

pairs (401), (312) and (200), (111) which are not fit well in the diffraction pattern collected at 25 kbar and 23°C (Fig. 5) are very poorly fit in the diffraction pattern collected at 34 kbars which also shows a similar discrepancy for the second order reflection of the (200), (111) pair. These discrepancies may indicate the presence of preferred orientation in KCN IV or may be due to an inadequacy in the assumed space group.

Results for measurements in phase IV at two different temperatures (Table IV) indicate that the C-N bond length contracts as the temperature is increased in phase IV although the value for bond length from the measurement at higher temperature ($1.02 \pm .06 \text{ \AA}$) is suspect due to the large uncertainty associated with it. Further increase of the temperature results in the transformation into the cubic phase III wherein the C-N bond length has lengthened to $1.23 \pm .02 \text{ \AA}$, a value which is slightly higher than the original value for the bond length $1.16 \pm .03 \text{ \AA}$ in phase IV at room temperature. This result could be independently checked by infrared spectroscopy. It is also apparent from Table IV that the C and N nuclei are nearly along the body diagonal of a slightly distorted cube of K^+ ions in the C_s^3 structure. This is the case if $x_N = z_N$ and $x_C = z_C$ and even though the ratio of x/z in these analyses was completely free the best fit to that data is for them to be close to unity.