The structure of the title compound, CsLiB$_6$O$_{10}$, comprises eight-coordinate Cs atoms and four-coordinate Li atoms, and an anion network of chains formed from B$_3$O$_7$ groups. The Cs and Li atoms occupy alternate sites in the channel along the $c$ axis.

**Abstract**

The structure of the title compound, CsLiB$_6$O$_{10}$, comprises eight-coordinate Cs atoms and four-coordinate Li atoms, and an anion network of chains formed from B$_3$O$_7$ groups. The Cs and Li atoms occupy alternate sites in the channel along the $c$ axis.

**Comment**

Borate crystals are of interest for the generation of coherent UV light because of their superior nonlinear optical properties. Various nonlinear optical borate crystals ($\beta$-BaB$_2$O$_4$ (BBO)) (Chen, Wu, Jiang & You, 1985), LiB$_3$O$_5$ (LBO) (Chen et al., 1989) and CsB$_3$O$_5$ (CBO) (Wu et al., 1993) have been found to date. Recently, we discovered a new borate crystal, CsLiB$_6$O$_{10}$ (CLBO) (Sasaki et al., 1995; Mori, Kuroda, Nakajima, Sasaki & Nakai, 1995), which has a different space group (I4d2) compared with LBO (Pn$\overline{2}a_1$) and CBO (P$\bar{2}1a_1$). CLBO, LBO and CBO contain the same basic unit in the borate network. It consists of a six-membered ring in which two of the B atoms are threefold coordinated and the third B atom is fourfold coordinated by O atoms. The borate network of CLBO surrounds eight-coordinate Cs atoms and four-coordinate Li atoms.
The title compound can be grown from stoichiometric melt and also from solution. Large high quality crystals can be obtained more readily than those of LBO, CBO and BBO. A superlarge CLBO crystal with dimensions of $13 \times 12 \times 10\, \text{cm}$ was grown in 12 days by means of the top-seeded Kyropoulos method (Sasaki et al., 1995).

![Fig. 1. Perspective view showing the coordination geometry of the Li atoms in the borate anion framework. Symmetry codes: (iii) $x + \frac{1}{2}, y - \frac{1}{2}, z$; (viii) $1 - y, x, -z$; (ix) $\frac{1}{2} + x, \frac{1}{2} + y, z - \frac{1}{2}$.](image1)

![Fig. 2. Molecular packing in the crystal showing the three-dimensional framework built up from triborate groups.](image2)

**Experimental**

Crystals of the title compound were grown by the top-seeded Kyropoulos technique in a platinum crucible by using a vertical cylindrical electric furnace. Starting materials were prepared from a mixture of Cs$_2$CO$_3$, Li$_2$CO$_3$ and B$_2$O$_3$ powders. Crystal growth was carried out at $1121\, \text{K}$ under an air ambient. The chemical formula of the obtained compound was determined by using inductively coupled plasma spectrochemical analysis.

**Crystal data**
- CsLiB$_6$O$_{10}$
- $M_r = 364.7$
- Tetragonal $I4_2d$
- $a = 10.494\, \text{(1)}\, \text{Å}$
- $c = 8.939\, \text{(2)}\, \text{Å}$
- $V = 984.4\, \text{Å}^3$
- $Z = 4$
- $D_x = 2.461\, \text{Mg m}^{-3}$

**Data collection**
- Rigaku AFC-5R diffractometer
- $\omega/2\theta$ scans
- Absorption correction: refined from $AF$

**Refinement**
- Refinement on $F$
- $R = 0.023$
- $\omega R = 0.035$
- $S = 2.37$
- 722 reflections
- 43 parameters

**Table 1. Fractional atomic coordinates and equivalent isotropic displacement parameters ($\text{Å}^2$)**

<table>
<thead>
<tr>
<th></th>
<th>$x$</th>
<th>$y$</th>
<th>$z$</th>
<th>$B_{eq}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Cs</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>2.396 (4)</td>
</tr>
<tr>
<td>O(1)</td>
<td>0.7982 (3)</td>
<td>1/4</td>
<td>1/8</td>
<td>1.94 (5)</td>
</tr>
<tr>
<td>O(2)</td>
<td>0.8022 (1)</td>
<td>0.4434 (1)</td>
<td>$-0.0059$ (2)</td>
<td>1.12 (2)</td>
</tr>
<tr>
<td>O(3)</td>
<td>0.6029 (2)</td>
<td>0.3557 (2)</td>
<td>0.0698 (2)</td>
<td>1.09 (2)</td>
</tr>
<tr>
<td>B(1)</td>
<td>0.5242 (3)</td>
<td>1/4</td>
<td>1/8</td>
<td>0.81 (4)</td>
</tr>
<tr>
<td>B(2)</td>
<td>0.7323 (2)</td>
<td>0.3508 (2)</td>
<td>0.0602 (3)</td>
<td>0.99 (3)</td>
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<tr>
<td>Li</td>
<td>0</td>
<td>0</td>
<td>1/2</td>
<td>1.32 (6)</td>
</tr>
</tbody>
</table>

**Table 2. Selected geometric parameters ($\text{Å}$, °)**

<table>
<thead>
<tr>
<th>Bond</th>
<th>$d$ (Å)</th>
</tr>
</thead>
<tbody>
<tr>
<td>B(1)—O(2)</td>
<td>1.467 (2)</td>
</tr>
<tr>
<td>B(2)—O(1)</td>
<td>1.389 (2)</td>
</tr>
<tr>
<td>B(2)—O(3)</td>
<td>1.363 (3)</td>
</tr>
<tr>
<td>O(2')—B(1)—O(2')</td>
<td>109.4 (2)</td>
</tr>
<tr>
<td>O(2')—B(1)—O(3')</td>
<td>106.67 (8)</td>
</tr>
<tr>
<td>O(2')—B(1)—O(3)</td>
<td>111.30 (9)</td>
</tr>
<tr>
<td>O(2')—B(1)—O(3)</td>
<td>111.30 (9)</td>
</tr>
<tr>
<td>O(2')—B(1)—O(3)</td>
<td>111.30 (9)</td>
</tr>
<tr>
<td>O(3)—B(1)—O(3)</td>
<td>111.5 (2)</td>
</tr>
<tr>
<td>O(2)—B(2)—O(3)</td>
<td>122.7 (2)</td>
</tr>
<tr>
<td>O(2)—B(2)—O(3)</td>
<td>122.7 (2)</td>
</tr>
</tbody>
</table>
CsLiB$_6$O$_{10}$

\[
\begin{align*}
O(2)-B(2)-O(1) & : 117.4(2) \quad B(2)-O(3)-B(1) : 123.6(2) \\
O(3')-B(2)-O(1) & : 119.8(2) \quad B(2)-O(3)-Li' : 123.9(1) \\
O(3')-Li-O(3') & : 142.9(1) \quad B(1)-O(3)-Li : 112.4(1)
\end{align*}
\]

Symmetry codes: (i) $y, x - \frac{1}{2}, \frac{1}{4} + z$; (ii) $y, 1 - x, -z$; (iii) $x, \frac{1}{2} - y, \frac{1}{4} - z$; (iv) $\frac{1}{2} - x, \frac{1}{2} - y, \frac{1}{4} + z$; (v) $x - \frac{1}{2}, y - \frac{1}{2}, \frac{1}{4} + z$; (vi) $y - \frac{1}{2}, \frac{1}{2} - x, \frac{1}{4} - z$; (vii) $\frac{1}{2} - y, x - \frac{1}{2}, \frac{1}{4} - z$; (viii) $1 - y, x, -z$; (ix) $\frac{1}{2} + x, \frac{1}{2} + y, z - \frac{1}{2}$.

The structure was solved by heavy-atom Patterson methods (Beurskens et al., 1992) and expanded by Fourier techniques (Beurskens et al., 1992). All atoms were refined anisotropically. All computations were performed using TExSAN crystallographic software (Molecular Structure Corporation, 1992).

The authors wish to thank Dr S. Sato, X-ray Research Laboratory, Rigaku Corporation, for making the four-circle X-ray diffractometer at their disposal.

Lists of structure factors and anisotropic displacement parameters have been deposited with the IUCr (Reference: OH1076). Copies may be obtained through The Managing Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

References


