The infrared spectrum of BCl$_3$ shows vibrational bands at 995, 480, and 244 cm$^{-1}$, while Raman bands appear at 995, 471, and 244 cm$^{-1}$. Is the geometry of the molecule trigonal pyramid (C$_3$v) or trigonal planar (D$_3h$)? Is your answer to this question consistent with chemical bonding principles (VSEPR)? Assign symmetry labels to the vibrational bands and identify the stretches and bends.

### C$_3$v Symmetry - BCl$_3$

The infrared spectrum of BCl$_3$ shows vibrational bands at 995, 480, and 244 cm$^{-1}$, while Raman bands appear at 995, 471, and 244 cm$^{-1}$. Is the geometry of the molecule trigonal pyramid (C$_3$v) or trigonal planar (D$_3h$)? Is your answer to this question consistent with chemical bonding principles (VSEPR)? Assign symmetry labels to the vibrational bands and identify the stretches and bends.

**E C$_3$v $\sigma_v$**

<table>
<thead>
<tr>
<th>$C_{C3v}$</th>
<th>$C3v$</th>
<th>$\Gamma_{uma}$</th>
<th>$\Gamma_{bonds}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$1 1 1$</td>
<td>$1$</td>
<td>$4$</td>
<td>$0$</td>
</tr>
<tr>
<td>$1 1 -1$</td>
<td>$2$</td>
<td>$3$</td>
<td>$1$</td>
</tr>
<tr>
<td>$2 -1 0$</td>
<td>$2$</td>
<td>$2$</td>
<td>$1$</td>
</tr>
</tbody>
</table>

$\Gamma_{uma} = \Gamma_{C3v}$

$\Gamma_{bonds} = (x^2 + y^2, xy)(xz, yz)$

$\Gamma_{vib} = \Gamma_{uma} - A_1 - A_2 - 2E$

$\Gamma_{stretch} = \Gamma_{bonds}$

$\Gamma_{bend} = \Gamma_{vib} - \Gamma_{stretch}$

This analysis predicts that there should be 4 IR and 4 Raman active vibrations. It also predicts that the IR and Raman vibrations should be coincident. This is not in agreement with the experimental data, so BCl$_3$ does not have trigonal pyramidal geometry.

This analysis also predicts that the stretches should have A1 and E symmetry, but since it has already been concluded that the molecule does not have C$_3$v symmetry this result will not be discussed further.
This analysis shows that there are 3 IR active modes (2E', A2") and 3 Raman active modes (A1', E'). It also show that there are two coincidences (2E'). Thus, D$_{3h}$ symmetry for BCl$_3$ is consistent with the spectroscopic data.

Thus the specific assignments are: A1' = 471; A2" = 480; E' = 995; E' = 244. From the analysis above it can be seen that the stretches occur at 995 and 471, and the bends are at 480 and 244 cm$^{-1}$.

VSEPR theory would predict a trigonal planar arrangement of chlorine atoms around the electron deficient boron, so the symmetry analysis and the bonding theory are in agreement with each other and the spectroscopic measurements.