Refinement of the Crystal Structure of Fluoborite, $\text{Mg}_3(\text{F,OH})_3(\text{BO}_3)$

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Summary

The crystal structure of fluoborite, $\text{Mg}_3(\text{F,OH})_3(\text{BO}_3)$, has been refined using X-ray data collected on an automatic diffractometer. The anisotropic refinement converged to a conventional $R$ of 0.029. The structural model proposed by Takéuchi as well as the space group $P \bar{6}3/m$ have been confirmed.

Fluoborite and nocerite were long considered to be two different mineral species, the former with chemical formula $\text{Mg}_3(\text{BO}_3)_2 \cdot 3\text{Mg}(\text{OH},\text{F})_2$, the latter with the chemical formula $\text{Mg}_3\text{Ca}_3\text{O}_8\text{F}_8$. Brisii and Eitel (1957) showed that infact nocerite is a fluoborate of magnesium, and is identical with synthetic $\text{Mg}_3(\text{BO}_3)_2 \cdot 3\text{MgF}_2$, the F-endmember of the fluoborite group. It was, therefore, concluded that nocerite and fluoborite differ only in their OH/F ratios. An increase of the lattice constant $a$ with replacement of F by OH was found by Segnit and Lancucki (1963) and by Flaminii (1966). Flaminii (loc. cit.) also showed that the $a$-lattice constant of nocerite from the type locality indicates that the mineral contains 8–9% $\text{Mg}_3(\text{BO}_3)_2 \cdot 3\text{Mg}(\text{OH})_2$.

The crystal structure of fluoborite was solved by Takéuchi (1950) on material from Tallgruvan, Sweden. However, the space group could not be definitely established, and the work is based on estimated...
intensities only. Therefore, a modern refinement of the structure was considered to be worthwhile. Using a "nocerite" from Nocera, Italy, it could also definitely prove that "nocerite" belongs to the fluoborite group.

The lattice constants were refined from 15 high order reflections \(2\theta = 45^\circ - 65^\circ\); Mo-\(K_\alpha\) radiation, graphite monochromator) by least squares methods (Table 1). They are in very good agreement with those published by Flamini (1966) for "nocerite".

<table>
<thead>
<tr>
<th>Space group</th>
<th>(P\bar{6}_3/m)</th>
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<tbody>
<tr>
<td>(a)</td>
<td>8.827(3) Å</td>
</tr>
<tr>
<td>(c)</td>
<td>3.085(2) Å</td>
</tr>
<tr>
<td>(V)</td>
<td>208 Å³</td>
</tr>
<tr>
<td>Cell content</td>
<td>(\text{Mg}_6(\text{F,OH})_6(\text{BO}_3)_2)</td>
</tr>
<tr>
<td>Specific gravity (meas.)</td>
<td>2.94 g. cm(^{-3}) (this work)</td>
</tr>
<tr>
<td>Specific gravity (calc.)</td>
<td>3.01 g. cm(^{-3})</td>
</tr>
</tbody>
</table>

Intensities (Mo-\(K_\alpha\) radiation, graphite monochromator) were measured on a Phillips PW 1100 computer controlled four-circle diffractometer by \(\omega\)-scans. The rate of scanning was 0.05°/sec, the scanning range 1°. For each reflection scans were made until the maximum number of scans (8) or the preset number of counts (3000) was reached. The background was measured at each side of the scan range for a time \(T\) according to the equation \(T = (T_{\text{scan}}/2) \cdot (\sqrt{I_{\text{back}}/I_{\text{int}}})\), where \(T_{\text{scan}}\) is the total scan time, \(I_{\text{back}}\) is the mean of two preliminary background measurements of 5 sec each at either side of the scan range in which the total number of counts \((I_{\text{int}})\) was stored.

Weak reflections with \((I_{\text{top}} - 2\sqrt{I_{\text{top}}}) < I_{\text{back}}\) were omitted. At the end of the refinement they were re-introduced with \(F_0 = 0\).

Three check reflections were measured every hour; no significant change in their intensities was observed.

556 reflections with all three indices positive were measured (up to 40°); the 403 reflections with \(I > \sigma (I)\) were used in the refinement. The intensities of 65 equivalent reflections \((I_{h0l} - I_{0kl})\) were averaged. The intensities were corrected for Lorentz and polarization effects, but no absorption correction was made because of the low value of the linear absorptions coefficient and the small size of the crystal \((0.08 \times 0.04 \times 0.27 \text{ mm})\). The statistical averages and the distribution