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Yusupovite, $Na_2Zr(Si_6O_{15})(H_2O)_3$, a new mineral species from the Darai-Pioz alkaline massif and its implications as a new microporous filter for large ions

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Abstract

Yusupovite, ideally $Na_2Zr(Si_6O_{15})(H_2O)_3$, is a new silicate mineral from the Darai-Pioz alkaline massif in the upper reaches of the Darai-Pioz river, area of the joint Turkestansky, Zeravshansky, and Alaisky ridges, Tajikistan. Yusupovite was found in a pegmatite composed mainly of reedmergnerite, aegirine, microcline, and polylithionite. It occurs as prismatic grains about 2 mm in size embedded in reedmergnerite; associated minerals are quartz, pectolite, zeravshanite, mendeleevite-(Ce), fluorite, leucosphenite, a pyrochlore-group mineral, neptunite, telyushenkoite, moskvinite-(Y), and shibkovite. Yusupovite is colorless, transparent with a white streak, has a vitreous luster, and does not fluoresce under ultraviolet light. Cleavage is perfect on {110}, parting was not observed. Mohs hardness is 5. Yusupovite is brittle with a splintery fracture. The measured and calculated densities are 2.69(2) and 2.713 g/cm^3, respectively. Yusupovite is optically biaxial (+) with refractive indices (λ = 589 nm) α = 1.563(2), β = 1.565(2), γ = 1.577(2); $2V_{meas}$ = 42(3)°, $2V_{calc}$ = 45°, strong dispersion: r > v. Yusupovite is monoclinic, *C*2/*m*, *a* = 14.5975(4), *b* = 14.1100(4), *c* = 14.4394(4) Å, β = 90.0399(4)°, *V* = 2974.1(3) Å^3. The six strongest reflections in the X-ray powder diffraction data [*d* (Å), I, (*hkl*)] are 7.05, 100, (020); 3.24, 96, (420); 3.10, 69, (241, $\bar{2}$41); 5.13, 53, (202, $\bar{2}$02); 6.51, 42, (201, $\bar{2}$01); 3.17, 34, (042). The chemical composition (electron microprobe) is: Nb_2O_5 0.39, SiO_2 58.84, ZrO_2 16.55, HfO_2 0.30, FeO 0.01, Y_2O_3 3.05, Cs_2O 2.58, K_2O 0.95, Na_2O 8.91, H_2O_{calc} 7.40, total 98.98 wt%, with H_2O calculated from structure refinement. The empirical formula (based on 17.5 O apfu) is $(Na_{1.76}K_{0.12}Cs_{0.11})_{\Sigma 1.99}(Zr_{0.82}Y_{0.17}Nb_{0.02}Hf_{0.01})_{\Sigma 1.02}(Si_{6.01}O_{14.98})(H_2O)_{2.52}$, *Z* = 8. The crystal structure of yusupovite was refined to R_1 = 3.46% based on 4428 observed reflections. In the crystal structure, there are six Si sites occupied by Si, two M sites occupied mainly by Zr with minor Y and Hf. Si tetrahedra form an epididymite Si_6O_{15} ribbon along [010]. Epididymite ribbons and Zr-dominant M octahedra share common vertices to form a heteropolyhedral Si-Zr-O framework. There are six interstitial sites partly occupied by alkali cations Na, K, and Cs. The three [7]-coordinated Na sites are occupied by Na at 95, 84, and 78%. The three A sites are occupied by K and Cs at 12, 18, and 16%. There are 10 W sites occupied by H_2O groups at 18–84%. Due to (K,Cs), Na and H_2O disorder, the symmetry of yusupovite decreases from orthorhombic, space group *Pbcm* (elpidite), to monoclinic, space group *C*2/*m*, and the *b* unit-cell parameter of yusupovite is doubled compared to the corresponding cell parameter in elpidite, $b_{yus} = 2a_{elp}$. Yusupovite, ideally $Na_2Zr(Si_6O_{15})(H_2O)_3$, is a dimorph of elpidite, $Na_2Zr(Si_6O_{15})(H_2O)_3$.

Keywords: Yusupovite, new mineral species, silicate, Darai-Pioz massif, Tajikistan, electron microprobe analysis, X-ray powder diffraction data, elpidite, crystal structure, alkaline pegmatite