Although the expressions for the α_j and β_j seem rather forbidding in appearance, in fact the 1620 can evaluate c in a very few seconds once the sum of the intensities is known. Furthermore if anomalous scattering is not important then α_4, α_5, α_6, β_4, β_5, β_6 are all zero.

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The crystal structure of β-K_3Bi*.

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K_3Bi undergoes a phase change at 280 °C. The low temperature form, α-K_3Bi, has the Na_3As, DO_{18}, type structure (Brauer & Zintl, 1937). The structure of the high temperature modification, β-K_3Bi, determined from powder patterns taken at 400 °C., is of the BiF_3, DO_3 type.

Samples of K_3Bi were crushed in a dry box and loaded into 0·3 mm. quartz capillaries. Powder photographs were taken at about 400 °C. in a Central Research Laboratories high temperature powder camera using Cu $K\alpha$ radiation ($\lambda = 1{\cdot}5418$ Å). These patterns were indexed as face-centered cubic with $a = 8{\cdot}805 \pm 0{\cdot}005$ Å. The density calculated on the basis of four K_3Bi formula units per unit cell is 3·17 g.cm.$^{-3}$.

The symmetry and composition of this phase suggest a structure of the DO_3 type of BiF_3 and this structure was ultimately confirmed. Among other compounds, Li_3Bi (Zintl & Brauer, 1935) and β-Li_3Sb (Brauer & Zintl, 1937) also have this same structure. The atoms occupy the following positions of space group O_h^5–$Fm3m$ (*International Tables for X-ray Crystallography*, 1952):

4 Bi in 4*a*: (0, 0, 0) + face centering,
4 K_I in 4*b*: ($\frac{1}{2}$, $\frac{1}{2}$, $\frac{1}{2}$) + face centering,
8 K_{II} in 8*c*: ($\frac{1}{4}$, $\frac{1}{4}$, $\frac{1}{4}$; $\frac{3}{4}$, $\frac{3}{4}$, $\frac{3}{4}$) + face centering.

The intensities of the first 14 lines of a typical powder pattern were estimated by visual comparison with a standard scale. After correction of the intensities by the Lorentz-polarization and multiplicity factors, structure factors were obtained for each of the 16 contributing forms. These data were used in a least squares refinement to obtain isotropic temperature factors for each species of atom and a scale factor. The atomic form factors of James & Brindley (1931) for neutral atoms were used in the calculated structure factors. The reliability coefficient, $R = \Sigma|F_o - F_c|/\Sigma|F_o|$, was 0·10 after these computations. The isotropic temperature factors which resulted are 2·2 Å^2 for Bi, 13·9 Å^2 for K_I, and 9·5 Å^2 for K_{II}. The powder pattern is listed in Table 1; the the intensities have been normalized so that the maximum I_0 is 100.

Table 1. *Powder pattern of* β-K_3Bi

hkl	d_o	d_c	I_o	I_c
111	5·07 Å	5·08 Å	75	66
200	4·36	4·40	62	40
220	3·10	3·11	100	160
311	2·647	2·655	89	77
222	2·540	2·539	27	22
400	2·195	2·200	45	34
331	2·013	2·020	48	46
420	1·964	1·969	30	39
422	1·795	1·797	55	71
511, 333	1·693	1·695	40	40
440	1·556	1·557	25	21
531	1·489	1·488	37	41
442, 600	1·468	1·468	19	22
620	1·396	1·392	27	26

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