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Shirozulite, $KMn^{2+}_3(Si_3Al)O_{10}(OH)_2$, a new manganese-dominant trioctahedral mica: Description and crystal structure

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ABSTRACT

Shirozulite is a new Mn-dominant trioctahedral mica from the Taguchi mine, Aichi Prefecture, Japan. The mineral occurs in tephroite-rhodochrosite ores in contact with a Ba-bearing, K-feldspar vein. Shirozulite formed during regional low-*P*/*T* metamorphism and, thereafter, suffered thermal metamorphism from a local granodiorite. Grains of shirozulite are up to 0.5 mm across and have a typical micaceous habit. Color: dark reddish brown. Cleavage: (001), perfect. Optical properties: biaxial negative, $2V_x$ = very small. Strongly pleochroic: X = pale yellow, Y = Z = pale brown, absorption X < Y ≈ Z. Refractive indices: $n_\alpha = 1.592(2)$, $n_\beta \approx n_\gamma = 1.635(2)$. The structural formula is $(K_{0.90}Ba_{0.09})(Mn^{2+}_{1.53}Mg_{0.94}Fe^{2+}_{0.20}Ti_{0.04}Al_{0.29})(Si_{2.54}\ Al_{1.46})\ O_{10}\ [(OH)_{1.97}F_{0.03}]$, and the end-member composition is $KMn^{2+}_3AlSi_3O_{10}(OH)_2$. Density: obs. = 3.20(3) g/cm^3 by pycnometer, calc. = 3.14(2) g/cm^3. Shirozulite is monoclinic, *C*2/*m*, 1M polytype, $a = 5.3791(7)$, $b = 9.319(1)$, $c = 10.2918(9)$ Å, $\beta = 100.186(9)°$, $V = 507.8(1)$ Å^3. The six strongest lines in the powder X-ray diffraction pattern are as follows: *d* (Å), *I* (%), (*hkl*): 10.16, 100, (001); 2.654, 96, ($\bar{1}$31); 3.386, 51, (003); 1.556, 48, ($\bar{3}$13); 2.467, 46, ($\bar{1}$32); 2.202, 36, ($\bar{1}$33). The crystal structure has been refined to an *R* value of 4.1% based on 663 observed reflections collected with Mo*K*α X-radiation from a single crystal. The mean bond lengths, tetrahedral rotation, and octahedral flattening angles are as follows: <T-O> = 1.668, <M1-O> = 2.118, <M2-O> = 2.103, <K-O>(inner) = 2.995, and <K-O>(outer) = 3.376 Å, $\alpha = 8.36°$, $\psi_{M1} = 58.5°$, $\psi_{M2} = 58.2°$. The apparent element distribution coefficient analyses among coexisting manganese or manganoan silicate minerals indicate that the trioctahedral mica structure cannot contain larger amounts of Mn^{2+} relative to Mg and Fe^{2+} than in olivine, pyroxenoid, and garnet.