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

G. Iezzi (1),* **G.D. Gatta** (1**), W. Kokelmann (2), G. Della Ventura (3), R. Rinaldi (4), W. Schäfer (5), M. Piccinini (6), F. Gaillard (1)

(1) Bayerisches Geoinstitut, Universität Bayreuth, Germany; (diego.gatta@uni-bayreuth.de), (2)ISIS, Rutherford Appleton Laboratory, Chilton, Didcot, U.K., (3) Dipartimento di Scienze Geologiche, Università di Roma Tre, Roma, Italy, (4) Dipartimento di Scienze della Terra, Università di Perugia, Italia, (5) Forschungszentrum Jülich, Germany, (6) Laboratori Nazionali di Frascati, I.N.F.N., Italy,* Now at: Dipartimento di Scienze della Terra, Università G. D.Annunzio, Chieti, Italy; (g.iezzi@unich.it), ** Now at: Dipartimento di Scienze della Terra, Università di Milano, Italy

$^{A}Na^{B}(NaMg)^{C}Mg_5Si_8O_{22}(OH,D)_2$ 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-of-flight 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 $P21/m$at both temperatures, as confirmed by the presence of b-type reflections ($h + k$= $2n$+ 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.