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Crystal structure of kanemite, $NaHSi_2O_5 \cdot 3H_2O$, from the Aris phonolite, Namibia

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ABSTRACT

Kanemite was studied by single-crystal X-ray diffraction. The mineral, ideally $NaHSi_2O_5 \cdot 3H_2O$, is orthorhombic (space group *Pbcn*); unit-cell parameters are $a = 4.946(3)$, $b = 20.502(15)$, $c = 7.275(3)$ Å, with $Z = 4$. The structure is solved and refined to an R value of 0.058 for 825 independent reflections. The arrangement of atoms consists of alternating (010) sheets of corrugated $[Si_2O_4OH]_n^{n-}$ and hydrated Na. The silicate sheets contain six-membered rings of $HOSiO_3$-SiO_4 units. Sodium atoms coordinate to six water molecules, forming layers of distorted octahedra. Residual electron densities were located that give reasonable positions for four H atoms. One H is part of a silanol group, and the other three H atoms are associated with water bonded to Na. Bonding between the silicate and Na sheets is through hydrogen bonding from H of the Na layer to O of the silicate sheet.