employed to calculate temperature factor $<\exp(\epsilon_{k}\tau_{0})>$ in order to avoid the inclinations of possible ambiguities arising from further approximations.

The results show that i) any models cannot satisfy the observed data sets unless potential parameters are regarded as temperature dependent (Mair's proposal for model A is preserved) and ii) model A is not good enough. Model B shows a great improvement of R-factor (from 2 to 1.2%) and the result of model C does not show any difference from model B at high temperature (higher than 423K), but in the temperature range from 325 to 373K near the transition temperature, model C is much better than model B since a remarkable improvement of R-factor is noticed (e.g. from 1.92 to 0.88% at 326K). Judging from the sufficiently low value of R-factors for the data at all the nine temperatures observed (R between 0.88 and 1.46%), we believe model C would be the best for this substance.

The integrated reflecting powers of forbidden Bragg reflections 410 and 430 in the crystals VgStI have been measured in a symmetric Bragg geometry on a single-crystal spectrometer at the CuK$_{\alpha}$ radiation. The vertical divergence of the primary beam made 10' and the horizontal one 3'. The calculated unmeasured patterns were in accordance with the experiment and the forbidden reflection intensities were measured in the unmeasured-free regions by means of the $\omega$-scan method. The 410 reflection maximum intensity was 20 c/s and the background 17 c/s; for the reflection 430 the values are 9.5 and 8, where 3 c/s is the fluorescent background of V and 5 the "diffraction" one. The primary beam intensity estimated by the forbidden 222 reflection in a perfect Si crystal was 2.10 c/s.

The obtained integrated reflecting power values are 1.74$\times$10$^{-10}$ and 1.37$\times$10$^{-10}$ for 410 and 430 respectively. The value of structure factors $P(410)=0.3020$ and $P(430)=0.1435$ have been computed upon the determinations are in good agreement with the results of B.Borie (Acta Crystallogr. A 27, 235, 1971) obtained by a somewhat other technique. The paper considers also the low temperature behaviour of these reflections.

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60.5-5 A NEUTRON DIFFRACTION STUDY OF THERMAL EXPANSION AND ANHARMONIC THERMAL VIBRATIONS IN SODALITE, Na$_4$Si$_3$Al$_3$O$_{12}$Cl.

By Richard K. McMullan, Chemistry Department, Brookhaven National Laboratory, Upton, New York 11973; and Subrata Ghose, Department of Geological Sciences, University of Washington, Seattle, Washington 98195.

Sodalite, Na$_4$Si$_3$Al$_3$O$_{12}$Cl is cubic, space group Fd3m, with $a = 8.882(1)$ Å at 295K, 292. The crystal structure consists of a cubo-octahedral framework of alternating AlO$_4$ and SiO$_4$ tetrahedra, with four- and six-membered rings; Cl occurs at the center of the cubo-octahedral cage and Na below the six-membered rings, both in tetrahedral coordination.

The unit cell dimensions and crystal structures of sodalite from Litchfield, Maine were determined from neutron diffraction data at 295, 500, 600, and 700K with $\chi(F^2)$ factors 1.5, 2.0, 1.9 and 1.8 respectively. The Al-Si order within the framework has been confirmed, the Al-O and Si-O bond distances being 1.710(4) and 1.620(4) Å at 295K. The thermal expansion of the tetrahedral framework, which is nonlinear, is principally effected through the increase of the Al-O-Si angles from 138.24(2)° at 295K to 140.25(3)° at 700K; concurrently, the Na-O distance increases from 2.356(1) to 2.400(1) Å. The antiharmonic thermal vibrations of the framework atoms are negligible, whereas those of Na and Cl increase considerably with temperature.

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60.5-4 ON THE STUDY OF FORBIDDEN REFLECTIONS IN VgStl.


The study of forbidden reflections in the Y$_2$Si$_2$O$_5$ (YgStl) crystal has been performed by a method of "unmeasured regions" described in a previous paper (Acta Crystallogr. A 36, 424-425, 1980). The results are presented in the paper and the discussion is restricted to the question of the feasibility of using this method in practice.