

employed to calculate temperature factor  $\langle \exp(i\mathbf{K}\cdot\mathbf{r}) \rangle$  in order to avoid the inclusions 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.

06.5-4 ON THE STUDY OF FORBIDDEN REFLECTIONS IN  $V_2Si$ . By A.I.Kolosovsky, Yu.A.Rosenberg, L.I.Kleshchinsky, V.M.Kiselev, Inst. of Transp. Engineers, 664074 Irkutsk and N.V.Shokhirev, Inst. of Chem. Kinetics, Sib. Branch of Academy of Sciences, 630090 Novosibirsk, USSR.

The integrated reflecting powers of forbidden Bragg reflections 410 and 430 in the crystals  $V_2Si$  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 umweganregung patterns were in accordance with the experiment and the forbidden reflection intensities were measured in the umweg-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  $2 \cdot 10^7$  c/s.

The obtained integrated reflecting power values are  $1.71 \cdot 10^{-10}$  and  $1.37 \cdot 10^{-10}$  for 410 and 430 respectively. The values of structure factors  $F(410) = 0.30 \pm 0.03$  and  $F(430) = 0.145 \pm 0.015$  computed upon these determinations are in good agreement with the results of B. Borie (Acta Crystallogr. A 37, 238, 1981) obtained by a somewhat other technique.

The paper considers also the low temperature behaviour of these reflections.

06.5-5 A NEUTRON DIFFRACTION STUDY OF THERMAL EXPANSION AND ANHARMONIC THERMAL VIBRATIONS IN SODALITE,  $Na_4Si_3Al_3O_{12}Cl$ . 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,  $Na_4Si_3Al_3O_{12}Cl$  is cubic, space group  $P\bar{4}3m$ , with  $a = 8.882(1)$  Å at 295K,  $Z=2$ . 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  $R(F^2)$  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 1.7407(4) and 1.6200(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  $138.24(2)^\circ$  at 295K to  $140.25(3)^\circ$  at 700K; concurrently, the Na-O distance increases from 2.356(1) to 2.400(1) Å. The anharmonic thermal vibrations of the framework atoms are negligible, whereas those of Na and Cl increase considerably with temperature.

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06.6-1 LESSONS FROM THE I.U.Cr. X RAY ATTENUATION PROJECT. D.C. Creagh, Department of Physics, Royal Military College, Duntroon, A.C.T. 2600, AUSTRALIA, and J.H. Hubbell, Radiation Physics Division, Centre for Radiation Research, National Bureau of Standards, Washington, D.C. 20234, U.S.A.

The I.U.Cr. X ray Attenuation Project which was inaugurated in 1978 under the auspices of the Commission for Crystallographic Apparatus is now almost finished. Some laboratories have yet to report their results and we are still receiving enquiries by laboratories wishing to join the project. It is our intention to provide specimen materials to these laboratories and to produce, at a later stage, addenda to the project reports which are now in the final stages of preparation.

This paper will discuss such important questions as:

- \* the need for complete sample characterization to ensure that the correct experimental configuration is chosen for the measurement;
- \* the strengths and weaknesses of different experimental configurations; and,
- \* the deficiencies of existing published data sets.

We are deeply saddened that the Chairman of the Commission for Crystallographic Apparatus, Sixten Abrahamsson, died before the presentation of the report on our project, in which he had taken a great interest.