Figure 4: Relation of the crystallographic unit cells for KCN III and KCN IV. $\vec{a}_1$, $\vec{a}_2$, $\vec{a}_3$ are the edges of the cubic cell for KCN III and $\vec{A}_1$, $\vec{A}_2$, $\vec{A}_3$ are the edges of the C centered orthorhombic cell coinciding with the cubic cell. The monoclinic unit cell of KCN IV with edges $\vec{A}_1'$, $\vec{A}_2'$, $\vec{A}_3'$ slightly distorted from the orthorhombic vectors may be pictured as the result of a rhombohedral distortion followed by a monoclinic distortion along the [111] axis of the cubic cell. The C and N atoms, shown as lying along a [111] axis in the above figure, lie in ordered positions in the $A_1'A_3'$ plane in the monoclinic cell of KCN IV.

Figure 5: TOF neutron diffraction pattern for KCN IV. The solid line shows the result of fitting the observed diffraction pattern assuming that KCN IV is described by the centered monoclinic space group Cm (C_s^3) (See Section IV). The inset above and to the left of the (001), (1$\bar{1}$0) monoclinic pair shows the result of doing the above fit to the data for the 30° scattering angle. The vertical lines just below the diffraction pattern give the monoclinic line positions while the positions of the observable Al_2O_3 lines due to the pressure cell are marked by the symbol A.