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# A sulfanilamide derivative containing a boronate ester group

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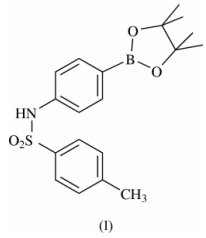
**Key indicators**

Single-crystal X-ray study
$T$ = 173 K
Mean $\sigma$(C–C) = 0.003 Å
$R$ factor = 0.040
$wR$ factor = 0.102
Data-to-parameter ratio = 12.4

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

A sulfanilamide derivative containing a boronate ester group, namely *N*-[4-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)-phenyl]-*p*-toluenesulfonamide, $C_{19}H_{24}BNO_4S$, crystallizes in the triclinic space group $P\overline{1}$. The Lewis-acid B atom lies in a trigonal planar environment where the OBO plane is roughly coplanar with the aromatic ring. No significant secondary intermolecular interactions are observed.




(I)

## Experimental

The title compound was prepared by addition of 4-(4,4,5,5-tetramethyl-[1,3,2]dioxaborolan-2-yl)phenylamine (200 mg, 0.91 mmol) in methylene chloride (3 ml) to a stirred solution of *p*-toluenesulfonyl chloride (86 mg, 0.45 mmol) in $CH_2Cl_2$ (3 ml). The reaction was heated at reflux for 18 h. Extraction with $CH_2Cl_2$ (3 × 5 ml) from water (10 ml) followed by removal of the solvent under vacuum afforded the desired compound as an off-white solid (yield 104 mg, 62%).

*Crystal data*

$C_{19}H_{24}BNO_4S$
$M_r$ = 373.26
Triclinic, $P\overline{1}$
$a$ = 6.6990 (10) Å
$b$ = 9.4253 (15) Å
$c$ = 16.492 (3) Å
$\alpha$ = 106.227 (2)°
$\beta$ = 91.189 (2)°
$\gamma$ = 105.430 (2)°
$V$ = 958.7 (3) Å$^3$
$Z$ = 2
$D_x$ = 1.293 Mg m$^{-3}$
Mo $K\alpha$ radiation
Cell parameters from 3627 reflections
$\theta$ = 2.3–25.2°
$\mu$ = 0.19 mm$^{-1}$
$T$ = 173 (2) K
Block, colourless
0.45 × 0.40 × 0.40 mm

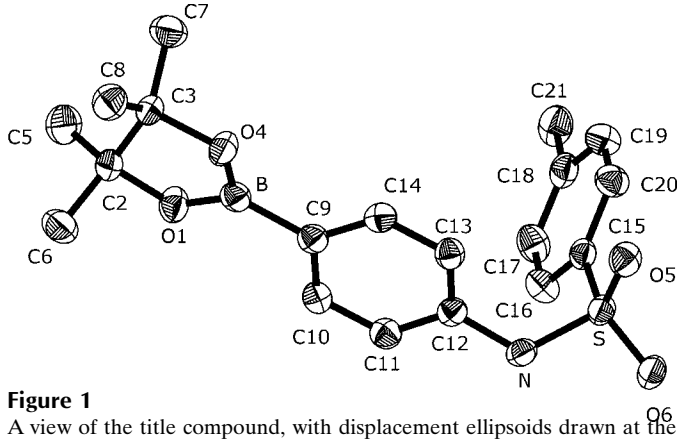



**Figure 1**
A view of the title compound, with displacement ellipsoids drawn at the 30% probability level. H atoms have been omitted for clarity.

*Data collection*

| | |
|---|---|
| Bruker *P*4/SMART 1000 diffractometer | 2829 reflections with $I > 2\sigma(I)$ |
| $\omega$ and $\varphi$ scans | $R_{int} = 0.019$ |
| Absorption correction: none | $\theta_{max} = 25.0^\circ$ |
| 4525 measured reflections | $h = -7 \rightarrow 7$ |
| 2986 independent reflections | $k = -11 \rightarrow 10$ |
| | $l = -19 \rightarrow 19$ |

*Refinement*

| | |
|---|---|
| Refinement on $F^2$ | $w = 1/[\sigma^2(F_o^2) + (0.0406P)^2 + 0.7629P]$ where $P = (F_o^2 + 2F_c^2)/3$ |
| $R[F^2 > 2\sigma(F^2)] = 0.040$ | |
| $wR(F^2) = 0.102$ | |
| $S = 1.05$ | $(\Delta/\sigma)_{max} < 0.001$ |
| 2986 reflections | $\Delta\rho_{max} = 0.40$ e Å$^{-3}$ |
| 240 parameters | $\Delta\rho_{min} = -0.25$ e Å$^{-3}$ |
| H-atom parameters constrained | |

All H atoms were placed in idealized positions and refined as riding, with C—H = 0.95–0.98 Å and N—H = 0.88 Å, and with $U_{iso}$(H) = 1.2–1.5$U_{eq}$ of the parent atom.

Data collection: *SMART* (Bruker, 1997–1999); cell refinement: *SMART*; data reduction: *SAINT* (Bruker, 1997–1999); program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *SHELXTL* (Sheldrick, 1997); software used to prepare material for publication: *SHELXTL*.

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## References

Bruker (1997–1999). *SMART*. Version 5.059. SAINT 6.02. Bruker AXS Inc., Madison, Wisconsin, USA.

Sheldrick, G. M. (1997). *SHELXS*97, *SHELXL*97 and *SHELXTL* (Version 5.1). University of Göttingen, Germany.