

Table I. Plane spacing and intensity of KCN III at 74°C and 22° kbar.

cubic hkl	d_{obs}	d_{calc}	$m F_{\text{hkl}} ^2_{\text{obs}}$	$m F_{\text{hkl}} ^2_{\text{calc}}$	
	(Å)	(Å)		Pm3m(0^1_h)	Free Rotation Model
100	3.807 ± .002	3.8080	16.38 ± 2.88	18.57	18.60
110	2.6912 ± .0011	2.6926	82.08 ± 5.64	79.79	79.00
111	2.1982 ± .0017	2.1985	5.84 ± 0.48	5.91	3.84
200	1.9049 ± .0007	1.9040	14.52 ± 1.74	14.49	16.09
210	*	1.7030	< 2.4	0.4	0.1
211	1.5538 ± .0016	1.5546	29.52 ± 2.64	30.87	27.02
220	*	1.3463	< 4.8	7.6	6.03
300 } 221 }	1.2694 ± .0028	1.2693	5.24 ± 3.32	5.51	6.45
310	*	1.2042	not observed	1.4	7.38
311	1.1498 ± .0016	1.1482	9.60 ± 2.40	9.68	8.82
Lattice Parameter = 3.8080 ± .0003 Å ⁰				Refinement Fitting Parameters	
Unit Cell Volume = 55.22 ± .01 Å ³					
B _K (Å ²)				2.6	2.23
B _{CN} (Å ²)				3.9	6.21
C-N Bond Length (Å)				1.23	1.2
R Value for fit (%)				4.1	11.5