

mate parameters $x=0.30$, $y=0.11$, $z=0.13$. Calculated structure amplitudes with Ca^{++} at 0, 0, 0; 0, 0, $\frac{1}{2}$; O' at $\frac{1}{2}$, $\frac{1}{2}$, $\pm z$ with $z=0.06$ and for an arrangement with Ca^{++} at 0, 0, $\frac{1}{2}$; 0, 0, $\frac{3}{4}$; O' at $\frac{1}{2}$, $\frac{1}{2}$, $\pm z$ with $z=0.19$ were almost equally in good agreement with observed values. The slight difference in agreement, however, favored the latter positions which place the water molecules at the corners of a square Archimedean antiprism about the calcium ion at the center of the co-ordination group.

This investigation is being continued in an effort to

establish the correct structure, and to note the effect on the structure as the radius of the central ion varies in the series $\text{CaO}_2 \cdot 8\text{H}_2\text{O}$, $\text{SrO}_2 \cdot 8\text{H}_2\text{O}$ and $\text{BaO}_2 \cdot 8\text{H}_2\text{O}$.

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The structure of the ferroelectric niobates and tantalates. By P. VOUSDEN, *H. H. Wills Physical Laboratory, Royal Fort, Bristol 8, England*

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The symmetries and parameters of the recently reported ferroelectric materials KTaO_3 , KNbO_3 , NaTaO_3 , NaNbO_3 (Matthias, 1949) have been measured by X-ray powder methods. At room temperature KTaO_3 is cubic and the other compounds are orthorhombic in symmetry. NaNbO_3 and KNbO_3 have tetragonal and cubic phases at higher temperatures similar to BaTiO_3 , but NaNbO_3 has no rhombohedral phase as low as -173°C .

Untwinned crystals of NaNbO_3 have been investigated by single-crystal methods. The unit cell has dimensions $\approx 5.6 \times 16 \times 5.6 \text{ \AA}$. and contains eight molecules. The space group is $P2_22_1$ and the structure has twenty-six parameters, most of which have been determined. The results show a displacement of the niobium ions by $\approx 0.1 \text{ \AA}$. along the long orthorhombic axis.

The space group conclusively shows the structure to be

non-polar unless the symmetry is really monoclinic (cf. Rochelle salt). However, optical and X-ray measurements have shown that any shear of the faces is $< 0.1'$, which is $< \frac{1}{300}$ of the orthorhombic distortion. The conclusion that orthorhombic NaNbO_3 is non-polar is most unexpected but can thus hardly be avoided.

A consistent explanation of the ion displacements can be given in terms of packing considerations alone. It is supposed that the orthorhombic distortion caused by the ferroelectricity allows ion shifts which reduce the misfit caused by the small sodium ion. It is this arrangement that can be shown to be non-polar. A detailed account of these researches will be published later.

Reference

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Crystal structure of 2,5-dimethoxy-2,5-dimethyl-1,4-dioxane.* By DEXTER FRENCH, *Chemistry Department, Iowa State College and Agricultural Experiment Station, Ames, Iowa, U.S.A.*

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This compound was of interest to us because of a report by Bergmann (1924) that it forms a crystalline iodine addition product which might be considered to be a simple model for the starch iodine complex. Preparatory to an examination of the iodine complex, a brief crystallographic investigation was carried out on the uncomplexed dioxane. Inasmuch as the iodine complex appeared to be too unstable to permit the use of ordinary diffraction techniques, the study was discontinued.

Inspection of the molecular structure of 2,5-dimethoxy-2,5-dimethyl-1,4-dioxane indicates the possibility of *cis* and *trans* stereoisomers, and it was hoped that the determination of the crystal symmetry might distinguish between these possibilities. However, the monoclinic space group $C2/c$ with four molecules per cell requires only that the molecule must have either a center of symmetry (*trans*, chair form for the dioxane ring) or a two-fold axis

(racemic mixture of *cis* forms; boat form for the dioxane ring).

Crystals of this compound are volatile; in the course of a few days' exposure to air the crystals were badly eroded although the diffraction patterns remained excellent. The unit-cell and space-group data were obtained by oscillation ($\text{Cu } K\alpha$) and Laue patterns:

$$a_0 = 11.4, b_0 = 6.4, c_0 = 13.2 \text{ \AA}; \beta = 95.7^\circ;$$

space group Cc or $C2/c$ with four molecules per unit cell. These values are in fair agreement with optical crystallographic data given by Nef (1904)

$$(a : b : c = 1.77246 : 1 : 2.00865, \beta = 84^\circ 13',$$

monoclinic holohedral). The space group Cc may be eliminated assuming that the previous assignment to the monoclinic holohedral class is correct.

References

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