

*American Mineralogist, Volume 84, pages 92–101, 1999*

## **Si, Al ordering in the double-ring silicate armenite, $\text{BaCa}_2\text{Al}_6\text{Si}_9\text{O}_{30}\cdot 2\text{H}_2\text{O}$ : A single-crystal X-ray and $^{29}\text{Si}$ MAS NMR study**

**THOMAS ARMBRUSTER\***

Laboratorium für chemische und mineralogische Kristallographie, Universität Bern, Freiestrasse 3, CH-3012 Bern, Switzerland

### **ABSTRACT**

The  $^{29}\text{Si}$  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 *Pnc2* [ $a = 18.660(2)$ ,  $b = 10.697(1)$ ,  $c = 13.874(2)$  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  $\text{H}_2\text{O}$  molecule. Barium is 12-fold coordinated by framework O atoms. Polarized IR spectra in the region of OH absorptions (between  $5700$  and  $1300\text{ cm}^{-1}$ ) were recorded on polished slabs of Wasenalp armenite and structurally related milarite from Val Giuf. In general, milarite and armenite show similar anisotropy of  $\text{H}_2\text{O}$  related absorptions.