

experiment. This indicates some distortion of the rhombohedral structure. Such a distortion leads to a centered monoclinic lattice of space group  $C_m (C_s^3)$ .

Two features of the monoclinic analysis of the KCN IV phase stand out. First the C and N atoms are ordered in the  $C_m(C_s^3)$  space group, allowing for the possibility that KCN IV is ferroelectric. There may be evidence for this in the fact that the (200), (111) monoclinic pair shows excess broadening over the instrumental line shape (Fig. 5). This may indicate some line broadening due to the presence of domains in the monoclinic structure. If this is so ferroelectric behavior would follow.

Second the temperature factors for the  $K^+$  and  $CN^-$  ions,  $B_K$  and  $B_{CN}$ , are smaller in KCN IV than KCN III. The large temperature factors in KCN III are probably due in large part to the molecular libration which is present in this disordered system, so it is not surprising that the value for  $B_{CN}$  decreases upon passing to KCN IV where the CN molecules are partially ordered. It seems likely that the rotational motions of the rod-shaped CN molecules are largely absent in KCN IV. This would imply the absence of the local dilatations of the  $K^+$  lattice present in a disordered system as KCN I.<sup>4</sup> This picture is consistent with our result that  $B_K \approx 0$  in KCN IV.

Some intensity discrepancies remain. For the two orders of the (001), (110) monoclinic pair which were observed, the observed intensity for the (001) line is lower than allowed by the fit using the space group  $C_m(C_s^3)$ . The observed intensity for the monoclinic