Since the general indexing and intensities match those of $R\bar{3}m$ (D^5_{3d}) (Fig. 3) fairly well, the distortion from the rhombohedral structure must be small. Since the best values for the rhombohedral unit cell constants indicate only a slight distortion from the cubic KCN III structure, let us start from a model of KCN III sketched in Fig. 4. The space group $R\bar{3}m(D^5_{3d})$ with the cyanide ions lying along the rhombohedral axis (Fig. 3) is close to the real structure, so we start with the C and the N atoms lying along a three fold [111] axis in the cubic cell. If $\vec{a}_1$, $\vec{a}_2$, $\vec{a}_3$ ($|\vec{a}_1| = 3.808$ Å) are the edges of the cube we can describe this structure with an orthorhombic cell with

$$\begin{aligned} \vec{A}_1 &= \vec{a}_1 + \vec{a}_2 \\ \vec{A}_2 &= \vec{a}_1 - \vec{a}_2 \\ \vec{A}_3 &= \vec{a}_3 \end{aligned} \qquad (6)$$

We now have a C centered orthorhombic structure with two molecules per cell and CN^- lying in the (010) plane. We get the $R\bar{3}m(D^5_{3d})$ space group by increasing the length of the cube diagonal so that the angle α is smaller than 90° ($\alpha = 86^\circ 42'$). A small change in a is required to agree with the rhombohedral lattice parameter, a = 3.7803 Å, given above. The C-centered orthorhombic cell becomes a C centered monoclinic cell whose basis vectors $\vec{A}_1$, $\vec{A}_2$, $\vec{A}_3$, are also given by Eq. (6) if $\vec{a}_1$, $\vec{a}_2$, and $\vec{a}_3$ in