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Packing systematics and structural relationships of the new copper molybdate markascherite and related minerals

Richard M. Thompson,* Hexiong Yang, and Robert T. Downs

Department of Geosciences, University of Arizona, 1040 E. 4th Street, Tucson, Arizona 85721, U.S.A.

Abstract

The structural relationships between the new mineral markascherite, ideally $Cu_3(MoO_4)(OH)_4$, and the related minerals szenicsite, antlerite, deloryite, flinkite, retzian, and cahnite are analyzed using hypothetical ideal closest-packed equivalents. Markascherite and the first three related minerals are based on cubic closest-packing (CCP) of anions, flinkite is based on stacking sequence ABAC, and retzian and cahnite are based on hexagonal closest-packing (HCP). However, models that are more realistic than those based on CP can be constructed for retzian and cahnite using small but systematic alterations of CP monolayers. A regular pattern of slight dislocations of some of the spheres in the monolayers creates dodecahedral interstitial sites when the monolayers are stacked, a feature not seen in perfect CP.

The use of ideal crystals removes all distortion from polyhedra in closest-packed minerals, allowing for comparison of structural similarities and differences. CCP minerals can have up to four nonequivalent stacking directions. Corresponding stacking directions in the minerals of interest are identified and used to compare the layers of cation coordination polyhedra perpendicular to these zones or face poles (stacking directions are presented in both direct space and reciprocal space). Such layers are natural structural subunits and provide insight into the relationships among these minerals.

Keywords: Markascherite, szenicsite, antlerite, closest-packing, deloryite, flinkite, cahnite, retzian