

The crystal structures of cesanite and its synthetic analogue—A comparison

A. PIOTROWSKI,¹ V. KAHLENBERG,^{1,*} R.X. FISCHER,¹ Y. LEE,² AND J.B. PARISE²

¹Universität Bremen, Fachbereich Geowissenschaften (Kristallographie),
Klagenfurter Strasse, 28359 Bremen, Germany

²Department of Geosciences, State University of New York, Stony Brook, New York 11794-2100, U.S.A.

ABSTRACT

Single crystals of a synthetic apatite-like phase with composition $\text{Na}_{6.9}\text{Ca}_{3.1}(\text{SO}_4)_6(\text{OH})_{1.1}$ were grown under hydrothermal conditions. This compound crystallizes in the hexagonal space group $P\bar{6}$ ($a = 9.4434(13)$ Å, $c = 6.8855(14)$ Å, $Z = 1$). The structure was solved by direct methods, and subsequently refined using 655 independent reflections ($R1 = 0.0542$). The chemical composition and the unit cell parameters indicated a close structural relationship with the mineral cesanite. A reinvestigation of the mineral showed that the natural and the synthetic phases are isostructural. Small differences result from the incorporation of both H_2O and $(\text{OH})^-$ into the structure of cesanite. Observed systematic absences revealed that the space group $P6_3/m$ allocated to cesanite in earlier studies is incorrect. The crystal structure of a cesanite with composition $\text{Na}_{7.0}\text{Ca}_{3.0}(\text{SO}_4)_6(\text{OH})_{1.0}(\text{H}_2\text{O})_{0.8}$ was successfully refined in space group $P\bar{6}$ ($a = 9.4630(8)$ Å, $c = 6.9088(5)$ Å, $Z = 1$, $R1 = 0.0468$ for 720 independent reflections [$I > 2\sigma(I)$]). The symmetry reduction can be attributed to ordering of the Na and Ca atoms among four symmetrically independent cation sites.