Table 4. *Comparison between the results of Krogh-Moe* (1964) *and the present results, which have been converted to his cell and space group Pmn*2_1

All parameters have been multiplied by 1000

Atom designation		This paper			From Krogh-Moe's paper		
This paper	From Krogh-Moe's paper	x'	y'	z'	x	y	z
Sr	Sr	0	288	0	0	289	0
O(1)	O(1)	0	728	415	0	728	454
O(2)	O(2)	359	858	953	359	857	064
O(3)	O(4)	365	225	356	365	226	335
O(4)	O(3)	223	632	353	221	631	335
B(1)	B(1)	378	173	041	379	174	976
B(2)	B(2)	248	677	006	246	671	963

individual isotropic temperature factors. Convergence was initially quite slow, but after three steps (a total of three adjustments of the scale factors by structure factor calculation and twelve cycles of least squares) Krogh-Moe's model refined to a result identical with ours.

The authors feel that the combination of more reasonable interatomic distances and angles, a lower *R* value of our structure with Krogh-Moe's data, and the ultimate refinement of his structure into ours with our data provides ample proof of the correctness of the structure as reported in the present paper.

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The Crystal Structure of the Copper(I) Cyanide Hydrazine Complex, $CuCN.N_2H_4$*†

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$CuCN.N_2H_4$ is orthorhombic, space group *Pbcm* with four formula units per unit cell. The lattice constants are $a=4{\cdot}684$, $b=9{\cdot}172$ and $c=7{\cdot}830$ Å. The CuCN portion forms planar zigzag infinite chains lying on the mirror. These chains are joined by the hydrazine molecules to form infinite puckered layers which nest together. The copper has four neighbors forming a quite distorted tetrahedron.

Introduction

Copper(I) cyanide forms addition compounds with a great many nitrogen-containing compounds. Because of the unusual structures shown by $KCu(CN)_2$ (Cromer, 1957) and $KCu_2(CN)_3.H_2O$ (Cromer & Larson, 1962) we have decided to investigate the structures of some of these addition compounds. The structure of $CuCN.NH_3$ has recently been published (Cromer, Larson & Roof, 1965) and we now report on the hydrazine complex, $CuCN.N_2H_4$.

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Table 1. *Final least-squares parameters for orientation* I *of* $CuCN.N_2H_4$

	x	y	z	$B_{11}\times10^4$	$B_{22}\times10^4$	$B_{33}\times10^4$	$B_{12}\times10^4$	$B_{13}\times10^4$	$B_{23}\times10^4$
Cu	0·2243 ± 4	0·3465 ± 2	$\frac{1}{4}$	197 ± 12	32 ± 3	155 ± 5	7 × 12	0	0
C	0·0319 ± 36	0·5328 ± 23	$\frac{1}{4}$	170 ± 81	58 ± 28	171 ± 41	−25 ± 81	0	0
N	0·0658 ± 30	0·1499 ± 18	$\frac{1}{4}$	225 ± 71	56 ± 23	197 ± 36	−13 ± 77	0	0
$-NH_2$	0·5215 ± 21	0·3232 ± 10	0·0398 ± 12	265 ± 48	47 ± 17	123 ± 19	−67 ± 44	83 ± 55	−69 ± 31

$g = 5{\cdot}43 \pm 0{\cdot}39 \times 10^{-6}$

Table 2. *Comparison of residuals for the three orientations*

(unobserved reflections omitted)

Orientation	$\Sigma\|\|F_o\|-\|F_c{}^*\|\|/\Sigma\|F_o\|$	$\Sigma w\|\|F_o\|-\|F_c{}^*\|\|/\Sigma w\|F_o\|$	$\Sigma w(F_o-F_c{}^*)^2$	$\sigma(\varrho)$
I	0·0738	0·0778	72·56	0·51 e.Å^{-3}
II	0·0796	0·0849	87·14	0·52
Disordered	0·0769	0·0802	77·09	0·50

Experimental

The compound $CuCN.N_2H_4$ is readily made by dissolving copper(I) cyanide in warm anhydrous or 64% aqueous hydrazine. When the solution cools, small crystals of the complex precipitate. The crystals are orthorhombic and show only the forms {010}, {100} and {001}.

Examination with a precession camera showed the crystals to be orthorhombic, space group *Pbcm*, if centric (reflections $0kl$ with k odd and $h0l$ with l odd were systematically absent). Lattice constants were obtained from a least-squares fit of 26 lines measured with a carefully aligned single-crystal orienter on a General Electric XRD-5 spectrogoniometer using Mo $K\alpha_1$ radiation ($\lambda = 0{\cdot}70926$ Å). The cell constants are $a = 4{\cdot}684 \pm 0{\cdot}001$, $b = 9{\cdot}172 \pm 0{\cdot}002$ and $c = 7{\cdot}830 \pm 0{\cdot}002$ Å. With four $CuCN.N_2H_4$ units per unit cell the calculated density is 2·401 g.cm^{-3}. The density measured by displacement in bromobenzene was 2·37 g.cm^{-3}. The linear absorption coefficient for Mo $K\alpha$ radiation is 64·8 cm^{-1}. Intensities for one-half of the hemisphere were measured out to $2\theta = 55°$ using Mo $K\alpha$ radiation and balanced filters. The fixed-counter, fixed-crystal technique was used. The crystal was 0·37 × 0·080 × 0·143 mm in size with the longest dimension parallel to the unit cell c axis which was also the rotation axis. Absorption corrections were quite small and hence were not applied. Equivalent F^2 were averaged and the observed F was the square root of this average. The average agreement of equivalent reflections was estimated by forming an index $\Sigma|F^2-\overline{F^2}|/\Sigma F^2$, where the summation was taken over all reflections which were observed more than once. This index was 0·081. A similar quantity, $\Sigma|F-(\overline{F^2})^{\frac{1}{2}}|/\Sigma(\overline{F^2})^{\frac{1}{2}}$, based on F, was 0·043.

Determination and refinement of the structure

If the space group is *Pbcm*, the copper atom and the cyanide group are required to be in special positions. A three-dimensional Patterson map was computed and the positions of all atoms except hydrogen were readily found. The copper atom and the cyanide group were

Table 3. *Observed and calculated structure factors for* $CuCN.N_2H_4$*, orientation* I

The column headings are l, $|F_o|/K$ and $F_c{}^*/K$ (see text). A minus sign preceding $|F_o|/K$ means 'less than'.

H= 0	K= 0	
2	68	-79
4	79	89
6	45	-47
8	24	21
10	18	-14
H= 0	K= 2	
0	53	-50
1	73	66
2	8	4
3	38	-39
4	26	-24
5	51	49
6	12	11
7	16	-14
8	-7	-3
9	17	14
10	-8	4
H= 0	K= 4	
0	79	-72
1	62	-59
2	52	53
3	26	29
4	49	-47
5	47	-41
6	28	24
7	10	9
8	16	-14
9	16	-12
H= 0	K= 6	
0	86	82
1	29	-30
2	47	-46
3	32	32
4	54	51
5	14	-14
6	34	-26
7	16	13
8	18	13
H= 0	K= 8	
0	-6	-3
1	38	38
2	18	-16
3	27	-29
4	-7	2
5	26	25
6	-7	-3
7	12	-10
H= 0	K= 10	
0	37	-40
1	14	-13
2	34	38
3	-8	4
4	28	-30
5	12	-13
H= 1	K= 0	
0	6	11
2	70	-70
4	14	15
6	14	-15
8	12	10
10	-10	0
H= 1	K= 1	
0	88	-71
1	49	50
2	71	72
3	39	-42
4	46	-51
5	23	26
6	31	31
7	17	-15
8	19	-17
9	-10	7
H= 1	K= 2	
0	32	27
1	16	-16
2	14	15
3	8	-10
4	-7	7
5	10	-12
6	-7	0
7	-8	-7
8	-8	-2
9	-9	-3
H= 1	K= 3	
0	26	-24
1	71	-68
2	18	19
3	59	60
4	13	-14
5	37	-38
6	9	9
7	27	23
8	-8	-4
9	-10	-11
H= 1	K= 4	
0	-6	-5
1	-5	-2
2	19	18
3	21	21
4	-6	-4
5	7	7
6	-8	6
7	13	10
8	-9	-2
9	-10	2
H= 1	K= 5	
0	73	71
1	7	8
2	68	-67
3	9	-9
4	48	49
5	-7	3
6	31	-30
7	-9	-3
8	21	16
9	-10	1
H= 1	K= 6	
0	-7	1
1	9	-8
2	27	-29
3	-7	0
4	-8	5
5	9	-8
6	-9	-8
7	-9	0
8	12	5
H= 1	K= 7	
0	19	-22
1	44	45
2	22	24
3	36	-37
4	15	-16
5	26	26
6	11	10
7	18	-15
8	-10	-6
H= 1	K= 8	
0	13	13
1	-7	-3
2	-8	6
3	-8	-1
4	-9	5
5	-9	-4
6	-10	-1
7	-9	-3
H= 1	K= 9	
0	29	-29
1	26	-28
2	23	25
3	22	24
4	21	-20
5	16	-16
6	14	13
H= 1	K= 10	
0	11	-12
1	-9	-2
2	-10	10
3	-10	9
4	-10	-6
5	-9	3
H= 1	K= 11	
0	26	29
1	12	-11
2	26	-26
3	-11	8
H= 2	K= 0	
0	28	-28
2	67	70
4	26	-31
6	22	26
8	18	-15
H= 2	K= 1	
0	44	-37
1	14	14
2	19	21
3	-6	-9
4	18	-19
5	10	9
6	12	11
7	-8	-3
8	-8	-4
9	-10	2
H= 2	K= 2	
0	19	17
1	80	-71
2	38	-40
3	65	70
4	15	16
5	33	-32
6	13	-12
7	29	29
8	-10	8
9	13	-9
H= 2	K= 3	
0	-6	-4
1	15	-13
2	-6	7
3	-7	6
4	-7	-4
5	9	-10
6	-8	2
7	-9	3
8	-9	-2
9	-9	-3
H= 2	K= 4	
0	45	42
1	36	35
2	46	-48
3	38	-42
4	28	29
5	13	12
6	22	-22
7	18	-18
8	12	11
H= 2	K= 5	
0	33	30
1	-7	5
2	22	-23
3	-7	-1
4	18	19
5	-8	5
6	14	-11
7	-9	0
8	-9	6
H= 2	K= 6	
0	26	-27
1	26	24
2	43	47
3	14	-14
4	21	-22
5	15	16
6	16	19
7	-9	-5
8	14	-11
H= 2	K= 7	
0	12	-10
1	9	9
2	-7	3
3	10	-9
4	-9	-5
5	-9	5
6	-9	3
7	-9	-4
H= 2	K= 8	
0	11	-14
1	45	-44
2	-8	-2
3	39	40
4	-9	-6
5	26	-24
6	-8	3
H= 2	K= 9	
0	-9	-6
1	-9	-7
2	11	9
3	-10	5
4	-9	-6
5	-10	-5
H= 2	K= 10	
0	25	25
1	-9	2
2	20	-23
3	-10	-8
4	18	17
H= 2	K= 11	
0	-11	10
1	-9	-1
H= 3	K= 0	
0	41	-37
2	-7	5
4	20	-20
6	-8	8
8	-9	-3
H= 3	K= 1	
0	51	45
1	33	-33
2	29	-31
3	22	24
4	26	28
5	17	-19
6	17	-18
7	11	9
8	-10	8
H= 3	K= 2	
0	27	24
1	36	-34
2	-7	-6
3	19	19
4	13	13
5	22	-23
6	-8	-6
7	-9	5
8	-9	2
H= 3	K= 3	
0	11	10
1	61	59
2	14	-13
3	42	-43
4	-8	8
5	34	35
6	-9	-5
7	17	-16
8	-9	4
H= 3	K= 4	
0	24	24
1	19	17
2	15	-15
3	-7	-4
4	15	16
5	13	15
6	-8	-8
7	-9	0
8	-10	5
H= 3	K= 5	
0	38	-37
1	-7	-4
2	29	29
3	-7	-1
4	24	-25
5	-9	-4
6	15	15
7	-9	-1
H= 3	K= 6	
0	27	-25
1	-8	5
2	-8	6
3	-9	-8
4	14	-15
5	-9	1
6	-9	6
7	-10	-3
H= 3	K= 7	
0	21	20
1	34	-33
2	14	-12
3	28	29
4	14	13
5	20	-19
6	10	-8
H= 3	K= 8	
0	-9	5
1	23	-21
2	-9	7
3	15	15
4	-8	1
5	15	-14
H= 3	K= 9	
0	14	15
1	19	21
2	17	-18
3	15	-16
4	-10	12
H= 3	K= 10	
0	12	9
1	-9	3
2	-10	-9
H= 4	K= 0	
0	51	49
2	27	-28
4	29	32
6	18	-17
H= 4	K= 1	
0	14	13
1	15	-14
2	19	-21
3	11	14
4	10	11
5	-9	-7
6	-10	-7
7	-10	6
H= 4	K= 2	
0	13	-14
1	35	33
2	-8	3
3	20	-22
4	-9	-8
5	21	22
6	-10	3
7	-10	-7
H= 4	K= 3	
0	-8	8
1	32	30
2	-8	-4
3	28	-30
4	-9	5
5	15	15
6	-9	-3
7	15	-13
H= 4	K= 4	
0	24	-24
1	23	-24
2	18	17
3	12	14
4	16	-16
5	17	-18
6	12	9
H= 4	K= 5	
0	13	-12
1	-8	0
2	14	15
3	-8	4
4	-10	-9
5	-9	2
6	-10	7
H= 4	K= 6	
0	32	30
1	15	-15
2	16	-16
3	13	15
4	19	20
5	-10	-8
H= 4	K= 7	
0	-10	6
1	17	-19
2	12	-12
3	14	15
4	-9	6
H= 4	K= 8	
0	-9	-2
1	18	19
2	-9	-6
3	13	-14
H= 5	K= 0	
0	17	17
2	26	-26
4	13	13
H= 5	K= 1	
0	-9	-16
1	13	13
2	22	21
3	11	-13
4	16	-13
5	-10	7
H= 5	K= 2	
0	-9	-2
1	21	20
2	-9	8
3	21	-20
4	-10	-2
5	12	10
H= 5	K= 3	
0	-8	-6
1	13	-12
2	-9	3
3	13	14
4	-9	-3
5	-9	-5
H= 5	K= 4	
0	11	-10
1	14	-14
2	13	13
3	15	16
4	-10	-7
H= 5	K= 5	
0	21	21
1	-9	2
2	22	-23
3	-9	-5
H= 5	K= 6	
0	14	10
1	-10	-11
2	16	-17
H= 6	K= 0	
0	-10	-10
H= 6	K= 1	
0	20	-18
1	-10	12

Table 4. *Magnitudes and direction angles, relative to the crystallographic axes, of the principal axes of the thermal vibration ellipsoids in* CuCN . NH$_2$

	Orientation I						Disordered cyanide group						Orientation II				
	Axis i	B_i(Å^2)	α	β	γ		Axis i	B_i(Å^2)	α	β	γ		Axis i	B_i(Å^2)	α	β	γ
Cu	1	1·7 ± 0·1	5 ± 9	85 ± 9	90												
	2	1·1 ± 0·1	95 ± 9	5 ± 9	90												
	3	3·8 ± 0·1	90	90	0												
(−NH$_2$)	1	2·0 ± 0·5	30 ± 15	90 ± 19	120 ± 15												
	2	1·0 ± 0·5	77 ± 19	26 ± 9	68 ± 15												
	3	3·9 ± 0·6	63 ± 11	116 ± 9	39 ± 10												
C	1	1·4 ± 0·7	22 ± 59	68 ± 59	90	CN(2)	1	1·5 ± 0·8	25 ± 15	67 ± 15	90	N	1	1·8 ± 0·9	35 ± 11	55 ± 11	90
(atom located at	2	2·1 ± 1·0	112 ± 59	22 ± 59	90	(atom located at	2	4·7 ± 1·3	113 ± 15	23 ± 15	90	(atom located at	2	6·2 ± 1·5	125 ± 11	35 ± 11	90
x = 0·03, y = 0·53,	3	4·2 ± 1·0	90	90	0	x = 0·03, y = 0·53,	3	5·0 ± 1·1	90	90	0	x = 0·03, y = 0·53,	3	4·4 ± 1·1	90	90	0
z = 0·25)						z = 0·25)						z = 0·25)					
N	1	2·1 ± 0·8	34 ± 139	124 ± 139	90	CN(1)	1	2·2 ± 0·9	38 ± 18	128 ± 18	90	C	1	1·9 ± 0·9	38 ± 15	128 ± 15	90
(atom located at	2	1·8 ± 0·8	56 ± 139	34 ± 139	90	(atom located at	2	0·5 ± 0·7	52 ± 18	38 ± 18	90	(atom located at	2	−0·3 ± 0·7	52 ± 15	38 ± 15	90
x = 0·07, y = 0·15,	3	4·8 ± 0·8	90	90	0	x = 0·07, y = 0·15,	3	4·1 ± 0·9	90	90	0	x = 0·07, y = 0·15,	3	3·9 ± 1·0	90	90	0
z = 0·25)						z = 0·25)						z = 0·25)					

clearly in the special position set 4(*d*) of *Pbcm*. The nitrogen of the hydrazine molecule was located in a general position. Subsequent refinement of this trial structure confirmed the choice of the centric space group. As in the case of CuCN . NH$_3$ there was uncertainty in the identity of the atoms in the cyanide group. In the present structure, however, there seemed to be no particular structural reason for choosing one orientation over the other.

One orientation of the cyanide group was arbitrarily chosen and a full-matrix least-squares refinement of all non-hydrogen atoms with anisotropic thermal parameters was made. The quantity minimized was $\Sigma w(F_o-F_c^*)^2$ where $w=w_E/(F_o+0{\cdot}02\ F_o^2)$, w_E is the weight based on counting statistics as given by Evans (1961) and

$$F_c^*=KF_c/\left\{1+g\left[\frac{2(1+\cos^4 2\theta)}{(1+\cos^2 2\theta)^2}\right]\mathrm{Lp}\ F_c^2\right\}^{\frac{1}{4}}$$

where K = scale factor, g = extinction parameter (Zachariasen, 1963), Lp = Lorentz and polarization factors and F_c is the ordinary calculated structure factor. Anisotropic temperature factors were in the form exp $\{-(B_{11}h^2+B_{22}k^2+B_{33}l^2+B_{12}hk+B_{13}hl+B_{23}kl)\}$. Form factors which are given in *International Tables for X-ray Crystallography* (1962) were used. For unobserved reflections, $w=0$. At the end of the refinement, $\Delta\xi_i/\sigma(\xi_i)$ was $<4\times10^{-3}$ for all parameters ξ and $<3\times10^{-4}$ for positional parameters.

The parameters resulting from this least-squares refinement, which we shall call orientation I, are given in Table 1. The refinement was repeated with the cyanide group inverted (orientation II) and, because there is so little structural difference between the two orientations, a third refinement was made with a disordered cyanide group. In the third refinement the two atoms in the cyanide group were assumed to be equal and to have a scattering factor equal to the average of those of carbon and nitrogen.

The R index and related quantities for the three refinements are given in Table 2. Orientation I is slightly favored. Moreover, for orientation II the thermal parameters for the nitrogen are quite large and for the carbon they are not positive definite. For the disordered orientation the thermal parameters are intermediate in value.

Table 3 gives the observed structure factors and those calculated with the parameters of Table 1. The R index of 7·38% (Table 2) is larger than we usually expect for an anisotropically refined structure, with little or no absorption error and with data obtained by counting techniques. A difference Fourier synthesis was computed but did not reveal the hydrogen atoms. There was, however, a peak of height 2·5 e.Å^{-3}, or about $5\times\sigma(\varrho)$, which remains unaccounted for. This peak was about 1 Å, in the z direction, from the copper atom. Another smaller peak of $\sim$1·25 e.Å^{-3} occurs at $\sim$0·25 Å from the copper atom in the mirror plane. Since the space group is not uniquely determined, least-

Table 5. *Interatomic distances and bond angles in* $CuCN.N_2H_4$, *orientation* I

Cu–C	1·93 ± 0·02 Å	C–N	1·17 ± 0·02 Å
Cu–N	1·95 ± 0·02	NH_2–NH_2	1·48 ± 0·02
Cu–2(–NH_2)	2·17 ± 0·01		
Angle		Angle	
N–Cu–C	129·8 ± 0·7	Cu–N–C	179·3 ± 1·5°
N–Cu–NH_2	98·8 ± 0·4	Cu–C–N	175·2 ± 1·6
C–Cu–NH_2	112·8 ± 0·4		
NH_2–Cu–NH_2	98·9 ± 0·6	Cu–NH_2–NH_2	114·2 ± 0·7

squares refinements were made in space groups of lower symmetry than *Pbcm*, namely $Pbc2_1$ (No. 29, non-standard setting) and $P22_12_1$ (No. 18, non-standard setting). Refinement was attempted in $Pbc2_1$ although it was realized that the copper network would have to remain the same as in *Pbcm*, the carbon and nitrogen atoms being free to move out of the mirror plane. This refinement was unsatisfactory, probably because of the near planarity of the Cu, C, and N atoms. Refinement was attempted in $P22_12_1$ with the thought that it would allow the copper lattice to change slightly, and this could perhaps be achieved without enhancing the $h0l$, $l \neq 2n$ and the $0kl$, $k \neq 2n$ reflections enough to make them observable. The least-squares calculations in $P22_12_1$ proceeded smoothly and converged to yield, within their standard deviations, the same results as the refinement in *Pbcm* and an *R* index of 7·71% for the anisotropic refinement.

Discussion

The thermal ellipsoids derived from the thermal parameters of Table 1 are given in Table 4. For the cyanide group the ellipsoids resulting from all three refinements are given. The ellipsoids for copper and hydrazine are essentially unchanged for the three cases. Clearly orientation I is the most reasonable with respect to the thermal motion.

A view of the structure as seen along **c** is shown in Fig. 1 and a view along **a** is shown in Fig. 2. The interatomic distances and angles are given in Table 5. There are no non-bonded atoms closer than 3·08 Å.

The structure is quite simply described. There are infinite zigzag chains of Cu–C–N–Cu–C–N– lying on the mirror. Thus these chains are planar. These chains are linked together by the hydrazine molecules forming infinite puckered layers which nest neatly together. In the other compounds studied there have been spiral chains of CuCN.

The copper atom has four neighbors in a quite distorted tetrahedron. The Cu–NH_2 distance of 2·17 Å is longer than usual. Most copper–nitrogen distances in these cyanide complexes have been 0·1 to 0·2 Å shorter. The N–N distance of 1·48 Å in the hydrazine molecule compares favorably with the value of 1·47 Å found in the dimethylhydrazines (Beamer, 1948), but is a little longer than the value of 1·447 ± 9 Å found in hydrazine monohydrate (Liminga & Olovsson, 1964).

All calculations were performed with an IBM-7094 computer using programs written by the authors.

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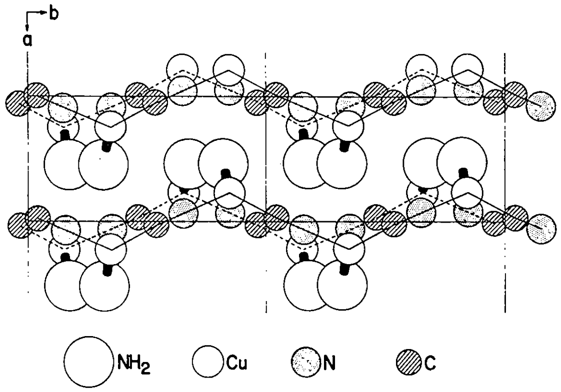

Fig. 1. A view of the structure as seen along **c**. Note how the puckered layers nest together.

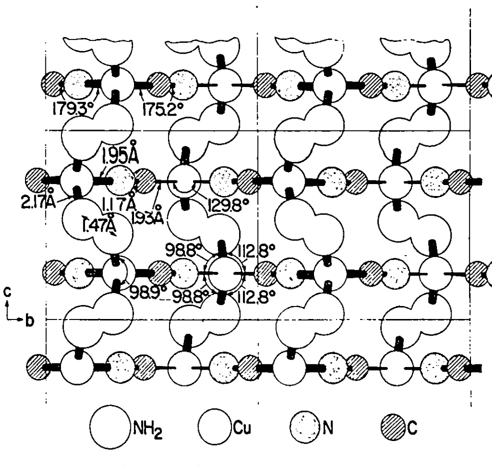

Fig. 2. A view of one of the puckered layers as seen along **a**.