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Key indicators

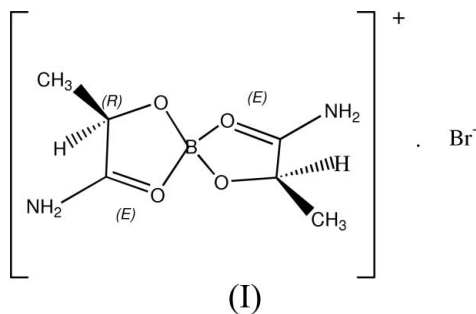
Single-crystal X-ray study
 $T = 293$ K
Mean $\sigma(\text{C}-\text{C}) = 0.008$ Å
 R factor = 0.032
 wR factor = 0.084
Data-to-parameter ratio = 11.4For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>.Bis[(*R*)-lactamido- $\kappa^2\text{O},\text{O}'$]boron(III) bromide

The title compound, $\text{C}_6\text{H}_{12}\text{BN}_2\text{O}_4^+\cdot\text{Br}^-$, contains one monomeric tetracoordinated boron complex cation, $[\text{B}(\text{C}_3\text{H}_6\text{NO}_2)_2]^+$, and one Br^- anion. The B coordination occurs *via* the amide and oxide O atoms [average B—O = 1.535 (6) and 1.415 (7) Å, respectively] and may be described as a distorted tetrahedral arrangement, with O—B—O angles in the range 104.2 (4)–116.8 (4)°. In the crystal structure, the cations and anions are linked by N—H \cdots Br and N—H \cdots O hydrogen bonds, generating a three-dimensional network.

Received 19 March 2007
Accepted 4 June 2007

Comment

Following our work on metal–amide crystalline complexes (Bekaert *et al.*, 2002*a,b*, 2003), we recently reported a new zinc complex with 2-hydroxypropanamide (lactamide), a bidentate ligand (Bekaert *et al.*, 2005). In the $[\text{Zn}(\text{lactamide})_3]^{2+}$ cation, the Zn atom, coordinated in a bidentate fashion *via* amide and oxide atoms O of each ligand, presents similar Zn—O bond lengths [2.074 (6) Å]. We now report a new boron complex, (I), with lactamide.



Compound (I) (Fig. 1) contains one monomeric four-coordinate boron complex cation, $[\text{B}(\text{C}_3\text{H}_6\text{NO}_2)_2]^+$, and one Br^- anion. The B atom is surrounded by two *R*-lactamide ligands, coordinated in a bidentate fashion *via* amide atom O1 (or O4) and oxide atom O2 (or O5). The B coordination may be described as a distorted tetrahedral arrangement with O—B—O angles in the range 104.2 (4)–116.8 (4)°. The two B—O (amide) distances are similar [average 1.535 (6) Å]. In the same way, the two B—O (oxide) distances are similar [average 1.415 (7) Å]; this difference can be explained by the ionic character of the B—O2 and B—O5 bonds. Among the two possible coordination modes (*N,O* or *O,O*) in metal complexes with lactamide or its derivatives described in the literature, the title compound presents an *O,O* mode like that described in the $[\text{Zn}(\text{lactamide})_3]^{2+}$ cation (Bekaert *et al.*, 2005).

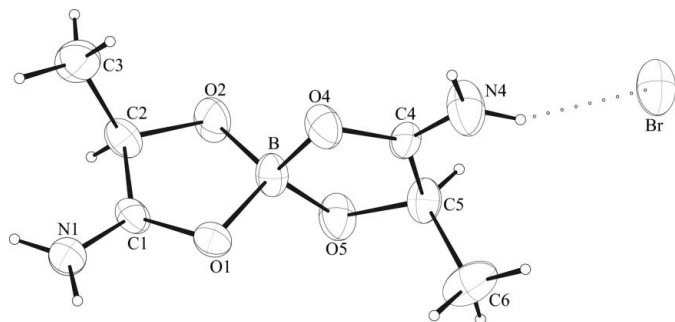


Figure 1
Perspective view of the asymmetric unit, showing atomic numbering. Displacement ellipsoids are shown at the 50% probability level for non-H atoms. The dotted line represents a hydrogen bond.

In the crystal structure, the individual complex cations are linked into chains running parallel to the *a* axis by inter-ion $\text{N}-\text{H}\cdots\text{Br}$ hydrogen bonds (Table 2 and Fig. 2). Such chains are crosslinked *via* the H1A(N1) atom, forming inter-cation $\text{N}-\text{H}\cdots\text{O}$ bonds with oxide atom O2. The crystal packing is completed by a further $\text{N}-\text{H}\cdots\text{Br}$ hydrogen bond.

Experimental

The title compound was prepared as follows. Boron tribromide (0.1 ml, 1.04 mmol) was dissolved in dry dichloromethane (10 ml) and carefully added to a solution of 2-hydroxypropanamide (0.200 g, 2.1 mmol) in dichloromethane (10 ml). The temperature rose, followed by the formation of a white precipitate. The white precipitate was rapidly filtered off and redissolved in boiling ethanol (5 ml). This solution was kept at 313 K for a week. Colourless needles slowly appeared in the solution; they were suitable for X-ray diffraction.

Crystal data

$\text{C}_6\text{H}_{12}\text{BN}_2\text{O}_4^+\cdot\text{Br}^-$	$\gamma = 116.858 (3)^\circ$
$M_r = 266.89$	$V = 281.99 (3) \text{ \AA}^3$
Triclinic, <i>P</i> 1	$Z = 1$
$a = 5.5806 (3) \text{ \AA}$	Mo $K\alpha$ radiation
$b = 6.0026 (4) \text{ \AA}$	$\mu = 3.64 \text{ mm}^{-1}$
$c = 9.7951 (6) \text{ \AA}$	$T = 293 (2) \text{ K}$
$\alpha = 98.823 (3)^\circ$	$0.35 \times 0.30 \times 0.10 \text{ mm}$
$\beta = 97.302 (4)^\circ$	

Data collection

Nonius KappaCCD diffractometer	2416 measured reflections
Absorption correction: multi-scan (SADABS; Sheldrick, 1996; Blessing, 1995)	1461 independent reflections
$T_{\min} = 0.235$, $T_{\max} = 0.560$	1452 reflections with $I > 2\sigma(I)$
(expected range = 0.292–0.695)	$R_{\text{int}} = 0.037$
	$\theta_{\text{max}} = 23.3^\circ$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.032$	$\Delta\rho_{\text{max}} = 0.54 \text{ e \AA}^{-3}$
$wR(F^2) = 0.084$	$\Delta\rho_{\text{min}} = -0.41 \text{ e \AA}^{-3}$
$S = 1.04$	Absolute structure: Flack (1983),
1461 reflections	654 Friedel pairs
128 parameters	Flack parameter: $-0.016 (10)$
H-atom parameters constrained	

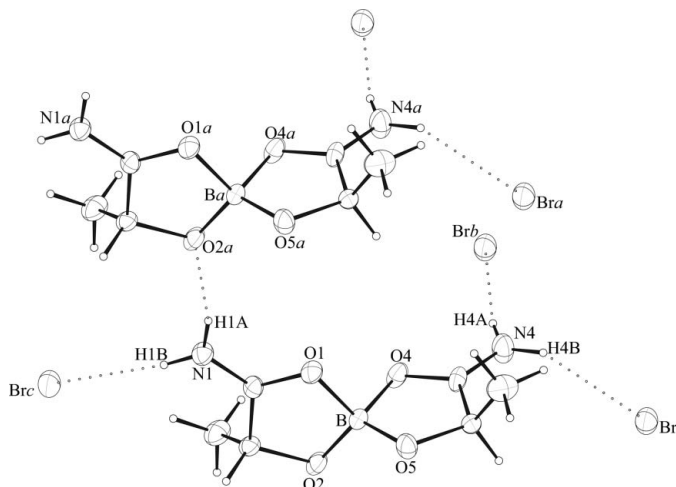


Figure 2
A view showing part of the $\text{N}-\text{H}\cdots\text{Br}$ and $\text{N}-\text{H}\cdots\text{O}$ hydrogen-bond network (dotted lines) in the title compound. Displacement ellipsoids are shown at the 30% probability level for non-H atoms. The suffixes denote atoms at the following equivalent positions: *a* ($x + 1, y + 1, z$), *b* ($x + 1, y, z$) and *c* ($x + 2, y + 1, z + 1$).

Table 1

Selected geometric parameters (\AA , $^\circ$).

B1—O5	1.405 (7)	O2—C2	1.408 (7)
B1—O2	1.425 (7)	C2—C3	1.506 (8)
B1—O4	1.534 (6)	O4—C4	1.286 (7)
B1—O1	1.536 (6)	N4—C4	1.282 (8)
O1—C1	1.275 (6)	C4—C5	1.512 (8)
N1—C1	1.289 (6)	O5—C5	1.418 (6)
C1—C2	1.514 (7)	C5—C6	1.489 (8)
O5—B1—O2	116.8 (4)	O2—C2—C3	113.2 (4)
O5—B1—O4	104.2 (4)	O2—C2—C1	102.7 (4)
O2—B1—O4	113.1 (4)	C3—C2—C1	113.7 (4)
O5—B1—O1	114.4 (4)	C4—O4—B1	108.2 (4)
O2—B1—O1	103.1 (4)	N4—C4—O4	122.5 (5)
O4—B1—O1	104.8 (4)	N4—C4—C5	124.9 (5)
C1—O1—B1	108.9 (3)	O4—C4—C5	112.6 (5)
O1—C1—N1	122.8 (4)	B1—O5—C5	112.4 (4)
O1—C1—C2	112.5 (4)	O5—C5—C6	112.7 (5)
N1—C1—C2	124.7 (4)	O5—C5—C4	102.5 (4)
C2—O2—B1	112.4 (4)	C6—C5—C4	113.4 (4)

Table 2

Hydrogen-bond geometry (\AA , $^\circ$).

$D-\text{H}\cdots A$	$D-\text{H}$	$\text{H}\cdots A$	$D\cdots A$	$D-\text{H}\cdots A$
N4—H4B ⁱ ···Br1	0.86	2.53	3.289 (5)	147
N1—H1A ⁱ ···O2 ⁱ	0.86	2.04	2.878 (5)	164
N1—H1B ⁱⁱ ···Br1 ⁱⁱ	0.86	2.49	3.341 (4)	173
N4—H4A ⁱⁱⁱ ···Br1 ⁱⁱⁱ	0.86	2.49	3.339 (5)	169

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

All H atoms were placed in idealized positions as riding atoms [$\text{C}-\text{H} = 0.98 \text{ \AA}$ (CH) and 0.96 \AA (CH_3), $\text{N}-\text{H} = 0.86 \text{ \AA}$ (NH_2), and $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C}, \text{N})$ (CH and NH_2) or $U_{\text{iso}}(\text{H}) = 1.5U_{\text{eq}}(\text{C})$ (CH_3)].

Data collection: *COLLECT* (Bruker–Nonius, 2004); cell refinement: *SCALEPACK* (Otwinowski & Minor, 1997); data reduction: *DENZO* (Otwinowski & Minor, 1997) and *SCALEPACK*; program(s) used to solve structure: *SIR97* (Altomare *et al.*, 1999);

program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *CAMERON* (Watkin *et al.*, 1996); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

The authors thank P. Retailleau, CNRS, Institut de Chimie des Substances Naturelles, Laboratoire de Cristallographie, 91198 Gif-sur-Yvette, France, for recording the X-ray diffraction.

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