

Neutron Diffraction Study of KCN III and KCN IV at High Pressure*

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The high pressure polymorphs of KCN, KCN III and KCN IV, have been investigated by neutron diffraction using a polycrystalline sample. Meaningful intensity measurements together with high resolution measurements of diffraction line positions confirm the structural description of KCN III but contradict the description of KCN IV suggested by previous high pressure x-ray work. The following picture emerges from our investigation. At a pressure of 25 kbar and at room temperature, KCN IV has a monoclinic structure with the C_s^3 space group in which the C and N nuclei are nearly along the body diagonal of a slightly distorted cube of K^+ ions. The conclusion from the x-ray work that KCN IV is rhombohedral is contradicted both by our intensity information and by the fact that several of the diffraction lines are displaced slightly from their exact rhombohedral positions. Increase of the temperature from 66°C to 74°C at a pressure of 22 kbar results in the transformation from phase IV into the cubic phase KCN III with the space group $Pm\bar{3}m$ (O_h^1) in which the CN^- molecules are ordered randomly along the eight equivalent $[111]$ directions. The temperature factors in KCN III are unusually large indicating a high probability of a CN^- ion

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