

jumping between equilibrium positions along the eight diagonal configurations.

I. INTRODUCTION

The pressure-temperature phase diagram of KCN has been reported¹⁻³ and is shown over a restricted P-T range in Fig. 1. Recent neutron diffraction measurements⁴ confirm that the I-V phase line shown by Pistorius et. al.² is in error as suggested in the note added in proof in that paper and thus it is not shown here. The structure of the high pressure phases of KCN have been examined via x-ray powder techniques^{5,6} in an opposed anvil type apparatus. It is these phases, KCN III and KCN IV, with which we will be concerned in this paper. Richter and Pistorius^{5,6} report KCN III as cubic, probably space group $Pm\bar{3}m (O_h^1)$ but their intensity data could not be used to help confirm this space group assignment. They made this assignment by analogy arguments from measurements on CsCN and TlCN. They also suggested that KCN III is disordered in that the CN^- ions either undergo a hindered rotation within the cubes of K^+ ions or that they randomly assume one of the 8 configurations along the 4 body diagonals. This latter structure could lead to a configuration entropy of $R \ln 8$. Neutron diffraction measurements^{4,7} in KCN I strongly suggest that the rotation model is incorrect. Pistorius⁵ reported the KCN IV structure to be rhombohedral with the space group $R\bar{3}m (D_{3d}^5)$. He suggested that the linear CN^- ions are oriented but not ordered along the body diagonal. Again the intensities of the x-ray lines could not