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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, $Ca_{\frac{1}{2}})_5Al_5Si_{19}O_{48}\cdot 12H_2O$, is very nearly that of mordenite. The crystal data of the two zeolites are as follows:

Dachardite (D)	*Mordenite* (M)
monoclinic[1]	orthorhombic
$a=18.73$ Å	$a=18.13$ Å
$b=10.30$ Å	$b=20.49$ Å
$c=7.54$ Å $\gamma=107°54'$	$c=7.52$ Å
Space group: *B2/m* or *Bm*	*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

[1] The first monoclinic setting is used in this paper for convenience.

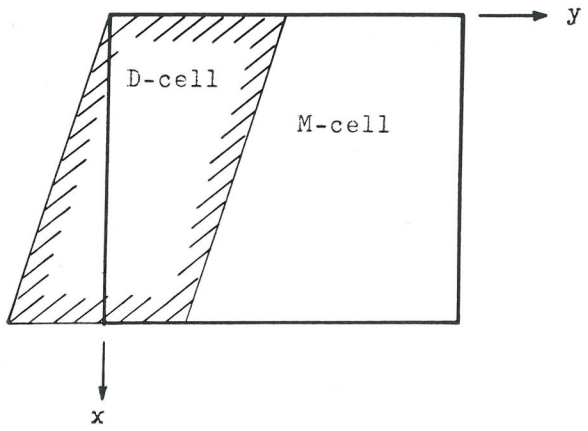


FIG. 1. Unit cells of D and M.

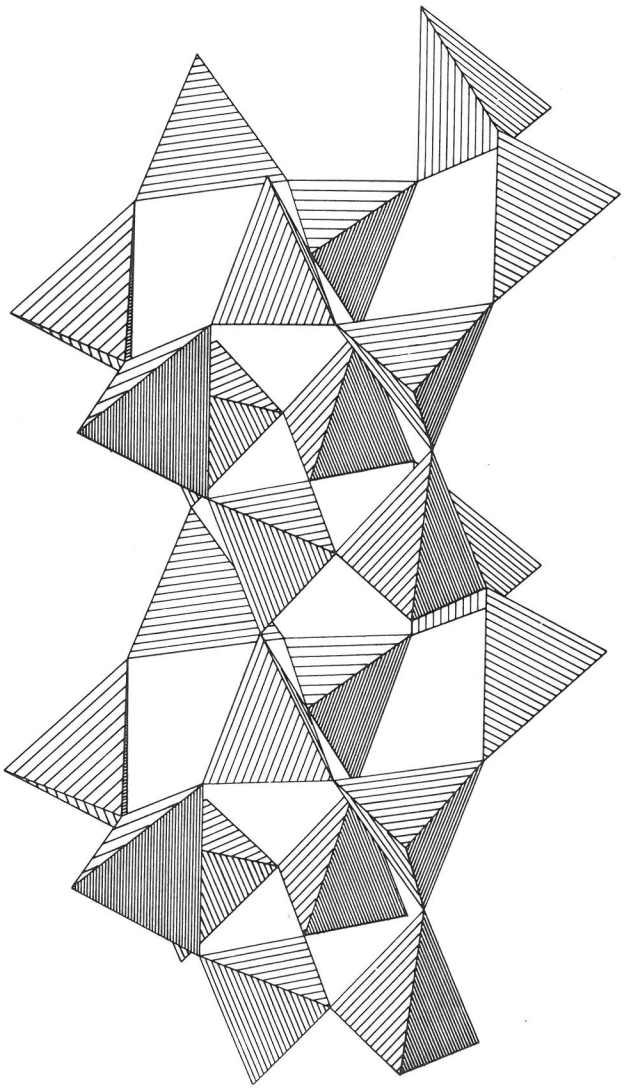
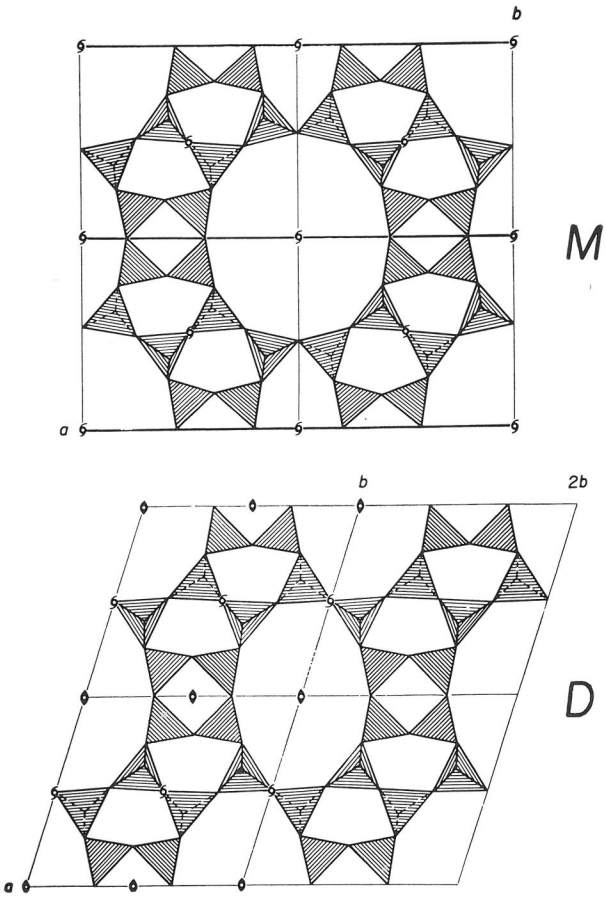


FIG. 2. Mordenite chain.



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.

FIG. 3. Projections of the framework structures of M and D.

REFERENCES

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