the r.h.s. of Eq. (6) are now taken to be the basis vectors for the rhombohedral cell.

There are three centered monoclinic space groups $C2(C_2^3)$, $C2/m(C_{2h}^3)$, and $Cm(C_s^3)$ which are subgroups of $R\bar{3}m(D_{3d}^5)$. $C2(C_2^3)$ and $C2/m(C_{2h}^3)$ give completely wrong intensities for all allowable positions of C and N and so we used the space group $Cm(C_s^3)$ with the C and N nuclei in the A_1A_3 plane of Fig. 4 which includes the primary rhombohedral axis of the undistorted cell. The nature of the monoclinic distortion from the rhombohedral can be inferred from the fact that the maximum "peak broadening" in the fit to the rhombohedral structure was observed for diffraction from planes normal to the principal diagonal of the rhombohedral structure. This implies a distortion of $\vec{A}_1$ and $\vec{A}_3$ but not of $\vec{A}_2$ in going to the monoclinic structure (Fig. 4). In what follows we describe the monoclinic cell with the parameters a, b, c, cosβ where, from Fig. 4,

$$\vec{A}_1 \rightarrow \vec{A}_1' \qquad A_1' = a$$

$$\vec{A}_2 \rightarrow \vec{A}_2' \qquad A_2' = b$$

$$\vec{A}_3 \rightarrow \vec{A}_3' \qquad A_3' = c \qquad \cos\beta = \frac{\vec{A}_1' \cdot \vec{A}_3'}{|\vec{A}_1' \cdot \vec{A}_3'|}$$

A fit of the KCN IV diffraction pattern to the space group $Cm(C_s^3)$ was done using the modification of our least squares fitting techniques described in Eq. (3) with the carbon nuclei at $(x_C, 0, z_C)$ and the nitrogen nuclei at $(x_N, 0, z_N)$. Symmetry requires that the C and N atoms lie in the plane pendicular to the unique