

The crystal chemistry of sogdianite, a milarite-group mineral

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ABSTRACT

The crystal structure of sogdianite, hexagonal, $a = 10.053(1)$, $c = 14.211(2)$ Å, $V = 1243.8(4)$ Å³, space group = $P6/mcc$, $Z = 2$, has been refined to an R index of 2.0% using 607 observed ($|F_o| > 5\sigma|F|$) reflections collected with an automated four-circle diffractometer using $\text{MoK}\alpha$ X-radiation. Site-scattering refinement and electron-microprobe analysis indicate the composition $(\text{Zr}_{0.76}\text{Ti}_{0.38}\text{Fe}_{0.73}\text{Al}_{0.13})_{\Sigma=2}(\square_{1.15}\text{Na}_{0.85})_{\Sigma=2}\text{K}[\text{Li}_3\text{Si}_{12}\text{O}_{30}]$. The T2 tetrahedron is completely occupied by Li, and all Al occurs at the octahedrally coordinated A site. The $\langle\text{A-O}\rangle$ bond length is compatible with all Fe being in the trivalent state. There is no significant positional disorder of the A-group cations, in accord with the absence of H_2O in sogdianite. Single-crystal X-ray precession photographs of sogdianite show the presence of diffractions that are incommensurate with the sogdianite diffraction pattern. The relative intensity of the incommensurate diffractions increases with the degree of apparent alteration of sogdianite (clear \rightarrow turbid \rightarrow murky), suggesting that sogdianite is altering to, or possibly exsolving, a second phase, probably zektzerite.