

monoclinic b axis. This is a more general requirement than that indicated by their location along the primary rhombohedral axis of the undistorted cell shown in Fig. 4. The structure factor $|F_{\vec{h}}|^2$ in Eq. (4) becomes

$$|F_{\vec{h}}|^2 = A_{\vec{h}}^2 + B_{\vec{h}}^2$$

with

$$A_{\vec{h}} = b_K e^{-B_K/4d_i^2} + \left[b_C \cos 2\pi(hx_C + lz_C) + b_N \cos 2\pi(hx_N + lz_N) \right] e^{-B_{CN}/4d_i^2}$$

and

$$B_{\vec{h}} = \left[b_C \sin 2\pi(hx_C + lz_C) + b_N \sin 2\pi(hx_N + lz_N) \right] e^{-B_{CN}/4d_i^2} \quad (7)$$

In the monoclinic cell $d_{\vec{h}}$ in Eq. (1) becomes²²

$$d_{\vec{h}} = (1 - \cos^2 \beta)^{\frac{1}{2}} / \left[h^2/a^2 + k^2(1 - \cos^2 \beta)/b^2 + l^2/c^2 - 2hl \cos \beta / ac \right]^{\frac{1}{2}} \quad (8)$$

All other parameters in Eq. (7) have been previously described. In the computer fit summarized in Eqs. (1), (4), and (7), the parameters $a, b, c, \cos \beta$, the lattice parameters for Al_2O_3 , $u, v, x_C, z_C, x_N, z_N, B_K, B_{CN}, \alpha, \gamma$, and δ were varied to yield a least square fitting to the data. This gives ten KCN crystal parameters using 53 peaks in the monoclinic structure. Most of these peaks are overlapping pairs or triplets but this analysis technique