

measurements by Williams (1961) also failed to produce a definite solution.

A comparison of the bond lengths in FeAl₃ and α -FeCuAl (Table 2) reveals that the largest differences between the two structures occur when an Al(2) or Al(4) atom is involved. This suggests that it is these sites which are affected most when the Cu atoms are introduced into the structure and thus it seems likely that these are the sites which are occupied by the Cu atoms in α -FeCuAl. This deduction is in agreement with the conclusions of Phillips (1953-54) although Black *et al.* (1961) were unable to detect Cu atoms in these sites.

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Short Communications

Contributions intended for publication under this heading should be expressly so marked; they should not exceed about 1000 words; they should be forwarded in the usual way to the appropriate Co-editor; they will be published as speedily as possible. Publication will be quicker if the contributions are without illustrations.

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On the detection of cyanide-ion rotation in potassium cyanide by neutron diffraction. By

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Recently, considerable interest has been shown in the study of the crystal structure of cyanides by neutron diffraction, in view of the fact that the neutron scattering amplitudes of carbon and nitrogen, apart from being significantly unequal, are comparable to and often exceed those of the metal atoms in contrast to their X-ray scattering factors (Bacon, 1963). This enables the carbon and nitrogen atoms to be distinguished and also accurately located in the presence of metal atoms. One of these investigations has been on potassium cyanide by Elliott & Hastings (1961), who, from a study of the neutron-diffraction powder data, concluded that at room temperature the cyanide ions in this cubic crystal (space group $Fm\bar{3}m$) are freely rotating (Pauling, 1930), rather than disordered, *i.e.* oriented at random along the eight [111] directions (Frenkel, 1935). This distinction in favour of the dynamic model against the static disordered model seemed somewhat surprising in view of the considerable difficulty we had in choosing between several models for cubic K₂Zn(CN)₄, even using single-crystal neutron data. The structure-factor calculations

of Elliott & Hastings on the basis of the static disordered model seem, however, to be in error.*

* *Note added on 1 September:* Elliott & Hastings in their reply to the editor say that there is indeed an arithmetical error in the calculation of their 111 intensities, but that correction of this would not have altered their conclusions. They also point out that they did not apply any Debye-Waller correction. While with the temperature factors used by us, our F_c 's on the basis of the dynamic model are in approximate agreement with the intensities calculated by Elliott & Hastings, removal of the temperature factors takes the calculated values for the dynamic model once again close to those for the static disordered model without temperature factors. In short, with or without Debye-Waller correction, distinction between the two models on the basis of powder neutron data seems difficult. It may be mentioned here that from the point of view of a diffraction experiment, it is not also possible to distinguish between a static disordered model and one in which the cyanide ions are undergoing hindered rotation and therefore the latter model can also be considered consistent with our data.

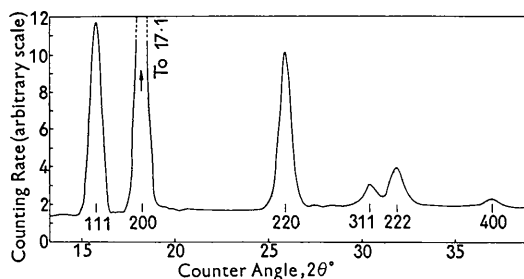


Fig. 1. Neutron diffraction powder pattern of potassium cyanide.

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

<i>hkl</i>	F_o^*	F_c	
		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:

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

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

A correction. By KARL E. BEU, *Development Laboratory, Goodyear Atomic Corporation, Piketon, Ohio, U. S. A.*

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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{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 $\bar{a} = 3.165190$ Å given by Delf for

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

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 $B_K = 2$ and $B_{C, N} = 5$ 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 same data but calculated in a different manner (Delf, 1963). Both \hat{a}_0 and \bar{a} agree within the stated confidence limits.

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