

Structural features of $\text{Ca}_8\text{Mg}[\text{SiO}_4]_4\text{Cl}_2$ – product of the people technical activity

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A sample of compound $\text{Ca}_8\text{Mg}[\text{SiO}_4]_4\text{Cl}_2$ was found by B.V. Chesnokov in the mine near Kopeisk (the Urals). The empirical formula on the base of electron-microprobe analysis: $(\text{Ca}_{7.06}\text{Mg}_{0.78}\text{Fe}^{3+}_{0.08}\text{Al}_{0.03})_{7.95} [\text{Si}_{4.02}\text{O}_{15.00}] [\text{Cl}_{1.26}\text{OH}_{0.36}\text{F}_{0.32}(\text{SO}_4)_{0.06}]_2$. Unit cell parameters of the cubic cell are: $a=15.040(4)$ Å, $V=3402.07$ Å³. X-ray single crystal data was collected using ENRAF-NONIUS diffractometer (Mo-radiation). Crystal structure was solved by direct methods and refined in the space group $Fd\bar{3}$ to $R_{\text{aniso}} = 2.6\%$ (495 reflections).

The main fragment of the structure is cluster made of four Si-tetrahedra and one central Mg-tetrahedron linked through the vertex. Average distances Si-O=1.63 Å, Mg-O=1.866 Å. Si-tetrahedra in pairs are oriented in opposite directions. Ca atoms form two types of polyhedra – regular octahedron (Ca-O=2.358 Å) and 8-fold polyhedra (average Ca-O=2.619 Å). Cl is a common vertex of six Ca bipyramids. The mixed framework is built of Si and Mg tetrahedra and Ca octahedra while Ca bipyramids occupy the holes.

The compound under consideration is hightemperature product of the burned rocks as a result of people technological activity.

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