

$$F_{\vec{h}} = \left[b_K e^{-B_K/4d_{\vec{h}}^2} + b_{CN} e^{-B_{CN}/4d_{\vec{h}}^2} \times 2\cos 2\pi \ell z \right] \times \left[1 + 2\cos(2\pi/3(-h + k + \ell)) \right] \quad (5)$$

This expression accounts for the equivalent origins in the hexagonal cell at (000), (1/3, 2/3, 2/3), (2/3, 1/3, 1/3). The fitting yielded a value for $z = 0.4041$, implying a CN bond length of 1.33 \AA . The results for the temperature factors for the K^+ ions and the CN group were respectively, $B_K = 1.67 \text{ \AA}^2$, $B_{CN} = 5.00 \text{ \AA}^2$. The solid line in Figure 3 represents the best fit of the KCN IV diffraction pattern to $R\bar{3}m(D_{3d}^5)$. The poor intensity agreement apparent from the figure is reflected in the rather large goodness of fit value, 8.93 (See Section III). The displacement of the (100) and (200) diffraction peaks from their exact rhombohedral positions (Table II) is evident from Fig. 3. The apparent line broadening for several of the diffraction peaks ((100), (110) and (200)) which was apparent in the fitting summarized by Eq. (1) (no constraints on intensities) is also evident in Figure 3.

The diffraction peak broadening discussed above could arise either from a domain size effect²¹ based on a short-range ordering of the CN^- molecule or from a distortion of the rhombohedral lattice to lower symmetry. The displacement of the (100) and (200) peaks from their positions in the rhombohedral lattice supplies a strong argument for the latter explanation.