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O-D···O bond geometry in OD-chondrodite

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ABSTRACT

The crystal structure of OD-chondrodite [$Mg_5Si_2O_8(OD)_2$, $P2_1/b$ (a unique), a = 4.74711(5), b = 10.34888(16), c = 7.90228(13) Å, α = 108.678(1)°] was refined to wR_p = 0.0218, χ^2 = 3.545 at ambient conditions using time-of-flight neutron powder data. The disordered H model proposed for OH-chondrodite on the basis of single-crystal X-ray data is confirmed. The occupations of the D1 and D2 sites are, respectively, 0.52(1) and 0.48(1). The long O5-D1 [1.076(4) Å] and O5-D2 [1.111(4) Å] bond lengths, which are two of the longest O-H(D) bonds observed in mineral structures, reflect the positional disorder of the O5 atom in the unshared OH-OH edge. Both D1 [1.968(4), 2.489(4) Å] and D2 [2.149(4), 2.251(4) Å] atoms are involved in two hydrogen bonds. A re-examination of the origin of positive OH frequency shifts in both F-bearing and OH-chondrodite at high pressure is warranted in view of the crystallographic data.