

pressure. We have scaled our results so that the TOF value for the intensity ($|F|^2$) of the (200) diffraction peak agrees with the literature value.^{7,17,18} Agreement is good except that the TOF value for the largest d-value peak (111) is slightly low. The good agreement with intensities obtained in previous powder neutron diffraction studies confirms the accuracy of our spectrum determination and the validity of the empirical correction discussed earlier.

For the KCN III pattern (Fig. 2) the diffraction peaks were well resolved and the peaks could be analyzed separately using Eq. (1) to determine the best value for the intensity of each peak. For the (110) diffraction peak there appear to be some small intensity "wings" above the background which may be due to thermal diffuse scattering, but no explicit allowance was made for this in the intensity analysis. The relative structure factors $|F_h^+|^2$ computed according to Eq. (2) were analyzed with a refinement program¹⁹ to determine the position of the CN^- ion in the unit cell and the Debye-Waller factors for the K^+ and CN^- ions. Scattering lengths of $b_K = .37$, $b_C = .665$ and $b_N = .94$ in units of 10^{-12} cm per atom were assumed for the respective nuclei.²⁰

Two different models were tried in the effort to determine the nature of the disordering of the linear CN^- molecules within the cubes formed by the K^+ ions in KCN III. Following Richter and Pistorius⁶ we first tried the space group $\text{Pm}\bar{3}\text{m}$ (O_h^1) in which the K^+ ions were placed at the origin and the C and the N atoms were averaged over the eight equivalent (g) positions at x_1, x_1, x_1 along the $[111]$ directions in the cubic unit cell. The eight CN scattering centers were each assigned a scattering length of $(b_C + b_N)/8$.