

structure factors for the diffraction peaks associated with the longer neutron wavelengths which were too low. In order to fit the measured intensities for well known cubic materials, the measured $I_0(\lambda)$ was adjusted for the longer neutron wavelengths by dividing it by $\sqrt{1 + (\lambda - 1.8)^2}$ for $\lambda > 1.8 \text{ \AA}$ and by unity for $\lambda \leq 1.8$ before using it in Eq. (1) to calculate relative structure factors. We are not sure why this empirical correction is necessary, but different detector efficiencies could account for it.

In further analyzing KCN IV, we modified the least squares fitting technique summarized in Eq. (2) in order to test particular space groups. In this case the term $\alpha_{\vec{h}}$ for the amplitude of the KCN peak with label \vec{h} in Eq. (1) is replaced by

$$\alpha_{\vec{h}} \rightarrow \frac{u\lambda_i^4 I_0(\lambda_i)}{S_i} \quad m_{\vec{h}} |F_{\vec{h}}|^2 \quad (3)$$

where u is an overall intensity scaling factor for KCN.

This analysis was particularly useful in refining the KCN IV structure since the KCN IV diffraction pattern contained overlapping peaks.

Since our intensity measurements are important to our interpretation of the diffraction patterns for KCN III and IV we present in Table III our intensity results for KCN I at room temperature and compare them with the powder diffraction results in the literature.^{7,17,18} Our measurements on KCN I were taken with the sample inside the pressure cell before application of