

can readily handle overlapping peaks. The results for the diffraction pattern taken at 25 kbar and 23°C are shown in Fig. 5 and Table IV. The monoclinic structure seems to account very well for the diffraction line positions. The fitting result for the monoclinic cell parameter, (Table IV) $\cos\beta = 0.0770 \pm .003$, rules out the possibility that the unit cell for KCN IV is orthorhombic. Some intensity discrepancies appear in the fit using the space group $Cm (C_s^3)$. It is evident from Fig. 5 that the observed intensity for the (002) peak of the monoclinic pair (002), (220) is significantly lower than allowed in the best fit (solid line). The inset at the lower right of Fig. 5 showing a restricted region of the fit to the data for the 30° scattering angle shows the same discrepancy for the (001) peak of the monoclinic pair (001), (110). The experimentally observed intensity for the monoclinic pairs of diffraction lines labeled (401), (312) and (200), (111) in Fig. 5 is larger than allowed in the fit to $Cm (C_s^3)$. The discrepancy for the (401), (312) and (200), (111) monoclinic pairs is far more serious in the fit to the diffraction pattern of KCN IV collected at 34 kbar and 23°C where it is also apparent that the observed intensity of the (400), (222) monoclinic pair is larger than allowed in the fit to C_s^3 . These discrepancies might be due to the presence of preferred orientation which, according to the latter examples, becomes more pronounced with pressure. The application or reduction of pressure in a solid pressure medium can give rise to preferred orientation. Indeed, we found that, after release of pressure, the intensities observed for the (111) and (222) peaks in KCN I were reduced by a factor of two with respect to their values prior to the application of pressure (Table III) while the intensities for the other peaks remained unchanged.

The temperature factors for the K^+ and CN^- ions, B_K and B_{CN} , are smaller in KCN IV than in KCN III, indicating that the