

NAYSi₂O₆: A NOVEL INOSILICATE WITH *VIERER* SINGLE CHAINS

Töbrens, D. M.¹ & Kahlenberg, V.¹

¹Institute of Mineralogy and Petrography, University of Innsbruck, Innrain 52, A-6020 Innsbruck, Austria
 e-mail: Daniel.Toebrens@uibk.ac.at

The existence of a sodium yttrium silicate with composition NaYSi₂O₆ has been first reported by CERVANTES-LEE (1981). In the course of an ongoing project on the phase relations in the system Na₂O-Y₂O₃-SiO₂ we have been able to determine the crystal structure of this compound from laboratory X-ray powder diffraction data. The symmetry is *P*2₁/*c* with unit cell parameters of *a* = 5.40787(2) Å, *b* = 13.69784(5) Å, *c* = 7.58431(3) Å, β = 109.9140(3)° at 25°C (*Z* = 4). The initial structure determination by simulated annealing using the program FOX was successful in space group *P*2₁. A subsequent analysis of the model by the MISSYM algorithm implemented in the program PLATON revealed an additional *c*-glide plane. Structure refinement with FULLPROF converged to residuals of R_{wp} = 7.2, χ² = 2.7, R_{Bragg} = 2.9 with an effective reflection / parameter ratio of 10. The structure was found to be a single chain silicate with a periodicity of four. The two symmetry dependent [Si₄O₁₂]-chains in the unit cell are parallel to *c*. A prominent feature is the strong folding of the chains within the *b,c*-plane resulting in Si-Si-Si-angles close to 90°. As a result, the intra-tetrahedral O-Si-O-angles within the chain are reduced (with an average value of <104.2(6)>°). On the other hand, the O-Si-O-angles involving only the non-bridging O-atoms are significantly larger (<O-Si-O>=122.2(9)°). The coordination of the Y³⁺-ions by O²⁻ is 7-fold in form of slightly irregular pentagonal bipyramids with oxygen atoms from four different chains contributing to the coordination polyhedron. Na⁺-ions are irregularly coordinated by 10 oxygens from two neighbouring chains. No disorder of the cations could be observed.

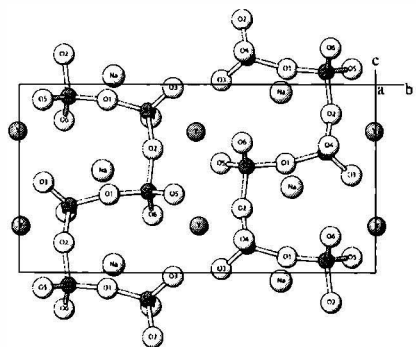


Fig. 1. Structure of NaYSi₂O₆ in projection || *a*

References

[1] CERVANTES-LEE, F. J. (1981): PhD thesis, University of Aberdeen, Scotland.