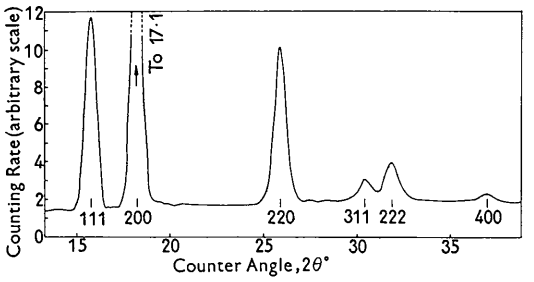

Fig. 1. Neutron diffraction powder pattern of potassium cyanide.

We have also collected the neutron diffraction powder data of potassium cyanide at room temperature and the experimental pattern is given in Fig. 1. This pattern was recorded at the Canada-India Reactor at a wavelength of 1·029 Å with the diffractometer described elsewhere (Chidambaram, Sequeira & Sikka, 1964). The sample was Baker A.R. grade potassium cyanide taken in a cylindrical thin-walled aluminum container of 10 mm diameter. The observed structure factors are given in Table 1.

Table 1. *Observed and calculated structure factors*

		F_c	
hkl	F_o*	DYN	DIS
111	3·65 (3·63)	3·72	3·66
200	5·92 (5·93)	5·94	5·91
220	4·46 (4·68)	4·52	4·54
311	1·18 (1·29)	1·21	1·17
222	3·70 (3·50)	3·43	3·55
400	2·38 (2·26)	2·62	2·32

* The values in parentheses are derived from the reported experimental intensities of Elliott & Hastings (1961).

The structure factors were calculated for the two models using the following formulae:

$$F_{\mathrm{DYN}} = 4b_{\mathrm{K}} \exp(-B_{\mathrm{K}} \sin^2\theta/\lambda^2) \pm 4\left[\sum_{i=\mathrm{C,N}} b_i \sin x_i/x_i\right] \exp(-B_{\mathrm{C,N}} \sin^2\theta/\lambda^2)$$

$$F_{\mathrm{DIS}} = 4b_{\mathrm{K}} \exp(-B_{\mathrm{K}} \sin^2\theta/\lambda^2) \pm 4\left[\sum_{i=\mathrm{C,N}} b_i \cos 2\pi hr_i/\sqrt{3}a \cos 2\pi kr_i/\sqrt{3}a \cos 2\pi lr_i/\sqrt{3}a\right] \times \exp(-B_{\mathrm{C,N}} \sin^2\theta/\lambda^2)$$

where $x_i = 4\pi r_i \sin\theta/\lambda$, r_i is the distance of C or N from the centre of gravity of the cyanide ion, and the $\pm$ sign in both formulae is chosen according as *hkl* are all even or all odd. A C–N distance of 1·16 Å was assumed and temperature factors of $B_{\mathrm{K}} = 2$ and $B_{\mathrm{C,N}} = 5$ were used which seemed to give the best agreement between the observed and the calculated structure factors as shown in Table 1. The F_o's have been normalized to the average of the two models.

The static disordered model seems to give slightly better agreement between F_o's and F_c's as compared with the dynamic model but it is not possible to say anything conclusive in favour of or against either model. Although least-squares refinement is likely to improve the agreement on both the models no such refinement has been attempted in view of the meagreness of the data. It may be mentioned here that neither the X-ray study of potassium cyanide by Siegel (1949) nor the Raman effect study by Mathieu (1954) could choose between the two models. The study of the heat capacity data (Messer & Zeigler, 1941) favours the existence of hindered rotation of the cyanide ions at room temperature. It appears possible to decide between the two models if high angle neutron diffraction data are collected with single crystals, and it is proposed to undertake such a study shortly.

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The evaluation of centroid lattice parameter data for tungsten by the likelihood ratio method. A correction.

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In a note added in proof in a recently published article (Beu, 1964, p. 1152) the number 3·165196 was inadvertently shortened to 3·16519, and this tends to obscure the meaning of the note. The note should read as follows:

$\hat{\hat{a}}_0$ calculated at 25 °C and corrected for refraction is 3·165196 ± 0·000018 Å (95% confidence limits). This is to be compared with $\bar{a} = 3{\cdot}165190$ Å given by Delf for the same data but calculated in a different manner (Delf, 1963). Both $\hat{\hat{a}}_0$ and $\bar{a}$ agree within the stated confidence limits.

Reference

Beu, K. E. (1964). *Acta Cryst.* **17**, 1149.