The midpoint of the CN bond was fixed at (1/2,1/2,1/2). In the refinement calculation[19] the thermal factors B_K, B_{CN} are given by the expression $e^{-B(h^2+k^2+\ell^2)/4a^2}$ 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 $1.23 \pm .02$ Å along one of the 111 directions. The thermal factors $B_K = 2.6$ Å^2, $B_{CN} = 3.9$ Å^2 are large, reflecting the large amount of molecular libration present in this disordered system. Using the relation

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

the linear motional amplitude $\langle \mu_x^2 \rangle^{\frac{1}{2}}$ is 0.18 Å and 0.23 Å 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" model[17] 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 $1.20 \sim 1.24$ Å. The results for the fit with a bond length of 1.2 Å are tabulated in Table I. The R value for