

Yusupovite, $\text{Na}_2\text{Zr}(\text{Si}_6\text{O}_{15})(\text{H}_2\text{O})_3$, a new mineral species from the Darai-Pioz alkaline massif and its implications as a new microporous filter for large ions

ATALI A. AGAKHANOV^{1,2}, LEONID A. PAUTOV², VLADIMIR Y. KARPENKO², ELENA SOKOLOVA^{3,*},
YASSIR A. ABDU³, FRANK C. HAWTHORNE³, IGOR V. PEKOV⁴ AND OLEG I. SIIDRA¹

¹Department of Crystallography, St. Petersburg State University, University Embankment 7/9, 119034 St. Petersburg, Russia

²Fersman Mineralogical Museum, Russian Academy of Sciences, Leninskii Pr-kt, 18-2, 119071 Moscow, Russia

³Department of Geological Sciences, University of Manitoba, Winnipeg, Manitoba R3T 2N2, Canada

⁴Department of Mineralogy, Moscow State University, Vorob'ovy Gory, 119991 Moscow, Russia

ABSTRACT

Yusupovite, ideally $\text{Na}_2\text{Zr}(\text{Si}_6\text{O}_{15})(\text{H}_2\text{O})_3$, is a new silicate mineral from the Darai-Pioz alkaline massif in the upper reaches of the Darai-Pioz river, area of the joint Turkestan, Zeravshan, and Alai ridges, Tajikistan. Yusupovite was found in a pegmatite composed mainly of reedmergnerite, aegirine, microcline, and polyolithonite. 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, moskvinit-(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/cm³, respectively. Yusupovite is optically biaxial (+) with refractive indices ($\lambda = 589$ nm) $\alpha = 1.563(2)$, $\beta = 1.565(2)$, $\gamma = 1.577(2)$; $2V_{\text{meas}} = 42(3)^\circ$, $2V_{\text{calc}} = 45^\circ$, strong dispersion: $r > v$. Yusupovite is monoclinic, $C2/m$, $a = 14.5975(4)$, $b = 14.1100(4)$, $c = 14.4394(4)$ Å, $\beta = 90.0399(4)^\circ$, $V = 2974.1(3)$ Å³. 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: Nb₂O₅ 0.39, SiO₂ 58.84, ZrO₂ 16.55, HfO₂ 0.30, FeO 0.01, Y₂O₃ 3.05, Cs₂O 2.58, K₂O 0.95, Na₂O 8.91, H₂O_{calc} 7.40, total 98.98 wt%, with H₂O calculated from structure refinement. The empirical formula (based on 17.5 O apfu) is $(\text{Na}_{1.76}\text{K}_{0.12}\text{Cs}_{0.11})_{\Sigma 1.99}(\text{Zr}_{0.82}\text{Y}_{0.17}\text{Nb}_{0.02}\text{Hf}_{0.01})_{\Sigma 1.02}(\text{Si}_{6.01}\text{O}_{14.98})(\text{H}_2\text{O})_{2.52}$, $Z = 8$. 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 H₂O groups at 18–84%. Due to (K,Cs), Na and H₂O disorder, the symmetry of yusupovite decreases from orthorhombic, space group $Pbcm$ (elpidite), to monoclinic, space group $C2/m$, and the b unit-cell parameter of yusupovite is doubled compared to the corresponding cell parameter in elpidite, $b_{\text{yus}} = 2a_{\text{elp}}$. Yusupovite, ideally $\text{Na}_2\text{Zr}(\text{Si}_6\text{O}_{15})(\text{H}_2\text{O})_3$, is a dimorph of elpidite, $\text{Na}_2\text{Zr}(\text{Si}_6\text{O}_{15})(\text{H}_2\text{O})_3$.

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