell refinement: *SMART*; data reduction: *SAINT* (Bruker, 2001); program(s) used to solve structure: *SHELXTL* (Bruker, 2001); program(s) used to refine

**Figure 1**

Molecular structure of (I). Atomic displacement ellipsoids are drawn at the 50% probability level.

structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

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