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, $(K, Na, Ca)_{5}Al_{15}Si_{19}O_{48}•12H_{2}O$, is very nearly that of mordenite. The crystal data of the two zeolites are as follows:

**Dachiardite (D)**
- monoclinic
- $a = 18.73 \text{ Å}$
- $b = 10.30 \text{ Å}$
- $c = 7.54 \text{ Å}$
- $\gamma = 107^\circ 54'$
- Space group: $B2/m$ or $Bm$

**Mordenite (M)**
- orthorhombic
- $a = 18.13 \text{ Å}$
- $b = 20.49 \text{ Å}$
- $c = 7.52 \text{ Å}$
- Space group: $Cmcm$ or $Cmc2$

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.
and indicated probable positions for the cations and some of the water molecules. The R-factor for the \( hko \) 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.