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Refinement of hydrogen positions in synthetic hydroxyl-clinohumite by powder neutron diffraction

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ABSTRACT

The structure of synthetic hydroxyl-clinohumite [$Mg_7Si_4O_{14}$·2Mg(OH)O] was refined for a deuterated sample using powder neutron diffraction data and the Rietveld technique [($P2_1/b$; $Z = 2$; a = 4.7488(1) Å; b = 10.2875(2) Å; c = 13.6967(3) Å; α = 100.63(1)°; V = 657.65(2) Å^3)]. The H atoms of the hydroxyl groups are disordered over two positions with an occupancy of approximately 0.5. This removes the possibility of a strong H-H interaction that was thought to destabilize the structure. The limited occurrence of hydroxyl-clinohumite in nature is the result of compositional rather than crystal chemical constraints.