

Direnzoite, [NaK₆MgCa₂(Al₁₃Si₄₇O₁₂₀)·36H₂O], a new zeolite from Massif Central (France): Description and crystal structure

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ABSTRACT

The crystal structure of direnzoite, a new natural zeolite found in the cavities of a xenolithic rock from the Massif Central (France) is reported. Apparently, direnzoite was formed throughout a process of hydrothermal crystallization within the vugs of a highly porphyric basalt. The determination of the crystal structure of this new zeolite was at the limits of the existing experimental techniques because of the paucity of available specimen, mainly composed of three tiny aggregates of fibrous microcrystals. The structure of direnzoite, solved by powder methods, was shown to be the K-dominant equivalent of the synthetic zeolite ECR-1 with a framework composed of layers of mordenite (MOR) and mazzite (MAZ) connected in a regular 1:1 stacking sequence with assigned framework topology EON. The chemical composition of direnzoite determined from the structure refinement is (Na_{0.94}K_{6.62}Mg_{1.42}Ca_{2.24})(Si,Al)₆₀O₁₂₀·36.8H₂O. The unit cell determined from the Rietveld structure refinement is $a = 7.57887(18) \text{ \AA}$, $b = 18.20098(57) \text{ \AA}$, $c = 26.15387(83) \text{ \AA}$, and the space group is *Pmnm*.

Six extra-framework sites and 14 water molecules were identified within the zeolite micropores. Three extra-framework sites are occupied by K⁺ ions. The others are occupied by Na⁺, Ca⁺⁺, and Mg⁺⁺. Although direnzoite and ECR-1 share the same framework, the distribution of their extra-framework cations is rather different. In direnzoite, there are no equivalent positions to C1, C2, and C4 positions found in ECR-1. Only sites C3 and C3b correspond respectively to K3 and Ca in direnzoite. In direnzoite, K1, K2, and Na correspond to water molecules sites (H₂O1, H₂O11, and H₂O8, respectively) in ECR-1.

Keywords: Zeolite, xenolith, synchrotron, powder diffraction, microprobe analysis