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H positions in leucophoenicite, $Mn_7Si_3O_{12}(OH)_2$: A close relative of the hydrous B phases

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ABSTRACT

The proton positions in leucophoenicite, ideally $Mn_7Si_3O_{12}(OH)_2$, have been determined by neutron powder diffraction under ambient conditions on a natural sample from Franklin, New Jersey. Refinement in the $P2_1/a$ space group gave $R_p = 2.0\%$ ($wR_p = 2.1\%$), $\chi^2 = 4.04$ for 110 refined parameters. The two non-equivalent protons form a pair of hydroxyl groups and make hydrogen bonds to the same O7 atom of the Si1 tetrahedron at distances of 1.99(1) and 2.09(1) Å. The H····H distance in leucophoenicite is 2.16(1) Å, which is more than twice the Van der Waal's radius of H (>2 Å) and so no proton positional disorder is expected in leucophoenicite. A comparison of the H environments is made between leucophoenicite and Phase B, Superhydrous B, and Phase A.