

The Crystal Structure of Sacrofanite, the 74 Å Phase of the Cancrinite Group

Paolo Ballirano^a, Elena Bonaccorsi^b, ^a*Department of Earth Sciences, University of Rome, Italy.* ^b*Department of Earth Sciences, University of Pisa, Italy.* E-mail: paolo.ballirano@uniroma1.it

Sacrofanite, $a = 12.903(2)$, $c = 74.284(8)$ Å, space group $P\bar{6}2c$, is the largest member known to date of the cancrinite group, displaying a 28 layer stacking sequence along the c axis. The members of this group share some structural features with zeolites, their structural cages hosting extra-framework ions as well as H₂O molecules. The crystal structure of sacrofanite has been modeled on the basis of HRTEM images collected by means of a JEOL 4000EX microscope and processed with the program CRISP. The obtained model has been successfully refined vs. synchrotron radiation data (collected at the X-ray Diffraction Beamline at the Elettra facility, Trieste, Italy) up to $R = 0.083$ for 2426 reflections, with a resolution of 0.96 Å. The layer stacking sequence has Zhdanov symbol $|12(8)21|12(8)21|$, and corresponds to ABCABACACABACBACBACABABACABC..., where A, B and C stand for the positions of the six-member rings in each layer. The topological symmetry is $P6_3/mmc$; however the ordering of Si and Al in the tetrahedral sites reduces the symmetry to $P\bar{6}2c$. The resulting framework is formed by two sequences of four cancrinite cages and two sodalite cages along $0, 0, z$, whereas sequences of one losod, one cancrinite, one losod, two sodalite, one liottite, and two sodalite cages develop along both $\frac{1}{3}, \frac{2}{3}, z$ and $\frac{2}{3}, \frac{1}{3}, z$. These cages host extra-framework cations and anions, as well as water molecules. The crystal chemical formula of sacrofanite, as obtained from the refinement, is $(\text{Na,K})_{98}\text{Ca}_{20}(\text{Si}_{84}\text{Al}_{84}\text{O}_{336})(\text{SO}_4)_{26}\text{Cl}_2 \cdot 8\text{H}_2\text{O}$.

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