



the C4–C5–C10 angle is larger. The conformational isomerism is also reflected in the behaviour of the boronic acid groups. In molecule *A*, the boronic acid group is rotated more with respect to the ring, as seen from the O2A–B1A–C4A–C5A torsion angle [94.82 (12)°]; in *B*, the boronic acid group displays a corresponding O2B–B1B–C4B–C9B torsion angle of –71.88 (13)°. Such flexible behaviour of a boronic acid group was found in other *ortho*-substituted arylboronic acids (Gainsford *et al.*, 1995; Ganguly *et al.*, 2003) but not for the closely related 2-formylphenylboronic acid (Scouten *et al.*, 1994), where the planar conformation is stabilized by an intramolecular hydrogen bond. Another difference is the conformation within B(OH)<sub>2</sub> groups, reflecting a specific crystal packing imposed by intermolecular hydrogen bonding. In molecule *A*, both OH bonds are *syn*-directed with respect to the ring, whereas in *B* they exhibit a *syn-anti* orientation.

The crystal packing diagram for (I), showing the effect of mirror symmetry, is depicted in Fig. 2. There are three classical O–H...O hydrogen bonds (the geometry and symmetry codes are given Table 2); the strongest hydrogen bonds, O3B–H3B...O11B<sup>iii</sup>, are formed between molecules *B* (motif *a* in Fig. 2) (Etter, 1990; Bernstein *et al.*, 1995), producing a centrosymmetric dimer [*R*<sub>2</sub><sup>2</sup>(14) graph-set descriptor]. Furthermore, molecules *B* are linked with one another by O2B–H2B...O3B<sup>ii</sup> hydrogen bonds between B(OH)<sub>2</sub> groups (motif *b*), forming centrosymmetric dimers [*R*<sub>2</sub><sup>2</sup>(8) rings] typical of arylboronic acids (Rettig & Trotter, 1977). Molecules *A* are linked to boronic acid O atoms of two adjacent molecules *B* by an O2A–H2A...O2B bridge [motif *c*, *D*<sub>2</sub><sup>2</sup>(7) graph-set descriptor]. The second-level motif *N*<sub>2</sub>(*ab*) = *C*<sub>2</sub><sup>2</sup>(9)[*R*<sub>4</sub><sup>4</sup>(20)] depicts a characteristic infinite chain of alternating fused rings. Other chains are represented by binary motifs *N*<sub>2</sub>(*ac*) = *C*<sub>3</sub><sup>3</sup>(15) and *N*<sub>2</sub>(*bc*) = *C*<sub>3</sub><sup>3</sup>(10). The hydrogen-bond network produces an infinite two-dimensional structure, where a larger ring depicted by the third-level graph-set descriptor *N*<sub>3</sub>(*abc*) = *C*<sub>4</sub><sup>4</sup>(15)[*R*<sub>8</sub><sup>8</sup>(30)] can be distinguished.

## Experimental

Compound (I) was obtained from Aldrich. Crystals of (I) suitable for single-crystal X-ray diffraction analysis were grown by slow evaporation of a saturated solution in ethyl acetate/toluene (1:1) (m.p. 375–377 K).

### Crystal data

C <sub>8</sub> H <sub>9</sub> BO <sub>4</sub>	Z = 6
<i>M</i> <sub>r</sub> = 179.96	<i>D</i> <sub>x</sub> = 1.389 Mg m <sup>-3</sup>
Monoclinic, <i>P</i> <sub>2</sub> <sub>1</sub> / <i>m</i>	Mo <i>K</i> α radiation
<i>a</i> = 8.2764 (2) Å	<i>μ</i> = 0.11 mm <sup>-1</sup>
<i>b</i> = 19.7124 (6) Å	<i>T</i> = 100 (2) K
<i>c</i> = 8.7321 (3) Å	Prism, colourless
<i>β</i> = 115.007 (3)°	0.46 × 0.32 × 0.21 mm
<i>V</i> = 1291.07 (7) Å <sup>3</sup>	

### Data collection

Oxford Diffraction KM-4 CCD diffractometer	23407 measured reflections
<i>ω</i> scans	3268 independent reflections
Absorption correction: multi-scan ( <i>CrysAlis RED</i> ; Oxford Diffraction, 2005)	2797 reflections with <i>I</i> > 2σ( <i>I</i> )
<i>T</i> <sub>min</sub> = 0.96, <i>T</i> <sub>max</sub> = 0.98	<i>R</i> <sub>int</sub> = 0.012
	<i>θ</i> <sub>max</sub> = 28.6°

### Refinement

Refinement on <i>F</i> <sup>2</sup>	<i>w</i> = 1/[σ <sup>2</sup> ( <i>F</i> <sub>o</sub> <sup>2</sup> ) + (0.0537 <i>P</i> ) <sup>2</sup> + 0.2342 <i>P</i> ]
<i>R</i> [ <i>F</i> <sup>2</sup> > 2σ( <i>F</i> <sup>2</sup> )] = 0.033	where <i>P</i> = ( <i>F</i> <sub>o</sub> <sup>2</sup> + 2 <i>F</i> <sub>c</sub> <sup>2</sup> )/3
<i>wR</i> ( <i>F</i> <sup>2</sup> ) = 0.094	(Δ/ <i>σ</i> ) <sub>max</sub> = 0.001
<i>S</i> = 1.12	Δ <i>ρ</i> <sub>max</sub> = 0.53 e Å <sup>-3</sup>
3268 reflections	Δ <i>ρ</i> <sub>min</sub> = –0.26 e Å <sup>-3</sup>
252 parameters	
All H-atom parameters refined	

Table 1

Selected geometric parameters (Å, °).

B1A–O2A <sup>i</sup>	1.3616 (11)	B1B–O3B	1.3677 (14)
B1A–C4A	1.592 (2)	B1B–C4B	1.5823 (15)
C5A–C10A	1.502 (2)	C5B–C10B	1.4825 (14)
C10A–O11A	1.1951 (17)	C10B–O11B	1.2204 (12)
C10A–O12A	1.3344 (17)	C10B–O12B	1.3280 (12)
B1B–O2B	1.3610 (13)		
O2A <sup>i</sup> –B1A–O2A	116.34 (12)	O2B–B1B–O3B	118.63 (9)
O2A <sup>i</sup> –B1A–C4A	121.50 (6)	O2B–B1B–C4B	118.41 (9)
C9A–C4A–B1A	119.48 (12)	O3B–B1B–C4B	122.67 (9)
C5A–C4A–B1A	123.59 (12)	C5B–C4B–B1B	122.76 (9)
C6A–C5A–C10A	120.73 (12)	C6B–C5B–C10B	117.27 (9)
C4A–C5A–C10A	117.65 (12)	C4B–C5B–C10B	121.05 (9)
O11A–C10A–O12A	124.97 (14)	O11B–C10B–O12B	122.72 (9)
O11A–C10A–C5A	123.66 (13)	O11B–C10B–C5B	124.87 (9)
O12A–C10A–C5A	111.37 (12)	O12B–C10B–C5B	112.42 (8)
		O2A–B1A–C4A–C9A	85.18 (12)
		O2A <sup>i</sup> –B1A–C4A–C5A	94.82 (12)
		B1B–C4B–C5B–C10B	–1.63 (15)
		C6B–C5B–C10B–O11B	–17.14 (15)
		C4B–C5B–C10B–O11B	165.22 (10)
		C6B–C5B–C10B–O12B	163.00 (9)
		O11B–C10B–O12B–C13B	–3.24 (14)

Symmetry code: (i) *x*, –*y* +  $\frac{1}{2}$ , *z*.

Table 2

Hydrogen-bond geometry (Å, °).

<i>D</i> –H... <i>A</i>	<i>D</i> –H	H... <i>A</i>	<i>D</i> ... <i>A</i>	<i>D</i> –H... <i>A</i>
O2A–H2A...O2B	0.883 (17)	1.901 (17)	2.7835 (11)	177.8 (16)
O2B–H2B...O3B <sup>ii</sup>	0.880 (19)	1.870 (19)	2.7451 (11)	172.8 (18)
O3B–H3B...O11B <sup>iii</sup>	0.858 (19)	1.87 (2)	2.7187 (11)	172.6 (18)

Symmetry codes: (ii) –*x* + 1, –*y*, –*z*; (iii) –*x* + 1, –*y*, –*z* + 1.

All H atoms were located in difference syntheses and refined freely [C–H = 0.931 (19)–0.996 (14) Å].

Data collection: *CrysAlis CCD* (Oxford Diffraction, 2005); cell refinement: *CrysAlis RED* (Oxford Diffraction, 2005); data reduction: *CrysAlis RED*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1990); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *DIAMOND* (Brandenburg, 1999); software used to prepare material for publication: *SHELXTL97*.

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Supplementary data for this paper are available from the IUCr electronic archives (Reference: JZ3006). Services for accessing these data are described at the back of the journal.

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