this fit was R =11.5% which is to be compared with R = 4.1% for the fit to Pm3m (0_h^1). The "free rotation" model appears to be a poor model for KCN III.

IV. ANALYSIS OF THE KCN IV PATTERN

The rhombohedral analysis of the KCN IV data exposed two serious problems. First, several of the diffraction peaks were broadened in excess of the instrumental broadening and their shape was not truly gaussian, so that the fitting program summarized in Eq. (1) could not yield the correct intensities. Second, the (100), (200) and (210) diffraction peaks were displaced from their rhombohedral positions by more than the experimental uncertainty (Table II). The observed diffraction peak positions for KCN IV given in Table II are very nearly consistent with a rhombohedral lattice with unit cell constants $a_{rh} = 3.7803$ Å, $\alpha_{rh} = 86^{\circ}42'$.

On the basis of high pressure x-ray measurements, Pistorius[5] concluded that the most likely space group for KCN IV was $R\bar{3}m(D_{3d}^5)$. Here the K^+ ion is at (0, 0, 0) and the cyanide ion lies along the rhombohedral axis but without distinction between the heads and tails of the CN^-'s. Using the modification of our fitting program summarized in Eq. (3) we tested this model. The CN^- group was treated as a single entity with a scattering length $b_{CN} = (b_C + b_N)/2$. This "CN atom" was placed at (0, 0, z) and (0, 0, $\bar{z}$) in the hexagonal cell for which the c axis coincides with the primary axis of the rhombohedral cell. The K^+ ion was placed at the origin as before. The expression for the structure amplitude in Eq. (3) becomes