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Superstructure of Challis mordenite with doubled monoclinic unit cell

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Abstract

A new superstructure was found in mordenite ($Na_{5.59}Ca_{1.80}Al_{9.19}Si_{38.81}O_{96}\cdot nH_2O$) from Challis Valley, Idaho—a zeolite widely used in previous studies. The occurrence of the superstructure reflections were observed in 12 specimens from two rock samples, at the midpoint of layers in the oscillation photographs around the **a*** and **b*** axes, but not around the **c*** axis. The apparent 2**a**, 2**b**, and **c** axes are orthogonal. In spite of yielding an apparent orthorhombic cell, careful observation of the intensities revealed that the superstructure is monoclinic with twice the volume of the orthorhombic cell: a' = 27.356(9), b' = 27.356(9), c' = 7.517(2) Å, γ' = 97.14(4)°, and V' = 5582(4) Å^3.

The presence of the superstructure was examined for specimens from ten other localities and a synthetic sample but there was no evidence for extra spots of the superstructure, indicating that the occurrence is not common.

The large displacement factors of O8 oxygen, and its associated 180° T-O-T angle that is energetically unfavorable, are basic to the mordenite structure. In the monoclinic superstructure the O8 oxygen is decomposed into several asymmetric O atoms by the symmetry reduction. The large displacement smearing of O8 oxygen perpendicular to the straight T-O-T, are explained by the superposition of decomposed O atoms.

The extra spots are predominantly observed in the reciprocal planes with l = odd in the same way as diffuse streaks. The observation of extra spots and diffuse streaks suggests that there are three kinds of domains in the mordenite, one in the ordered form and two others in the random form of $c/2$ linear displacements. The domain in the ordered form represents the superstructure. Thus, we propose a model for the superstructure in which the $c/2$ displacement occurs alternatively in the two basic unit cells slightly modified in the superstructure, yielding the periodic arrangements.

Keywords: Mordenite, superstructure, monoclinic cell, diffuse streak, linear displacement, ordered form