# Single-crystal X-ray diffraction study of melanophlogite from Sakhalin, Far East Russia

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Melanophlogite is one of silica clathrate minerals, which contain various gas molecules in their cage-like framework structures.

We recently discovered new localities of melanophlogite in the South Sakhalin, Far East Russia. In Nevelsk, melanophlogite occurs in calcareous concretion of the Miocene mudstone in association with autochthonous fossils of chemosynthetic fauna such as Conchocele sp. and Acharax sp. Associate minerals are opal and chalcedony, and melanophlogite occurs as aggregates of cubic crystals of sizes up to 0.1 mm.

In “Zamiraylova head” cape, melanophlogite occurs in hydrothermal veins filling fissures of a small basaltic volcanic body. The vein consists of microcrystalline quartz, opal, aragonite, calcite, and pyrite. A lot of cubic pseudomorphs of chalcedony after melanophlogite occur in voids of these veins, while unaltered melanophlogite crystals were only found at the center of thick vein. The same kind of hydrothermal veins are also distributed in a basaltic volcanic body in Kuznetsova cape.

Presence of methane in the samples from “Zamiraylova head” cpae was confirmed by C-H stretching mode of the Raman spectra at ~2900 $cm^{-1}$. Single-crystal X-ray diffraction experiment at room temperature (23˚C) revealed that its crystal structure is consistent with previously reported model, i.e., three-fold twinning of the pseudo-cubic tetragonal structure with space group *P*42/*nbc* (#133). At 100˚C, all reflections arising from 2x2x1 super-cell disappeared and the structure could be refined using cubic *Pm*-3*n* (#223) space group. When it was cooled down to 70˚C, additional reflections reappeared at positions slightly shifted from those expected for 2x2x1 super-cell, indicating a possible presence of long-range order or incommensurate phase between alpha-beta transition of melanophlogite.

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