

were green and pale yellow in colour respectively. The former crystals were found to have lost 2-3% in weight while the latter had gained 2-3%, during firing.

When examined under the microscope crystals of both colour were found to be biaxial. X-ray single-crystal rotation photographs showed the structure to be orthorhombic, but a simpler structure cell than that reported by Goodman (1953) fitted the data. For both green and yellow crystals the calculated dimensions were

$$a = 17.51, b = 17.81, c = 7.73 \text{ \AA},$$

compared with Goodman's values

$$a_0 \sim 25, b_0 \sim 25, c_0 \sim 7 \text{ \AA}.$$

The measured density was approximately 6.6 g.cm.^{-3} , and this suggests that the new unit cell contains 20

molecules, compared with the 40 molecules proposed for the larger cell.

Permittivity values were also measured at various temperatures for slices cut from some of the larger yellow crystals. Sharp maxima, of the order of 15,000, were obtained in the permittivity/temperature curves at 570° C. (the Curie temperature found by Goodman (1953)) for directions of measurement lying in the principal cleavage plane of the crystals. When similar measurements were made in a direction perpendicular to the cleavage plane no maxima were obtained.

Further studies of single crystals of orthorhombic lead niobate are being made by electrical, X-ray and optical methods, and it is hoped to describe the results in detail in a separate paper.

Reference

GOODMAN, G. (1953). *J. Amer. Ceram. Soc.* **36**, 368.

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The structure of TiF_3 .^{*} By STANLEY SIEGEL, Argonne National Laboratory, Lemont, Illinois, U.S.A.

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Ehrlich & Pietzka (1954) have reported the unit cell of TiF_3 as rhombohedral with $a = 5.52_3 \text{ \AA}$ and $\alpha = 58.88^\circ$. Our measurements indicate similar values:

$$a = 5.519 \pm 0.002 \text{ \AA}, \alpha = 59.07 \pm 0.07^\circ.$$

Powder patterns recorded with $\text{Cu K}\alpha$ radiation ($\lambda\alpha_1\alpha_2 = 1.5417 \text{ \AA}$) in a camera of 19 cm. diameter show the pseudo-cubic character of the cell. Several maxima are not resolved, and microphotometer tracings give weak indications only of the multiple nature of these lines.

The extinctions and structure reported here are consistent with the space group $R\bar{3}c$. The cell contains two molecules with

$$\begin{aligned} & 2 \text{ Ti in } 0, 0, 0; \frac{1}{2}, \frac{1}{2}, \frac{1}{2}, \\ & \text{and } 6 \text{ F in } \pm(x, \frac{1}{2}-x, \frac{1}{4}); \pm(\frac{1}{2}-x, \frac{1}{4}, x), \\ & \pm(\frac{1}{4}, x, \frac{1}{2}-x), \text{ with } x = -0.183 \pm 0.011. \end{aligned}$$

TiF_3 is therefore isostructural with VF_3 reported by Jack & Gutmann (1951). Each titanium atom occupies the center of a slightly distorted octahedron formed by six fluorine atoms, with $\text{Ti}-6 \text{ F} = 1.97 \pm 0.02 \text{ \AA}$. The fluorine atoms lie in planes normal to the $[111]$ direction and an octahedron is formed from three fluorines in each plane on either side of a titanium atom. The normal distance between a titanium atom and a fluorine plane is 1.13 \AA . The fluorine-to-fluorine distances within the octahedra are 2.78 ± 0.02 and $2.79 \pm 0.02 \text{ \AA}$.

The X-ray data are presented in Table 1. Reflections extending to $\sin^2 \theta = 0.93$ are observed on the film. However, maxima suitable for intensity purposes range up to $\sin^2 \theta = 0.40$ only.

^{*} Work performed under the auspices of the U.S. Atomic Energy Commission.

Table 1. Observed and calculated data

hkl	$(\sin^2 \theta)_o$	$(\sin^2 \theta)_c$	$I_o^{\frac{1}{2}}$	$I_c^{\frac{1}{2}}$
110	0.03934	0.03959	110	154
211	0.07840	0.07808	46	45
$10\bar{1}$	0.07933	0.08028	32	34
210	0.1090	0.1091	40	49
222	0.1196	0.1154	10	7
200	0.1582	0.1199	81	75
220	0.1582	0.1584	22	23
$20\bar{1}$	0.1909	0.1905	68	66
321	0.1956	0.1957	50	54
$21\bar{1}$	0.1992	0.2001	21	20
332	0.2330	0.2320	37	33
310	0.2398	0.2384	14	16
$2\bar{1}\bar{1}$	0.2674	0.2408	35	39
422	0.3124	0.2675	25	29
220	0.3213	0.3123	*	—
432	—	0.3211	*	—
421	—	0.3400	*	—
433	0.3475	0.3445	*	—
$31\bar{1}$	—	0.3475	*	—
$21\bar{2}$	—	0.3500	*	—
330	0.3572	0.3511	*	—
$41\bar{1}$	0.3572	0.3562	*	—
$30\bar{1}$	0.3602	0.3562	*	—
431	0.3602	0.3607	20	21
$32\bar{1}$	0.3931	0.3926	14	15
	0.3978	0.3991		

* Not resolved in intensity.

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References

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