N. V. ZUBKOVA,\* I. V. PEKOV,\* N. V. CHUKANOV,\*\* A. V. KASATKIN,\*\*\*
D. A. KSENOFONTOV,\* V. O. YAPASKURT,\* S. N. BRITVIN,\*\*\*\*
D. Yu. PUSHCHAROVSKY.\* REDEFINITION OF LEMANSKIITE:
NEW MINERALOGICAL DATA, CRYSTAL STRUCTURE
AND REVISED FORMULA NaCaCu5(AsO4)4Cl·3H2O

\*\* Moscow State University, Moscow, Russia

\*\* Institute of Problems of Chemical Physics RAS, Moscow, Russia

\*\*\* Fersman Mineralogical Museum, RAS, Moscow, Russia

\*\*\*\* Saint Petersburg State University, Saint Petersburg, Russia

Refinement of the crystal structure of lemanskiite (R = 0.019), studied for the first time, has allowed redefining this mineral: to carry out refinement of its formula; redefine crystal system, space group and parameters of its unit-cell. X-ray powder diffraction pattern of lemanskiite has been correctly identified, the IR spectrum was obtained for its pure sample — free from pollutions by other phases. It is shown that lemanskiite is not a dimorph of lavendulan NaCaCu<sub>5</sub>(AsO<sub>4</sub>)<sub>4</sub>Cl·5H<sub>2</sub>O but contains less H<sub>2</sub>O in comparison with the latter. Studied sample of lemanskiite has been picked up from the oxidation zone of Perseverancia deposit (Guanaco, Antofagasta, Chile). Its empirical formula is Na<sub>0.98</sub>(Ca<sub>0.98</sub>Sr<sub>0.03</sub>)<sub>Σ1.01</sub>Cu<sub>5.07</sub>As<sub>3.97</sub>O<sub>15.97</sub>Cl<sub>1.03</sub>·3H<sub>2</sub>O. The idealized formula of lemanskiite may be written as NaCaCu<sub>5</sub>(AsO<sub>4</sub>)<sub>4</sub>Cl·3H<sub>2</sub>O. The mineral is monoclinic,  $P2_1/m$ , a = 9.250(2), b = 10.0058(10), c = 10.0412(17) Å,  $\beta = 97.37(3)^\circ$ , V = 921.7(3) Å<sup>3</sup>, Z = 2. Lemanskiite represents a new structure type in the lavendulan group. Crystal structure of lemanskiite is based on the heteropolyhedral layers built by clusters of four distorted Cu-centered tetragonal pyramids, linked by edges, and eight AsO<sub>4</sub> tetrahedra connected also with the Cu-centered squares not involved in the clusters. Na-centered trigonal prisms and Ca-centered seven-fold polyhedra, connected with heteropolyhedral layers from both sides of each layer, are linked in the interlayer space by shared edges.

Key words: lemanskiite, lavendulan, lavendulan group, arsenate, crystal structure, oxidation zone, Perseverancia mine, Chile.