The Tobermorite-Like Layer in Non-Tobermorite Minerals. Elena Bonaccorsi, Stefano Merlino.

The tobermorite-like layer (TLL) is a characteristic feature in all the structures of the natural and synthetic compounds of the tobermorite group [1]. In those structures eptahedra of calcium cations, characterized by 'a pyramidal part on one side and a dome part on the other side joining the equatorial oxygen atoms', form columns through edge sharing; the columns are connected each other, once again through edge sharing, and adjacent columns present the pyramidal apical ligands on opposite sides of the resulting infinite layers. These layers, decorated with wollastonite chains on both sides, build up the 'complex layers' which are the basic structural module in all the phases of the tobermorite group (Fig. 1).


Byzantievite, ideally Ba(Ca,REE,Y)\(_2\)(Ti,Nb)\(_3\)\((\text{SiO}_4)\)\(_3\)\((\text{PO}_4)\)\((\text{SiO}_4)\)\(_3\)\((\text{BO}_4)\)\(_2\)\(\text{O}_2\)\((\text{OH})\)\(_3\)((\text{H}_2\text{O})\)\(_5\), is the only mineral which contains three different oxyanions: (BO\(_4\)), (SiO\(_4\)) and (PO\(_4\)). They occur in the ratio 9:5:3. Byzantievite occurs in the moraine of the Dara-i-Pozz glacier, the Alai mountain ridge, Tien-Shan Mountains, northern Tajikistan. Byzantievite has no natural or synthetic analogues. The crystal structure of byzantievite, a \(9.1202(2), c 102.145(5)\) \(\text{Å}\), \(\gamma 120\)°, \(V 7357.9(5)\)\(\text{Å}^3\), sp. gr. \(R3\), \(Z=3\), \(D_{calc} 4.151\) \(\text{g/cm}^3\), was solved by direct methods and refined to an \(R\) index of 13.14%. In the crystal structure, there are fifty cation sites. Twenty-three sites are fully occupied and twenty-seven sites are characterized by partial occupancy: six sites are more than 50% occupied and twenty-one sites are less than 50% occupied. In the crystal structure of byzantievite, there are two distinct parts that alternate along the \(c\) axis. Part one is characterized mainly by fully occupied cation sites and part two, mainly by partially occupied cation sites. Part one has a local inversion centre whereas part two does not. Hence the crystal structure of byzantievite lacks an inversion centre. For better understanding of this framework structure, we describe it as sheets of polyhedra stacked along \{001\}. Sheet a is composed of [12]-coordinated Ba atoms. Ti-dominant octahedra and B-triangles share common vertices to form sheet b. [8]-coordinated (Ca,REE, Y) polyhedra and B triangles share common vertices and edges to form sheet c. Sheet d is composed of [10]-coordinated (Ca,REE, Y) polyhedra and P tetrahedra. Sheet e is formed by [8]-coordinated (Ca,REE, Y) polyhedra, Si tetrahedra and B...