

The midpoint of the CN bond was fixed at $(1/2, 1/2, 1/2)$. In the refinement calculation¹⁹ the thermal factors B_K , B_{CN} are given by the expression $e^{-B(h^2+k^2+l^2)/4a^2}$ prior to squaring in the structure factor where a is the lattice parameter for KCN III. The results of the refinement fitting are given in Table I. The position of the CN group resulting from the refinement was $x_1 = 0.407$ yielding a C-N bond length of $1.23 \pm .02 \text{ \AA}$ along one of the 111 directions. The thermal factors $B_K = 2.6 \text{ \AA}^2$, $B_{CN} = 3.9 \text{ \AA}^2$ are large, reflecting the large amount of molecular libration present in this disordered system. Using the relation

$$B_{K,CN} = 8\pi^2 \langle \mu_x^2 \rangle_{K,CN} \quad (4)$$

the linear motional amplitude $\langle \mu_x^2 \rangle^{1/2}$ is 0.18 \AA and 0.23 \AA for the K^+ and CN^- ions, respectively. The R value for the first ten peaks, of which only seven are clearly visible above the background was 4.1%. The large thermal factors reduced the amplitude of the peaks associated with the smaller lattice spacings below the statistical fluctuation in the background.

Next we tried a "free rotation" model¹⁷ in which the K^+ ions were again fixed at the origin and the CN group was treated as a single entity which moved freely on the surface of a sphere whose center was at $(1/2, 1/2, 1/2)$ and whose radius was one half the CN bond length. The best fit resulted for bond lengths in the range $1.20 \sim 1.24 \text{ \AA}$. The results for the fit with a bond length of 1.2 \AA are tabulated in Table I. The R value for