SINGLE-CRYSTAL MEASUREMENTS ON PARACELSIAN

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ABSTRACT. The cell dimensions and space group of paracelsian have been determined and these have been compared with those of topaz and danburite. There is a close similarity between paracelsian and danburite.

PARACELSIAN, BaO·Al₂O₃·2SiO₂, was first described in detail by Spencer (1942). His goniometric measurements showed that the crystals have orthorhombic morphology but his optical measurements could be rationalized only if the crystals were assumed to have lower symmetry. Twinning and striations, indicating lower symmetry, were observed.

X-ray measurements have now been made on several crystals obtained from Spencer’s original material. All of these were found to be single crystals with the following crystal properties:

From precession photographs (not assumed to be orthorhombic) From Geiger-counter spectrometer (assumed to be orthorhombic)

\[
\begin{align*}
  a \sin \beta &= 9.02 \pm 0.09 \text{Å} & a' &= 9.076 \pm 0.005 \text{Å} \\
  b &= 9.50 \pm 0.09 \text{Å} & b &= 9.583 \pm 0.005 \text{Å} \\
  c \sin \beta &= 8.47 \pm 0.09 \text{Å} & c' &= 8.578 \pm 0.005 \text{Å} \\
  \beta &= 90^\circ \pm 0.5^\circ & \text{using } \text{CuK}_\alpha, \lambda &= 1.54050 \text{Å} \\
  \text{using } \text{MoK}_\alpha, \lambda &= 0.7107 \text{Å} & \text{CuK}_\alpha, \lambda &= 1.54434 \text{Å}
\end{align*}
\]

Using the density found by Spencer, 3.31, there are 4(calc. 3.95) units of BaO·Al₂O₃·2SiO₂ in the unit cell. The more accurate measurements give \( a' : b : c' = 0.9471 : 1 : 0.8952 \) which compare well with Spencer’s goniometric axial ratios \( a : b : c = 0.9470 : 1 : 0.8956 \).

Comparison of intensities on single-crystal photographs showed that the crystals are monoclinic. There are pseudo-mirror planes of symmetry parallel to (100) and (001), and the mismatch of intensities over these planes is very small. The crystals therefore are very markedly pseudo-orthorhombic. Systematic absences were found only for reflections with \( h \) odd in \((h00)\), \( k \) odd in \((0k0)\), \( l \) odd in \((00l)\), \( h \) odd in \((h0l)\). In addition systematic absences for reflections with \((k+l)\) odd in \((0kl)\) were at first found. However, long-exposure photographs revealed a few very weak reflections with \((k+l)\) odd in \((0kl)\). The space group is therefore \( \text{P}2_1/\text{a} \), assuming that reflections with \( k \) odd in \((0k0)\) are truly absent; if not, the

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space group is P2/a or Pa. The crystals are in pseudo space groups Pna or Pnam.

Optical measurements, kindly carried out by W. S. MacKenzie of this Laboratory, showed that \( a \approx X, \ b = Z, \ c \approx Y, \ 2V = 52.7^\circ + 0.5^\circ \) (sodium light), optically negative. Spencer found that \( a = 1.5702, \ \beta = 1.5824, \ \gamma = 1.5869, \) optically negative, \( 2V = 50^\circ \ 35' \) (sodium light). MacKenzie found that the isogyres in convergent polarized light were single, and no peculiar effects (as described by Spencer) occurred upon rotation of the crystal in convergent polarized light.

Spencer pointed out the "very remarkable agreement between the (goniometric) angles of paracelsian and those of topaz and danburite." Comparison of the X-ray properties of the crystals further extends this agreement.

By interchanging the x and y axes of paracelsian, we have the following comparison:

<table>
<thead>
<tr>
<th></th>
<th>Paracelsian</th>
<th>Top</th>
<th>Danburite</th>
</tr>
</thead>
<tbody>
<tr>
<td>Axial ratios</td>
<td>1.056 : 1 : 0.9456</td>
<td>1.0570/2 : 1 : 0.9540</td>
<td>1.0888 : 1 : 0.9614</td>
</tr>
<tr>
<td>a</td>
<td>9.58Å</td>
<td>4.64Å</td>
<td>8.75Å</td>
</tr>
<tr>
<td>b</td>
<td>9.08Å</td>
<td>8.78Å</td>
<td>8.01Å</td>
</tr>
<tr>
<td>c</td>
<td>8.58Å</td>
<td>8.38Å</td>
<td>7.72Å</td>
</tr>
<tr>
<td>Space group</td>
<td>Pbnm (pseudo)</td>
<td>Pbmm</td>
<td>Pbmm</td>
</tr>
<tr>
<td>Composition</td>
<td>BaAl₂Si₂O₈</td>
<td>Al₃P₂Si₁₁O₂₇</td>
<td>CaB₂Si₂O₈</td>
</tr>
<tr>
<td>No. of units in</td>
<td>4</td>
<td>2</td>
<td>4</td>
</tr>
<tr>
<td>unit cell</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

The structures of topaz (Pauling, 1928; Alston and West, 1928) and danburite (Dunbar and Machatschki, 1930) are known, whereas the structure of paracelsian is unknown. Comparison of the properties given above suggests that the structure of paracelsian may be similar to that of topaz or that of danburite (there is no obvious relation between the structures of topaz and danburite). It appears more likely that the structure of paracelsian is similar to that of danburite, with the calcium replacing the barium and the aluminium replacing the boron. If this were true, then the increased axial lengths\(^1\) of paracelsian would be expected because the ionic radii of barium and aluminium atoms are respectively larger than the radii

\(^1\) Note added in proof. The structure of paracelsian has now been determined and it is indeed similar to that of danburite. Full details will be published elsewhere.
of calcium and boron atoms. The increase in the axial lengths is approximately that to be expected from the theoretical ionic radii.

The structure of celsian, which has the same chemical composition as paracelsian, is similar to that of orthoclase (Taylor, Darbyshire and Strunz, 1934). There is no obvious relation between the axial lengths and space groups of paracelsian and celsian.

Weissenberg and precession photographs have been taken in preparation for a structure determination.

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References


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