

LETTER

Crystal structure of a new high-pressure polymorph of topaz-OH

MASAMI KANZAKI*

Institute for Study of the Earth's Interior, Okayama University, Misasa, Tottori 682-0193, Japan

ABSTRACT

A new high-pressure form of topaz-OH (denoted here topaz-OH II) was obtained at 14 GPa and 1400 °C. The X-ray diffraction pattern of this phase can be indexed by an orthorhombic cell with $a = 4.72318(5)$, $b = 8.91480(9)$, and $c = 2.77276(3)$ Å. The lengths of a and b are similar, but c is approximately a third of that for a previously reported topaz-OH (denoted topaz-OH I). The structural formula of topaz-OH II can be written as $(\text{Al}_{0.68}\text{Si}_{0.32})(\text{O}_{0.66}(\text{OH})_{0.34})_2$, suggesting significant cation disorder in the structure. The crystal structure of topaz-OH II is solved using powder synchrotron X-ray diffraction data, and refined with constraints provided by a separate multi-nuclear NMR study. The structure has similarities with topaz-OH I and diaspore (α - AlOOH) structures, having partially occupied double edge-shared octahedral chains, and 2×1 tunnels with partially occupied tetrahedral and octahedral sites.

Keywords: Crystal structure, high-pressure studies, phase transition, order-disorder