

an analysis of domain line broadening for single crystal x-ray diffraction carried out by Evenson and Barnett.²¹ Although the resultant fit reproduced the observed line shapes fairly well it could not account for the displacement of observed peak positions discussed above. This fit also could not account for the observed intensity for the diffraction line with rhombohedral indexing (221). This discrepancy was pointed out for the monoclinic analysis since the monoclinic pair (401), (312) corresponds to the rhombohedral (221) line in the undistorted cell. The goodness of fit ratio for this analysis (5.3) was significantly worse than the corresponding ratio for the monoclinic analysis (3.7).

V. DISCUSSION AND CONCLUSION

The KCN III phase seems to be understood reasonably well. The crystal structure is cubic with the space group $Pm\bar{3}m(O_h^1)$. The diffraction peak intensities are well represented assuming a disordered crystal with the CN^- ion randomly distributed over the 8 diagonal configurations. The temperature factors are unusually large indicating a high probability of the CN^- ion jumping between equilibrium positions. The large motional amplitude for the K^+ ions may be caused by local dilatations accompanying the rotational motions of the CN^- ion. This dynamical picture is very similar to that proposed for KCN I.⁴

The KCN IV phase is more difficult to definitively interpret. There is some displacement of the (100) and (200) peaks from their exact rhombohedral positions ($\sim .014 \text{ \AA}$ and $.007 \text{ \AA}$, respectively) which, although small, is well outside the accuracy of the