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Low-T neutron powder-diffraction and synchrotron-radiation IR study of synthetic amphibole $Na(NaMg)Mg_5Si_8O_{22}(OH)_2$

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^ANa^B(NaMg)^CMg₅Si₈O₂₂(OH,D)₂ amphibole was hydrothermally synthesized at 850 °C and 0.3 GPa. SEM, EPMA, and X-ray powder-diffraction data showed the experimental product to consist of a high amphibole yield (90–95%), plus minor quartz and rare enstatite. Neutron powder-diffraction data were collected using a time-offlight diffractometer at room T and at 8 K, respectively, and structure refinement was carried out using the Rietveld method. The space group of the amphibole is P21/matboth temperatures, as confirmed by the presence of b-type reflections (h + k = 2n + 1)1). FTIR OH- and OD-stretching spectra at both room and low T(30 K) show two main absorptions, which are assigned to two non-equivalent OH groups in the structure, and a third lower-frequency band, assigned to A-site vacant environments (local cummingtonite environments). At room- and low-T, the cell parameters are (in Å): a9.7188(1) and 9.7016(2), b17.9385(3) and 17.8953(4), c5.2692(1) and 5.2574(1); β (°) is 102.526(1) and 102.597(2). Cell volumes (Å3) are 896.78(2) at room T and 890.80(2) at 8 K, with a relative reduction of less than 1%. Accurate structural positions for the hydrogen atoms were obtained from diffraction data. The O5A-O6A-O5A and O5B-O6B-O5B angles, diagnostic of the A- and B-chains kinking along c, are 190.0° and 159.2° at 293 K and 193.8° and 156.8° at 8 K, respectively. The orientation of the thermoelastic strain ellipsoid was calculated and the principal unit-strain tensor components are reported. A comparison between the low-temperature data reported here and the high-temperature data for a similar amphibole composition, reported by Cámara et al. (2003) up to 643 K, is presented.