

ordering of the  $\text{CN}^-$  molecules is more complete in this phase. The value for  $B_{\text{CN}}$  in the fit to the diffraction pattern collected at 25 kbar,  $23^\circ\text{C}$  ( $B_{\text{CN}} = 2.80 \text{ \AA}^2$ , Table IV) gives a linear motional amplitude for the CN ion  $\langle \mu_x^2 \rangle_{\text{CN}}^{1/2} \sim .19 \text{ \AA}$  (Eq. (4)) which is to be compared with the values  $B_{\text{CN}} = 4.0 \text{ \AA}^2$ ,  $\langle \mu_x^2 \rangle_{\text{CN}}^{1/2} \sim .24 \text{ \AA}$  for KCN III. The value for  $B_{\text{K}}$  in phase IV is essentially zero in contrast to the large  $B_{\text{K}} = 2.7 \text{ \AA}^2$  found in phase III. (The result that the thermal factor for the potassium ion  $B_{\text{K}}$  has been reduced to zero in each of the above fits means that, in the course of the fitting, the statistical error for this parameter exceeded its value.) We suggest the following explanation for this result. In KCN I the large motional amplitude for the  $\text{K}^+$  ions is associated with the local dilatations accompanying the rotational motions of the  $\text{CN}^-$  ion. This also seems a reasonable picture for KCN III. In KCN IV the ordering of the  $\text{CN}^-$  molecules is more complete, and it is likely that these rotational motions are largely absent. Consequently the local dilatations of the  $\text{K}^+$  ions should be absent also.

Results for the computer fit to a third diffraction pattern for KCN IV (22 kbars,  $66^\circ\text{C}$ ) are also summarized in Table IV. Comparison of the value for the C-N bond length  $1.02 \pm .06 \text{ \AA}$  with that obtained for the room temperature measurement at 25 kbars,  $1.16 \pm .03 \text{ \AA}$ , indicates that the C-N bond contracts somewhat as the temperature is increased in phase IV.

An attempt was made to fit the KCN IV data (25 kbars,  $23^\circ\text{C}$ ) using the rhombohedral space group  $R\bar{3}m (C_{3v}^5)$ . This introduced an additional positional parameter in comparison with the fit to  $R\bar{3}m(D_{3d}^5)$  since the C and N positions are now allowed to vary individually. However the fit was essentially different from that described for the space group  $R\bar{3}m$  since the fitting program was modified to include the effect of preferential line broadening due to a domain size effect following