

## Slyudyankaite, $\text{Na}_{28}\text{Ca}_4(\text{Si}_{24}\text{Al}_{24}\text{O}_{96})(\text{SO}_4)_6(\text{S}_6)_{1/3}(\text{CO}_2)\cdot 2\text{H}_2\text{O}$ , a new sodalite-group mineral from the Malo-Bystrinskoe lazurite deposit, Baikal Lake area, Russia

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### ABSTRACT

The new sodalite-group mineral species slyudyankaite, ideally  $\text{Na}_{28}\text{Ca}_4(\text{Si}_{24}\text{Al}_{24}\text{O}_{96})(\text{SO}_4)_6(\text{S}_6)_{1/3}(\text{CO}_2)\cdot 2\text{H}_2\text{O}$ , was discovered in altered lazurite-bearing metasomatic rock at the Malo-Bystrinskoe gem lazurite deposit, Baikal Lake area, eastern Siberia, Russia. The associated minerals are diopside, calcite, fluorapatite, phlogopite, lazurite, and pyrite. Slyudyankaite forms green to pale blue isolated anhedral equant grains up to 0.5 cm across and their aggregates. The streak is white and the luster is vitreous. Slyudyankaite is brittle, with a Mohs hardness of 5½. Cleavage and parting are not observed. Density measured by flotation in heavy liquids is equal to 2.46(2) g·cm<sup>-3</sup>. Density, calculated using the empirical formula and unit-cell volume refined from single-crystal XRD data, is 2.454 g·cm<sup>-3</sup>. Slyudyankaite was characterized using the IR, Raman, ESR, near infrared (NIR), visible (Vis), and ultraviolet (UV) absorption, XPS and photoluminescence spectroscopy methods. The chemical composition is (wt%, electron microprobe, H<sub>2</sub>O and CO<sub>2</sub> determined by selective sorption of ignition products, CO<sub>2</sub> confirmed by quantitative IR spectroscopic method, sulfate sulfur determined by wet chemical analysis): Na<sub>2</sub>O 19.28, K<sub>2</sub>O 0.12, CaO 5.13, Al<sub>2</sub>O<sub>3</sub> 27.01, SiO<sub>2</sub> 33.25, SO<sub>3</sub> 10.94, S 1.75, Cl 0.10, CO<sub>2</sub> 1.42, H<sub>2</sub>O 0.90, −O≡(Cl, HS)−0.03, total 99.87. The empirical formula is  $\text{Na}_{27.57}\text{Ca}_{4.05}\text{K}_{0.11}(\text{Si}_{24.52}\text{Al}_{23.48}\text{O}_{96})(\text{SO}_4)_{6.06}\text{S}_{2.42}^0\text{Cl}_{0.12}(\text{CO}_2)_{1.43}\cdot 2.21\text{H}_2\text{O}$  where S<sub>2.42</sub><sup>0</sup> is the total sulfide sulfur, mainly occurring as neutral S<sub>6</sub> and subordinate S<sub>4</sub> molecules, according to the structural data. XPS spectroscopy confirms the presence of sulfide sulfur in neutral form. The crystal structure was determined using single-crystal X-ray diffraction data and refined to  $R = 0.0428$ . Slyudyankaite is triclinic, space group P1,  $a = 9.0523(4)$  Å,  $b = 12.8806(6)$  Å,  $c = 25.681(1)$  Å,  $\alpha = 89.988(2)$ °,  $\beta = 90.052(1)$ °,  $\gamma = 90.221(1)$ °,  $V = 2994.4(2)$  Å<sup>3</sup>,  $Z = 1$ . Slyudyankaite contains two kinds of sodalite cages occurring in the structure in a ratio of 3:1. Cages of the first kind are completely occupied by SO<sub>4</sub><sup>2-</sup> anions and extra-framework cations, whereas cages of the second type contain only neutral molecules (S<sub>6</sub>, CO<sub>2</sub>, H<sub>2</sub>O, and minor S<sub>4</sub>). The strongest lines of the powder X-ray diffraction pattern [ $d$ , Å ( $I$ , %) ( $hkl$ )] are: 6.45 (11) (004, 112, 020), 3.716 (100) (204, 220, 116, 132), 2.878 (12) (136, 028, 044), 2.625 (23) (208, 240), 2.431 (6) (209), 2.275 (6) (048), 2.143 (12) (0.012, 336), 1.784 (7) (444, 1.14, 356, 172).

**Keywords:** Slyudyankaite, sodalite group, microporous materials, polysulfide groups, crystal structure, X-ray diffraction, spectroscopy