The crystal structure of low melanophlogite

Takeshi Nakagawa[1], Kuniaki Kihara[2]

[1] Natural Science and Technology, Kanazawa Univ, [2] Dept. of Earth Sci., Kanazawa Univ.

The crystal structure of low natural melanophlogite was first determined using single crystal X-ray diffraction data at room temperature. The structure is tetragonal with space group P42/nbc and unit-cell a=26.818(2) and c=13.365(1) angstrom, which is the (2x2x1) superstructure of high-temperature cubic melanophlogite and includes four formula units. This low temperature form is a displacive variant of the cubic high form. The bond angles for Si-O-Si are distributed in the rather large range from about 145 to 171 degree with the mean of 159.4(3) degree. The oxygen thermal vibrations are highly anisotropic with a wide variety of mean square displacements. A positive correlation is indicated in the relationship between the Si-O-Si bond angles and the mean square displacements.