Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

2-(*p*-Tolyl)-1,3,2-benzodioxaborole

George Bramham,[a] Andrei S. Batsanov,[b]* Todd B. Marder[b] and Nicholas C. Norman[a]

[a]School of Chemistry, University of Bristol, Bristol BS8 1TS, England, and [b]Department of Chemistry, University of Durham, South Road, Durham DH1 3LE, England

Correspondence e-mail: a.s.batsanov@durham.ac.uk

Key indicators

Single-crystal X-ray study
T = 120 K
Mean σ(C–C) = 0.002 Å
R factor = 0.040
wR factor = 0.128
Data-to-parameter ratio = 13.2

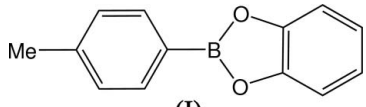
For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

Received 31 January 2006
Accepted 2 February 2006

The title molecule, $C_{13}H_{11}BO_2$, adopts a planar conformation and a stack/herringbone packing motif in the solid state.

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).



(I)

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)°].

Experimental

To a stirred light-yellow solution of $[Co(PMe_3)_3(BO_2C_6H_4)_2]$ (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 $CoCl_2$. 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). ^{11}B NMR: δ 31.9. EI–MS *m*/*z* 210 (M^+).

Crystal data

$C_{13}H_{11}BO_2$
M_r = 210.03
Monoclinic, $P2_1/c$
a = 17.7405 (10) Å
b = 4.9935 (4) Å
c = 12.3989 (16) Å
β = 100.80 (1)°
V = 1078.93 (17) Å^3
Z = 4
D_x = 1.293 Mg m^{-3}
Mo *Kα* radiation
Cell parameters from 687 reflections
θ = 10.3–24.0°
μ = 0.09 mm^{-1}
T = 120 (2) K
Plate, colourless
0.22 × 0.15 × 0.05 mm

Data collection

Bruker SMART 6000 CCD area-detector diffractometer	1654 reflections with $I > 2\sigma(I)$
	$R_{int} = 0.071$
ω scans	$\theta_{max} = 27.5^\circ$
Absorption correction: none	$h = -23 \rightarrow 17$
9171 measured reflections	$k = -6 \rightarrow 6$
2486 independent reflections	$l = -16 \rightarrow 16$

Refinement

Refinement on F^2	All H-atom parameters refined
$R[F^2 > 2\sigma(F^2)] = 0.040$	$w = 1/[\sigma^2(F_o^2) + (0.0681P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.128$	
$S = 1.02$	$(\Delta/\sigma)_{max} < 0.001$
2486 reflections	$\Delta\rho_{max} = 0.25$ e Å^{-3}
189 parameters	$\Delta\rho_{min} = -0.19$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

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) Å and Csp^2—H = 0.95 (2) to 1.00 (2) Å.

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

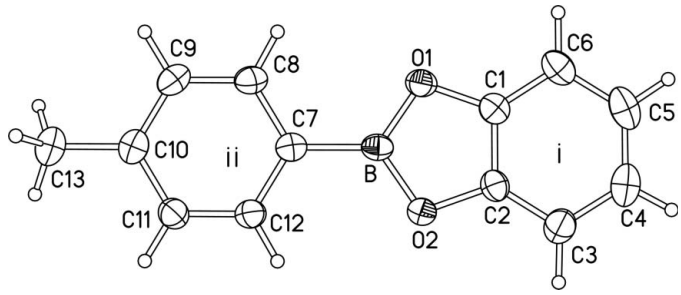


Figure 1
Molecular structure of (I). Atomic displacement ellipsoids are drawn at the 50% probability level.

The authors thank the EPSRC for financial support and Frontier Scientific Inc. for generous gifts of diborane(4) compounds.

References

Adams, C. J., Baber, R. A., Batsanov, A. S., Bramham, G., Charmant, J. P. H., Haddow, M. F., Howard, J. A. K., Lam, W. H., Lin, Z. Y., Marder, T. B., Norman, N. C. & Orpen, A. G. (2006). *Dalton Trans.* In the press (DOI 10 1039/b516594f).

Bruker (2001). *SMART* (Version 5.625), *SAINT* (Version 6.02A) and *SHELXTL* (Version 6.12). Bruker AXS Inc., Madison, Wisconsin, USA.

Dai, C. Y., Stringer, G., Corrigan, J. F., Taylor, N. J., Marder, T. B. & Norman, N. C. (1996). *J. Organomet. Chem.* **513**, 273–275.

Zettler, F., Hausen, H. D. & Hess, H. (1974). *Acta Cryst.* B**30**, 1876–1878.