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Short Communications

Contributions intended for publication under this heading should be expressly so marked; they should not exceed about 500 words; they should be forwarded in the usual way to the appropriate Co-editor; they will be published as speedily as possible; and proofs will not generally be submitted to authors. Publication will be quicker if the contributions are without illustrations.

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The crystal structure of Rb_2ThF_6.

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A preliminary survey of the system RbF–ThF_4 (Thoma, 1957) revealed the existence of a compound with the formula Rb_2ThF_6. Examination of the compound by means of the polarizing microscope showed it to be uniaxial positive with indices of refraction

$$N_E = 1{\cdot}494 \pm 0{\cdot}003 \quad \text{and} \quad N_O = 1{\cdot}472 \pm 0{\cdot}003$$

(Landau, 1957). Optical investigations of materials of the above composition quenched from the temperature range 800 °C. to 400 °C. exhibited no phase changes and constant optical properties.

Debye–Scherrer diffraction films were taken of powdered samples using a 114·6 mm.diag. cylindrical camera and Cu $K\alpha$ ($\lambda = 1{\cdot}5418$ Å) radiation. The data thus obtained were indexed and found to best fit a hexagonal cell whose lattice parameters are $a_0 = 6{\cdot}85 \pm 0{\cdot}020$ Å and $c_0 = 3{\cdot}83 \pm 0{\cdot}020$ Å. The density was pycnometrically measured as 5·45 g.cm.$^{-3}$ which may be compared with an X-ray density of 5·56 g.cm.$^{-3}$ calculated with one molecule of Rb_2ThF_6 per unit cell. No systematic absences of reflections were observed from the powder X-ray diffraction data.

The lattice dimensions, crystal symmetry, and diffracted X-ray intensity distribution of Rb_2ThF_6 indicate a close structural relationship with β_1-K_2ThF_6 (Zachariasen, 1948). Presuming these two compounds to be isostructural, the atoms were placed in those positions deduced by Zachariasen in accordance with the space group $C\bar{6}2m$, namely,

2 Rb in $(\frac{1}{3}, \frac{2}{3}, \frac{1}{2})$; $(\frac{2}{3}, \frac{1}{3}, \frac{1}{2})$.
1 Th in (0, 0, 0).
3 F in $(x, 0, 0)$; $(0, x, 0)$; $(\bar{x}, \bar{x}, 0)$ where $x = 0{\cdot}640$.
3 F in $(x, 0, \frac{1}{2})$; $(\bar{x}, \bar{x}, \frac{1}{2})$; $(0, x, \frac{1}{2})$ where $x = 0{\cdot}220$.

Table 1 shows the satisfactory agreement of observed and calculated intensities, the latter calculated from the formula

$$I \propto |F|^2 . p . (1 + \cos^2\theta)/\sin^2\theta \cos\theta ,$$

where F is the structure amplitude, and p is the multiplicity factor.

Table 1. *Comparison of observed and calculated intensities for* Rb_2ThF_6

hk·l	*d* (Å)	*I* (obs.)*	*I* (calc.) $\times 10^{-5}$
10·0	5·92	16	18
00·1	3·82	0	0·3
11·0	3·43	33	36
10·1	3·23	30	37
20·0	2·97	4	3
11·1	2·79	3	2
20·1	2·35	21	23
21·0	2·25	5	3
30·0	1·98	13	12
21·1	1·94	25	26
00·2	1·92	0	4
10·2	1·83	5	3
30·1	1·756	2	0·9
22·0	1·710	6	5
11·2	1·676	10	9
31·0	1·644	0	1
20·2	1·615	0	1
31·1	1·511	10	9
40·0	1·489	0	0·6
21·2	1·460	0	1·7
40·1	1·344	8	3

* Peak intensities observed from an X-ray diffractometer tracing of a sample prepared by the method of McCreery (1949).

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