

Compositional variability and crystal structural features of guanacoite

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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, $\beta = 100.44(1)^\circ$, $V = 624.1(5)$ Å³, $P2_1/c$, 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 $\text{MoK}\alpha$ X-radiation. The chemical formula based on the refinement is $(\text{Cu}_{0.85}\text{Mg}_{0.15})_2\text{Mg}_2(\text{Mg}_{0.83}\text{Cu}_{0.17})(\text{OH})_4(\text{H}_2\text{O})_4(\text{AsO}_4)_2$. The structure model obtained is in good agreement with the previous structure determination, although the occupancies of the three M sites ($M = \text{Mg}$ 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 $\text{Cu}_2\text{Mg}_2(\text{Mg},\text{Cu})(\text{OH})_4(\text{H}_2\text{O})_4(\text{AsO}_4)_2$ to $(\text{Cu},\text{Mg})_2\text{Mg}_2(\text{Mg},\text{Cu})(\text{OH})_4(\text{H}_2\text{O})_4(\text{AsO}_4)_2$ 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