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The crystal structure of jonesite, $Ba_2(K,Na)[Ti_2(Si_5Al)O_{18}(H_2O)](H_2O)_n$: A first example of titanosilicate with porous double layers

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ABSTRACT

The crystal structure of jonesite, $Ba_2(K,Na)[Ti_2(Si_5Al)O_{18}(H_2O)](H_2O)_n$ (monoclinic, $P2_1/m$, a = 10.618(2), b = 25.918(4), c = 8.6945(14) Å, β = 127.633(3)°, V = 1894.8(6) Å^3, Z = 4) from the Benitoite Gem Mine, San Benito County, California has been solved by direct methods from a crystal twinned on (001) and refined to R_1 = 0.045 (wR = 0.119, S = 1.028) using 3308 unique observed reflections ($|F_o| \geq 4\sigma_F$). The structure is based upon porous double layers of distorted $Ti\Phi_6$ octahedra (Φ = O, H_2O) and TO_4 tetrahedra (T = Si, Al) parallel to (010). The layers consist of two sheets of corner-sharing $Ti\Phi_6$ octahedra and Si_2O_7 groups each. The two adjacent sheets are linked along b by T_4O_{12} tetrahedral rings that are disordered over two positions. The double layer has an open structure characterized by eight-membered tetrahedral rings with apertures (free diameters) of 3.37×3.37 and 3.33×3.33 Å^2, for two symmetrically non-equivalent rings. K^+ cations and H_2O molecules are located in the pores of the double layers. Ba^{2+} cations are between the double layers and provide their linkage into three-dimensional structure. Jonesite is a first example of titanosilicate with porous double-layer structure.