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Compositional variability and crystal structural features of guanacoite

Atsushi Kyono*

Division of Earth Evolution Sciences, Graduate School of Life and Environmental Sciences, University of Tsukuba, Tennodai 1-1-1, Tsukuba, Ibaraki 305-8572, Japan

Abstract

Guanacoite with high Mg content from the type locality (El Guanaco mine, Chile) was investigated to elucidate the crystal-chemical characteristics of this arsenate mineral. In this study, WDS X-ray intensity maps revealed that guanacoite single crystals from the investigated specimen show distinct and characteristic compositional zoning, which varies cyclically along [100], which is in the direction of the elongation of the prismatic crystals (Witzke et al. 2006); the boundaries separating different compositional regions lie perpendicular to the prism faces. The crystal structure of a selected fragment [a = 5.459(2), b = 16.808(9), c = 6.917(3) Å, β = 100.44(1)°, V = 624.1(5) Å^3, $P2_1/c$, and Z = 2], was solved using direct methods and refined to an R index of 3.09% for 1385 observed [$I_o > 4\sigma(I_o)$] reflections measured at 103 K using Mo$K\alpha$ X-radiation. The chemical formula based on the refinement is $(Cu_{0.85}Mg_{0.15})_2Mg_2(Mg_{0.83}Cu_{0.17})(OH)_4(H_2O)_4(AsO_4)_2$. The structure model obtained is in good agreement with the previous structure determination, although the occupancies of the three M sites (M = Mg or Cu) are distinctly different, i.e., the sites are considerably richer in Mg, especially M1 and M3. These structural results suggest that guanacoite's chemical formula should be enlarged from the Cu-rich composition $Cu_2Mg_2(Mg,Cu)(OH)_4(H_2O)_4(AsO_4)_2$ to $(Cu,Mg)_2Mg_2(Mg,Cu)(OH)_4(H_2O)_4(AsO_4)_2$ to include the Mg-rich members (Mg up to 3.395 apfu). It appears that the chemical variability of guanacoite is mainly due to Mg-Cu substitution on the M1 and M2 sites.

Keywords: Guanacoite, copper magnesium arsenate hydrate, crystal structure, chemical analysis, Jahn-Teller distortion