The crystal structures of clinohedrite $Ca[ZnSiO_4]\cdot H_2O$ and herstmannite $(Mn, Mg)Mg(OH)_2[ZnSiO_4]$

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(Submitted November 25, 1977)

Dokl. Akad. Nauk SSSR **238**, 1348–1350 (February 1978)

PACS numbers: 61.60.+m

The refinement of the crystal structure of clinohedrite $Ca[ZnSiO_4]\cdot H_2O$ (a = 5.131, b = 15.928, c = 5.422 Å, β = 103.39°, Z = 4, Cc) (Refs. 1 and 2)[1)] and the appearance of an article[4] on a new zinc silicate, herstmannite $(Mn, Mg)Mg(OH)_2\cdot[ZnSiO_4]$ (a = 8.185, b = 18.65, c = 6.256 Å, Z = 8, Bbcm), with a similar crystal-chemical formula, has stimulated the comparison of their crystal structures.

Crystal-chemical analysis reveals that, despite the different parameters and symmetries of these two minerals, in the structure of clinohedrite we can choose a pseudoorthogonal unit cell ($\mathbf{a}' = \mathbf{a} - \mathbf{c}$, $\mathbf{b}' = \mathbf{b}$, $\mathbf{c}' = \mathbf{a} + \mathbf{c}$): a' = 8.29, b' = 15.93, c' = 6.55 Å, α = 90, β = ~93, γ = 90°, in which the parameters a and c are close to the corresponding parameters of herstmannite, while the difference between the parameters b and b' is due to the different structures of the cation (octahedron) layers, appearing clearly in the new "redrawn" xy projection of clinohedrite (Fig. 1) when it is compared with the corresponding projection of herstmannite.

In the structure of clinohedrite (Fig. 2A) the cation layer consists of zigzag Ca-bands extending along the diagonal **a**−**c** and joined together only by hydrogen bonds. But in the structure of herstmannite (Fig. 2B) along the same **a**−**c** direction there are extended (Mn, Mg)-bands with a different configuration, joined into a single layer by Mg-octahedra. The width of this layer is greater than that of the layer in clinohedrite by half the edge of an Mg-octahedron. Since two cation layers are fitted into the period b of both minerals, the difference between the periods b and b' of herstmannite and clinohedrite is the length of one edge of an Mg-octahedron (about 2.94 Å).

The anion matrices of $Ca[ZnSiO_4]\cdot H_2O$ and $(Mn, Mg)Mg(OH)_2[ZnSiO_4]$ consist of cubic close-packings of O atoms. The filling of the octahedral and tetrahedral cavities is such that in both structures we observe alternation of the above-mentioned octahedral and identical (Fig. 3) tetrahedral Zn−Si layers along the b(b') direction, each of them being formed by Zn-metachains of a rare "metagermanate" type, joined together by Si-orthotetrahedra.

The difference between the formulas of clinohedrite $Ca[ZnSiO_4]\cdot H_2O$ and herstmannite $(Mn, Mg)Mg(OH)_2[ZnSiO_4]$, expressed in an excess of Mg^{2+} cations over Ca with a corresponding replacement of a neutral H_2O particle by

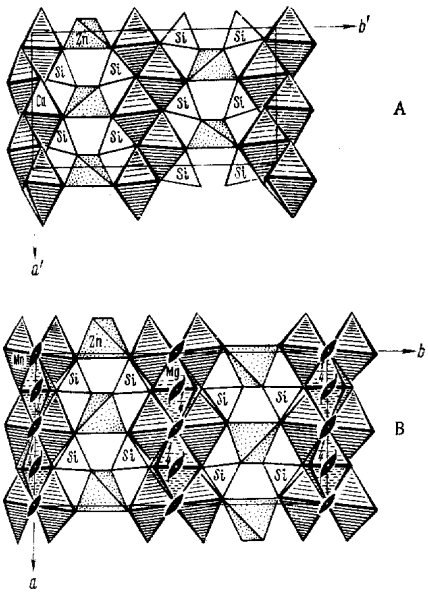

FIG. 1. Showing xz-projections of structures. A) Clinohedrite $Ca[ZnSiO_4]\cdot H_2O$; B) herstmannite $(Mn, Mg)Mg(OH)_2\cdot[ZnSiO_4]$.

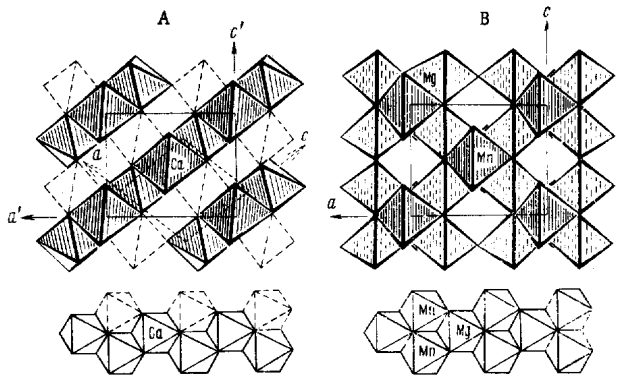

FIG. 2. Fragments of structures (cation layers and bands). A) Clinohedrite; B) herstmannite.

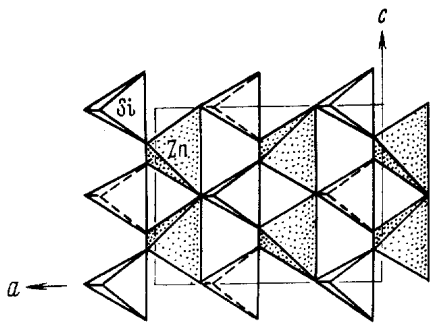

FIG. 3. Tetrahedral Zn−Si layer in structures of clinohedrite and herstmannite.

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$(OH)_2^{2-}$, is reflected in a difference between the cation structures of the minerals, though their overall structures are similar.

[1)]During the preparation of this article the authors became acquainted with an article by Venetopoulos and Rentzeperis,[3] who give the results of an independent refinement of the crystal structure of clinohedrite.

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[4]P. Moore and T. Araki, Am. Miner. 62, 51 (1977).

Translated by S. E. Hall