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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. KOCKELMANN,[2] G. DELLA VENTURA,[3] R. RINALDI,[4] W. SCHÄFER,[5] M. PICCININI,[6] AND F. GAILLARD[1]**

[1]Bayerisches Geoinstitut, Universität Bayreuth, D-95440 Bayreuth, Germany
[2]ISIS, Rutherford Appleton Laboratory, Chilton, Didcot, U.K.
[3]Dipartimento di Scienze Geologiche, Università di Roma Tre, Largo S. Leonardo, Roma, Italy
[4]Dipartimento di Scienze della Terra, Università di Perugia, Italy
[5]Forschungszentrum Jülich, D-52425 Jülich, Germany
[6]Laboratori Nazionali di Frascati, I.N.F.N., Frascati, Italy

## ABSTRACT

$^{A}Na^{B}(NaMg)^{C}Mg_5Si_8O_{22}(OH,D)_2$ 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 $P2_1/m$ 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): *a* 9.7188(1) and 9.7016(2), *b* 17.9385(3) and 17.8953(4), *c* 5.2692(1) and 5.2574(1); β (°) is 102.526(1) and 102.597(2). Cell volumes (Å$^3$) 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 discussed.