

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

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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 H<sub>2</sub>O 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  $(\text{Na,K})_{98}\text{Ca}_{20}(\text{Si}_{84}\text{Al}_{84}\text{O}_{336})(\text{SO}_4)_{26}\text{Cl}_2 \cdot 8\text{H}_2\text{O}$ .

**Keywords:** crystal structure, HRTEM, synchrotron radiation