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Si, Al ordering in the double-ring silicate armenite, $BaCa_2Al_6Si_9O_{30}\cdot 2H_2O$: A single-crystal X-ray and ^{29}Si MAS NMR study

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ABSTRACT

The ^{29}Si MAS NMR spectrum of armenite from Wasenalp (Valais, Switzerland) indicates complete Si, Al ordering. The same chemical shifts (−82.3, −95.0, and −101.8 ppm) were also measured for armenite from Rémigny (Quebec, Canada), however, the intensity ratios of the NMR bands for the latter sample differed. A full sphere of X-ray single-crystal data on an optically homogeneous domain of armenite from Rémigny was collected on a three-circle diffractometer equipped with a CCD area-detector. The crystal structure was refined in the acentric space group *Pnc*2 [a = 18.660(2), b = 10.697(1) c = 13.874(2) Å] to R1 = 3.6% based on 4275 reflections. These results confirm complete Si, Al ordering. Mean Si-O distances range between 1.615 and 1.629 Å; mean Al-O distances between 1.734 and 1.742 Å. Calcium is sevenfold coordinated by six framework O atoms and one H_2O molecule. Barium is 12-fold coordinated by framework O atoms. Polarized IR spectra in the region of OH absorptions (between 5700 and 1300 cm^{-1}) were recorded on polished slabs of Wasenalp armenite and structurally related milarite from Val Giuf. In general, milarite and armenite show similar anisotropy of H_2O related absorptions.