THE CRYSTAL STRUCTURE OF DACHIARDITE

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ABSTRACT

Structural work on mordenite suggested a possible structure for dachiardite, a rare zeolite. This trial structure has been confirmed by 2-dimensional Fourier syntheses.

The crystals are monoclinic with space group $B2/m$ or $Bm$. The framework structure of dachiardite is closely related to the mordenite structure. There are comparatively wide channels along both the $b$ and $c$ axes.

Dachiardite is a rare zeolite which occurs in association with mordenite on Elba, Italy. Its composition, $(K, Na, Ca)_{5}Al_{5}Si_{19}O_{48} \cdot 12H_{2}O$, is very nearly that of mordenite. The crystal data of the two zeolites are as follows:

<table>
<thead>
<tr>
<th>Dachiardite (D)</th>
<th>Mordenite (M)</th>
</tr>
</thead>
<tbody>
<tr>
<td>monoclinic$^1$</td>
<td>orthorhombic</td>
</tr>
<tr>
<td>$a = 18.73$ Å</td>
<td>$a = 18.13$ Å</td>
</tr>
<tr>
<td>$b = 10.30$ Å</td>
<td>$b = 20.49$ Å</td>
</tr>
<tr>
<td>$c = 7.54$ Å</td>
<td>$c = 7.52$ Å</td>
</tr>
<tr>
<td>$\gamma = 107^\circ 54'$</td>
<td>$\gamma = 107^\circ 54'$</td>
</tr>
<tr>
<td>Space group: $B2/m$ or $Bm$</td>
<td>Space group: $Cmcm$ or $Cmc2$</td>
</tr>
</tbody>
</table>

The relationship between the unit cells of D and M, as illustrated in Fig. 1, was first noted by Gottardi (1960).

The structure of M is based on characteristic chains shown in Fig. 2 (Meier, 1961). These chains can be linked in two different ways to give the aluminosilicate frameworks of M and D. Figure 3 shows the resultant frameworks in projection along [001]. The trial structure of D (involving framework atoms only) gave an initial R-factor of 0.37 for the $hk0$ reflections. Two-dimensional Fourier and difference maps confirmed the general features of the framework.

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$^1$ The first monoclinic setting is used in this paper for convenience.

Fig. 1. Unit cells of D and M.

Fig. 2. Mordenite chain.
and indicated probable positions for the cations and some of the water molecules. The R-factor for the $hk0$ reflections of the structure with cations and water has been reduced to 0.22 in the course of 4 cycles of refinement by means of difference maps. (The R-factor for the aluminosilicate framework alone is 0.30). Fourier projections along [010] and [100] were also computed and helped to confirm the structure.

The structure of D is penetrated by a 2-dimensional system of comparatively wide channels. The main channels run parallel to the $c$ axis and are interconnected by channels parallel to the $b$ axis. The free openings of these channels are about 4 Å. The observed twinning of D can be readily explained on the basis of the aluminosilicate framework.

Three-dimensional refinement using low-temperature data of the sodium form of D is in progress. A more detailed account of our work will be published in Zeitschrift für Kristallographie.

References


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*Fig. 3. Projections of the framework structures of M and D.*