Papers of M H F Wilkins: annotated copies of Rosalind Franklin's DNA notebooks

Contributors

Franklin, Rosalind, 1920-1958 Wilkins, Maurice, 1916-2004 Ashton, Jennifer

Publication/Creation

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CAMBRIDGE.

17 May 1976

19. MAY 1976

Professor M. H. F. Wilkins, F.R.S.,
MRC Biophysics Research Unit,
King's College,
26-29 Drury Lane,
London, WC2B 5RL.

Dear Professor Wilkins,

I enclose xerox copies of the Rosalind Franklin notes which you requested from Dr. Klug. In due course, you will receive a bill for them from Head Office.

Yours sincerely,

Jennie Ashton

J. Ashton (Mrs)
Secretary to Dr. A. Klug

Encs.

12. NOV. 1992

Dear Maurice,

Herewith copies from Int. Tables of the 3 non-mirroring monoclinic space group. Please call me if I can be of any further help.

best wishes

David.

KING'S COLLEGE LONDON

THE RANDALL INSTITUTE

Telephone message for

From Morris Wilkins

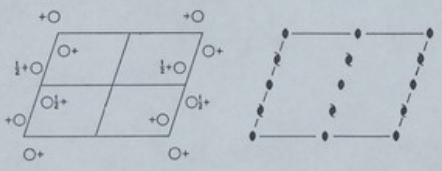
Date _____

Time 4.10

Taken by Sonia

Please ring him

at 081-858 1817

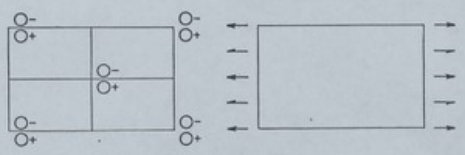


1ST SETTING Origin on 2; unique axis *c*

Number of positions, Wyckoff notation, and point symmetry			Co-ordinates of equivalent positions	Conditions limiting possible reflections
			(0,0,0; $\frac{1}{2}$,0,$\frac{1}{2}$)+	
4	*c*	1	*x*,*y*,*z*; $\bar{x}$,$\bar{y}$,*z*.	General: *hkl*: $h+l=2n$ *hk*0: $(h=2n)$ 00*l*: $(l=2n)$
2	*b*	2	0,$\frac{1}{2}$,*z*.	Special: as above only
2	*a*	2	0,0,*z*.	

Symmetry of special projections

(001) *p*2; $a'=a/2$, $b'=b$ (100) *pm*1; $b'=b$, $c'=c/2$ (010) *c*1*m*; $c'=c$, $a'=a$



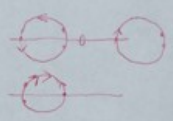
Origin on 2; unique axis *b* 2ND SETTING

Number of positions, Wyckoff notation, and point symmetry			Co-ordinates of equivalent positions	Conditions limiting possible reflections
			(0,0,0; $\frac{1}{2}$,$\frac{1}{2}$,0)+	
4	*c*	1	*x*,*y*,*z*; $\bar{x}$,*y*,$\bar{z}$.	General: *hkl*: $h+k=2n$ *h*0*l*: $(h=2n)$ 0*k*0: $(k=2n)$
2	*b*	2	0,*y*,$\frac{1}{2}$.	Special: as above only
2	*a*	2	0,*y*,0.	

Symmetry of special projections

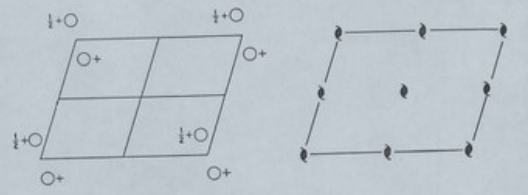
(001) *cm*1; $a'=a$, $b'=b$ (100) *p*1*m*; $b'=b/2$, $c'=c$ (010) *p*2; $c'=c$, $a'=a/2$

packing



$P2_1$
C_2^2

No. 4 $P\,1\,1\,2_1$ 2 Monoclinic



1ST SETTING

Origin on 2_1; unique axis c

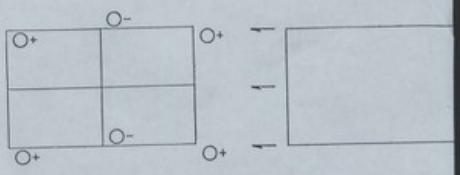
Number of positions, Wyckoff notation and point symmetry			Co-ordinates of equivalent positions	Conditions limiting possible reflections
2	a	1	x,y,z; $\bar{x},\bar{y},\frac{1}{2}+z$.	hkl: No conditions $hk0$: No conditions $00l$: $l=2n$

Symmetry of special projections

(001) $p2$; $a'=a$, $b'=b$

(100) $pg1$; $b'=b$, $c'=c$

(010) $p1g$; $c'=c$, $a'=a$



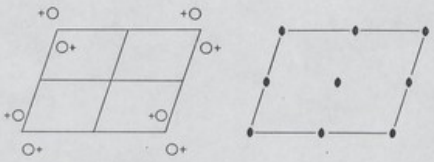
Origin on 2_1; unique axis b

Number of positions, Wyckoff notation, and point symmetry			Co-ordinates of equivalent positions
2	a	1	x,y,z; $\bar{x},\frac{1}{2}+y,\bar{z}$.

Symmetry of special projections

(001) $pg1$; $a'=a$, $b'=b$

(100) $p1g$; $b'=b$, $c'=c$



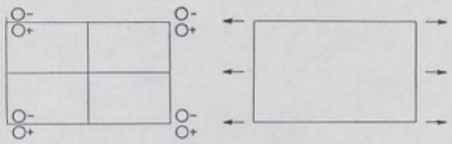
1ST SETTING

Origin on 2; unique axis c

Number of positions, Wyckoff notation, and point symmetry			Co-ordinates of equivalent positions	Conditions limiting possible reflections
				General:
2	e	1	x,y,z; $\bar{x},\bar{y},z$.	hkl: } No conditions $hk0$: } $00l$: }
				Special:
1	d	2	$\frac{1}{2},\frac{1}{2},z$.	No conditions
1	c	2	$\frac{1}{2},0,z$.	
1	b	2	$0,\frac{1}{2},z$.	
1	a	2	$0,0,z$.	

Symmetry of special projections

(001) $p2$; $a'=a, b'=b$ (100) $pm1$; $b'=b, c'=c$ (010) $p1m$; $c'=c, a'=a$



Origin on 2; unique axis b

2ND SETTING

Number of positions, Wyckoff notation, and point symmetry			Co-ordinates of equivalent positions	Conditions limiting possible reflections
				General:
2	e	1	x,y,z; $\bar{x},y,\bar{z}$.	hkl: } No conditions $h0l$: } $0k0$: }
				Special:
1	d	2	$\frac{1}{2},y,\frac{1}{2}$.	No conditions
1	c	2	$\frac{1}{2},y,0$.	
1	b	2	$0,y,\frac{1}{2}$.	
1	a	2	$0,y,0$.	

Symmetry of special projections

(001) $pm1$; $a'=a, b'=b$ (100) $p1m$; $b'=b, c'=c$ (010) $p2$; $c'=c, a'=a$

C'

19 Jan 53 → 27 July 53

NB

14 Oct 52 → 19 Jan 53
has no entries ??
Notebook Missing ?

R.E.F.

Jan 53 use of models in later stages of A analysis

DNA Crystallographic Calcns. etc 1953

Tues Feb
p 15 3.2.53. disc of 11 p repeat
∞ model ? concat argument about tilt of bases ?

✓ p 3. 19.1.53. diads in A
✗ date ? Chargaff data

J. Callender says colloq at end of Jan → p 20 First B mention 10.2.53

10.2.53. p. 22 Density + water content. assumes 22 nucleotides.

23.2.53 p. 28 B helix 23.2.53 51C Photo.
p. 34 if B is helix A is similar in compressed form.
helical analysis — plug words "at last" — p. 36 2 chains in A favours 2 chains in B
p. 38 Density of B is 3 chains

pre WC p. 37 missing data on ll = 1 & 2.
8.3.53 – 18.3.53 p. 39 – p. 42

p35 extraordinary note by A Klug about RF missing point about bases.

In Jan 53 models for P-P distance + ovalap of bases. Suggest a trio bases bases

29.1.53 has difficulty with base-base contact

3 2 53 probably after colloquium. probably 11 p chain. difficulty of bases in contact centimetres all in ∞ structure

correctly gets 2·5 spacing for inclined bases with fully extended chain. But rejects!

10. 2.53 up till now no helix + but now turns to B but hardly does anything + goes back to A.

Seems no sign of helices in A up till WC. Tho' p 34 she says A is similar to B.

[Data do not speak for themselves.]

But July 25 2 chain helix in B then in a modified form must also exist in A since they A ⇌ B is readily reversible

14 Oct 52
was last date
in other notebook

19 Jan 53

19.1.53

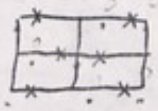
Results of superposition of 3-dimensional Patterson of crystalline Na DNA

Space group C 2

- axes found in superposition function
- mirror planes impossible ∴ asymmetric C

Axial sections

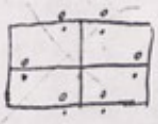
one axial section contains principal maxima (c:0)



the other no important maxima (c: ½)

Peaks at heights 13/30 → 17/30

v strong, also in pseudo-hexagonal array



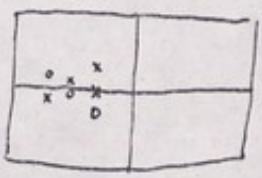
[N.B. hexagons appear canted, ∴ superposition method is not capable of eliminating central peak. But ½ cell reconcile centres w density ⅔ would have pseudo-cell of side a = b ≈ 13 Å]

Possible structure having chains along a+c diagonal

but fibres can't be built this way - unreasonable

∴ search for alternative - gives:-

Figure of 8 structure (in projection)



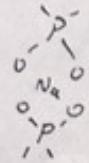
7 peaks on chain in one cell.
2 pairs of chains / unit cell
(2 pairs / full cell)
i.e. 56 nucleotides / full cell

Consistent w density data if

½ ≈25% H_2O

⅔ 2 P atoms per peak

i.e. 2 chains "back to back"



i.e. chains are ⊥ pairs, one upside-down w.r.t the other

Patterson peaks representing Zphosphates

If pairs are all ⊥ // orient^{n} ⊥ resol^{n} is poor, maxima will give distances between mid-pt of pairs

i.e. : : gives : o :

If pairs ⊥ one another, no central maxima

i.e. : .. gives : ::

does this indicate that pairs at c=8 are inclined to other pairs at ⊥ give weaker peaks?

Peak at 4·3 Å on section c=2 would then be P-P distance with pair?

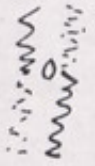
but in that case Na is not directly between P-P, or resolution would be destroyed by 2 Na-P peaks

disc. of diads
Chargaff
rose again
idea

Peak at left 0 lies on axis

∴ 2 P atoms attached to similar nucleotides

- apart from this, symmetry does not control nucleotide sequence except that in a "back-to-back" pair of chains top half of one is similar to bottom half of other



Each chain of peaks is unit cell

∴ can't reconcile nucleotide sequence with Chargaff's analysis

~~if all chains are same, sequence must be~~ A B C D D C B

N.B. Symmetry axis does not affect sequence within one chain

Distance between neighbouring peaks 5.7Å (= 3 dimension)

Nearest to agreement with Chargaff analysis would be

4 purines, 3 pyrimidines, with 2 purines & 2 pyrimidines occupying equivalent positions

- c.f. Broomhead, & similar XRD structures of adenine & guanine

tilting discussion 5·7 spacing
phosphate of nucleotides but not for chain inclined to axis.

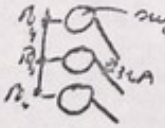
Construction of models

Scale $\frac{1}{2}'' : 1\text{Å}$ (as for Patterson diagrams)

Backbone chain

PO_4 tetrahedra - wooden balls, tetrahedrally pierced (Fraser) placed in contact.
Sugar ring constructed (wire) on Furberg model

Constructed models using only phosphates & sugar rings
show that it is possible to construct straight-chain model
with P-P = 5·7 Å, & all sugar rings in identical pos"n
Pyrimidines for pos" of base chain, are then inclined @ 25-30° to backbone
- this would have inter-base plane spacing ~ 5·0 Å
Base-planes can be tilted on this model to give inter-plane
spacing 3·4 Å but then is the v little overlap, i.e. v little
van der Waals attraction



∴ if P-P distance 5·7 Å, not straight chain
- this (among other things) eliminates a-c diagonal structure

Putting Pyrimidine rings ⊥ & in full contact we can have
3 phosphates in straight line, & P-P distance ~ 5·7 Å
but 4th must lie well off this line to bring 4th
pyrimidine into contact
(system involves some distortion of N_3 bonds)
[linked to sugar]

PTO

If next base is a purine then next P out-of line could bring 6-ring of purine into contact with pyrimidine

This arrangement for 1 or 3 P has sugar ring nearly || to P chain

⇒ 3 base rings either ⊥ or inclined to chain

Backbone chain and symmetry at c = 0

Consider 2 pairs of chains 1, 1′ and 2, 2′, separated by $b = \frac{1}{3}$

1 is related to 1′ and 2 to 2′ by dyad axis

1 —— 2 and 1′ to 2′ by rotation through 180°

Construct wire model of chain corresponding to Patterson peaks

i.e. 7 steps of each 5.7Å, with 3 successive sets of 3 [illegible]° & reasonable angles

→ angle 0-1-2 ~ 100°

angle 2-3-3′ ~ 110°

For accurate model these angles would be equal, since 3-3′ ∥ 1-0 etc.

∴ angles 100 - 110°

Suppose length of pyrimidine nucleotide is in a-c plane

Then for a-c diagonal part of structure (i.e. peaks 1'-0-1)

(Some of this tilting is going in correct direction)

$\sin^{-1} \frac{3.4}{5.7} = 36\frac{1}{2}°$

∴ if ~~plane~~ plane of pyrimidine is ⊥ a-c plane, it makes

$\angle 36\frac{1}{2}°$ with phosphate chain

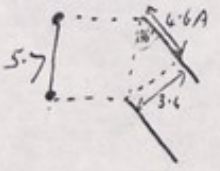
$\angle 36\frac{1}{2} + 41 = 77\frac{1}{2}$ with fibre axis

Unlikely the ∠ between base & backbone is so small

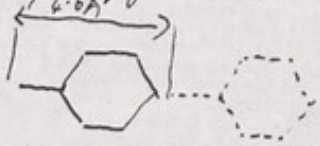
∴ more probable base is also inclined to a-c plane

- this would make its length more nearly ⊥ to both backbone chain & fibre axis

In general, if all P-sugar are equivalent, then $c_1 - c_1' = 5.7\,A$



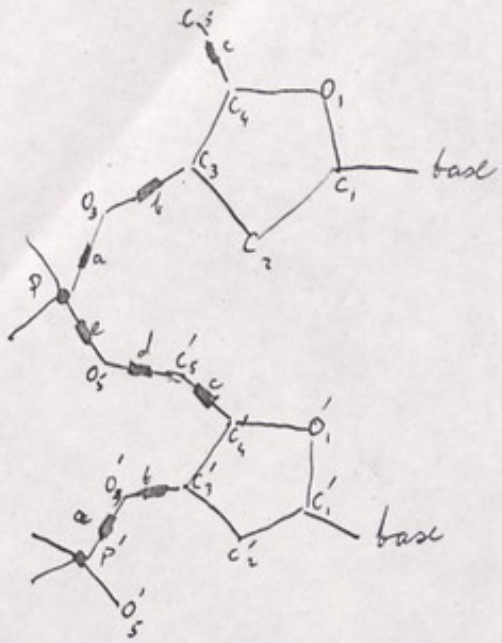
i.e. no overlap of ⊥ pyrimidines



∴ sugar rings must be skew to one another,

with ⊥ distance between bonds C_1N — $C_1'N'$ ~ 3.4 A

- bases then ∥ one another but differently oriented



Free rotation at a, b, c, d, e

26 Jan

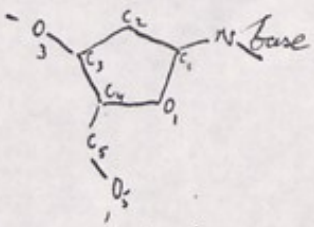
26.1.53

Wire model of backbone chain and sugar rings

Scale 1" : 1 Å

Sugar ring constructed as : Furberg and Beevers + Cochran

i.e. 4 atoms coplanar and C_3' ½ Å out of plane, bringing O_3 on to plane



All free rotation obtained by making joint with certain zones [illegible]

PO_4 tetrahedra

Requirements

1. Neighbouring P on chain 5.7" apart
2. 2 un-bound O of PO_4 facing away from sugar
3. $P\begin{matrix}O\\-O\end{matrix}-$ near vertical plane (Fraser, but this was not for structure A)
4. Possibility of placing neighbouring bases parallel at ~ 3.4 Å between planes

Observations

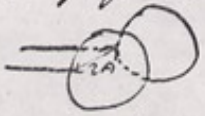
Distance apart of P P' determined by rotations b, c, d, esp. c

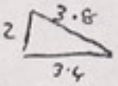
Distance apart of C_2 C_5' —— —— a, b, e

(closest approach ~ 1.2")

Fully extended chain gives P – P ~ 6.8 Å

If r d w contact d ~ 3.4 Å between bases, rise pyramides are ~ 3 Å : diameter of C, N bonds, seen in projection ⊥ plane of rings, must'nt be > ~ 2 Å apart





∴ separation distance between N and N' > 3.8 Å

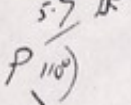
29.1.53

It doesn't seem to be possible to put 3 P groups i.e. in spacing 5.7 Å and have C,N bonds ~ 90° for 11 bases at 3.4 Å resp.

Is it possible for 3 P making bond of 110°?

If so, perhaps structure has groups of 2 or 3 bases in 11 context, and break of contact when chain turns a corner i.e. not helical

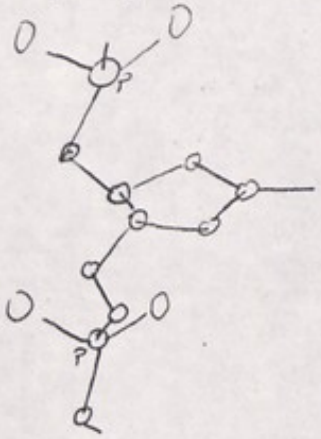
"chain turns at a corner" (non-helix)



= this config° it is easy to avoid steric hindrance of sugar rings. Not easy for P 5.7 P 5.7 P

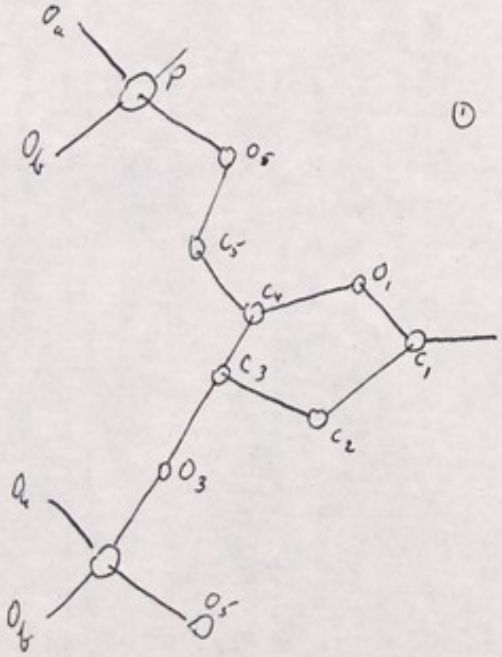
Arrangements of backbone chain with P-O:5'

1. Sugar rings ~ ⊥ P-P makes it easier to avoid steric hindrance



This leaves $P\langle^{O}_{O}$ directed to <u>one side</u> of sugar ring

2. Sugar rings ~ ∥ P-P — again $P\langle^{O}_{O}$ to one side



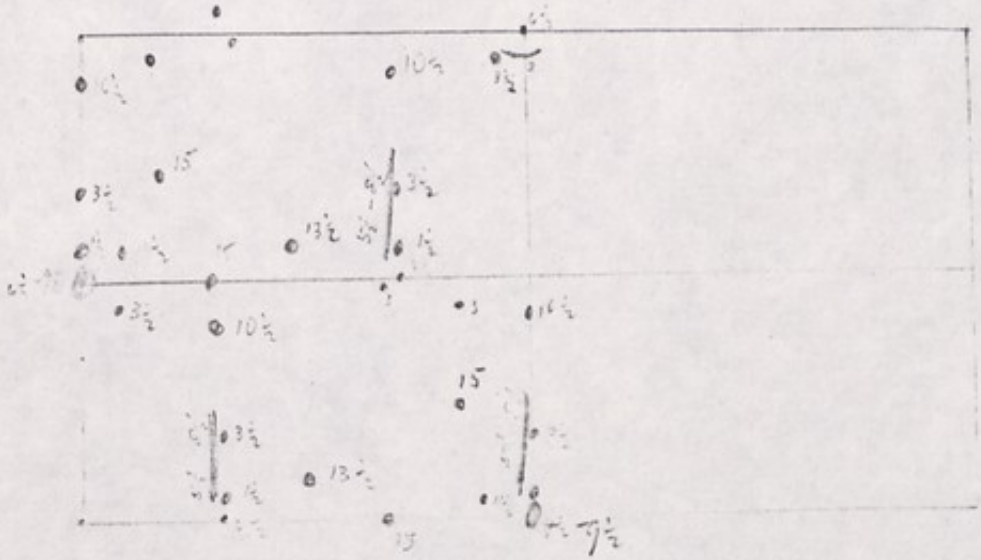
Steric factors

① Make C_5 equidistant from O_3 and O_b

② C_3 tilted away from O_a, but <u>not</u> equidistant betw. O_a and O_5 ∴ this would make C_2 approach $O_{5'}$
∴ compromise

③ $P-O_{5'}-C_5-C_4$ co-planar
This keeps $O_{5'}$ at max. (& equal) distance from O_1 and C_3

M 9 B



2 Feb 12

2.2-53 1

Objection to α structure

Part of chain -1, 0 - 1 lies along a - c diagonal
P-P of pair at 0 must lie in a - c plane, ∴
Patterson shows that this must be ∥ along a - c diagonal
i.e. ∥ same direction as chain
∴ impossible

Superposition

To obtain function which gives members of atom-pairs
& not their centres, must take account of fact that
V_g is not strictly an axial section but on either side of it
Suppose P-P distance in pair = 4.5 Å
& corresponds to peak on section $\frac{3}{c}$ a = 5 cms
the axes at c = 1½, a = 2½ cms
This is MgB

3.2.53

MgB doesn't help solve the problem of how
the a - c diagonal streak is related to the ¼ - cell
heavy peak, nor does it show poss. alternative form
for chain

3.2.53

M2g

Peak of height 13 repeats at $\frac{1}{3}$ of away . . . by placing V_g not at height 0 but at height 13

i.e. put OMg on 0/13 M2 , and giving

Mg displacement ÷ 8.3 cms, of M_2 $\frac{1}{2}$ shift where necessary

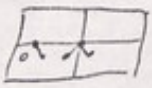
axes are then at height $-13 \div Mg$ (and a = 0)
$\angle(2,7)$

. . draw Mg C derived fm MG with axes at height 17

and M2 B " " M_2 with axis at 0/17

Principal positions of c:2 vectors – Patterson

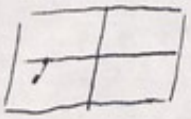
Sections 0–2 (twice)



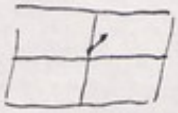
N.B. not at 0

∴ not 11 pairs

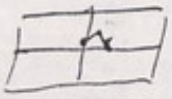
Sections 10–12



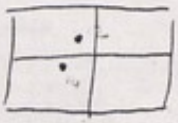
Sections 3–5 (or 2–4)



Sections 14–16



Sections 12–14



11 P chain
why not ref to 11th el. reflection?

This is the correct argument but she has not realised that a helix gives base sep^n less because at smaller radius on helix
But this is not a helix

If there are 11 nucleotides per chain

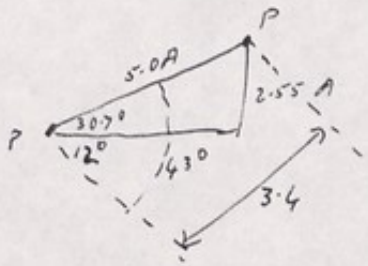
near inter-P spacing along c-axis is 2.55 A

calculated value or ref to exp value?

If P.P : 5.0 A

and inter-nucleotide base spacing 3.4 A

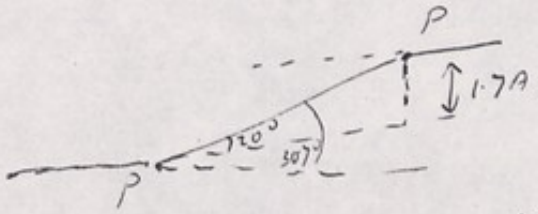
this makes bases inclined at ~ 12° to ⊥ to fibre axis



but then no contact ∴ bases too small

no overlap?
There would be some?
p.6. pyrimidine ~3A diam

or if chain is

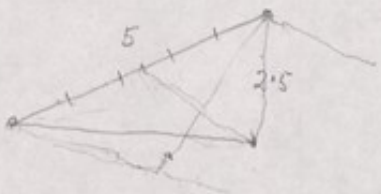


bases inclined ~ 11° to the axis

but only 20° to P-P chain

∴ impossible

rejected because she assumed bases were same distance apart along chain as are the phosphates.



5 Feb 53 16

23

5.2.5-3

"chain steps"

Possible steps in chain

Predominant near-origin peaks in P are ~5A

① within 2 peak 122 - strongest of all but c=15
(∴ general rule)

∴ suppose this is important step in chain

also ② step along a-c diagonal (within 3

or ③ within 2, peak 75 (similar to ①, with a-sgt reversed)

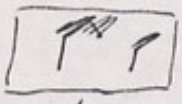
If there are the 3 poss. chain steps, the total number of ②+③ is equal to no. of ①

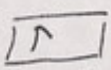
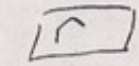
∴ total translation in 'a' = 0

There is no horizontal translation of ~5A

2 consecutive ① can occur (within 2½ of 5)

or 3 " ①

or ① followed by ③ i.e. a  possible

but not ① followed by ② but not  or 

N.B. angle of ① in a-b plane is somewhat variable

- probably some peaks lie nearer 'b' axis, to account for resolution power on 'b' axis than 'a' although 'b' axis is further from main maxima

since by

② can be followed by ③ but not by ①

and ③ can be followed by ① (~~similarly~~) but not by ②

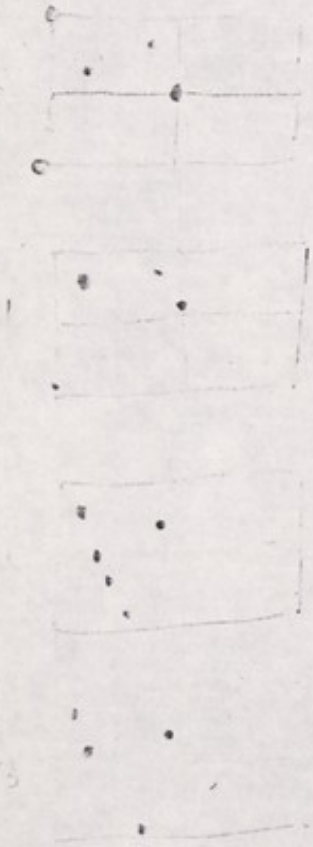
but ~~②~~ ③ following ① giving peak c~5, b~½ which fulfils in hole

Ponte seguenze n/posto ① ② e ③

① - ① - ① ② - ② - ② ③ - ③ - ③

① - ① - ③

1/12



(cont'd from opp.)
The nuggets Harker puts cob ~~a = 8-0~~

M 11

Peak on section 2, $a = -4.8$ cms $b = 3.3$ cms

Possible posⁿ of peaks in -ve region of Patterson marked in, and made when they coincide with +ve region of 2nd sheet, they were marked with dotted lines on M 11

M 12

Suppose M 11 vector occurs twice consecutively. Then M 11 is multiple, 2 structures being related by V_{11}

∴ M 12 is M 11 displaced V_{11} on itself

$a = -3.5$ $b = 3.5$

M 12 Axes on section 7, with a ~ -2.0 cms?

7.2.53

Try M 13, using peak at height 4, a ~ 3.0 cms b = 0 in M 11

distance of this peak from peak on section 1, ?

9.2.53

Possible posⁿ of axes in M 11

c = 4	a = 3.5 cms	c = 11	a = -3.5 cms
c = 7	a = -0.5	c = 8	a = +0.5
c = 1	a = -2.5	c = 14	a = +2.5 — no : gives peak on wrong a-c diag. on section 4
c = 4½	a = 0		

gives Harker peaks c = 7 a = 4.8 } v good
∧ c = 11 a = -4.8 }

gives 2 Harker peaks differing by c = 4, a = 10 cms

∴ superposition of a-c section on itself, with displacement c = 4, a = 10 gives poss. vector ∴ least poss. posⁿ of axes

B.

note question mark

2 Sentences only

10.2.53

13 Mar

Structure B

Evidence for 2-chain (or 1-chain helix) ?

49c - general trend is as for right contorsion helix (which differs from right dextrorsum chain in integral no. residues/turn only in contrib^n of high order $\bar{J}$'s & the latter)

and this is indistinguishable from double helix with residues in each having same ζ-value, since 2-ch. chain has opp. signs in ξ & η terms (eq 1-2), & eq^n 2 contains only R^2, ξ^2, η^2 & $\tan\psi, \eta/\xi$

13.3.53. Axes derived from other possible pairings of VII' derived from V II

$\frac{1}{2}a-5$	$\frac{1}{2}(c+2)$	$a-10$	$c+4$	Hardin peaks
-4·7	6	-14·4	14	✗ ✓
-4·0	6½	-13·0	15	✗ ✓
7·0	6½	9·0	15	✗ ?
4·8	7	4·6	16	✗ ?
6·0	3	7·0	8	✗
0	3	-5	8	✗

Back on the Pattersons!

Possible pos's of Harker peaks of V_{11} and axes in M_{11}

Harker peaks are a , c
and a-10 , c+4
then axes is at $\frac{1}{2}(a-5)$ and $\frac{1}{2}(c+2)$

Observed	a - 10 (ans)	c+4	$\frac{1}{2}(a-5)$	$\frac{1}{2}(c+2)$	
	1·4	$4\frac{1}{2}$ +	3·2	$(1\frac{1}{4})$ $1\frac{1}{2}$	
no V'	21·0	$6\frac{1}{2}$ -	13·0	$(2\frac{1}{4})$ 2	
	11·6	$9\frac{1}{2}$ +	8·3	$(3\frac{3}{4})$ 4	IID
	23·0	$10\frac{1}{2}$ -	14·0	$(4\frac{1}{4})$ 4	IIC
	12·8	$13\frac{1}{2}$ -	8·9	$(5\frac{3}{4})$ $5\frac{1}{2}$	MIIE
	26·0	$13\frac{1}{2}$ +	15·5	$(5\frac{3}{4})$ 6	
	19·8	20	12·4	9 ✓	II 13

M 9 11

M 9 shows a vector V 11 having one end in common with end of V 9

∴ pair M 9 on M 11 with origin at a : 2·4 as 6·6·8

and O M 9 11 is O M 9 on 2 9 M 11

i.e. axes on M 11 at a : 2·4 c : 1

if true axes are M 9 axes

M 911 blue for axes on M 9 axes

presumably A structure

M. Wt

Wt. primitive unit cell 11.2×10^3

Vol. " " " 12230 Å^3

Suppose partial sp. vol. DNA is 0.55 (as did Riley)

Vol. of 22 nucleotides is $\frac{0.55 \times 330 \times 22 \times 10^{24}}{6.03 \times 10^{23}}$: 6620 Å^3

∴ vol. assoc. water = 12230 − 6620 = 5610 Å^3

≈ 45.8 % of volume

∴ Wt % of water is $\frac{45.8}{45.8 + 54.2 \times \frac{1}{0.55}} = \frac{45.8}{45.8 + 98.7} = \frac{45.8}{144.5}$: 31 %

?

Density of water in Na DNA

Dry density 1.63 sp. vol. .615

Density + 35% (wgt) of water = 1.52 (wgt) i.e. sp. vol. .658

vol. 1.35 g of ~~mixture~~ wet DNA : .889 cc

∴ vol. of .35 g water : .274 cc ∴ vol. DNA is wet.

i.e. density of water : 1.28 g/cc v high

Suppose density of water : 1.00 g/cm³

Vol of 1.35 g wet Na DNA: .615 + 0.35 : .965 cc

density : $\frac{1.35}{.965}$: 1.40 g/cc

Suppose density of water 1.00 ∴ of mixture 1.52 i.e. vol 1.35 g : $\frac{1.35}{1.52}$ g : 0.89 cc

sp. vol. DNA : 0.89 − 0.35 = 0.54

Suppose partial sp. vol. DNA 0.55

∴ ——— H_2O 1.00

Then for 40% H_2O, 1.4 g ~~occupies~~ occupies 0.55 + 0.40 : 0.95 cc

$d = \frac{1.4}{.95} : 1.475$

35% H_2O $d : \frac{1.35}{0.90} : 1.50$

30% H_2O $d : \frac{1.30}{0.85} = 1.53$

12 Dec ? 24
Feb ?
12.12.53

a - c diagonal

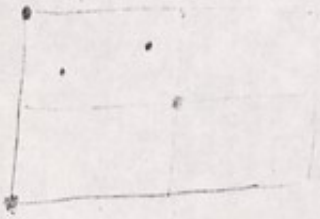
All Patterson peaks streak along forward a - c diagonal

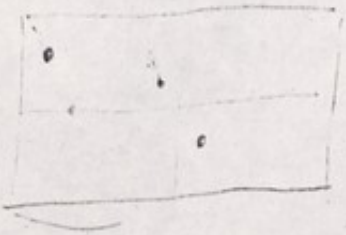
- this suggest possibility of disorder in direction of diagonal

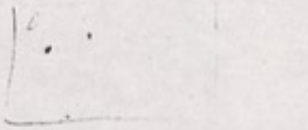
M11C

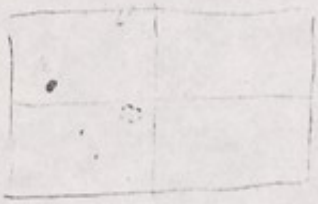
No good
- Leets 1 – 4 almost nothing

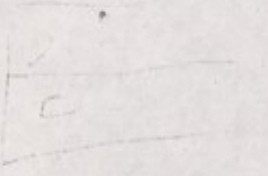
M12 (

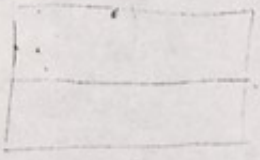


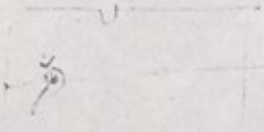


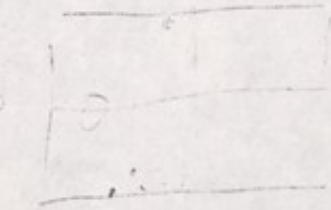


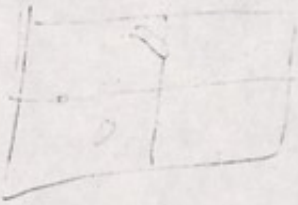


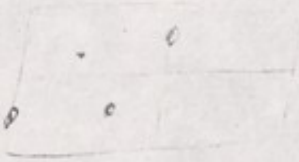


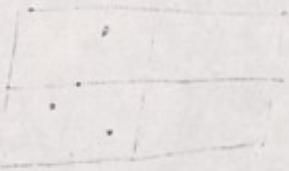


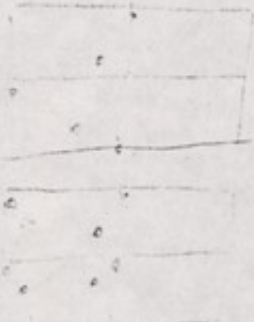


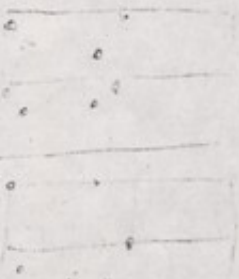








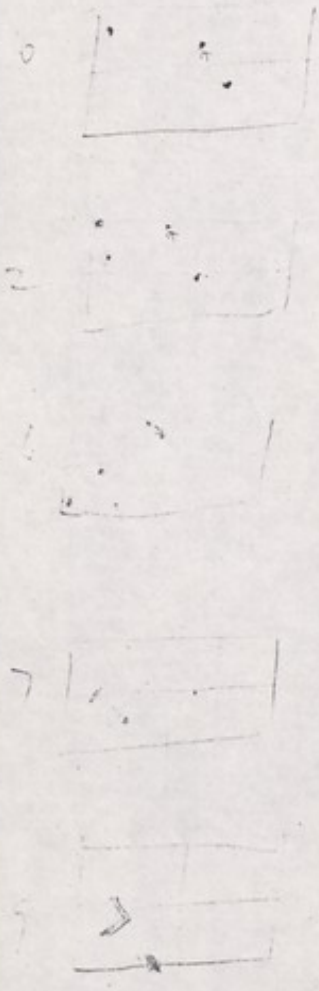




M Ag. 13. 11

O M 13 on 1711, with MB reflected across ~~the a axis~~ B plane
(i.e. turned over short axis

spots used are reflection 0
and 1 on with 28
(marked with red arrow.)



Sections.

11 13.11

Possible position - Spars

Search for V_{13}' will meet 6 position. Then axis lies ½ way between this and sheet 0

Section 16 – no : 7 & 8 not axial

Section 13 -> bad axial sections

25 "

26 "

5 less bad axial sections 2/3, 17/8

P 28 – 38 incl. taken out for copying

2 Mar 99

24 Feb

Vi brief entry on 10.2.53. P20 with much crossed out MW

28

See further notes of Structure B on 23-2-53 P 28

A.K.

23.2.53

13 days after the 2 sections about NB 49 C possibly indicating a helix. MW

Structure B

Photograph 51 C

3·4 A are − 158·5 mm on projection

∴ 158·5 : 2R tan 2θ where R is effective specimen-film distance for projection

For d : 3·40 A, θ (CuKα) : 13° 4′ tan 2θ : 0·491

$$R = \frac{158.5}{2 \times 0.491} = 161.4 \text{ mm} \qquad 2R = 322.8$$

Equator mm	tan 2θ	θ	d (Å)	1/d	λ/d	~~θ~~ mm on Optical chart	Conversion factor
20·2	·0625	1° 48′	24·5	·041	·0629	12·6	(·624 ~~·619~~)
54·7	·1695	4° 49′	9·16	·109	·168	33·6	·614
82	·254	7° 8′	6·19	·162	·249	50·7	·618
to 100	to ·310	8° 37′	to 5·13	·195	·300	61·7	·617
						mean	·616
120	·372	10° 12′	4·34	·230	·355		
to ~~152~~ 152	to ·470	12° 36′	3·52	·284	·438		

These equatorial maxima do not correspond to maxima ∝ $J_0^2(x)$,

which are approximately at 0, a, 2a, 3a | min. $\bar{J}_0(x)$ for x 3·83 10·18
max. $\bar{J}_0(x)$ for x 7·02 13·32

Best fit, assume 1st max. is missing (9·16 A reflexion is v weak)

Then max. at $\frac{\lambda}{d}$: ·27, ~~·405~~ ·391, and ·149 ·27

since $2\pi R r \triangleq$ ~~7·124~~ 7·0 for $R \cdot \frac{2\pi\theta}{\lambda} \cdot \frac{1}{d} : \frac{\lambda}{27}$ ~~·405~~ ·175

$\therefore r \triangleq \frac{\text{~~7·124~~}\ 7.0}{2\pi \times 175}$: ~~6·32~~ 6·36

page 2 of 39

39

5th layer line

1st diffuse spot

$2l$: 88 to 100 mm $\tan 2\theta$: .2725 to .310 θ 7°37′ to 8°37′

d : 5.80 to 5.10 $\frac{1}{d^2}$: .0298 to .0385

$c^2 \frac{1}{d^2} = \left(\frac{5}{34}\right)^2 \left(\frac{6.34}{3.45}\right)^2$: .02165

$\therefore \left(\frac{\xi}{\lambda}\right)^2$: .0082 to .0169 $\frac{\xi}{\lambda}$: .0905 to .130

ξ : .139 to .200

1st max. for $J_5^2(x)$ has $x \sim 6.5$

$\therefore$ if $r = 6.36A$, $R = \frac{\xi}{\lambda} = \frac{6.5}{2\pi \times 6.36}$: .163

- fits better with max. $\doteq J_3(x)^2$,

or J_5, and $r = 9.4A$, giving $\frac{\xi}{\lambda}$: .113 which agrees with measurement MW MW

3rd layer line

1st streak of spots

$2l$: 49 to 65 mm $\tan 2\theta$: .152 to .201 θ : 4°19′ to 5°41′

d : 10.24 to 7.76 $\frac{1}{d^2}$: .00953 to .01665

$\frac{11}{c^2} : \left(\frac{3}{34}\right)^2$: .00780

$\therefore \left(\frac{\xi}{\lambda}\right)^2$: .00153 to .00885, $\frac{\xi}{\lambda}$: .0391 to .0940

1st max. for $J_3^2(x)$ has $x \sim 4.2$

$\therefore R = \frac{\xi}{\lambda} = \frac{4.2}{2\pi \times 6.36}$: .105

for $r = 9.4A$ $R = \frac{\xi}{\lambda}$: .071 reasonable fit MW

but equator, taking $r = 9.4A$ MW

MW

Trying to fit one value of r only

should have maxima at $\frac{1}{9.4 \times 2\pi}$ (3.83, 7.02, 10.18, 13.32) $\doteq \frac{\xi}{\lambda}$

i.e. at .065, .119, .172, .226 and zero at 2.40 and zero at .0406

or ξ : .100, .183, .265, .348

and zero at ξ : .0625 i.e. exactly on observed strong peak

hence bad fit MW

step in right direction – adding J_n for different values of r.

MW

2 helices of different radius for simple case of whole number of residues per turn.

Following Cochran Crick + Vand (Acta Cryst. 5 581, 1952)

term $J_n(2\pi Rr)e^{in(\psi+\frac{1}{2}\pi)}$ becomes $J_n(2\pi Rr)e^{i(n\psi - n\phi + \frac{1}{2}n\pi + 2\pi l z/c)}$

(in present case, $l = n$)

For equator $I = \left[J_0(2\pi Rr_1) + J_0(2\pi Rr_2)\right]^2 = J_0^2(2\pi Rr_1) + J_0^2(2\pi Rr_2) + 2J_0(2\pi Rr_1)J_0(2\pi Rr_2)$

For n^{th} layer line, $I = FF^* = J_n^2(2\pi Rr_1) + J_n^2(2\pi Rr_2) + J_n(2\pi Rr_1)J_n(2\pi Rr_2)\left(e^{in(\phi - 2\pi z/c)} + e^{-in(\phi - 2\pi z/c)}\right)$

$= J_n^2(2\pi Rr_1) + J_n^2(2\pi Rr_2) + 2J_n(2\pi Rr_1)J_n(2\pi Rr_2)\cos\left[n(\phi - 2\pi z/c)\right]$

Here terms in $J_n J_n'$ may give negative contribution to intensity

but on any layer-line, moving out from the meridian, when the first maxim appears in a J_n contribution (i.e. for the J_r term corresponding to largest value of r) there is no negative term in I, since all other J_n terms are small and +ve

∴ even for complex helical structures, first maxima should give maxim diameter.

roughly correct but really not right. it assumes that nucleotide is radial (all in same phase) k. maybe she did not realise it was an assumption MW

On equator, first max. (in J_0^2), excluding central max, involves -ve J_0, ∴ max. diameter can't necessarily be got from equator

In general

$$F_n = e^{in(\psi + \frac{\pi}{2})} \left[J_n(x_1) e^{in\alpha_1} + J_n(x_2) e^{in\alpha_2} + \dots + J_n(x_p) e^{in\alpha_r} \right]$$

where $\alpha_q = \phi_q - 2\pi z_q / c$

& $x_q = 2\pi R r_q$

& $I = FF^* = \sum_{p}^{p} J_n^2(x_p) + \sum_{p \neq q}^{pq} J_n(x_p) J_n(x_q) \cos[(\alpha_p - \alpha_q)]$

& same argument applies

i.e. first max. give outside radius

but later max. & equatorial non-central max. complicated

2-strand helix with pairs of groups at opp. ends of diameter

~~$J_n(x_p) = J_n(x_q)$~~ $x_1 = x_2$, $\alpha_1 - \alpha_2 = n\pi$

diad along fibre axis?
MW

yes

∴ layer-lines absent for n odd

& $I = 4 J_n^2(x)$ for n even

page number?

(42)

Conclusion

Structure B does not fit single helical theory, even for low layer-lines. ξ-values of first maxima are too small for single-stranded helix, & even more so for multi-stranded. i.e. we would have Jn on 1st l.l. for n strands equally spaced.

Closing radius of helix so that layer-line maxima fit for single-strand (i.e. r = 9·4 Å) gives v bad fit for equator (OK but one should not worry too much because one is simplifying MW)

Outer shape / \ \ / emerging from 3·4 reflection indicates repeat at 3·4 Å is v important — i.e. view \/ /\ represents structure

factor of whole figure, which exists only for c = n × 3·4, & figure repeats for 3·4 n spot as for helix

For r = 9·4 Å
She seems to take lack of agreement between 3rd & 5th l.l. with equator to rule out 'single helix' model.
Over hasty rejection
MW

Note underlining of if ! MW

(ie J5 on 5th layer line
(On R.E.F's terminology there could still be two chains, unrelated by the symmetry)
See P. 46 QK.

Structure B if helix is right-hand helix

i.e. 2-strand, fitting 5th layer-line max. to $J_{10}(x)$, and requires $r \sim 17A$ which is much too big

Suppose ~~diameter~~ radius of outer helix 8·5 A

This gives 3rd layer-line max. at $\xi/\lambda = .0805$

at 5th ——— ——— $\xi/\lambda = .122$

– these values are reasonable, because max $\simeq J_3$ / J_5 is near outer edge of peak

For equator, we then have max. at $\xi/\lambda = .072, .132, .190, .250$

and 1 zero for $\xi/\lambda = .045$

– this still has zero rather near the 2·5A equator spot

Length of helix of diameter radius 8·5A / pitch 34A

$l^2 = 34^2 + (8.5 \times 2\pi)^2 = 1156 + 2850 = 4006$

$l = 63.3$

∴ distance between atoms on 8·5A radius helix $= \frac{63.3}{10}$

$= 6.3A$

Intensity of inner \ / compared with rest of photograph suggests the outer helix (~8·5A) is heavy part of structure, i.e. P

~~good argument.~~ This is not our argument about radial nucleotide MW

For radius 10A

$l^2 = 1156 + 3950 = 5106$ $\quad l = 7.15A$

For radius 9·4A $l^2 = 1156 + 3490 = 4646$ $\quad l = 6.82A$

A + B similar! 34
MW

[1] right-hand helix as above = basis of structure B, the structure A is probably similar, with P-P distance along fibre axis < 3·4 A, probably 2-2·5A

similar with respect to P-P dist
MW

(c.f. 2A indicated by pos" of P-P peaks = Pattern
d 2·5A " " 11th layer line reflection)

a.K

Now with radius 8·5 A she seems to feel discrepancy of 3rd & 5th with equator less serious & is prepared to consider the model.
evidently 'similar' does not mean that A is helical see Klug
MW

24.2.53 5

NB only Second day on B. MW

Single-strand helix for structure B rules out atom-pairings for structure A (with 7 pairs in fibre period)

∴ single strand has 3.4 A ± c between neighbouring P

∴ structure A has less

This is correct A.K.

If Suppose important translation in Patterson is

$c = \frac{1}{11}$ $b = \pm\frac{1}{11}$ $a = \frac{2}{11}$ (corresp. approx. to Patterson peak)

Then important reflections are those for which

$$h\left(-\frac{2}{11}\right) + k.\left(\pm\frac{1}{11}\right) + l.\frac{1}{11} = 1$$

$$-2h \pm k + l = 11$$

$$-2h \pm k = 11 - l$$

i.e. on 11th layer-line and expect only 0, 0, 11

and mass of reflections on layer-lines 6, 7, 8, without (001) ⇒ does not indicate steps of $\sim\frac{1}{7}$ in c

These reflections are due to the bases. And he REF missed this. A.K. A.K.

← That seems extraordinary. Klug says she missed the bases. MW MW says octaz

Structure B

7th layer-line

2ℓ : 12.2 – 13.8 mm to 2θ : .378 to .427

θ : 10° 21′ to 11° 34′ d : ~~3.691~~ 4.28 to 3.84 Å

$\frac{1}{d^2}$: .0546 to ~~.0377~~ .0678

$\left(\frac{J_7(x)}{C x^2}\right)$: $\left(\frac{\text{P}(3)}{\text{P}(4)}\right)^2$: .0424 $\therefore \left(\frac{\xi}{\lambda}\right)^2$: .0122 to .0254

ξ/λ : .110 to .159

J_7 max. for $J_7(x)$ has $x \sim 9.0$

$\therefore$ for $r \sim 8.5$,

$R = \xi/\lambda = \frac{9}{2\pi \times 8.5}$: .168

for $r = 9.4$ ξ/λ : .152

N.B. Here we expect observed max. to be displaced outwards : Lorentz etc

9th layer-line shd also have max. of same value as 3rd

i.e. ξ/λ : .039 to .094

– this is apparently absent

3-chain or 2-chain helix?

Chains are not equally spaced, : this wd mean n^{th} layer-line contains $3n$s ✓

∴ 3-chain helix is highly improbable (could be possible if suitably spaced)

∴ chains wd be non-equivalent (2 chains ~~change~~ wd be equivalent)

Also : structure A believed to have 2 chains / unit cell (symmetry or other evidence) MW

i.e. B has 2 chains because A has 2 chains.

by density B must be 2 or 3. MW

R.F.T. wd at least making the correct correction A Y

At last

why missing? was it because of spottiness or l.l.? MW

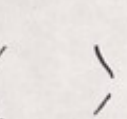
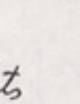
Structure B, 51 c

Layer. Indx	I_r max ξ/λ obs	ξ/λ for r: 9.4	ξ/λ for r: 8.0	ξ/λ for r. 85
0	~~0.905 - 0.130~~ 0.041	.065 zero 0.0406	.076 zero 0.048	zero 0.045
1				
2	MW			
3	0.391 - 0.940	0.071	.083	.0805
5	0.905 - 0.130	0.113	.133	.0122

next page is 5 May MW
This is last B discussion.

N.B.
Outer Pattern  emanating from 3·4 spot is not repeat of pattern  from origin. If it were they would cross on 5th layer-line

OK
(or is it confused?)
HW

Inner  meets  on 5th layer-line OK

$J_{10}(x)$ has first max. for $x \sim 11.8 = 2\pi Rr$

Observed max. on equator, $R = .162$ to $.195$

$\therefore r = 11.6$ to 9.6 OK

Here observed max. is displaced inwards ∴ 3rd max. of J_0 for $r = 9.6$ Å has $R = .172$

Density

Volume of cylinder radius 10 Å, height 34 Å : $\pi \times 100 \times 34 = 10700$ Å^3

Vol. dry nucleotide (density 1·63) = 336 Å^3

∴ no. nucleotides / cylinder : $\frac{10700}{336} = 32$

need to ignore low water content B patterns! MW

Since some fairly dry fibres give structure B, density of cylinder ≈ prob. mean density of dry Na DNA. water lying mainly outside cylinder.

∴ this suggests 3 chains

but not easy to reconcile w structure A

For helix of radius 8·5 Å Vol. cylinder : $\pi \times 8.5^2 \times 34 \simeq 7700$ Å^3

no. nucleotides : $\frac{7700}{336} = 23$

Patterson?

5. 3. 53

M 11

Uses peak on section 2 units, it seems, must be a P-P peak. Other superpositions may be fruitless
∴ used part of Patterson not due to P-P

V 11 is clearly multiple – or, more probably, peak is due to agglomeration of near-equal vectors. ∴ should be several valid positions for axes (as described 9.2.53)

∴ take M11B and M11D and look for possible chain common to each – allowing shift + b-direction of one relative to other

To find correct posn of M11B wrt M11D, look for the 4 origin peaks in each
– these are at height 8 in 110 in M11B and 3, 5 in M11D
(M11c no good, as shown by fact that origin peaks are lost)

M11B can be put on M11D in 4 ways
1/ axes of 0 on 11B may overlap. height 15 on 11D
∴ ~~rotate through 90°~~ put 0-7 on 15-7
i.e. on 15-8 upside-down
2/ 11B and 11D may give different enantiomorphs
– this amounts to 0-7 on 0-7 rotated and upside-down

i.e. posn's are
i) 0-7 on 0-7
ii) 0-7 on 0-7 rotated and upside-down
iii) 0-7 on 15-8 upside-down
iv) 0-7 on 15-8 rotated

M11D 0-7 on M11B 15-8 upside-down

11D 0-7 at ~~≈ -11 cms~~ ~~quite good fit for 3-5, quite good for 10~~
-16.3 3, 5, 8, 10 all fit, ~~but bad for 8~~ general fit good
. Impossible : predicted 5 not considered as predicted 0

M11D 0-7 on M11B 15-8 ~~rotated~~ rotated

11D 0-7 at ≈ +3.5 cms - gives 5-10 nearly coincident, 3 & 8 quite good
(2.7 cms given)
11D 8-15 on 11B 0-7 rot. . general fit good

M11D 0-7 on M11B 0-7

M11D at -15.7 cms → good fit for 3, 5, 8, 10 but using v small peaks
general fit good on 0-7, bad on 15-8
M11D at -8.7 cms

M11D 0-7 on M11B 0-7 rotated and upside-down

~~11D 0-7 at ≈ 21.5 cms gives 3 & 5 good~~
~~General fit poor~~

M11 superpositions 16.3.53

~~M11B & M11E both have origin peaks of height 8 & 10~~
~~Their have different 'a' values, ∴ must relate to different chains~~
~~How can M11E 8-15 be fitted to M11B?~~

M11B has origin peaks at 8 & 10, M11E at 5, 7
Their have different 'a' values, ∴ either belong to diff. chains
or to diff parts of same chain

A. Diff. chains, same heights

M11E 0-7 on M11B 8-15 upside-down

a: 0 b: +7.9 cms
general fit — other peaks less good

M11E 0-7 on M11B 8-15 rotated

a: b/2, b: 11.8 cms good on both tests

M11E 0-7 on M11B 0-7

a: 1/2 b: −1.0 cms

a: 0. b: −8.2 cms ~~origin~~ 0 peaks good
a: 0 b: +8.5

M11E 0-7 on M11B 0-7 rotated and upside-down

20 April

20.4.53

Post Watson-Crick

Is structure A triclinic?

2-axis can't pass through DNA chain : asymmetric sequence

but myoglobins always show peak on axes

If peaks are P, axis can only be pseudo-axis

i.e. array of P monoclinic, but true symmetry triclinic

In this case, whole Patterson is wrong

: each reflection is unresolved pair, (hkl) and $h\bar{k}\bar{l}$)

[If structure is triclinic & P's & monoclinic will Patterson give & correct P-P vectors?]

If structure truly monoclinic

either chains don't go through axes

i.e. no peaks on axes

or sequence of phospho-ester links is 3 3 5 5 3 3 .. etc

this is symmetric about phosphorus atom

but unsuitable a) : widens from asymmetric degradat

b) : prob. unions & get 3Å equally spaced bases, distance ∂ 3.4Å

21 April

inspection of pattern suggest equal spacing

~~spac~~ pseudo halving

21. 4. 53

Intensities of structure A suggest equally spaced chains (pseudo-halving of cell)

Then unit has true diad $\frac{1}{2}$-way between planes

+ pseudo-diad through chain, relating phosphates only

- can we arrange units so that pseudo-diad applies to whole structure and true diad does not?

Pseudo-diad passing through P is only possible if chains are equally spaced.

Vertical distance between 2 chains would then be ~ same as shorter vertical distance in Crick model.

Shapes of Patterson peaks

All peaks are stretched along a.c axis

- can this be due to P ··· Na ≈ that direction ?

- well-resolved ~~peak~~ peaks on C=2 suggest that Na does not lie half-way between 2 P's

Shapes of P-P, Na-Na, and P-Na peaks were calculated by approximating f^2 curve (or $f_P f_{Na}$) by $e^{-a^2 s^2}$ and taking account of artificial temperature factor used

Results

P-P	r(A)	0	0.5	1.0	1.5	2.0	2.5	3.0
P-P	P(-)	115.2	108.0	88.8	64.0	40.4	22.6	10.9
Na-Na		66.3	59.4	42.6	24.1	11.4	4.3	1.3
P-Na		85.2	78.5	61.8	41.3	23.5	11.4	4.7
P-P + Na-Na		181.5	167.4	131.4	88.1	51.8	26.9	12.2
2 (P-Na)		170.4	157.0	123.6	82.6	47.0	22.8	9.4
Shape of peaks for P-Na distance 3.0A		190.9	190.2	178.4	170.7	175.4	183.9	182.6
Shape of peaks for P-Na 2.5A		204.3	214.4	213.0	211.7	208.8	~~197.3~~ 4169.2	
Shape of peaks for P-Na 2.0A		228.5	250.0	255.0	245.1	222.2	183.9	135.8

Isolated Patterson peaks mostly have max. dimension

approx. twice min. dimension

½-peak width of P-P + Na-Na (Patterson) ~ 1.5 × 2 Å

∴ this is minimum dimension.

∴ ∅ ½-peak width of P—Na combination must be ~ 3.0 × 2 Å

∴ this requires P - Na distance ~ 2.0 Å

7 May

7.5.53

Attempts to adapt Watson and Crick model to structure A

Modifications introduced

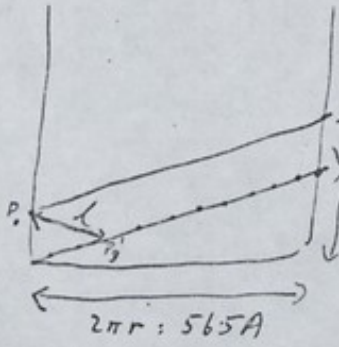
1/ P–P distance decreased from 7.0A to 5.3A
(as suggested by peaks on sections 2-3)

2/ 11 nucleotides per turn instead of 10
(as suggested by meridional peak on 11th layer-line)

3/ 2 chains of helix are equally spaced
(as suggested by pseudo-helical symmetry of cell
and indication on Patterson that only part of structure
repeats at half-cell height

4/ P on radius 9A instead of 10A
(as indicated by cylindrical Patterson)

Suppose chains equally spaced
and P's vertically above one another on chains
Draw schematically un-unwrapped helix



Suppose $P_0 P_3'$ are linked through
three C_3's of same purine-pyrimidine
complex. Then on W & C model
$P_0 - P_3' = 15.2A$

To obtain length of arc l on un-wrapped helix, consider helix of same radius, of which $P_3' P_0$ are is a part
Then this helix makes 3/11 of a turn ∴ height $\left(\frac{1}{2} - \frac{3}{11}\right) \times 28A = \frac{5}{22} \times 28A$
i.e. whole turn ∴ height $\frac{5}{22} \times 11/3 \times 28 = 5/6 \times 28 = 23.4A$
∴ length of whole turn $= \sqrt{56.5^2 + 23.4^2} = \sqrt{3192 + 548} = \sqrt{3740} = 61.2A$
∴ length of arc $l = 3/11 \times 61.2 = 16.8A$

8.5.53

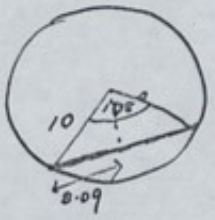
Length of P.P' bracketed through C_3's to same P_4-P_3 complex

Crick says 15.2 A
but this is inconsistent w other data of his model - too small

$C_1 - C_1' = 11A$
$C_1 - P \sim 3.5A$ (from wire model)
and these are fairly nearly co-linear
$\therefore PP' \sim 18A$
- this is consistent with other W & C data

When chain contracts to form structure A, $P - C_3$ can't decrease much - contraction must occur between C_3 & P on other side
$\therefore PP'$ still ~ 18 A

If $P_0 P_0'$ are vertically above one another, distance 15 A



x,y cpt of P_0P_3' is 16.18
3 cpt $(15.0 - 3\times3.4) = 4.8$ A
$\therefore P_0P_3' = \sqrt{16.18^2 + 4.8^2} = \sqrt{261.8 + 23.0} = 16.8$ A

If P_0 rotated ~ 1 A behind P_0' on helix
$P_0P_3' \sim 17.6$ A

11- Blue Book : Section A

Difficulties

Can they have one block / primitive cell

. . how account for 13 A water in C form?

and how account for pseudo-bonds

Density

Vol. dry nucleotide, density 1·63 g/cc, ÷ 336 A^3

Partial sp. vol. 0·55 (Kahler, J. Phys. Coll. Chem. 52 1948 676)

Suppose partial sp. vol. ÷ structure A is 0·55

the 330 g occupy $0.55 \times 330 = 181.5$ cc

1 nucleotide occupies $\frac{181.5 \times 10^{24}}{6.03 \times 10^{23}}$ $Å^3$ $= 296$ $Å^3$

1 molecule H_2O occupies $\frac{18 \times 10^{24}}{6.03 \times 10^{23}}$ $= 29.85$ $Å^3$

Vol. of complete unit cell 24650 $Å^3$

1 nucleotide + 4 H_2O .. 415 $Å^3$ giving 59 nucleotides / unit cell

.. 5 .. .. 465 55

6 475 51·5

7 505 48·5

8 535 45·7

9 565 43·3

Structure B. Suppose 24·5A reflection is (100) of hexag. close-packed rods

Then vol. unit cell: $\frac{2}{\sqrt{3}} \times 24.5^2 = 694$ $Å^3$ $\times 34 = 694 \times 34$ $Å^3$

Suppose this contains 20 nucleotides, i.e. M.Wt $= 20 \times 330 = 6600$

Then density due to nucleotides only is

$$\frac{6600}{6.03 \times 10^{23} \times 694 \times 10^{-24} \times 34} = 0.465 \text{ g/cc}$$

∴ if true density is 1·52 g/cc

water content must be $\frac{1.52 - 0.465}{0.465} \times 100 = 227\%$ of dry weight!

If 40 nucleotides = unit cell

water content is $\frac{1.52 - 0.93}{0.93} = 63.5\%$ of dry weight

still high, but more reasonable

11 May

11.5.53

Equatorial reflections in structure B

Main reflection ~ 24.5 Å

If this is inter-helical distance, density is much too low

Some inter-penetration of chains in one direction must be possible, the spacing in other direction being 24.5 Å

but nucleo-protein gives a same spacing, 24.5 Å

and in this case, as W & C model inter-penetration quite impossible

spacing measured on R & W's published photo

Distances in mm

	① R-W	② Structure B	Ratio ①/②
equatorial	15.4	7.5	2.05
1st layer line	21.7	10.3	2.1
3.4 Å reflection	111	57	1.95

12 May

12. 5.07

Density calculations (see above) suggest packing is such that there are 2 helices per unit cell

(i.e. not hexag. close-packing
- reasonable ∵ helix hasn't got hexag. symmetry

M. Wt. of 20 nucleotides 6600
+ 50% H_2O 9900

∴ X-section of unit cell, for density 1.50 is

$$\frac{9900 \times 10^{16}}{6.03 \times 10^{23} \times 1.50 \times 34 \times 10^{-8}} \text{ Å}^2 = 322 \text{ Å}^2$$

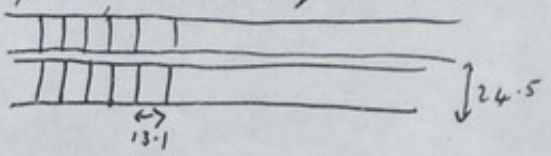
If hexag. close-packing, $\frac{\sqrt{3}}{2} a^2 = 322$ $a^2 = 372$
$a = 19.3$

If distorted, $a b \sin\gamma = 322$
and $b \sin\gamma = 24.5$ (∵ strong reflection)
∴ $a = 13.1$ A - impossible for W & C model

Or Unit cell contains 2 helices
and $a = 26.2$ A.

This is only slightly distorted from graphite-like structure, giving inter-helical distance ~ 16 A

∴ Helices in sheets, with inter-sheet sep^n 24.5A and inter-penetration giving other dimension $\frac{322}{24.5} = 13.1$A



In nucleo-protein, then 13.1 A must have to expand, and 24.5A stays const.

W + C modified for structure A

Cylindrical Patterson ~~below~~ suggests helix of diameter 18A

∴ suppose P_1' on helix of radius 9.0A

and 11 residues per chain (∵ 11th layer-line reflection)

Horizontal opt of P–P on 10A, 10-residue helix : $20 \sin 18° = 6.18$A

9A 11-residue helix : $18 \sin \frac{32.73°}{2} = 5.07$A

P–P for B : $\sqrt{6.18^2 + 3.4^2} = \sqrt{38.19 + 11.56} = \sqrt{49.65} = 7.05$A

—— A : $\sqrt{5.07^2 + 2.55^2} = \sqrt{25.70 + 6.53} = \sqrt{32.23} = 5.68$A

∵ near inter-base distance is const. ∠ of tilt ~40°.

Suppose ∠ of tilt 40° and $C_1' - C_1'$ const. at 11 Å

then horiz. opt of $C_1' - C_1' = 11 \cos 40° = 8.4$A

∴ ~~C_1' lies on ⊙ of radius 4.2A~~

Suppose P_n and P_n' lie vertically above one another

($\frac{1}{2}$-height peak suggests this is approx. true)

Then on ⊙ containing all C_1''s, ~~chord~~ chord subtending $\frac{3 \times 360°}{11}$

at centre is of length 8.4A

radius : $\frac{4.2}{\sin 49.1°} = 5.55$A

[for structure B, equivalent radius is $\frac{5.5}{\sin 54°} = 6.8$A

∴ radial extension of sugar + phosphate ~ same in both cases]

Horizontal opt of $C_1' - C_1'$ is then $5.55 \times 2 \sin \frac{360}{2 \times 11} = 3.12$A

Total $C_1' - C_1' = \sqrt{3.12^2 + 12.55^2} = \sqrt{9.73 + 6.53} = \sqrt{16.26} = 4.03$ A

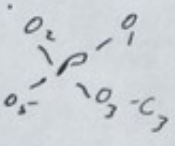
Model giving approx right distances & reasonable v of w

C_2 equidistant from O_1, O_5-

~~P - O_3 - C_3 - C_2 coplanar, & in vertical plane.~~

~~Also coplanar with O~~

giving max. v d W distances for C_2O_2 & C_2O_5-



~ planar

P - O_5- - C_5- - C_4

P - P 5·7 Å C_1' - C_1' 4·0 Å

C_1' N points ~ 40° upwards (when O_3 - C_3 is below P)

Helix of radius 9.0 ~~Å~~ A Pitch 28.1 A

Length of one turn : $\sqrt{(2\times 9\pi)^2 + 28.1^2}$: $\sqrt{56.55^2 + 28.1^2}$: $\sqrt{3198 + 790}$

: $\sqrt{3988}$: 63.15 A

x - cpt of vector on cylindrical Pattern

: 2 X 9 sin $\frac{360 \times n}{11 \times 2}$: 18 sin 16.35 n

x_1 : 18 X ·2815 : 5·07

x_2 : 18 X ·5407 : 9·74

x_3 : 18 X ·7559 : 13·60

x_4 : 18 X ·9098 : 16·37

x_5 : 18 X ·9898 : 17·80

Distances of atoms from axis in projection

with base tilt 4 0°

① r	② 2πr	③ 2πr × .088	$J_0(3)$
0·78	4·9	0·43	·95
1·31	8·2	0·72	·87
1·88	11·8	1·04	·75
2·28	14·3	1·26	·65
2·63	16·5	1·45	·55
2·73	17·2	1·51	·51
2·88	18·1	1·59	·46
3·06	19·2	1·69	·40
3·11	19·5	1·72	·39
)3·35	21·0	1·85	(·31)·16
3·86	24·3	2·14	·14
3·92	24·6	2·16	·13
4·09	25·7	2·26	·08
4·10	25·8	2·27	·07
4·12	25·8	2·27	·07
4·44	27·9	2·45	·02
·54	28·5	2·51	$\overline{\cdot 05}$
·55	28·6	2·51	$\overline{\cdot 05}$
4·90	30·8	2·71	$(\overline{\cdot 15})\,\overline{\cdot 08}$
·10	32·1	2·82	$\overline{\cdot 19}$
·67	35·6	3·13	~~$\overline{\cdot 20}$~~ $\overline{\cdot 21}$
·67	35·6	3·13	$\overline{\cdot 21}$

t/21

19 May 53

19.5.53

Intensities in structure A

If one helix per lattice point, then ~~equatorial~~, intensities depend only on structure factor of helix

∴ can't explain large diff. I for (130) and (200)
is this wrong, → large error in Patterson?

To calculate equatorial intensities, only require radial distance of each atom.

Suppose base complex tilted 40°.

Drawing (1" : 1Å) gives $C_1' - C_1'$: 11.2 Å

∴ (see 2 pages back) these lie on helix of radius 5.67 Å

Suppose tilt is about "diad" of complex. Then draw foreshortened complex by reducing distance of each atom from diad by factor $\cos 40° = 0.766$. This gives projection

Then measure distance of each atom from axis.

Intensities & positions of 1st equatorial reflection

Continuous transition from ~17 Å in near-dry DNA through 19 Å for structure A → >24 Å

This suggests that reflection has same significance in 2 phases
i.e. related to inter-unit distance in both cases

Intensity appears to have min. at ~19 Å
- c/ dry rather dry photo 34 in which reflect ~17-18 Å
is stronger than normal 19 Å in structure A

[Dry photo 34 has meridional arc of larger spacing than structure B (of ~36 Å) ?]

Spacing on photos showing A+B (e.g. 75, 5,) ~20 Å + intensity high

52 & 53 are same specimen as 51, at higher RH (92%)
- they have same equatorial spacing

4.6.53

Tilt of bases in structure A

6, 7, and 8 layer-lines suggest $\sim 25°$

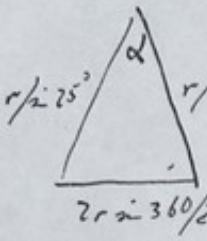
$\therefore$ $c/3$ mean values are 0.56, 0.48, .44 for these layer-lines

i.e. $\tan^{-1}$ 29°, 26°, 24°

Suppose tilt 25°, find ∠ between planes of neighbouring bases

i.e. ∠ between ⊥'s to planes of bases

These lie on cone of semi-vertical angle 25°



$\alpha = 2\sin^{-1}\left(\sin\frac{360}{22}\sin 25\right)$

$= 2\sin^{-1}\cdot 2818 \times \cdot 4226 = 2\sin^{-1}\cdot 11.9$

$\doteq 2 \times 6°\,50'$

$\doteq 13\frac{1}{2}°$

3.

4

2

5

2.

3.

1

4.

5.

Harker peaks for helix of radius 9A (structure A)

	'a'		'c'	$\delta = \frac{1a}{22} \times 254$	'c' co-ordinates in A	'c' co-ordinates in section
1.	$18 \sin \frac{360}{22}$	$= 18 \sin 16.36° : 18 \times .2818 : 5.07$	$c/11$	0.6	3.2, 17.2	
2.	$18 \sin 360 \times \frac{3}{22}$	$: 18 \sin 49.1° : 18 \times .7559 : 13.6$	$3c/11$	1.6	9.3, 23.2	
3.	$18 \sin 360 \times \frac{5}{22}$	$: 18 \sin 81.85° : 18 \times .9899 : 17.8$	$5c/11$	2.1	14.9, 0.8	
4.	$18 \sin 360 \times \frac{2}{11}$	$: 18 \sin 65.5° : 18 \times .9100 : 16.4$	$7c/11$	1.9	19.8, 5.8	
5.	$18 \sin 360 \times \frac{1}{11}$	$: 18 \sin 32.72° : 18 \times .5404 : 9.74$	$9c/11$	1.2	24.2, 10.1	

δ is : c-b sections are not $\perp$ to fibre axis.

$\pm \delta$ depending on orientation (or hand) of helix

Examination of inter-helical vectors on 3-dimensional chart orientation & hand to be as indicated opposite, & this gives + δ

27 July 53

24.7.53

Suppose the 2 levels on which P atoms lie are related by vector V_1

and suppose a vector v on Patterson is a P – X interaction, where X is any atom (e.g. N_a)

then there is a similar vector $V_1 - v$

Suppose V_1 has $x = -1$ A
$y = 0$
$z = 13$ A (= section 14)

then find which Patterson peaks, un-accounted for by P-P vectors, occur in pairs v and $V_1 - v$. These will be P – X vectors

e.g. v section 10, $x = 6$ A $y = 0$
$V_1 - v$ section 4

v section 12 $x \sim 8$ A, $y \sim 7$ A
gives section 2 $x \sim -9$ A $0 \sim -7$

Extra page Includes

Loose sheet
A.K.

Attempt to explain (0011) by arrangement of two-plane groups

$$F_{00l}^{hkl} = \sum_3 f^2 \omega 2\pi l z$$

Suppose 7 groups at heights $0, \frac{5}{30}, \frac{10}{30}, \frac{13}{30}, \frac{17}{30}, \frac{20}{30}, \frac{25}{30}$

Take amplitudes 20 for $\frac{5}{30}, \frac{10}{30}, \frac{13}{30}$ (steps 10, 20, 26)

and " 10 " 0

and vary heights (3-values) to find: —

Possible arrangements giving strong 00l

① Heights $0, 5, 8\frac{1}{2}, 13\frac{1}{2}$ $F_{0011} = 54$ $F_{007} = 52$ $F_{003} = 19$ $F_{009} = -18$

② " $0, 5\frac{1}{2}, 11, 13\frac{1}{2}$ $F_{0011} = 78$ $F_{005} = 36$ $F_{006} = 25$

③ " $0, 5\frac{1}{2}, 10\frac{1}{2}, 13\frac{1}{2}$ $F_{0011} = 60$ $F_{006} = 36$ $F_{0012} = 26$ $F_{009} = 30$

Two 2-3-4 Heights $0, 10, 20, 26$ gives $F_{0011} = 12$, $F_{0012} = 46$ $F_{005} = 20$ $F_{006} = 34$ etc

① & ③ fit Pattern less well than ②

∴ conclude that (0011) is not due to pinacoidal groups

Consider each peak being 2 cyclic $\sim 2\Lambda$ groups ∴ C

Then heights $1, 4, 6, 7\frac{1}{2}, 9\frac{1}{2}, 12\frac{1}{2}, 14\frac{1}{2}$

gives $001 = \bar{3}$ $002 = \bar{2}$ $003 = \bar{8}$ $004 = \bar{13}$ $005 = 1$ $006 = 5$ $007 = 6$

$008 = 2$ $009 = 3$ $0010 = 5$ $0011 = \bar{37}$ $0012 = 4$ $0013 = \bar{22}$ $0014 = \bar{13}$ $0015 = 7$

found in notebook, undated
?Feb 1953? A K

3 chains

Non-equivalents unlikely

if equivalent must be equally spaced ∴ this is ruled out

But both indicate 2

2 chains

suggested by 1 chain : 2 chains in structure A

equally spaced ruled out

But unequally spaced 2 are still equivalent

THE NOTEBOOK CONTINUES FOR PERHAPS ANOTHER 50 PP. BUT SINCE THESE NUMBERED LAT ROMAN APPEAR TO BE CLASS NOTES AND NOT EXPERIMENTAL WORK, AND I HAVE RUN OUT OF TIME, I AM NOT INCLUDING PHOTOCOPIES OF THE FINAL PAGES.

X·22·99

1

R. FRANKLIN
NOTE BOOK
1952

Revised Monoclinic Cell

$a^* = 7.9\,10^{-2}$. $b^* = 4.25\,.10^{-2}$.

Zero layer spot.	ξ observed	ξ calc.	Index	Intensity	
3	0·159	0·158	200	Very very Strong	2
4	0·1825	0·18	220	Very Weak	1
5 (β?)	0·216	0·214	050	Very Weak	1
6	0·241	0·234 0·241	240 310	Fairly Strong	5
7	0·282			Very Weak	* 1
8 (β)	0·304	0·308 0·300	170 090 } 260	Very Weak	2
9	0·317	0·316 0·317	400 410 & 350	Fairly Strong	7
10	0·33	0·327	420	Strong	8
11	0·357	0·358	440	Weak	2
(β) 12	0·373	0·376	280	Weak	1
13	0·389	0·3825 0·395	090, 450, 370 190	Weak	5
14	0·407	0·407	460	Strong	8
15	0·427	0·425	0,10,0	Fairly Strong	5

P 47 Sep 52
P 17 18 Nov 51
48 Dec 52
48 Monoclinic
P 52 13 Feb
53 28 Feb
54 Mark 3

020
(130)
200
220
140
310
300
240 150
070
060
350
420
440
080
460
0·40
510
0·42
540
560
530

ξ = 27·0
320
check
(060)
(270)
ξ·40 Check
2 measured ξ.

Plate VIII

$d_{hkl} = \frac{\sqrt{3}}{2} \cdot a \cdot \frac{1}{(h^2+hk+k^2)^{\frac{1}{2}}}$

Assume 2nd spot 11·3 A° = d_{110}.

$d_{110} = a/2$.

$\therefore a = 22{\cdot}6$.

$d_{100} = \sqrt{3} \cdot a/2 = 19{\cdot}6$ A°. Therefore on the Rotograph

$\therefore$ A symmetrical

	h k l	$\sqrt{h^2+k^2+hk}$	d_{theory}	$d_{observed}$	2x mms	Intensity	No. of Refl.	ϵ
1	0 1 0	1	19·6	19·5 ?	5·5 ?	Fairly Strong	1	0·09
3	1 1	$\sqrt{3}$	11·3	11·3	9·5	Very Strong +	3	0·15
4	2 0 0 2	2	9·8	9·7	11·00	Very Weak	4	0·18
7	2 1 1 2	$\sqrt{7}$	7·4	7·4	14·5	Fairly Strong	6	0·24 (2×1)
9	3 0 0 3	3	6·53	6·33		Very Weak	7	0·28 (0·32)
2	2 2	$\sqrt{12}$	5·65	5·64		Fairly Strong	9	0·31
13	3 1 1 3	$\sqrt{13}$	5·41	5·47		Strong	10	0·33
6	4 0 0 4	4	4·9	5·0		Weak	11	0·35
9	3 2 2 3	$\sqrt{9}$	4·5	4·59		Weak	13	0·389
1	4 1 1 4	$\sqrt{21}$	4·27	4·37		Strong	14	0·40
1	5 0 0 5	5	3·92	4·17		Fairly Strong	15	0·427

$d = \lambda/\epsilon$. $\epsilon = \lambda/d$

Additional Observed Effects:-

2x	Intensity	$d\lambda = \epsilon$	No. of Refl.	$d\lambda = \beta$	2x mms	Intensity	$d\lambda = \epsilon$	No. of Refl.	$d\lambda = \beta$
5 ∴	Very Weak		5	$\pm\epsilon$	21·5	Weak		11	
	Very Weak		7		22·5	Weak		12	β of 14
13	Very Weak		8	β of 10	23·5	Weak		13	
15	Fairly Strong.		2	β of 3	24·7	Strong		14	
9·1	Fairly Strong		9		25·9	Fairly Strong		15	
9·9	Strong		10						

3

cms. 2x	θ_B^c	θ_B°	log sin θ_B°	$\lambda = K\alpha_{12}$ / d A°	No of L Reflexn	$\lambda = p$ / d_A°
0·550 (0·57)	0·04583 *	2° 37½′	1·33916	19·503	1	
1·10 (1·12)	0·0916 *	5° 15′	1·03857	9·7588	4	
1·45	0·12083 *	6° 55½′	0·91872	7·4079	6	
1·70	0·1416 *	8° 7′	0·85022	6·3270	7	
1·83	0·1525	8° 44′	0·81863	5·8829	8	$q = 0·3$ 5·3248
1·91	0·15916 *	9° 7′	0·80013	5·6377	9	
1·99	0·16583 *	9° 30′	0·78239	5·4008	10	
2·15	0·17916 *	10° 16′	0·74902	5·0106	11	190 = 270 $q = 0·373$
2·25	0·1875	10° 45′	0·72927	4·7885	12	4·3351
2·35	0·19583 *	11° 13′	0·71104	4·5926	13	
2·47	0·20583 *	11° 47½′	0·68962	4·3713	14	-
2·59	0·21583 *	12° 22′	0·66924	4·1706	15	150° $q = ·216$
13·	0·1083 *	6° 12½′	0·96601	8·2484	5	7·4749
0·860	0·0716 *	4° 6′	1·14571	12·494	2	11·309

$\log \frac{\lambda K\alpha_{12}}{2}$ = T·95097 $\quad \lambda_\beta$ = 1·617 A°

$\log \frac{\lambda\beta}{2}$ = T·90768

NB Intensity alternates ... zero line ?

—

Second layer line lies between $2y_2$ = 7·5 and 7·75 mms.
This gives limits of c as 27·7 and 29·2 and 27·9 and 29·5
Mean 28·55

1st layer line lies between 3·70 & 3·8 mm's. Giving c between 28·98 and 28·32 A° Mean 28·6.

Therefore taking c = 28·5 A° gives $z_1 = 0·0627$.

$z_2 = ·1254$

1·86

4

1st layer line.

2x.	ξ	d_A λ=kx12	No. of Reflex.	Intensity	d_{obs}	σ^2	σ	d_{hkl} calc
5·5.	0·0916	16·06	1	Strong		·01236	0·1112	101 16·1
9·5 9·25	0·158 0·150	10·48	2	Strong		·02894	0·1702	111 10·45
10·5	0·170	9·85	3	Weak	8·96	·03284	0·1812	
1·5	0·185	9·16	4	Very Very Weak		·03814	0·1952	201 9·22
4·5	0·241	7·18	5	Weak		·0619	0·2485	211 7·14
5·5	0·25	6·92	6	Weak	6·27	·0664	0·258	301
17·2	0·28	6·22	7	Weak		·0822	0·287	301 6·32

Disc is tail of spot on 2nd layer line

Disc is spread of spot 2/3 way

$3_1^2 = 0·00391+5$

NB $d_{221} = 5·52$

$\frac{1}{d_{hkl}} = 1/\left(\frac{4}{3}\frac{(h^2+hk+k^2)}{a^2} + \frac{l^2}{c^2}\right)^{\frac{1}{2}}$ $\therefore d^2_{hkl} = 3a^2c^2/c^2(h^2+hk+k^2)+l^2 \cdot 3 \cdot a^2$

$\therefore 3_2^2 = 0·0157$

2nd layer line.

2x	ξ	d_A λ=kx12	No. of Reflex.	Intensity	d_{hkl} Monoclinic	σ^2	σ	d_{obs}
5·25	0·0875 0·085	12·4	1	Strong	(012) $\bar{2}02$	·0206	·1439	
6·25 ECK	0·110	11·1	2	Fairly Str.	02$\bar{2}$	·0257	·1605	
·5	0·17	8·45	3	Fairly Str	$\bar{3}12$	·0446	·2115	7·65
·1	(0·20) 0·198	7·7	4	Str. Fairly	$\bar{1}52$ ~~242~~	·0537	·232	6·9
4·1	0·236	6·82	5	Strong	202	·0687	·262	
·5	0·265	6·1	6	Weak	~~$\bar{4}42$~~	·0859	·292	5·55
3·8	0·3	5·5	7	Strong	~~$\bar{4}42$~~ ~~242~~	·1057	·325	
·2	~~0·31~~ 0·315	5·35	8	~~Strong~~	~~$\bar{3}12$~~ ~~162~~	·1117	·334	

NB 131 to $\xi_1 = 1194$

1st hexagonic

Index	d_{calc}	d_{obs}	Intensity	Monoclinic hkl	ξ
101	16·1	16·05	Strong	021	0·09
~~111~~	~~10·45~~	~~10·48~~	Strong	$\bar{2}21$	0·15
201	9·22	9·15	Very Weak	~~$\bar{2}31$~~ $\bar{1}41$	~~0·17~~
211	7·14	7·18	Weak		
301	6·32	6·22	Weak		

2nd hexagonic

2x	No of Refl.	ξ	σ	$\lambda = fx.$ d	hkl.	Intensity
21·5	9	·35	·3492	4·8	~~$\bar{5}30$~~ (~~$\bar{4}60$~~) ~~472~~	Weak.
23·5	10	·372	·3995	4·46	352	Fairly Strong
24·8	Abt. 11	·4	·4195	4·26	422 ~~$\bar{4}22$~~	Fairly Strong

Calculated Values of $\zeta_{6,7,8}$ from ζ_1 & ζ_2.

$\zeta_6 = 0·3762$

$\zeta_7 = 0·4389$

$\zeta_8 = 0·5016$.

These measurements can also be related to a C centred rectangular cell. $a = 22 \cdot 6\ A^\circ$ $b = 39 \cdot 2$

$a^* = 7 \cdot 95\ 10^{-2}$

$b^* = 4 \cdot 56 \cdot 10^{-2}$

& $2c^* \cos\beta^* = 7 \cdot 5\ 10^{-2}$

Now apparent c value $= c^* \sin\beta^*$. ie $\frac{1}{28 \cdot 5} = 6 \cdot 27\ 10^{-2}$

$\Rightarrow \frac{7 \cdot 5}{6 \cdot 27} = \frac{2c^* \cos\beta^*}{c^* \sin\beta^*}$ Hence $\tan\beta^* = 1 \cdot 672$. ie $\beta^* = 59°8'$

ie $\beta = 121°$ & $c^* = 24 \cdot 45$.

ie $\gamma = 180 - \beta^*$

2nd layer line meas. suggest $2b^* = 4 \cdot 1 \cdot 10^{-2}$

ie $b = 43 \cdot 5$.

$d_{020} = 21 \cdot 75$.

$\varepsilon_{020} = 82 \cdot 10^{-2}$

Origin for 1st layer line is $c^* \cos\beta^*$ in direction $-a^*$ ie $3 \cdot 75 \cdot 10^{-2}$

Reflex No	Intensity	ξ	hkl
1	Strong	0·09	021
2	Strong	0·15	$\bar{2}21$
3	Very Weak	0·168	131 & T41
4	Very Weak	0·185	(check)
5	Weak	0·241	331
6	Weak	0·25	
7	Weak	0·28	311

6th layer line $2x = 12 \cdot$ mms.

$\therefore \xi = 0 \cdot 21$

If $3_6 = \cdot 375$ (calc) $3_6^2 = 0 \cdot 1415$

Hence $\sigma^2 = 0 \cdot 1815$ $\sigma = 0 \cdot 426$.

$\therefore d = 4 \cdot 18$.

Now $d_{006} = 4 \cdot 08$.

~~This also explains diffuse streaks from origin~~

4th layer line Origin for 7th layer line is $7 \cdot c^* \cos\beta^* \rightarrow -a^*$ from 00.

ie $26 \cdot 25\ 10^{-2}$ $\xi = 0 \cdot 23$ $d = \frac{1}{6 \cdot 27 \times 25 \cdot 3} = 0 \cdot 439$.

+ max $\cdot 2$. d 127. NB ~~dec~~

8th layer line

Origin for 8th layer line. ie $30 \cdot 00 \cdot 10^{-2} \rightarrow -a^*$ from. $\xi = \cdot 2 - \cdot 25$

$3_8 = \cdot 50$ $\bar{6}28$. $\bar{1}38$ $\bar{2}58$ 468

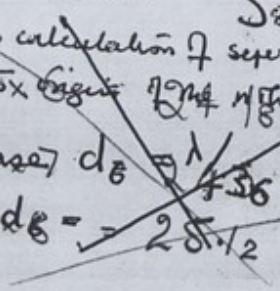
Observed Values "Centres" of Heavy Top Arcs.

$\xi_6 = 0.21$ $\zeta_6 = 0.39$ $\therefore d = 4.03$ (0 = 0.443)

$\xi_7 = 0.22$ $\zeta_7 = 0.45$ $d = 3.50$ (0 = 0.509)

$\xi_8 = 0.230$ $\zeta_8 = 0.52$ $d = 3.14$ (0 = 0.568)

NB This calculation of separation of planes is not valid unless ξ_n & ζ_n are referred to origin of 24 mm nett. Then $d = \lambda / \sqrt{\xi_n^2 + \zeta_n^2}$ recorded as these measurements



If this be case, d_6 since ξ's referred to origin of Arc (nett = zero value $\xi = 24.5$)

Then $d_6 = 28.12$. i.e. $d_{006} = 4.08$ (Intercept unit $d \times n$)

$d_{007} = 3.6$

$d_{008} = 3.06$

NB If measure centration of much young spots 8. get $\zeta_y = 3.7$ cm

Hence $d = 3.27$. ?

The above spots lie on a line making intercepts

$\xi_6 = 20.8\,10^{-2}$ $\xi_7 = 21.8\,10^{-2}$ & $\xi_8 = 22.7.\,10^{-2}$.

Both the theoretical value of ζ_6 ζ_7 & ζ_8 respectively

is ~~22~~ $\zeta_6 = 0.3762$ $\zeta_7 = 0.4389$ $\zeta_8 = .5016$

as calculated from observed ζ_1 & ζ_2.

Going. ξ_6. $\bar{5}36$. $\bar{3}56$, $\bar{2}56$ or $\bar{1}46$

ξ_7 $\bar{6}07$, $\bar{1}37$

ξ_8 $\bar{5}58$ $\bar{1}18$

RANGE OF THREE TOP SPOTS.

Extremes of 6th 7th & 8th arcs in Top left to Bottom right, have the following ξ & ζ values;-

6 $\xi_1 = .175$ $\zeta_1 = 0.42$ $\xi_2 = .25$ $\zeta_2 = 0.37$.

7 $\xi_1 = .175$ $\zeta_1 = 0.48$ $\xi_2 = 0.25$ $\zeta_2 = 0.44$

8 $\xi_1 = .2$ $\zeta_1 = 0.54$ $\xi_2 = .25$ $\zeta_2 = 0.475$

NB Best line through these spreads photographically has $\theta = 64°7'$.

Can make Spot 1 zero. (110) & 2nd spot (220). Then in my decline 8
q_{010} is $b^* = 4.7.10^{-2}$. & $a^* = 6.5.10^{-2}$.
and $c^* \cos\beta^* = 1.16.10^{-2}$ $2c^* \cos\beta^* = 2.3$.

Zero layer line

Spot	Index
1	110
3	220
6	330
9	440
14	550

1st layer line

Spot	Index	q.
1	111	0.9
2	$\bar{2}21$	0.15
3.	221	0.17.
4	$\bar{3}11$?	0.185
5.	$\bar{1}51$.	0.241.
6	331	0.25
7	340	0.28

~~1st layer line~~

∴ 6th layer line has org = $6.90.10^{-2}$ in $-ve\ a^*$.

3.5
1.7

2nd layer line

Spot	Index	q
1	102	0.0875. (Check)
2	112	0.10
3	$\bar{3}02$	0.17
4	322	0.198
5	322 / 052	0.236
6		0.268

Intercept. 1st layer. $= -1.15.a^*$
Intercept 2nd layer $= -2.3$.

$e^{-q^2 s}$

$1, e^{-\frac{\pi x^2}{a^2}}$

a

Suppose line joining A, B C & 2nd 200 line spot is really 202 line

Then $\tan\beta^* = 7.5600$. ie $\beta^* = 82° 28'$

Hence intercept c^* $c = c_{app} \cdot \sin\beta^* = 28.2$.

Hence Intercept on 1st layer line $= \lambda/28.2 \cos\beta^*$

$= .83 \cdot 10^{-2}$

Constrain Hallowell 200 = 16.
But 8.2 = 110.

NB Obtain $2c^*\cos\beta^*$ by assuming 1st spot on 2nd layer line to be 202. Then $\varepsilon_{200} - \varepsilon_{1st\,spot\,2nd\,line}$ gives displacement of 2nd line origin from zero line origin ie gives $2c^*\cos\beta^*$.

Correction to Previous Monoclinic Lattice

$c^*\cos\beta^* = 3.525\,10^{-2}$. $2b^* = 8.5\,10^{-2}$. $a^* = 7.9\,10^{-2}$.

ie $b = 4.282\,5$ A° $a = 22.6$ A°

NB More careful measurement shows ε_{202} to be 0.0875. Since $\varepsilon_{11.34°} = .158$. this gives the above value of $c^*\cos\beta^*$. This means $\varepsilon_{006} = 21.150\,10^{-2}$ (ie displacement of 6th order 6th nett)

And $\varepsilon_{005} = 17.625$.

Calculation of c^* and β^* Both these values depend on the apparent value of c. as determined by separation of the layer lines. This is not certain due to spread in meridional direction.

If centre of spot C(6) be considered as locating 006. Then

$\zeta_6 = 39.10^{-2}$ ie $\zeta_1 = 6.5.10^{-2}$

Now ζ_5 observed = 32.5 10^{-2} ie suggesting $\zeta_1 = 6.5.10^{-2}$

ζ_4 observed $= 26.10^{-2}$ suggesting $6.5\,10^{-2}$

Centre of spot B. gives. $\zeta_7 = 4.6.10^{-2}$ ie $\zeta_1 = 6.57$ $[\zeta_7 = 45.5]$

or $= 4.5\,10^{-2}$ $\zeta_1 = 6.43$. $[\zeta_1 = 6.5]$

Centre of spot A (measured or squared drafted) $\zeta_8 = 51.10^{-2}$ ie $\zeta_1 = 6.4$

But darkest spot scales at $\zeta = 52\,10^{-2}$ ie $\zeta_1 = 6.5$.

Week 13th

Crowds of Spots between 2nd & 6th layer lines.

5th? $2x = 12.5$ mms $2y = 20$ Fairly Strong. (12.5-12.75)

$\xi_1 = .21$ $\zeta = .325$ 505 or 255.

4th? $2x = 116$ mms $2y = 15.75$ Strong.

$\xi = .25$ $\zeta = .26$.

NB Tabulated from ξ_1 & ζ_2. $\zeta_5 = 0.3135$ $\zeta_4 = 0.2508$

13th March

Consider Lattice vector $\xi = 15.8\,10^{-2}$ as 200. ξ 100 $= 7.9.10^{-2}$

110 4th layer line spot as 111.

If 1st spot on 2nd layer line is $\bar{2}02$. Then displacement from origin of 002 is $15.8 - 8.75$. ie $7.05.10^{-2}$.

So $c^* \cos\beta^* = 3.525.10^{-2}$

If this is the case then ~~if first spot is 200~~, can't get 1st spot 1st layer line as 111. since its ξ value falls short of the 10R line. ie if 1st spot is 200. then next spot is 5.

Suppose first spot 100, second spot will be 020. 3rd 120 & 4th 200. This gives $010 = 10.1\,10^{-2}$. But ~~020~~ this is absent. Could be C centered. Then 020 should be present ie $\xi = 20.2$. But this absent. ∴ First spot (11.3A°) is ≠ 110.

Suppose 11.3 A° = 020. next spot is 120. the next 200. Take d 200 as in case above = 7.4 quite thus a strong reflection. This also does not fit the rest of the spots. ie 11.3 ≠ 020.

If $\zeta_1 = 0.065$. Then $C = 27.45$ ie $\sin\psi_1 = 0.065$ ∴ $\psi = 3°\,44'$

$y_2 - y_1 = 30 \tan\psi = 30 \times 0.0644 = 1.9542$ ie $2y_1 = 3.908$ mms.

$\zeta_3 = 0.13$. $\sin\psi_2 = 7°\,28'$ ∴ $2y_3 = 6.4\,3111 = 7.86$ mms

11

1st layer line

Spot	ξ_{obs}	ξ_{calc}	Index
1	0·0916	0·092	021
2	0·150	0·150	$\bar{2}20$
3	0·170	0·170	131
4	0·185	0·178	$\bar{1}41$ $\bar{2}31$
5	0·241	0·241 02395	151 $\bar{3}31$
6	0·25	0·245 0·255	$\bar{2}51$ 241
7	0·28	0·283 0·281	$\bar{2}60$ $\bar{4}08$

check ?

2nd layer line:-

1	0·0875	0·0878	$\bar{2}02$
2	0·1	0·11	022
3	0·17	0·17 0·172	$\bar{1}42$ $\bar{3}12$ or 122
4	0·198	0·196	132
5	0·236	0·238 0·244	$\bar{3}42$ 302 $\bar{4}02$
6	0·265	0·265 0·261	062 $\bar{5}22$ · 232 152
7	0·3	0·299	$\bar{4}42$
8	0·31 0·315	0·310 0·315	312 $\bar{3}62$
9	0·35	0·348	$\bar{5}32$ 082 082
10	0·38 (75)	0·374 0·38	$\bar{3}52$ $\bar{3}82$
11	0·4	0·395 0·40	422 362

5th layer line

Spot	ξ_{obs}	ξ_{calc}	Index
1	·21	·215	505 or $\bar{2}55$

4th layer line

1	·26(5)	·254 or ·256 ·26	134 054 $\bar{5}14$

$\bar{2}64$

6th layer line

Spread		·2115	006
Spot		·29	116
		·138	$\bar{1}16$
		·26	$\bar{6}06$

$6c^* \cos\beta^* = 0.2115$

7th layer line:

Spread		·172	$\bar{1}17$
Spot		·214	$\bar{3}57$
		·224	$\bar{4}57$
		·228	$\bar{6}07$
			047

$7c^* \cos\beta^* = 24.675\,10^{-2}$

8th layer line

		·23	$\bar{6}38$
		·239	138
		·208	$\bar{1}18$

$8c^* \cos\beta^* = 28.200^{-2}$

Zonal lines

$a^* \perp c$

$c^* \perp a$

$\beta^* = 180 - \beta$

$b^* \parallel b$

001 + h0l strongest
Incl. layer β^*.

Calculation of apparent c. $\lambda_{K\alpha_{12}} = 1.786\,A^\circ$

$\zeta_6 = 39.\,10^{-2}$ Whence $c = 27.46$

$\zeta_7 = 45.6\,10^{-2}$ — $c = 27.46.$

$\zeta_8 = 52.\,10^{-2}$ — $c = 27.46.$

$\zeta_5 = 32.5.\,10^{-2}$ — $c = 27.46.$

$\zeta_4 = 26.\,10^{-2}$ — $c = 27.46.$

$\zeta_2 = ?$ fall in gap above $13.\,10^{-2}$. $c = 27.46.$

$\zeta_1 = ?$ On above $\zeta_6 - \zeta_4$ suggest $6.5\,10^{-2}$ $c = 27.46.$

NB ζ_1 has $2\eta_1$ observed between 3.9 and 3.70. Above value gives $2\eta = 3.9$

ζ_2 has $2\eta_1$ twice 7.8 and 7.8. Above calc. value gives $2\eta = 7.86$ mms.

Calc. of β^* (i) $c^* \cos\beta^* = 3.525\,10^{-2}$ $\zeta^*_{(alp)} = c^* \sin\beta^* = 6.5\,10^{-2}$

Whence $\tan\beta^* = 6.5/3.525 = 1.8425.$

Hence $\beta^* = 61^\circ\ 30'\ 35''.$

(ii) The negative slope of the line joining $\bar{2}02$ and 200 is $\tan\beta^*$

Whence $\tan\beta^* = \zeta_2/\zeta_{200} - \zeta_{\bar{2}02} = \dfrac{13.\,10^{-2}}{7.05.\,10^{-2}}$

NB $\zeta_2 = 2.c^*\sin\beta^*$ and, $\zeta_{200} - \zeta_{\bar{2}02} = 2c^*\cos\beta^*$

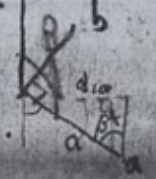
is same value as above. Since these are the observed values from which the values of $c^*\cos\beta$ & $c^*\sin\beta^*$ were calculated.

Calculation of c. $c^* = 6.5\,10^{-2}/\sin\beta^*$ $\therefore 27.46.\sin\beta^* = \lambda/c^* = d_{001}$

$\lambda/c^* = 24.125.A^\circ$ i.e. 24.1 & $d_{001} = 24.1.$

NB $\lambda/a^* = 22.6\ A^\circ = d_{100}$

$\lambda/b = 42.2A^\circ = d_{010} = b$



$d_{100}/a = \cos\beta$

i.e. $c = 27.45\,A^\circ$, $b = 42.2A^\circ$ $a = 25.75\,A^\circ$

13

Suppose spot 3 zero line be 100. Then consider line thro' this point & A, B, C. give 106, 107 & 108.

and values of $6c^*\cos\beta^* = (21 - 15\cdot8)10^{-2} = 5\cdot2 \therefore c^*\cos\beta^* = 0.86 * 10^{-2}$

$7c^*\cos\beta^* = (22 - 15\cdot8)10^{-2} = 6\cdot2$ " $= 0.885$

$8c^*\cos\beta^* = (23 - 15\cdot8)10^{-2} = 7\cdot2$ $\therefore c^*\cos\beta^* = 0.9$

Mean value 0.883.

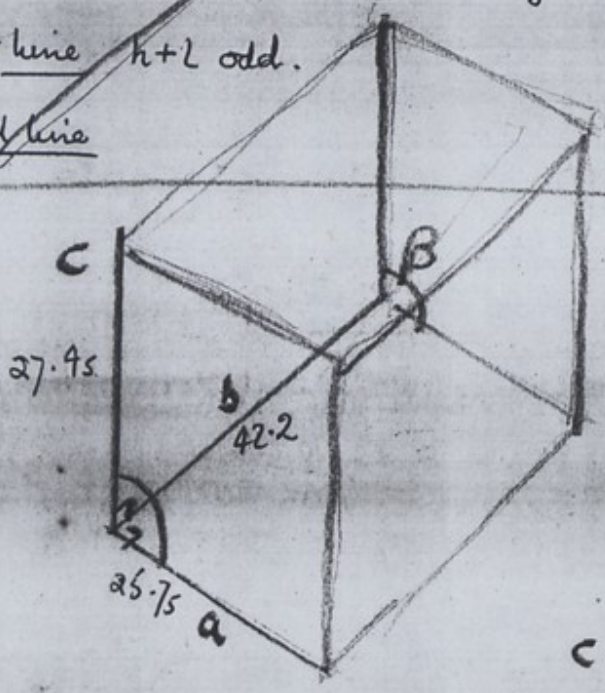
This however leads to no satisfactory indexing of 1st & 2nd layer lines. & further provides no explanation of line joining spot 6 (6) to origin.

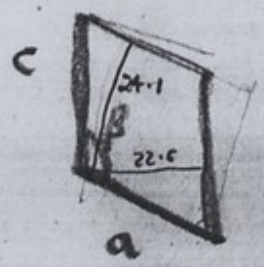
Absent Reflections

Zero line:— h+k odd. Missing 130.

1st line h+l odd.

2nd line





Number of Monomers per Unit Cell

Davidson gives 330 as average Mol wt. for a nucleotide. So assuming One (23) Sodium atom per nucleotide, tacked on to phosphate ion, we have Av. M.Wt. = 353.

Then, if Molecular mass associated with each cell be M.

$$M = \frac{V(\text{in } A^{\circ 3})\,\rho}{1.6604}$$ ρ = density of polymer in gms/cc

Further M should be an integral multiple of 353.

Now $V = abc\sin\beta$.

$V = 22.6 \times 42.2 \times 27.45 \times \sin\beta$ $= 26.2 \cdot 10^3\ A^{\circ 3} \cdot \sin\beta$

$a.b.c\sin\beta$ = 25.75 · 42.2 · 24.1 = $23.0.10^3.A^3$ $= 26.2.10^3\ A^3$??

Density? Dry wt. figure given by Astbury is 1.65 gms/cc. !! The value here must be lower ∴ specimen has taken up water, further than is water necessary for the order observed. However Astbury's figure not necessarily true value.

Let N be number of Monomeres per unit cell then

$$N = \frac{V\rho}{1.6604 \cdot 352}$$ $= 44.8\rho$.

~~$44.8\ \rho = 39.4.\rho$~~

ρ gms/cc	N
1.65	~~74.65~~
0.406	16
0.813	32
1.625	64

Now Unit cell is C centered. Suppose then ~~8~~ 8. Whose spacing d = 3.15 indicates 8 planes to the unit cell, does give the reflection from nearest approach of base rings. Then unit cell may be assumed 8 monomers high. Simplest packing is one chain down each corner and one at centre. Total 2 chains unique to each cell. ie Only 16 nucleotides weight associated with the unit cell. This would mean $\rho = 0.406$.

A reasonable assumption is that whatever the value of N it must be some multiple of 8, Due to the height of the unit cell,

and the strength of the 3.15 reflection. On this premise density may have values as listed. Further since cell appears to be C centered, N should appear as a multiple of 16. This values of ρ so calculated show that 2 chains per unit cell (of single nucleotides one above the other) is unlikely. 4 chains may be possible, 8 chains most likely.

The reflections are spread out in such a way as to suggest plate like units. Suppose then the monomers to be condensed in planar tetranucleotides. 64 monomers could then be arranged in the cell as 2 chains (unique) of 8 tetranucleotides in height.

—

Calc. Suppose 60% water by weight combining with nucleic acid of density 1.65.

From layer line measurement $c = 27.45$.

Now $27.45/8 = 3.43$.

Suppose then that height of effective nucleotide = 3.43 A

Davidson gives mean molecular weight of nucleotide as 330.

Suppose that fibre contains water such that each nucleotide is associated with 60% water by weight

∴ Molecular weight of wet nucleotide = 825.

Dried effective density of fibre = 1.19 gms/cc.

∴ Let volume of 1 gm of fibre be x cc's. Then $\rho_{\text{wet fibre}} = \frac{1}{x}$ gms/cc

Now 1 gm fibre = $3/5$ gm water + $2/3$ gms nucleic acid (dry weight).

If density of water 1 gm/cc. Then Volume $x = \frac{3}{5} + \frac{2}{5} \cdot \frac{1}{1.65}$

i.e. $x = 0.8425$. ie $\frac{1}{x} = 1.19$.

Suggested Cell Dimensions.

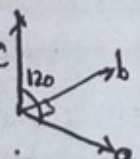
From consideration of zero layer line spacings, arrangement is very near to hexagonal. $a = 22.6\ A^\circ$.

Area of cell base $= \frac{\sqrt{3}}{2} a^2 = 442.5$ sq A°.

Considering a section $3.43 A^\circ$ high, we have, per unit cell.

a mass. $442.5 . 3.43 . 1.19$ gms.

But since ab plane inclined to fibre axis



with $d_{001} = 24.1$.

One should consider height of nucleotides w.r. to this. Height of 24.

ie if 8 nucleotides/cell height then Effective height $= \frac{24.1}{8} = 3A$

if 6 nucleotides Effective height $= 4\ A^\circ$.

Then Mass associated with slice of cell $3A^\circ$ high $= 442.5 . 3 . 1.19$

Hence number of wet nucleotides in this section $= \frac{442.5 . 3 . 1.19}{1.6604 . 825}$

$= 1.15$.

In section $4A^\circ$ high. $N = \frac{442.5 . 4 . 1.19}{1.6604 . 825.}$ ie $1.15 . \frac{4}{3} = 0.3834$

$= 1.532$.

Volume of nucleotide, taking dry wt. $= 356\ A^{\circ 3}$.

∇. 1 nucleotide associated 42% water. of density 1.0 (as measured).

has volume of ~~#70~~ A^3. $979\ A^\circ$.

Volume unit cell. abc. 27.3510^3.

ie No. nucleotides/unit cell 27.9 ie 28.

Primary cell. 14 nucleotides.

$2d \sin\theta = \lambda$. 1.5

$\sin\theta = \lambda/42 = 0.0366$

18th. Nov. 51

Number of Nucleotides / Unit Cell: —

Mol. Wt. Dry. Nucleotide - Average . 353.

Vol. 1 Dry Nuc. $\frac{353 \cdot 1 \cdot 6604}{1 \cdot 65}$ $\left[V = \frac{M, 1 \cdot 6604}{\rho}\right]$

$= 355 A^3$.

If Combined with 42% by weight of water, density 1

Vol. assoc. water $= \frac{\cdot 42 \cdot 353 \cdot 1 \cdot 66}{1}$

$= 246 A^3$

Vol. Wet. Nuc. $= 601 A^3$

Vol. Cell $= 26 \cdot 2\,10^3 A^3$

No: Nuc's / cell $= 43 \cdot 6$. $\simeq \pm$ ~~48~~

ie 24 units / lattice point.

* In the light of later knowledge - suggest it really is 44. ie 22 µ lattice µ

① 8 nucleotides in height of cell. 3 CHAINS/helix

② 6 nucleotides in Wt. 4 CHAINS/cylinder.

Correction Av. molecular Wt. 330. (Goldwin Thymonucleic Davidson

ie Dry Vol. 332. ∴ Wet. Vol. 562.

Water Assoc. 230.

ie Number / cell. 46·5. ie $\pm$ 48.

Thus corresponds to 8 molecules of water per nucleotide

---

* No. nucleotides / cell = 44. ie 22 units/lattice point. Arranged on helix in two strands of 11 nucleotides each strand.

23rd Nov. 51

1st spot now quite clear on micro-photographs.

R.F. measurements on zero layer line. Derived from taking 2nd spot as 11·3 A° :—

Spot	d A°	log d.
1	19·0	1·279
2	11·3	1·053
3	7·45	0·872
4	7·02	0·846
5	6·26	0·797
6	5·66	0·753
7	5·43	0·735
8	5·23	0·719
9	5·02	0·701
10	4·51	0·654
11	4·36	0·640
12	4·10	0·614

Previous spacings derived from Shethouse Film :-

Spot	d A°	
1	19·5	
(2)	(12·49 β 073)	Missing
3	11·3	
4	9·75	Missing
(5)	(8·25 β 076)	Missing
6	7·41 (7·02 ?)	
7	6·33	
8	5·88	Missing
9	5·64	
10	5·41	
11	5·01 (5·23 ?)	
12	4·79	Missing
13	4·59	
14	4·37	
15	4·17	

ie 3 Missing & 2 new ones.

On zero layer line $\lambda / d_{hk0} = \xi_{hk0}$

On l layer line $\lambda / d_{hkl} = \sqrt{\xi^2_{hkl} + \zeta^2_{hkl}}$.

Using Bunn Chart can get fit with new values as;-

$0\overset{1}{2}0$, $2\overset{2}{0}0$, $3\overset{3}{1}0$ (050), $1\overset{4}{5}0$ (320) $0\overset{5}{6}0$ (250) $4\overset{6}{0}0$ (410) $4\overset{7}{2}0$ (260)

$1\overset{8}{7}0$? $5\overset{9}{8}0$ (450 500) $2\overset{10}{8}0$ (370 520) 190 (090 540)

Taking a reciprocal nett. $a^* = \lambda/2.11.3 = 7.9.10^{-2}$ and $b^* = \lambda/2.19 = 4.7$
Can index 2nd layer, choosing 1st reflection to be $\bar{2}02$
and ~~from this fixing~~ in so doing fixing β^* (same value as before). Following values ensue.

Reflection	Index.
1.	$\bar{2}02$
2.	022 if $\xi_2 = 0.117$ (and not ·10)
	$\bar{2}12$ if $\xi_2 = \cdot 10$. ~~Not feasible because 022 is the same~~
3.	$\bar{3}12$ or $\bar{2}32$
4.	042
5	$\bar{1}52$ or $\bar{2}10$ $[\xi = 23.6\,10^{-2}]$
	202 $[\xi = 23.0\,10^{-2}]$
6	$\bar{4}22$ or 232
7	$\bar{2}62$ or 242 (poor fit)
8	312 (poor fit)
9	$\bar{5}30$
10	$\bar{4}62$ ($\bar{3}72$ $\bar{5}42$)
11	$\bar{5}52$ 272 422.

Not feasible because $\xi_{102a} > \xi_{\bar{2}12}$ and so 022 would be missing

1st layer lines 1st spot cannot be indexed. (previously 021 but with smaller b, 021 now too far away)

2nd.	$\xi = \cdot 158$	$\bar{2}21$	
	$\xi = 150$	121	$\bar{1}31$
4th.	131	$\bar{2}31$	
5th	231	$\bar{1}51$.	

INSERTED BETWEEN [19 AND 20] IN R. FRANKLIN NOTEBOOK

Suppose Empty 8·0000 GT 1390
$\pm 1.10^{-4}$.
Full volume 2·0000 $\pm 10^{-4}$.

TON

Suppose add ·005 g./cc of stuff having density, in water, of 1·82.
Then for volume of solution
1cc solvent + $\frac{\cdot 005}{1\cdot 82}$ weighs 1·005

$\therefore$ $\rho_{solution} = \frac{1\cdot 005}{1 + \frac{5.10^{-3}}{1\cdot 82}} = \frac{1\cdot 005}{1\cdot 00276} \doteq 1\cdot 00275$

NCES

D ∴ 2ccs. 2·0050

So expected difference is $50\,10^{-5}$ gms. & we can weigh correct $\pm 5\,10^{-5}$ & accuracy possible here of 10%

GHTS

If stuff still only has density 1·63. $\rho_{sol} = \frac{1\cdot 005}{1\cdot 00306}$
i.e. $4\cdot 5\,10^{-5}$ gm.
$\rho_{sol} = 1\cdot 00225$

Difference being $50\,10^{-5}$ gms & we only have an accuracy of $\pm 5\,10^{-5}$ i.e. 10%

$\frac{1\cdot 010}{1\cdot 0055}$
$\frac{1\cdot 005}{}$

TATLOCK LTD.

Diff $= 0\,1000\,10^{-5}$

·019/cc. ·01 $\frac{5}{10}$ $\frac{1}{2}$%

N . GLASGOW i.e. 10 c.c. solution · 1 i.e. 100 milligrams
H . MANCHESTER Weigh sp. gr. tube & dry stuff & weigh ~~add solution to certain higher weight~~

Make up 5 ccs. solution
i.e. Preferably ·05 g. i.e. 50 milligrams. & thus

Cylindrical Patterson.

Consider only the first two layer lines and equator.

Equator:—

d	1/d
·8	0·0513
·3	0·0885
7(	0·1025
·25	0·1212
·41	0·1350
·33	0·1580
88	0·170
54	0·1775
41	0·1850
01	0·1995
79	0·2090
59	0·2180
37	0·2285
·17	0·2400

1st layer line:—

6·1	0·0622
10·48	0·0955
9·85	0·1015
9·15	0·1092
7·18	0·1392
6·92	0·1445
6·22	0·1610

2nd layer line:—

12·4	0·0807
11·12	0·900
7·7	0·130
6·82	0·1465

d	1/d
6·1	0·1640
5·5	0·1820
5·35	0·1870
4·8	0·2085
4·46	0·2240
4·26	0·235

Projected Micro-Film.

Plate 10A. Magnification ~~unknown~~ not measured. 2nd spot zero layer line taken as 11.3 A°. Rest of plate calibrated from this value.

Zero layer line

		Corrected (= 5 F). 10 cms
2nd Spot.	$2x_2 = 2.95$ cms.	$2x_2 = 2.74$ cms $\quad x_2 = 1.37$ cms
1st. Spot.	$x_2 - x_1 = 0.9$ cms.	$x_1 = 0.747$ cms.
3rd Spot.	$2x_3 = 6.1$ cms. $\quad x_3 = 3.05$.	$x_3 = 2.12$ cms.

1st. layer line

$2y_1 = 1.65$. $\quad y_1 = 0.825$

$[2x_1 + (x_2 - x_1)]$

1st Spot. $2x_1 = 3.1$ cms $\quad x_1 = 1.125$ cms

2nd Spot. $x_2 - x_1 = 0.85$ cms. $\quad x_2 = 1.975$

3rd Spot. $x_3 - x_1 = 1.9$ cms. $\quad x_3 = 3.025$

$2x_1 = 2.25$	$x_1 = 0.78$ cm
	$x_2 = 1.37$ cm.
	$x_3 = 2.10$ cm.
	$y_1 = 0.573$ cm $z = 0.056$

2nd layer line $\quad 2y_2 = 3.2$ cms. $\quad y_2 = 1.6$ cms.

1st doublet i) $2x_1 = 2.1$ cms. $\quad x_1 = 1.05$ ii) 2.5 cms $\quad x_2 = 1.25$

Next Strong Spot. $2x_3$? $= 6.0$ cms. $\quad x_3 = 3.0$

	$x_1 = 0.73$ cms.
	$x_2 = 0.87$ cms.
	$x_3 = 2.08$ cms.
	$y_2 = 1.11$ cms. $z = 0.11$

3rd layer line

$2x_1 = 6.05$ cms. $\quad x_1 = 3.025$

$2x_2 = 6.75$ cms. $\quad x_2 = 3.375$

$x_1 = 2.1$ cms
$x_2 = 2.34$ cms.

4th layer line

$2x_1 = 6.65$ cms $\quad x_1 = 3.325$

$2x_2 = 7.1$ cms. $\quad x_2 = 3.55$

$2x_3 = 7.7$ cms $\quad x_3 = 3.85$

$x_1 = 2.31$
$x_2 = 2.465$
$x_3 = 2.67$

1st layer line	$2x_1 = 5.55$ cms.	$x_1 = 1.925$ cms
	$x_1 = 2.775$	
2nd layer line	$2x_1 = 4.50$ cms	$x_1 = 1.56$ cms
$x_1 = 2.25$	$2x_2 = 5.6$ cms	$x_2 = 1.940$ cms
$x_2 = 2.8$		
3rd layer line	$2x_1 = 3.2$ cms.	$x_1 = 1.11$ cms
$x_1 = 1.6$	$2x_2 = 4.80$ cm.	$x_2 = 1.67$ cm.
$x_2 = 2.4$		
$x_3 = 3.05$	$2x_3 = 6.1$ cms.	$x_3 = 2.12$ cm.
4th layer line		
$x_1 = 2.35$	$2x_1 = 4.7$ cms.	$x_1 = 1.63$ cm.
	$2x_2 = 5.9$ cms.	$x_2 = 2.05$ cm.
$x_2 = 2.95$		

Magnification Factor M.

Bernal Chart 1. (Proc Roy Soc) is for a Flat Plate SFD = 10cms.

Now $\sin\theta_B = \lambda/2d$ ∴ For calibration spot. $\sin\theta_B = \frac{1.539}{22.6} = 0.0682$

i.e. $\theta_B = 3° 54\frac{1}{2}'$. Whence $2\theta_B = 7° 49'$. (Checked)

Thus on zero layer line with SFO = 10cms. $x = 10.\tan 7°.49'$

$= 1.3728$

i.e. $2x = 2.745$ cms.
(10 cms.)

Thus to reduce above measurements of projected plate to fit Chart 1. Must use factor of $1/1.44$. $M = 1/1.44$

Zero layer line Spacings.

1st Spot. $x_1 = \frac{1.975}{2.475} - 0.9 = 1.075$. Corrected $x_1 = 0.8750$.

$\tan 2\theta_B = 0.0750$ i.e. $2\theta_B = 4°.16'$ i.e. $\theta_B = 2°.8'$

$\lambda = 1.88630$ $d = 17.6$ A° $\sin\theta = 1.42919$ $d = 20.67$ A°

Plate 108 Zero layer line. Projected. $2x_2 = 4.05$ cms.

23 $x_2 - x_1 = 0.9$ cms.

$\frac{1}{F}$ Factor Magnesium Plate 3. $\frac{1}{F}$ where $F = 4.05/2.715 = 1.4$

$x_1 = 1.125$. x_1 (corrected 10 cm) $= 0.7625$.

$\tan 2\theta = 0.07625$. $2\theta_8 = 4° 22'$.

T·88630 : $\lambda/2$
1·41914 : corr $2° 11'$
1·30544 20.2 A°,

$d_1 = 20.2$ A°.

To find ξ values of 10 A spots and hence index, necessary to assume ζ values to be same as those on the Oct 3rd plate. i.e. $c = 27.45$ A°. Since measurements on 10 A are not possible

Now $c = l\lambda/\zeta$: i.e. $\zeta = l\lambda/c$. Whence:- (for $\lambda = 1.539$ A°

	Observed on Plate 10 A	
$\zeta_1 = 0.056$	0.056	} These do agree within limits
$\zeta_2 = 0.112$	0.11	} of measurement.
$\zeta_3 = 0.168$		
$\zeta_4 = 0.224$		
$\zeta_5 = 0.280$		
$\zeta_6 = 0.336$		
$\zeta_7 = 0.392$		
$\zeta_8 = 0.448$		
$\zeta_8/\lambda = 0.292$		

Values of ξ as measured off from Bernal Chart 1.

Zero $\xi_1 = 0.075$ ($x_1 = 0.747$ cm) $d = 20.5$ A°
$\xi_2 = 0.137$ ($x_2 = 1.37$ cm)
$\xi_3 = 0.21$ ($x_3 = 2.12$ cm)

1st $\xi_1 = 0.078$
$\xi_2 = 0.137$.
$\xi_3 = 0.205$

2nd $\xi_1 = 0.073$
$\xi_2 = 0.087$
$\xi_3 = 0.203$

3rd $\xi_1 = 0.207$
$\xi_2 = 0.230$ ✓
42 C

4th $\xi_1 = 0.225$
$\xi_2 = 0.240$
$\xi_3 = 0.260$ 42 C 21 A

5th $\xi_1 = 0.1935$
$d = 20$ A° $\xi_1 = 0.0$
$d_9 = 19.5$ $\xi_1 = 0.07$
$d_{10} = 19.2$ $\xi_1 = 0.08$

GT $\xi_1 = 0.16$ $\xi_2 = 0.195$

JK $\xi_1 = 0.130$ $\xi_2 = 0.180$ $\xi_3 = 0.215$

BR $\xi_1 = 0.185$ $\xi_2 = 0.22$ 24

Plate 21A. Magnification factor M. $2x_{10-2} = 5.05$ cm. $M = \frac{1}{5.05/2.795} = \frac{1}{1.84}$.

1st layer line x cm.

$2x_{10} = 2.85$	$2x_{10} = 3.1$	$2x_{10} = 4.45$	$2x_{10} = 4.9$	Dbl.
$2x_{20} = 1.55$	$2x_{20} = 1.685$	$2x_{20} = 2.42$	$2x_{20} = 2.665$	Dbl.
$x_{20} = 0.775$	$x_{20} = 0.8425$	$x_{20} = 1.21$	$x_{20} = 1.3325$	
$\xi_1 = 0.0778$	$\xi_2 = 0.0843$	$\xi_3 = 0.121$	$\xi_4 = 0.133$	

$x_{10} = 3.825$	$x_{10} = 4.175$	$2x_{10} = 13.3$	NB All ξ agree with 42c.	
$x_{10} = 2.08$	$x_{10} = 2.27$	$2x_{10} = 7.24$		Dbl.
$\xi_5 = 0.202$	$\xi_6 = 0.222$	$x_{10} = 3.62$		
		$\xi_7 = 0.347$		

$\zeta_1 = 0.056$.

2nd layer line x cm.

$2x_{10} = 2.85$	$2x_{10} = 3.35$	$2x = 5.75$	$2x = 6.45$.	$2x = 7.6$	Dbl.
$2x_{20} = 1.55$	$2x_{20} = 1.82$	$2x_{10} = 3.125$	$2x_{10} = 3.501$	$2x_{20} = 4.13$	
$x_{10} = 0.775$	$x_{10} = 0.91$	$x_{10} = 1.5625$	$x_{10} = 1.75$	$x_{20} = 2.065$	
$\xi_1 = 0.0778$	$\xi_2 = 0.091$	$\xi_3 = 0.156$?	$\xi_4 = 0.174$	$\xi_5 = 0.201$	

$2x = 9.85$	$2x = 10.45$.	$2x = 13.95$		
$2x_{10} = 5.35$	$2x_{10} = 5.68$	$2x_{10} = 7.58$	Dbl.	$\zeta_2 = 0.112$.
$x_{10} = 2.675$	$x_{10} = 2.84$	$x_{10} = 3.79$		
$\xi_6 = 0.261$	$\xi_7 = 0.275$	$\xi_8 = 0.36$		All but ? agree 42c.

All line x cm.

$2x_{10} = 8.35$	$2x_{10} = 8.8$	$2x_{10} = 9.7$	
$2x_{20} = 4.53$	$2x_{20} = 4.78$	$2x_{20} = 5.27$	$\zeta_4 = 0.224$
$x_{10} = 2.265$	$x_{10} = 2.39$	$x_{10} = 2.635$	
$\xi_1 = 0.22$	$\xi_2 = 0.234$	$\xi_3 = 0.255$.	All agree 42c.

5th line x cm. Mean Values Top & bottom.

$\bar{x} = 3.225$	$\bar{x} = 3.425$	$\zeta_5 = 0.280$.	
$2x_{10} = 1.75$	$2x_{10} = 1.865$		dbl.
[redacted]	[redacted]		
$\xi_1 = 0.176$	$\xi_{11} = 0.185$		

6th line Bottom:- $2x_1 = 4.5$ $2x_2 = 5.6$ $2x_3 = 6.6$

Top:- $2x_1 = 4.2$ $2x_2 = 5.4$ $2x_3 = 6.5$ Top Closest

$\zeta_6 = 0.336$ $2\bar{x}_1 = 4.35$ $2\bar{x}_2 = 5.5$ $2\bar{x}_3 = 6.55$

1 $2x_{10} = 2.36$
$x_{10} = 1.18$
$\xi_1 = 0.13$

2 $2x_{10} = 2.99$
$x_{10} = 1.495$
$\xi_2 = 0.157$

3 $2x_{10} = 3.56$
$x_{10} = 1.78$
$\xi_3 = 0.182$

7th line Bottom:- $2x_1 = 3.7$ $2x_2 = 5.2$ $2x_3 = 7.0$ Top Furthest

Top:- $2x_1 = 4.0$ $2x_2 = 5.8$ $2x_3 = 7.0$

$\zeta_7 = 0.392$ $2\bar{x}_1 = 3.85$ $2\bar{x}_2 = 5.5$ $2\bar{x}_3 = 7.0$

1 $2x_{10} = 2.09$
$x_{10} = 1.045$
$\xi_1 = 0.13$,

2 $2x_{10} = 2.99$
$x_{10} = 1.495$
$\xi_2 = 0.164$

3 $2x_{10} = 3.81$
$x_{10} = 1.905$
$\xi_3 = 0.198$

8th line Bottom:- $2x_1 = 4.6$ $2x_2 = 6.3$ $2x_3 = 8.6$

Top:-

1 $2x_{10} = 2.5$
$x_{10} = 1.25$
$\xi_1 = 0.160$

2 $2x_{10} = 3.43$
$x_{10} = 1.715$
$\xi_2 = 0.190$

3 $2x_{10} = 4.67$
$x_{10} = 2.335$
$\xi_3 = 0.24$

$\zeta_8 = 0.448$

INSERTED FACING [P. 24]
IN R. FRANKLIN NOTEBOOK

Theoretical Formulae for the Strength of the diffracted beam:-

P. 560.-562. International Tables. II.

Rotation Photograph.

If E = Total Energy in a given reflected beam, when crystal has been rotating for time t.

& I = Total energy incident / sec in collimated beam.

& p' = Number of planes, owing to crystal symmetry, contributing to reflection

$\mathcal{A}$ = Absorption factor. depending on θ, λ and crystal size & shape.

Then $$\frac{E}{I} = \mathcal{A} \cdot \frac{N^2 e^4 \lambda^3 V}{4\pi m^2 c^4} \cdot t \cdot \frac{1+\cos^2 2\theta}{\sin 2\theta} \cdot \frac{\cos\theta}{\sqrt{\cos^2\varphi - \sin^2\theta}} \cdot p' F^2$$

$F = F_0 e^{-M}$ where $F_0 \equiv$ Structure Factor of the unit cell. (dependent on (hkl) alone).

M is the temp. factor, $M = 8\pi^2 \overline{u^2}_x \left(\frac{\sin\theta}{\lambda}\right)^2$. An appx mean value of M may be used, assuming that $\overline{u^2}_x$ is the same for all atoms. (The mean square displacement of the atoms from their average positions, measured ⊥ to the reflecting planes being $\overline{u^2}$.

Factor A $\equiv \frac{1+\cos^2 2\theta}{\sin 2\theta}$ Factor B $\equiv \frac{\cos\theta}{\sqrt{\cos^2\varphi - \sin^2\theta}}$.

Where φ is the angle between reflecting plane and axis of rotation. (NB Any plane not containing axis of rotation ie any spots other than zero layer line, will rotate with lower effective angular velocity and so give stronger reflections. Hence must be ~~decreased~~ increased by factor B.) to give observed value. ie Observed intensity needs to be decreased.

equator correspond to zero layer reflections.

Thus if we are concerned only with relative intensities I_R we have

$$\frac{1+\cos^2 2\theta}{\sin 2\theta} \cdot \frac{\cos\theta}{\sqrt{\cos^2\varphi - \sin^2\theta}} \cdot F^2 = I_R .$$

But $I_{observed}$ must also be reduced by factor C, due to obliquity of incidence on photographic film, giving false increase. Thus

$$F^2_{observed} = I_{obs} \cdot C \cdot \frac{\sqrt{\cos^2\varphi - \sin^2\theta}}{\cos\theta} \cdot \frac{\sin 2\theta}{1+\cos^2 2\theta} .$$

Let $\frac{\sqrt{\cos^2\varphi - \sin^2\theta}}{\cos\theta} = D_1$ (Cox & Shaw. 1930. Proc. Roy. Soc. A. Vol. 127 P71)

$$\frac{\sin 2\theta}{1+\cos^2 2\theta} = D_2 = 1/A .$$

Obliquity factor C. For Cu $K_{\alpha 12}$ and Monocoucha Film.

From data obtained by RF. we arrive at following table of values relating C to angle of incidence i.

NB Angle of incidence will be constant for each layer line and $i = \sin^{-1} y/r$ r = radius of camera.

C/	i°/	C/	i°/
1.000	0	0.944	37.2
1.000	11.4	0.817	40.0
.992	14.3	0.784	42.8
.984	17.1	.759	45.7
.971	20.0	.733	48.6
.956	22.8	.709	51.4
.939	25.7	.682	54.3.
.917	28.5		
.893	31.4		
.868	34.3.		

Factor A. $\left(\frac{1+\cos^2 2\theta}{\sin 2\theta}\right)$

27

θ°	A	x mms Zero layer	x mms 1st line.				
0	∞	0	∅	/	/	/	/
1	57.272	1.045	∅	∅	/	/	/
1.5	38.162	1.57	∅	∅	/	/	/
2	28.601	2.095	∅	∅	/	/	/
2.5	22.860	2.62	0.786	∅	/	/	/
3	19.029	3.1416	1.83	∅	/	/	/
3.5	16.289	3.67	2.485	∅	/	/	/
4	14.231	4.19	3.14	x=0	/	/	/
4.5	12.628	4.71	3.83	2.03	/	/	/
5	11.344	5.24	4.26	2.97	/	/	/
6	9.411	6.29	4.85	3.72	0.6	/	/
7	8.025	7.34	6.00	5.1	3.55	x=0 θ=6.55	
8	6.980	8.39	7.25	6.3+	5.2	2.68	
9	6.163	9.44	8.16	7.4	6.6	4.83	
10	5.506	10.45	9.23	8.65	7.85	6.45	
12	4.510	12.58	10.22	9.82	9.12	7.97	
14	3.791	14.65	12.4	12.0	11.5	10.7	
16	3.244.	16.75.	14.5	14.2	13.75	13.1	
			16.6	16.35	15.95	15.3	

Zero layer line Camera Radius $r = 30$ mm.

Now $r2\theta^c = x$. $\therefore \theta^c = x/2r$ ie $\theta^\circ = 90\frac{x}{\pi r}$ ie $x = \frac{\pi r\theta}{90}$

ie $x = \frac{\pi}{3}\theta^\circ$ mms.

1st layer line $\zeta^2 = 1 + \sin^2\phi - 2\sin\phi\cos\left(\frac{x}{r}\right)^c$ (Bunn p149)

Now $d = \lambda/\sqrt{\zeta^2+\zeta^2}$ $\therefore \zeta^2 = \frac{\lambda^2}{d^2} - \zeta^2$ But $\zeta^2 = \cos^2\phi$

$\therefore \lambda^2/d^2 - \cos^2\phi = 1 + \sin^2\phi - 2\sin\phi\cos\left(\frac{x}{r}\right)^c$ Now $\lambda^2/d^2 = 4\sin^2\theta$

$\therefore 4\sin^2\theta = 2\left(1 - \sin\phi\cos\left(\frac{x}{r}\right)^c\right)$ $\therefore \cos\left(\frac{x}{r}\right)^c = \frac{1-2\sin^2\theta}{\sin\phi}$

$\therefore \cos\left(\frac{x}{r}\right)^c = \cos 2\theta/\sqrt{1-\zeta^2}$ $\therefore x = \pi/6 \cdot \cos^{-1}\left(\cos 2\theta/\sqrt{1-\zeta^2}\right)$

			8th layer line.
x=0 θ=8·125			
4·02	x=0 θ=9·88		
6·116	1·91	x=0 θ=11·68	x = ∞ for θ = 13·5° A = 3·975
9·3	7·3	3·00	
12·2	10·6	8·4	~~3·27~~ 4·19
14·6	13·4	10·9	9·43

θ/	A/
13·5°	3·975
11·68	4·67.
9·88	5·57
8·125	6·87
6·55	

1st layer line $(1-\zeta^2)^{\frac{1}{2}} = (0.99686.)^{\frac{1}{2}}$ ~~$= 1.0 \quad \therefore x = \frac{\pi}{6} \cos^{-1}(\cos 2\theta)$~~

$= 0.998 \quad \therefore x = \frac{\pi}{6} \cos^{-1}\left(\frac{\cos 2\theta}{0.998}\right)$

2nd layer line $(1-\zeta^2)^{\frac{1}{2}} = (0.9875)^{\frac{1}{2}} = 0.9925$

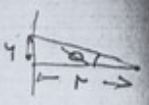
3rd $(1-\zeta^2)^{\frac{1}{2}} = 0.985$ 4th 0.974 5th 0.960 6th 0.941.

7th 0.918 8th 0.892.

Factor D_1

$r = 30$ mms

α_1 & α_{12}



	ϕ	$\tan\phi$	$r.\tan\phi = y$ mms.	$y \times 5/3$
3_1	3° 13′	·056	1·68	2·80
3_2	6° 26′	·112	3·36	5·60
3_3	9° 41′	·17063	5·12	8·53
3_4	12° 57′	·2299	6·89	11·49
3_5	16° 16′	·2917	8·75	14·58
3_6	19° 38′	·3567	10·70	17·83
3_7	23° 5′	·4262	12·78	21·31
3_8	26° 37′	·5011	15·03	25·05

Coca Shaw Chart. 5cm = 1.

First Layer.	x mm.	D_1
0·3	0·5	0·2
0·6	1·0	0·3
·90	1·5	0·4
1·2	2·0	0·6
1·50	2·5	0·7
1·8	3·0	0·75
2·10	3·5	0·8
2·4	4·0	0·85
2·70	4·5	
3·0	5·0	0·9
4·80	8·0	0·95
6·6	11·0	9·75

2nd layer	x mm	D_1
0·6	1·0	·2
1·0	1·75	·3
1·50	2·5	·4
1·8	3·0	·5
2·4	4·0	·6
3·450	5·75	·7
3·90	6·5	·75
4·50	7·5	·8
5·4	9·0	·85
6·90	11·5	·9
10·50	17·5	·95
15·30	25·5	·975

3rd layer

x mm	D_1	
1	·15	0·6
1·75	·2	1·05
2·25	·25	1·350
2·75	·3	1·650
3·0	·35	1·8
3·5	·4	2·10
4·0	·45	2·4
4·75	·5	2·850
5·5	·55	3·30
6·25	·6	3·750
7·0	·65	4·20
8·5	·70	5·10
9·5	·75	5·70
11·0	·8	6·6
13·5	·85	8·10
17·5	·9	10·5
26·0	·95	15·6
39·0	·975	23·4

4th heights			5th line		6th line		7th line		8th line	
			xmms	D_1	xmms	D_1	xmm		xm	D
1·5	0·9	·15	2·0	1·2 ·15	2·5	1·5 ·15	3·0	1·8	3·[illegible]	2·28 ·15
2·25	1·35	·2	3·0	1·8 ·2	3·7	2·22 ·2	4·5	2·7	5·3	3·18 ·2
3·0	1·8	·25	3·8	2·28 ·25	4·7	2·82 ·25	5·7	3·4	6·5	3·9 ·25
3·5	2·10	·3	4·5	2·7 ·3	5·5	3·3 ·3	6·8	2·88	8·0	4·8 ·3
4·2	2·52	·35	5·20	3·12 ·35	6·5	3·9 ·35	8·0	4·8	9·0	5·4 ·35
5	3·0	·4	6·0	3·6 ·40	7·7	4·62 ·4	9·0	5·4	10·5	6·30 ·4
5·75	3·45	·45	7·0	4·2 ·45	8·8	5·28 ·45	10·5	6·30	12·5	7·50 ·45
6·5	3·9	·5	8·2	4·92 ·5	10·0	6·0 ·5	12·0	7·20	14·0	8·4 ·5
7·5	4·5	·55	9·2	5·52 ·55	11·5	6·9 ·55	14·0	8·4	16·0	9·6 ·55
8·75	5·25	·6	11·0	6·6 ·6	13·0	7·8 ·6	16·0	9·6	18·5	11·10 ·6
10·0	6·0	·65	12·5	7·5 ·65	15·0	9·0 ·65	18·5	11·1	22·0	13·2 ·65
11·5	6·90	·7	14·5	8·9 ·7	17·5	10·5 ·7	21·5	12·90	25·5	15·0 ·7
13·0	7·8	·75	16·5	9·9 ·75	20·5	12·0 ·75	24·5	14·70	29·5	17·7 ·75
15·5	9·3	·8	19·5	11·7 ·8	24·5	14·4 ·8	29	17·4	35	21·0 ·8
17·85	10·71	·85	23·5	14·1 ·85	29·5	17·7 ·85	37	22·2	46	27·6 ·85
24·0	14·4	·9	31·0	18·6 ·9	39·[illegible]	·9	52	31·2	[illegible]	
37·5	22·5	·95	51·0	30·6 ·95	[illegible]	·95	[illegible]			
65·[illegible]	[illegible]	·975	[illegible]	·975						

Above values of x must be multiplied by 3/5 & scale then down to Stubbins radius.

Factor C Let Angle of Incidence be Ω then we have :-

l :	1	2	3	4	5	6	7	8
Ω :	3°13′	6°26′	9°41′	12°57′	16°16′	19°38′	23°5′	26°37′
C :	1·0	1·0	1·0	0·995	0·987	0·973	0·953	0·932

Plate 42 C. Projected Measurements.

Zero layer line 2x. Rm's.

Spot:	1	2 (11·3)	3	4	5	6	7	8	9	10
2x:	2·62	4·45	6·72	6·95	9·0	9·32	9·62	10·25	Projection Measure	11·4
Spot	11[b]	12[c]								
2x	12·95	12·55								
1st. layer: [Top:]	1	2	3	4	5	6	7	8	9	10
2x top	2·45 (a)	2·75 (b)	4·32 (a)	4·52 (b)	5·15	6·65	7·8 (a)	8·2 (b)	11·78 (a)	12·4 (b)
2x Bottom	2·40	2·75	4·30	Missing	Missing	6·60	7·7	8·1	11·62	12·3
2x Mean	2·425	2·75	4·31			6·625	7·75	8·15	11·70	12·35
2nd layer:	1 (a)	2 (b)	3 (a)	4	5	6	7	8	9	10
2x Top.	2·25	2·45	2·82	5·0	5·7	6·62	8·9	9·32	$x_9 - x_8$ 0·5	11·5
Spot.	11.	12	13							
2x Top.	12·1	14·4	15·5.							
2x Bottom	2·25	2	3	4	5	6	7	8	9	10

42C layer line ζ values:- M = 1/1.62.

1st $2y = 1.75$cm. Projected $x_{10} = 0.75$ cm $y = 0.875$, $y_{10} = 0.54$, $\zeta = 0.055$

2nd $2y = 3.50$cm. $x_{10} = 0.695$ cm $y = 1.75$. $y_{10} = 1.08$ $\zeta = .105$

3rd $2y = 5.40$ cm. $x_{10} = 2.0$ cm $y = 2.70$, $y_{10} = 1.670$ $\zeta = .160$

4th $2y = 7.45$cm $x_{10} = 1.906$ $y = 3.725$. $y_{10} = 2.30$, $\zeta = .220$

% difference from Stubbins values. 1st 2% 2nd 6½% 3rd 5% 4th 1.8%

NB 1st and 4th layer lines agree exactly 2nd and 3rd have low ζ values. [c = 27.96 A°. (1+4)]

Further Measurements. 42E

Ist Spot. 1st layer line. $2x = 2.15$. $M = \frac{1/2.15}{1.6} = 1/1.344$

$2y_1 = 1.55$.	$2y_{10} = 1.154$	$y_{10} = 0.577$.	$\zeta = 0.057$	As measured from Bernal chart.
$2y_2 = 3.12$.	$2y_{10} = 2.32$	$y_{10} = 1.16$	$\zeta = 0.112$	
$2y_3 = 4.8$.	$2y_{10} = 3.57$	$y_{10} = 1.785$	$\zeta = 0.170$	
$2y_4 = 6.6$.	$2y_{10} = 4.92$	$y_{10} = 2.46$.	$\zeta = 0.230$,	

These figures do not disagree significantly with a period of = 27.0. A° ie Stubbins confirmed. (ie Period is 27.5 A° with accuracy ± 2%)

Structural Details.

1/ Furberg found in cytidylic that the ~~P-O3~~ P–$O_{3'}$ bond is roughly

1/ Furberg says that in cytidylic acid the Phosphate group is in the trans position to the d-ribose ring. & that therefore in DNA if this is still so, the bond from $O_{3'}$ to the P atom will be roughly // to the axis of the molecule.

2/ Also in cytidine he finds the $O_{5'}$ is near the plane of the Pyrimidine ring.

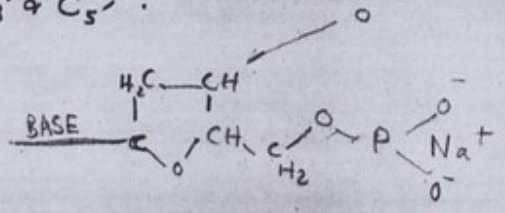
3/ Bruce finds C=O dioclinous such that C=O roughly ⊥ to fibre axis.

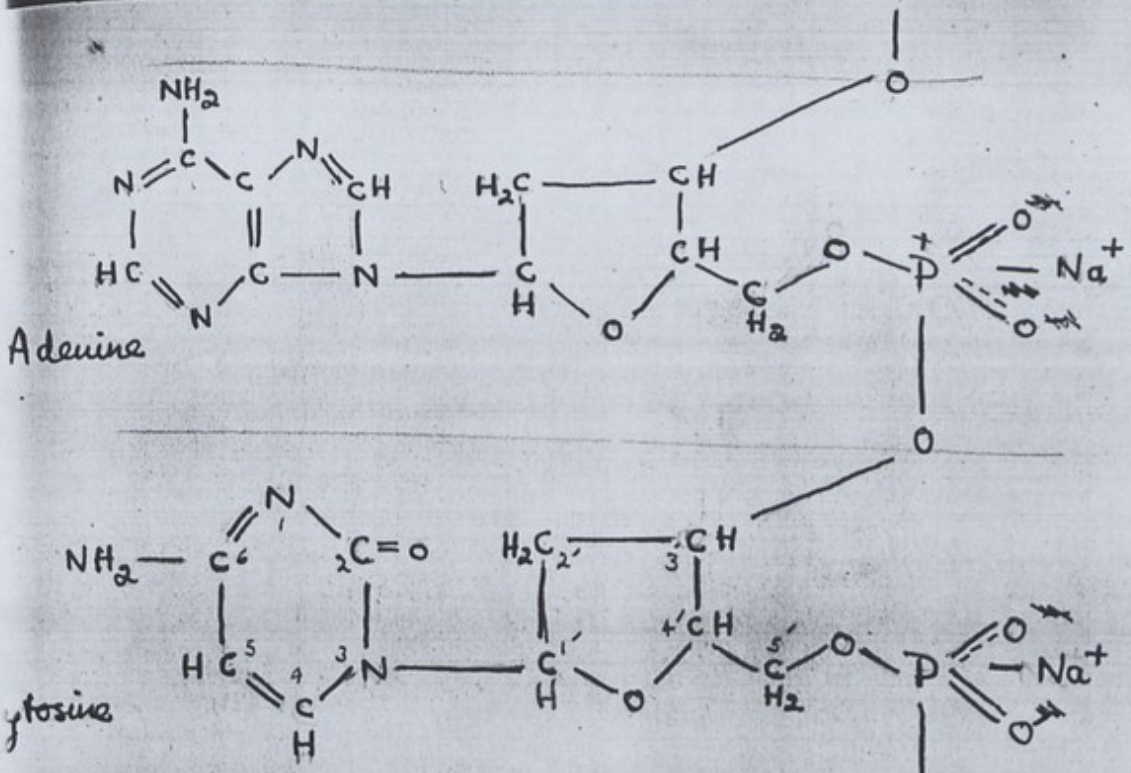
4/ Davidson prints thymine as though 6 position had C=O. The H going on the N_1. He prints uracil the same way, and refers to thymine simply as 5-methyl-uracil.
{What about C_6 = O & N_1 – H in Guanine ? if this is correct}

{These structural suggestions are incorporated in the diagramatic representation of Sodium DNA formula opposite.}

5/ Only two positions on D-2-desoxyribose ring available for esterification ie the OH groups on $C_{3'}$ & $C_{5'}$.

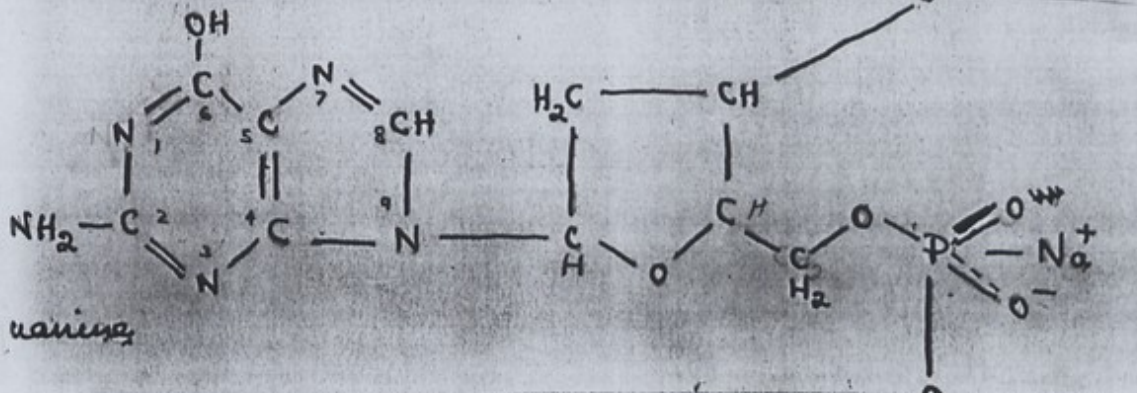
6/ Base very weakly at N. Ie to sugar ring.



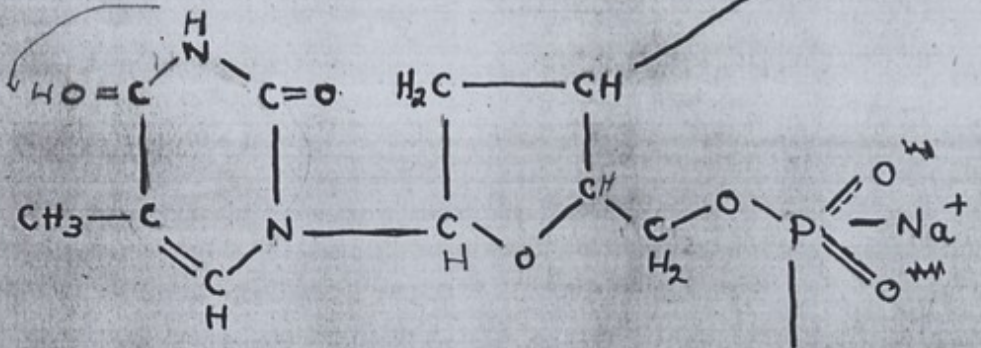


Adenine

ytosine



uanine



Thymine

37 BLANK

Calculation of Molecular Weight of the Nucleotides

O = 16. H = 1. C = 12. P = 31. Na = 23. N = 14.

If consider the Phosphate as $NaPO_3$, then the Sugar only has 20's.

Thus. Phosphate: Na 23, P 31, O_3 48 } 102. Sugar: 7H 7, C_5 60, O_2 32 } 99.

So that the constant contribution to each nucleotide from sugar and phosphate is 201.

Purines:— Adenine: C_5 60, H_4 4, N_5 70 } 134. Guanine: C_5 60, H_4 4, N_5 70, O_1 16 } 150.

Pyrimidines: Cytosine: C_4 48, H_4 4, N_3 42, O_1 16 } 110. Thymine: C_5 60, H_5 5, N_2 28, O_2 32 } 125.

a) On view of a statistical tetranucleotide the molecular wt. of an "average multiple" would be obtained by adding the wt. of the four bases & dividing by four, this gives base contribution of 129·75. i.e. Average Weight 330·75.

b) Taking Chargaff's figures for base content i.e. A = 1·6 : G = 1·3 : C = 1·0 . T = 1·5 we may arrive at an average weight of base compt. thus. $\{134.1.6 + 150.1.3 + 110.1.0 + 125.1.5\}/5.4$ i.e. $(214.4 + 195 + 110 + 187.5)/5.4 = 706.9/5.4 = 130.91$.

i.e. Average Wt. = 331·9.

~~Cytosine~~ Possible wts./Unit Cell of 11 Nucleotides.

On basis of a). 3638·25. On basis of b) 3650·9.

On basis of 3A + 3G + 2C + 3T we have c) 3658. i.e. Differences are less than 1% Approximately 2/3 %.

39

To calculate Number of Nucleotides / Unit Cell.

Volume of 1 dry nucleotide is $V = \frac{M \cdot 1 \cdot 6604}{\rho}$

$\rho = 1.63$ g/cc. dry density of NaDNA according to Astbury.

$\therefore V = 330 \cdot 1 \cdot 66 / 1 \cdot 63 = 336$ A°.

Then wish to know 1) the % composition, by weight, of water in the crystalline state. 2) The density of this water.

Can then calculate Volume of associated water & hence volume of a "wet" nucleotide.

Volume of Unit Cell $V = abc \sin\beta^*$. ie $V = 22.39 \cdot 8 \cdot 28 \cdot 1 \cdot \sin 83\frac{1}{2}°$

" " " " 0.9936

$V = 24450$ A^3.

Suppose 22 nucleotides / lattice point ie 44 per c-centered cell.

Volume Wet nucleotide $= 24450/44 = 556$

ie Volume of associated water $= 220$ A°. If A% is water content at density ρ

$$220 = \frac{A}{100} \cdot \frac{330 \cdot 1 \cdot 66}{\rho} \quad \text{ie} \quad \frac{A}{\rho} = \frac{220}{3 \cdot 3 \cdot 1 \cdot 66} \simeq \frac{20}{\cdot 498}$$

ie $A/\rho \cong 40$.

Thus if $\rho = 1$. $A = 40\%$.

Consider Water Uptake of 43·6%. Increase of 330·436 mol. units ie 144 m.

1 water mol = 18 m. ie ≡ 8 molecules of Water / Nucleotide.

$\therefore$ M of Wet Nuc. = 474. ie $V_{\text{wet nuc}} = 474 \times 1 \cdot 6604 / \rho$. Take $\rho = 1 \cdot 55$.

$= 507 \cdot 5$ A°.

$\therefore$ No: wet nucs / cell $= 24450/507 \cdot 5 = 48 \cdot 2$ ie 24·1 per Primitive Cell.

Water Uptake 21·8%. Increase of 72 m. ie ≡ 4 molecules of Water / nucleotide.

$\therefore$ M. of Wet Nuc = 402. ie $V_{\text{wet nuc}} = 431$ A°. taking $\rho = 1 \cdot 55$.

$\therefore$ No. of wet. nucs/cell = 56·8. ie 28·4 per Primitive Cell.

Density – Temp. Data for CCl_4. Ref. Int. Critical Tables Vol III P. 27-28

$$d_t = [d_s \pm 10^{-3}\alpha(t-t_s) + 10^{-6}\beta(t-t_s)^2 + 10^{-9}\gamma(t-t_s)^3] \pm 10^{-4}\Delta.$$

$t_s = 0°C$. d = density in gm./m2. = spc. gravity $t/4$ (in vacuo).

$d_s = 1.63255$. $\alpha = -1.9110$ $\beta = -0.690$. γ = No value.

Limit of error .0002. Applies over range 0°C – 40°C.

d_t.	t.
1.63255	0°
1.62682	3
1.62109	6
1.61536	9
1.60962	12
1.6039	15
1.5981	18
1.5924	21

Considering 2nd term only.

Chloroform $CHCl_3$.

$d_s = 1.52643$. $\alpha = -1.8563$

$\beta = -0.5309$.

Range −53 to +55. $\gamma = -8.81$.

Calculation of Number of Atoms in a Unit Cell.

Adenine unit = 10 + 12 atoms.
Cytosine unit. = 8 + 12
Guanine " = 11 + 12
Thymine " = 9 + 12.

Take Chargaffs figures of
A = 1.6 G = 1.3 C = 1.0 T = 1.5

Amount of A present if have 44 dry units per unit cell is $\frac{44}{5.4} \times 1.6 = 8.15 \times 1.6 = 13$.

Number of G = 10.6 C = 8.15 T = 12.2.

∴ So take A = 13. G = 11. C = 8 T = 12

∴ 286 + 253 + 160 + 252 ie 851 atoms.

$CHCl_3$	1.5376	−6°C
		−5°C
		−4°C
	1.5320	−3°C
		−2°C
		−1°C
	1.5264	0°C

		+1°C
		+2°C
	1.5208	+3°C
		+4°C
		+5°C
	1.5153	+6°C
		+7°C.

Over range −10°C to +10°C.

$10^{-6}\beta(t-t_s) \not> .0005$. (value t=10°C)

and so may be neglected.

Hence change in d_t for 1°C over this range is simply $10^{-3}.\alpha$.

ie. 0.0018 ≅ 0.002.

41

Calculation of H_2

Chargaff's data (Fed prev. Wilkins was reptent) gives:- for Calf-Thymus DNA.

	Moles/mole P	Hydrogen bonding Group.	Max. No: of H bonds Possible.	Max H bonds per Mole P
Adenine	0·28	NH_2	2	0·56
Guanine	0·21	NH_2. C=O.	3	0·63
Cytosine	0·21	NH_2 C=O.	3	0·63
Thymine	0·26	C=O C-OH.	3.	0·78
	0·96			2·60

Assume 5 k. cals. per H bond.

Then Energy / Mole. P $\simeq \frac{2 \cdot 6 \cdot \times 5}{2} \times \frac{1}{0 \cdot 96} = 6 \cdot 8$ k. cal/mole P

ie Max. H bond energy per mole of nucleotide = 6·8 k cals

Number of Nucs/Unit Cell. Volume of Wet Nuc = $\frac{M \cdot 1 \cdot 6604}{P}$.

Take N = 402, 420, 438, 456, 474

of 4, 5, 6, 7, 8, mols of water/nuc.

of 21·8, 27·3 33·0, 38·2, 43·6 % Water content.

Hence Sum Vol Unit Cell = 24450. $A^{\circ 3}$.

Number = $\frac{1}{M_{wet}} \cdot 24450 \cdot \frac{1 \cdot 521}{1 \cdot 6604}$ taking Wet Density 1·521. at 75 %.

$\therefore = 1/M \cdot 22420$.

Hence No: 55·8, 53·5, 51·2, 49·1 and 47·4 per Unit Cell

ie Per Primitive cell. $\simeq$ 28, 21·75, 25·6, 24·55 and 23·7.

No = $\frac{24450 \cdot \rho}{1 \cdot 6604} \cdot \frac{1}{M_{wet}} = 54$ $\rho = 1 \cdot 471$

M_{wet}.	No
402	54·0
420	51·6.
438	49·5.
456	47·5
474	45·7.

Bruce's notes on Structure of D.N.A.

"If, in crystalline D.N.A. the molecules exist in a spiral (helix) config. one may consider the form it might take by virtue of the chemical forces stabilizing the molecule.

a) In the spiral (helix) of chain b) In the crystal lattice.

On examination of the chemical formula reveals three types of forces which could contribute to this stabilization.

1) Van der Waals attractions between the Base rings which are planar, and a general attraction whenever the sugar residues approach other nucleotides?

2) Hydrogen bonding between the NH_2, OH, NH and C=O groupings.

3) Electrostatic attractions between the Na ions & phosphate Oxygens.

In order to asses the relative importance of these possible forces the total energy involved in each one should be calculated.

(i) $U_1 \equiv$ the Van der-Waal attraction energy per nucleotide between adjacent bases in a system where they are stacked directly above each other. eg. Astbury's Model. This value might be obtained from the crystal energy of say Benzene, in which the contribution of hydrogen bond energy is not required.

Thus. for $C_6(CH_3)_6$ 1. Latent Ht. of fusion 30·4 cal/gm. at 165·5°C.
2. " " " Vap. 12·9 k.cal/mole at 536·7A°.

Cohesive Energy $= L_1 + L_2 - R\bar{T}$?

ie $U_1 = \frac{30.4 \times 1.62}{103} + 12.9 - 1.987 . 536.7 . 10^{-3}$

$= 4.9 + 12.9 - 1.1. = 16.7.$ k. cal./mole.

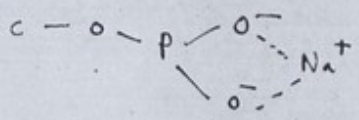
ie. Maximum Van-der-Waal Energy per nucleotide ~ 16·7 kilo-calories/mole.

(ii) $U_2 \equiv$ the hydrogen bond energy per nucleotide. This may be calculated very approx from the known energies of the $NH_2 \ldots OC$ bonds etc, if the number of such H bonding groups per nucleotide is known. ie a knowledge of the model proportions and tautomeric forms of the purines & pyrimidines is required. Calculation not understood.

Refs 1. M.E. Spaght. S.B. Thomas. G.S. Parks. J. Phys. Chem. 36 882 (19
4} 2. F.H. MacDougall. L.I. Smith. J.A.C.S. 52 1998. (1930).
These refer to Van-der-Waal Energy calculation.

(iii) U_3 = The Energy of electrostatic attraction. For this must know the Na/P ratio. and the co-ordination number of the oxygen atoms around the Sodium ion. ie →

A.



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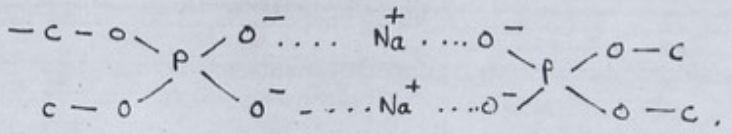

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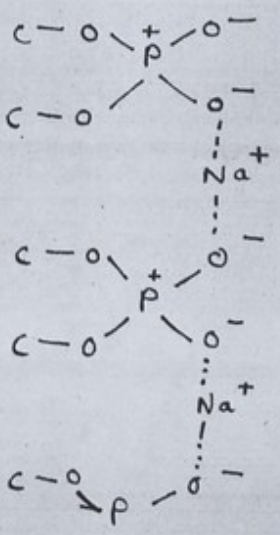

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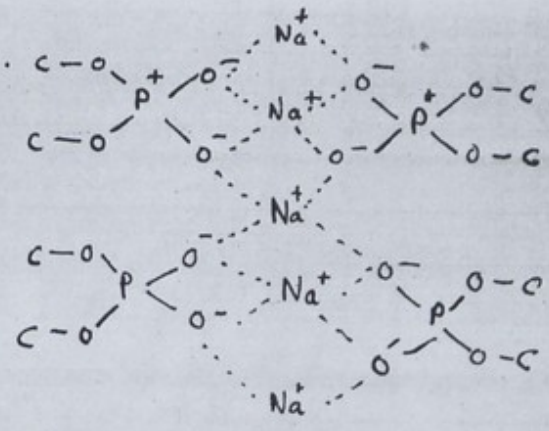
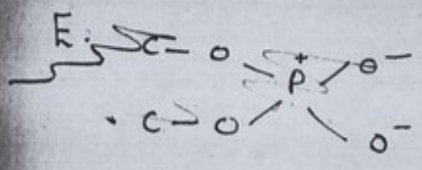
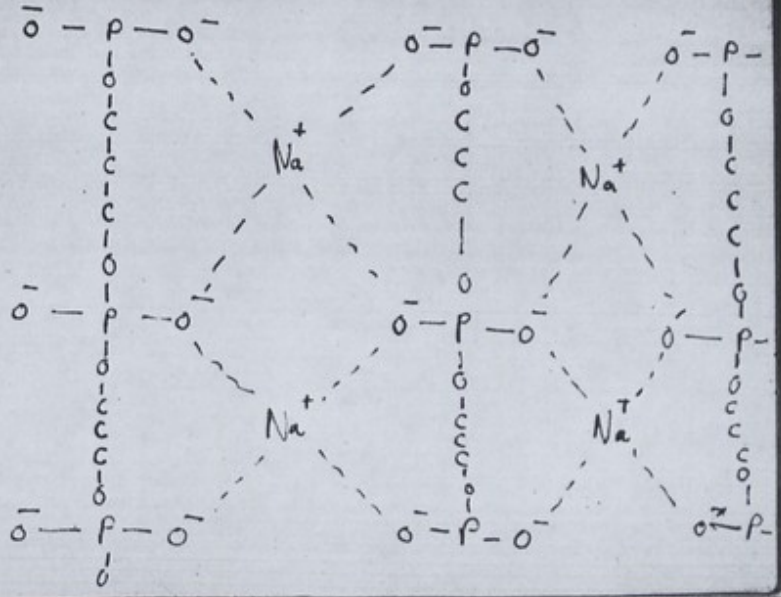


E.



Planar Tetrametaphosphate.



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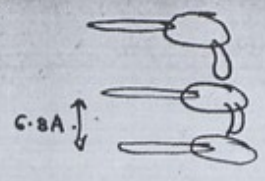
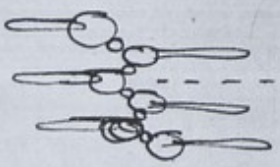
Models ① Fully extended chain (not previously reported)
can be built with 1 bases, 6·8 A° apart



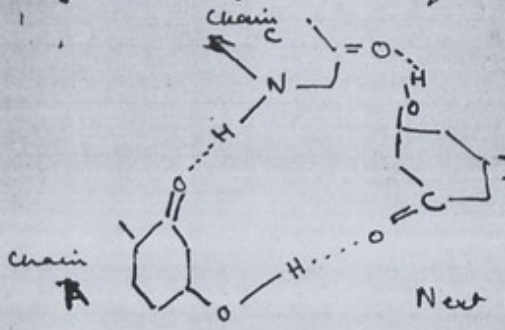
② Twisted helix modes.



Plots of 1+2 available.

Formation of H. bonds

Suggested arrangement (basic model).



Ring formation.

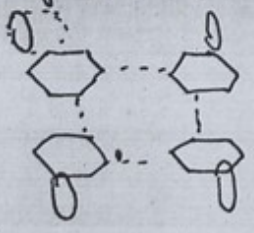
All bases may be fitted

Next layer sits on top giving

max. V.de Waal energy. 3 chain arrangement as shown most

most :. Helix.

Four chain arrangement can be built by putting sugars alternate
each side in vertical array.

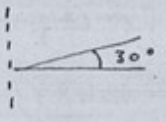


Brief Summary of Main Conclusions & Results on D.N.A. (Bruce)

46

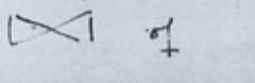
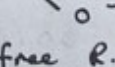
From I.R. Spectra.

1. Purine & Pyrimidine rings preferentially oriented ⊥ to direction of shear.

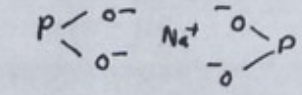


Results set upper limit of 30° from ⊥. (probably nearer to 20°).

Refs. Nature.

2. Absorption bands corresponding to symmetrical & antisymmetrical vibrations of  indicate equivalence of the P–O⁻ bonds. (This done on free R.N.A.). Birefringence shows  plane is within 30° of ⊥.

Ref. Progress in Biophysics.

3. Failure of NH, NH_2 & C–OH of bases to exchange with D_2O at room temp. indicates that solution leaves the H–bonds intact in solution must ∴ involve rupture of  type of attraction. eg⁵ phosphates outside.

Also means that the unit structure, coiled chain or associated chains, is held by H. bonds & V.d. Waal forces. Ref. Thesis.

4. Energy to be expected from;- a) H bonds ~ 7 K.cal./mole of nucleotide

b) V.d.W. (Bases) ~ 16 K.cal./mole of nucleotide.

c) Na – Phosphate bonds. No exact calculations but estimated considerable, say ~ 20 - 30. K.cal per mole of nucleotide.

(No reference. Wilkins.)

47 Density Determinations Sept. 52.

~~Dry~~ Small pieces of DNA. (~~Dry~~ batch from Signer + Swander) made into gels with distilled water. & allowed to dry slowly in the lab under a cover glass. As they dried, prodded into round blobs. Six such dried blobs then placed over P_2O_5 for 2 days. ie Drying started Monday. First weighed Tuesday morn

Blob 1 0.0015 gm. ($\frac{1}{3}$ dry at)

Blob 2 { 0.0012 (+3)
0.0013 (−5)

Blob 3 { 0.0009 (+8)
0.0010 (−0)

Blob 4 0.0008 (−1½)

Blob 5 { 0.0012 (+5)
0.0013 (−5)

Blob 6 { 0.0014 (+8)
0.0015 (+1)

Weighed again Tuesday evening

Blob 1 0.0014 (+6) . 0.0015 (−1)
2. 0.0012 (+5), 0.0013 (−3)
3. 0.0010 (+2)
4. 0.0008 (−0)
5. 0.0012 (+8)
0.0013 (−1)
6. 0.0015. (+2).

Next Weighed Wednesday Afternoon

1 .0014 (+2)
2. 0012 (0)
3. ·0010 (−2)
4. ·0008 (−3)
5. ·0012 (+7)
6. ·0015 (−1).

∴ deemed dry weight reached. (AT ROOM TEMP. ie 20°C)

Floatation Expt

Blob 4. Sinks in CCl_4 at 20°C. { density of CCl_4 (Analar) checked at 19½°C and found to be 1.594 ± 1
NB Should be 1.595 at 20°C. if pure.

Floating	Sinking	
8½.	9 + 10	10½ °C.

Movement over range 9–10°C so slow could not distinguish direction

Blob 6 Floats at 20°C. presume dust or trapped air.

Blob 5 20°C Sinks.

Floating ←	→ Sinking	
14	14½ + 15½	16.

Blob 2 20°C Sinks.

Floating ←	→ Sinking	
15½	16 + 17	17½.

Dry Wt. of Blobs. Expt. 2. Dec. '52

FRIDAY Evening

Zero. 0

1. 0·0032 gm.
2. 0·0020 gm (host)
3. 0·0023 gm. (flat)
6. 0·0013 gm. (Irreg)
7. 0·0018 gm. (flake)

Dry Wt. of Blobs - Jan 5th:

Zero - 10.

1 0·0032 (+2 div).
3 0·0023 gm.
6 0·0013 gm.
7 0·00185.

5 0·0012. (+3 div)
4 0·0008 (−2 div).

Jan 8th

Floatation Expt.

Blob 1. Sinks at 20°C in CCl_4.

Floating | Sinking

3°C ~~2½°C~~ | ~~3½°C~~ 4°C – 4½°C

~~3–3½~~ 4°C.

Blob 3

Blob 5 20°C Sinks Rapidly.

Floating | Just Sinking

3°C | 5°C.

4°C

Blob 6

Floating | Sinking

13°C. | 14°C.

Blob 4 21°C sinks rapidly.

Floating | Sinking

0°C — 3°C | 4°C — 5½.

3½.

Blob 1 Repeat.

Floating | Just Sinking

3°C | 5°C.

4°C

Humidity Data.

Sat. Salts:—

$H_3PO_4 \frac{1}{2}H_2O$.	24°C.	9%
$ZnCl_2 . 1\frac{1}{2}H_2O$. (Unstable).	20°C.	10%
~~$KC_2H_3O_2$~~		
$LiCl . H_2O$.	20°C.	15%
$KC_2H_3O_2$	20°C	20%
$NaCl$.	16°C	30%
$CaCl_2$	20°	32%

SULPHURIC ACID:—

Density of Acid.	RH.
1·7.	3·2
1·6	8·5
1·5	18·8.

From this second set of expts. we consider the density of NADNA to be equal to that of CCl_4 at 4°C. $\rho = 1.625$.

ρ at 5°C = 1.623 ie At this range 1°C = 0.002 gm/cc³.
ρ at 3°C = 1.627

These blobs then placed over Sulphuric Acid of high concentration. $\rho = 1.7$.
cf. % Humidity.
NB Zero of Balance not rep.
left to equilibrate from. Jan 10th to Feb. 3rd. 53 Around – 5.

Weights.	Water Uptake	Blob
0.0031+ 2div.		1
0.0024 + 3 div.		3
0.0019 + 1 div.		7
0.0013 – 2div.		6.

NB 0.0001 ≡ 8 div of div.

Feb 3d – 5th left to Equilibrate with Sat. Soln of Sodium Chlorate ie 75%.
Lab 20° – 21°C

Blob	Weights	% Water Uptake
1	0.0042 – 1div.	
3	0.0032 ± 0div	
7	0.0024 + 2 div.	
6	0.0018 ± 0 div.	

Density Measurement Blob 1 – 5°C | Sink | Float –7° – 6m6½.
Blob 8 | Sink 16°C | Float 14°C 15° Chloroform.

Feb. 6th	Blob	Weights
% Uptake	1	0.0041 + 2 div. Rechecked 0.0041 + 1 div.
10/31 = 32.3%	3	0.0033 – 1 div.
35%	7	0.0025 – 1div
30.5%	6	0.0018 + 2div.
42%		

NB During course of weighings zero seems to have wandered by 4 div.
Lab 22°C

Feb 10th Density: Floatation expt on Blob 1. done before weighing. Rest of blobs weighed before floated.
Lab 21½°C.

Blob 1	Sink.	Float.		Weight: 0.0041 –3d	0.0033–5 d	0.0025+0 d	0.0018–2
	8	7½ 6.	→ 7½	Blob: 1	3	7	6.

After 4 mins on Pan. 0.0039 – 1d.

Blob 6	Sink	Float
	33	32°C.

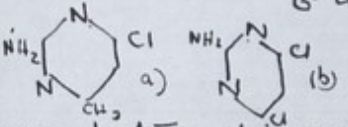
Blob 1 Check. Sink –3 | Float –5

T.O

1 Acta. Vol 1. Part 1. Pp. 1-48. March 1948.

Clews & Cochran :- Structure of Pyrimidines a) 2-amino. 4 methyl 6-chloropyrimide

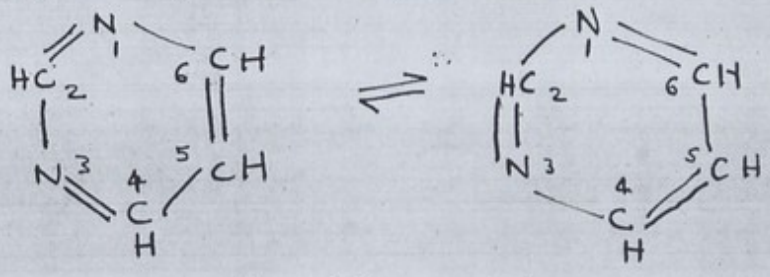
a & b) 2 amino. 4,6 dichloro pyrimidine



Notes on Structure

1 Pyrimidines in general. 6 mem. heterocyclic ring. 2 N atoms

Resonance can occur between a number of structures; including the two Kekulé structures I. & II ie C-C & C-N bonds in ring have approx 50% double bond character.



2 Thus NH_2 · pyrim · tautomerism may occur through migration of a H from NH_2 to a Ring N.

3 Cell is Monoclinic $P2_1/a$. $a \simeq 16$ $b \simeq 4$ $c \simeq 10$ $\beta \simeq 108°$

4 The Rings lie tilted out of the ac plane by 31° (ie line joining C_2 & C_5 is at 31° to 010)

5 The Cl's are packed together about axes // to b axes. & run along // to b.

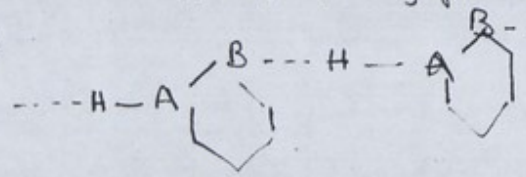
Certain Cl-Cl distances are abnormally short, possibly due to formation of hydrogen bonds.

6 Also N in amino group to N in neighbouring ring is short.

ie $N_2 - N_3' = 3.37 A°$ & $N_2 - N_1'' = 3.21$. These are suggested (All other interatomic distances are > than 4 A°) as hydrogen bonds N — H ····· N and are almost co-planar with the ref molecule. Pauling quotes distances of 2.98A & 3.20A² for this type of bond in Ammonium Azide & 3.38 A for a weak bond in crystalline Ammonia. This type of hydrogen bonding explains the tautomerism of the pyrimidines not on the Kekulé model above but due to fact that the chemical & physical properties ~~of~~ would

intermediate between ---H—A ring system to B---H—A next ring system B

51 ie

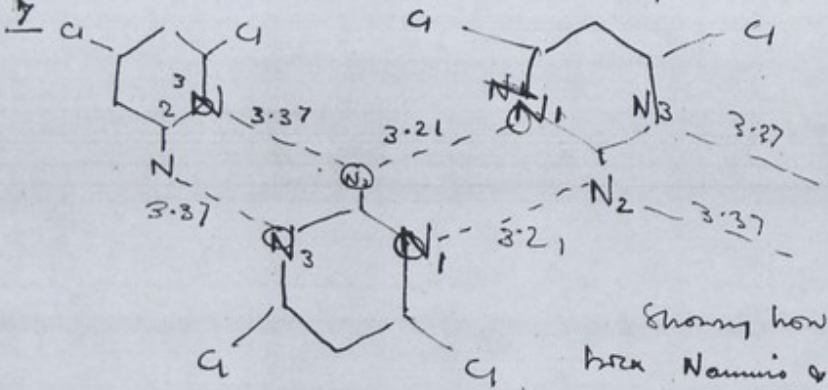


and

—H---A⁓⁓B—H---A⁓⁓B—

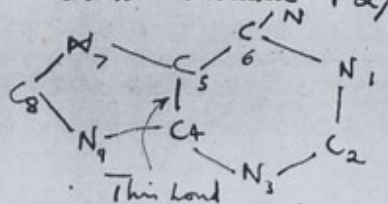
The hydrogen bond system in the pyrimidines described by Clews-Cochran seems to present an example of such a mesohydric structure both intermolecular sharing of the tautomeric hydrogen.

7



Showing how hydrogen bonds between Nammo & N_3 ring are longer than Nammo & N_1 ring.

Acta VII. 1. Part 6. June Broomhead. Structure of Adenine hydrochloride.
Cell is Monoclinic P2/c. a = 8·8. b = 4·8. c = 19·5. β = 114°
4 Molecules & Two H_2O's in each cell.



This bond longer 1·44 than other ring C-C distances = 1·32. ± 0·05.

1 Molecule tilts out of 010 plane so that line C_6 to N_3 makes 37° and C_8 to N_1 makes 19°. with ac plane.

2 ⊥ distance mix planes of corresponding Purines in adjacent unit cells is 3·2 A°

3 Short Van-der-Waals contacts N_3 to N_3' = 3·22A in same cell
& N_3 to N_3' = 3·18 A in adjacent cell.
Also N_3 to C_2' = 3·38. N_1 links to a Water by Hydrogen bond 2·87A.
N_7 from N_{10} adjacent mole. same cell by 2·99A°.
& N_{10} " N_7 " " next cell. 3·38A°.

The Water molecule is bonded to 2 N's & 2 Cl's which form a distorted tetrahedron round it. 52
Condneles that hydrogen bonds involving all the N's as well as the Cl & H_2O mols. & the major forces holding the mols. together & determining the structure.

Density Measurements

① Place some chloroform under hat & saturate with 75% RH.
② Look up Coeff. Expansion of Chloroform.
③ Make more blobs.

Feb. 13 Blob. 1. Straight from Equilibrating tank. Float $2\frac{1}{2}$ | Sinks $3\frac{1}{2}$. 3-

Check by Rotachid about 5min afterwards. Float $1\frac{1}{2}$ | Sinks 2

Repeat. Float $\frac{1}{2}$ | Sinks 1. $\frac{3}{4}$

* Provisional "75% Density" taken as that of Chloroform at 3°C. ± 1°C. ie 1.521 ± 0.002 g/cc.

Weights — Obtained

Blob.	
1	0.0041 + 1 div.
3	0.0032 + 1 div.
6	
7	

Sep. Funnel. Ran off Wet CH_3Cl_3 Float 1 | Sink $1\frac{1}{2}$ · CH_3Cl_3 very turbid.

Floatation Expts. Feb. 20th. Blobs dried over P_2O_5 4 days. Transfered from drying vessel straight into floatation expt.

Blob (a). Supersat. 15°C. (b) 10°C + (c) 24°C. Conclusion: Not dried sufficiently.

Weighing Feb 25th

Blob	Wt
a	0.0010 g − 1 div.
b	0.0108 g + 4 div.
c	0.0091 g − 1 div.
d	0.0043 g + 4 div.
e	0.0076 g + 2 div
f	0.0071 g ~~± 0 div~~ − 1 div.

Pt 1

Blob	Wt
g	.0051 − 2 div. g.
h	.0080 + 1 div g
i	.0057 − 2 div g.
j	.0088 − 2 div. g
K.	.0055 − 3 div. g.

Pt 2.

Floatation Expt Just Sinking Temps: Feb 25th (After weighing. But from P_2O_5 Pot 1)

a). Floating def at 2°C — Sinking definately at 8°C. Just Floats over range 3 – 6.° C.

b) First Sinks 12°C. Tends to stick to them. indicating blob still a little wet.

c) Just sinks 22°C.

d) " " 13°C.

e) " " 11°C.

f) " " 9°C

Floatation Expt Feb 28th. 1st Batch. Blob. 75%. Equilibrated. 3 weeks. Floating In. CH_3Cl_3. which had been sitting under water for 2 weeks.

Weighings Pot I. Feb 28th. to 1/100 R m.g.

a) 0.0010 g. + 5 div or 0.0011 – 5 div.

b) 0.010 g +3 div.

c). 0.0091 — 2div.

d). 0.0043 + 1 div.

e) 0.0076 – 3div.

f) 0.0071 — 2 div.

Floating Expt. March 3rd.

Blob	Sinking Temp.
a).	4 – 5°C.
b)	10°C or little less. ie ≃ ½ – ¼ °C.
c).	Still floating at 19°C. though only just.
d)	10°C – 9°C.
e)	8°C. NB Blob e) dropped in when T > 10°C. Therefore sank immediately, spending negligable time in surface. Then cooled down to 5°C & prevented from rising to surface. Blob quite dry, no sticky edges. Expt repeated by cooling to 0°C & leaving blob in ∅ near the surface. Find just sinks temp. of 10°C. Clearly water must be condensing on the surface. Also edges of blob became sticky.
f).	Following above technique. 6°C – 8°C.

this March 5th. Pot II 51 — 2d.

g. [0051 - 2] ~~0514 milligramm~~.
h. [0080 + 1] 80 ~ 79 + 6
i. [0057 - 2] 56 + 2
j. [0088 - 2] Lost & found on floor. 88 − 6. = 87 + 2(3).
k. [0055 - 3] 54 + 3.

March 26th. Pot II Zero at +1. div. Pot I

g. a) 10 − 2d.
h. b) ·0105 − 2d.
i. c) ·0089 − 3d.
j. d) ·0042 ~ − 1d.
k. e) ·0074 + 6.d.
f). ·0069 + 1.

Density Floatation Expt.

a). Dust sinks at 4°C.
b) " " " 7-8°C
c) " " " 19°C. Dry
d) " " " 9°C
e) " " 8°C. NB Density of Chloroform at 30°C
f). " " 6°C. is ~~1.470~~ 1.4707 ≏ 1.471.

Put to equilibrate at 75% Both Pots End of March 25-26°C.

Those observations May 17th.

Weighing (% Water Uptake)

a) 0·0013 + 3d. (0·0014 − 5 div)
b) 0·0143 + 1d.
c) 0·0121 − 2d.
d) 0·0058 − 2d.
e) 0·0101 + 1d.
f). 0·0098 − 4d.

3+5d is $\frac{3+25}{9.75}$ = 37½%
3+3d is $\frac{38.375}{104.75}$ = 36.6%
16.125/88.625
16.125/41.875
26.375/74.75
23.375/69.125

Floatation Chloroform from Bottle.

a) 28½°C.
b) 30 − 29½°C.
c) 35
d) 30½
e) 31½
f).

% Water Uptake

a) 37% b) 36·6% c) 36·3% d) 38·6% e) 35·3%
f). 34%.

Determination of Density of Chloroform. May 17th.

55 Wt. of Picnometer. 22·8719. (Polished clean)

" " " 22·8938 (Washed repeatedly with ether)

" " " 22·8918. (Polished again with clean handkerchief)

Wt. of Pic + Chloroform. 59·602 / 59·602 | ∴ Wt. Chloroform = 36·710

Wt. of Pic after Washings with ether. (Chloro. emptied). 22·881

Wt. of Pic + Water = 47·751 Temp. 21·7°C.

Wt. of Water = 24·880.

Density Chloroform = $\frac{36·71}{24·88}$ = 1·474 (Slide Rule)

Suppose take pic empty as 22·892
The Water 24·859
∴ ρ = 1·480.
Error of 0·4%.

NB At. 21·7°C, ρ theoretically = 1·486.
(Experimental value in Error by 0·8%)

B166(a) X-rayed ~~Dust~~ Just before. coronation. Gives Powder diagram. Suggests structure A.
Put back in 75%, bottles. Weighed after 4 days. ·0013+3d. ie no change in weight.

B166 C & d Put with Sodium Carbonate ie 92% to equilibrate. JUNE 4th.

Floatation Expt. June 4th Chloroform from sheeted bottle. Heated in water bath to 30°C.
B166(a). Just sinking at 26°C. But later began to sink again. Drying out?
Sinking quite rapidly at 21°C.
Thereafter just sinking at 12°C.

5b

blob. b) Just begins to float on 32°C.

to

a) Just began to float on 35°C

Flotation Expt June 5th. Blob (a) Will not sink at room temp. Chloroform. (21°C) leave it standing for 2–3 mins whilst fetch beaker of hot water ± (70°C). Still will not sink. (stay down when put down to bottom of T.T.) Heat to 35°C rising rapidly sinks. Rises ± 30°C. quite definite. Finds some level about 2/3 rd's up tube. Neither floats or sinks. Therm reading 29°C. Then suddenly at 28°C it starts to sink. Will not float if brought to surface. Just sinks to bottom. Is this a "water logging" phenomena? or a drying out of water & collapse of structure.

~~Could test by leaving blob standing in Chloroform at room temp.~~

Blob ~~Blob~~ then just floats off at 10–11°C. [11.5 definately sunk.].

Blob (e). Just floats at 37–38°C. Straight from equi. bottle 75% 2–3 mins in Chloroform. Blob in Chloroform for {10 minutes. 15. No sign of blob (a) phenom. (≃ 20°C).

Repeated heating opt. Took it to 40°C. Found would not begin to float until 27°C. After 30 mins just floats at ~~30~~ 19°C.

Weighed Blob (e) ~~wet~~ at 1½ after removal from Chloroform. .0095 + 3D.

Blob. (d). X-rayed. Powder diagram A. 75%. Weighed straight from camera.

(d) Wt .0055 + 0d. (ie lost .0003 mg; probably drying out in dark room.) [12.30 am. June 8th]

Blob C At 92% Since Wed: ie ≃ 5 days. Wt Increased to .0135 + 4d.

Dry Wt. .0089 – 3d. ie Increase .0046 +7d. ie $\frac{46 \cdot 875}{88 \cdot 625} \cdot 100\%$ ie 53%.

Blob C. put in Camera & Exposure started. Eve. Monday. 8th June. 92% RH.

Weights 9th June (Afternoon). Rest of Blobs (except f.) put in 92% RH. Monday. Afternoon.

(a) .0016 + 1d.
(b) .0167 ± 1d
(c) In Camera.
(d) .0069 – 4d.
(e) .0119 + 4d.

Density liquids

NB Blob C taken off tube Wed. Morn. Liquid blown over from bubbler. Wt. .0181 – 1d.

Bromo-benzene. 1.4991 at 15°C
Iodo-benzene 1.832 at 20°C
n-Amyl-Iodide. 1.517 at 20°C

Floatation Expt Blob c. Wt. ·0176 = 2d. After (15 min / 20) at 92% previously inset in Camera

Blob d i) June 10th. Wt. ·0066 ~~+0d~~ = 1d.
Placed in Camera. Wed (11th) afternoon. 92%

ii) Friday June 12th. Blob d. Weighed from Camera. ·0059 (60) +1d.
Blob replaced in Constant Humidity Container. Zero out. Setting at −9: Above value set at 0. ∴ Real Reading ·0061 to ·00615.

July 6th Weights of Pt 1. at 92%. (1 Month + at 92%)
Lever Slip Balance & zero unit ~~·2755gms~~. [·2755g.]

Blobs
a) (·0016 +1d) [·2771.] : ·2770+5d.
b) (·0167 −1d) [·2922] : ·2918 +0d.
c) Boiled in Bromo-benzene. : ·2872 +0d.
d) (·0069 −4d) [·2824] : ·2822 [·2821+0]
e) (·0119 +4d) [·2874] : ·2872 +2d.

Density
Allyl Bromide (3 bromopropene) 1·398. Bpt. 71°C. Insoluble Water.
n-Amyl bromide. ~~+264~~. 1·246, Bpt. 128°C. Insoluble water.
Cyclo hexyl bromide. 1·3290. Bp 163°C Insoluble " .
(Phenyl cyclo hexane).

Flotation Expt

① July 8th. Allyl Bromide. Blob (a), Floats quite all way up to 25°C.
n-Amyl bromide. Blob (b) Sank rapidly at < −10°C.
Blob re-weighed · ·2916 — 3d.

Cyclo-hexyl bromide. Blob. e), & Blob (a) both sink.

Powder 100gms. p-Bromotoluene C_7H_7Br. $d_{0°C} = 1.4313$. $\alpha = -1.25$.
Range of expt. 30 − 100°C. Limit of Error ±·0005. [NB $\rho = 1.35$ @ 45°C]
Handbook gives $\rho = 1.3898 \left(\frac{20}{4}\right)$. Melting Point. 28°C. Insoluble in water.

1 Yale Journal of Biology & Medicine. VXIX. No 6. July 1947. Kurt. G. Stern.
Nucleoproteins and Gene Structure.

58

NB Calculation of length of NaDNA Model:

Av. Molecular Wt. of a nucleotide = 330. 20 such in ## 34A°. (Two chains per molecule)

∴ Wt of length 34A° = 330 × 20 = 6600.

Suppose Molecular Wt of 10^6. Then Molecular length = $\frac{10^6}{6600} \times 34$.

Thus for 8 million mol. wt. should have particle length

of $41.20.10^3$ A.

$= 10^3 . \frac{34}{6.6}$

$= 5.15.10^3$ A.

P941 Suggests that nucleoproteins are linked-units of DNA° Protein.

July 16th Weights of Pot 1 at 92 %. Lever Slip: Balanced to zero with .(·2755.)

Blobs. a). 0·2772 −2d.

b) 0·2921 + 2d.

c) 0·2874 − ## 0

d) 0·2823. + 0.

e) 0·2878 − 6d.

Floculation Expt. Blob (a). Alkyl Bromide Floats even at 32°C.

So density is < 1·398 − [·002 × 32 ie ·064] [if α is cf. CCl_4] *. But it must be much smaller wf. expansion.

ie < 1·334.

Now Cyclo Hexyl bromide has ρ. 1·329. require + 005. ie ≏ −2°C if α of CCl_4.

Blob (b) Cyclo-hexyl bromide.

Total Stock of ("non-pulling") Figure of Schwendler. 0·5333(0)d.

16 Sept. yesday Weighed out (directly on pan). 0·05 Y? taking up water rapidly. Visibly as steady drift on ·00001 scale (eye scale). [0·0620. after 10 mins in lab air.]

Placed in bottle with glass Lid. Tried Wt. (+ lid) = 9·7115 −2d. (≡ 9·71147.)

(Rinsed bottle with) Lap lft. (10) gram ≡ Bottle + ·288Y + 3d ie Bottle 9·71127 and no drift.

Repeat right way round. 9·7116 + 6d and a little drift

9·7117 − 1d.

Ultracentrifuge 200,000 g. ω = 54,000 r.p.m. Mean Radius 65 mm.

59 Height of column 12mm.

[CROSS-OUT IN RED]

$\frac{54,000}{60} \times 2\pi = \omega$ radians/sec.

Centrifugal force = $m \cdot \omega^2 r$.

∴ Check on values above. Cent. Force on 1 gram = $\frac{54^2 \cdot 10^6 \cdot 4 \cdot \pi^2 \cdot (6.5)}{36 \cdot 10^2}$ =

= ~~$\frac{(13.0)^2 \cdot 6 \cdot 4 \cdot 7}{4^2} \cdot 10^4 = 1,1,3,27,\pi^2 \cdot 10^4$~~

∴ Mean Force = 208,000.10^3 dynes.

If taken r_1 = 70mm. & r_2 = 60mm

Then $F_1 = 2.24 \cdot 10^8$ dynes. } Field at either end of 1cm cell.
$F_2 = 1.92 \cdot 10^8$ dynes. }

Nett Gradient per 1cm is $0.32 \cdot 10^8$ dynes. ie 0.32 dynes/A°.

Therefore Tension produced in a 5000A° molecule is 1600 dynes. ie 1.63 grams wt.

~~If ions at end were fixed. But is free to move against a viscous drag.~~

Macro-Expt

Consider a 10μ fibre stretching under 10 gram weight load.

Xsection = $\pi(5 \cdot 10^{-3})^2$ $\pi \cdot 25 \cdot 10^{-6}$ sq cms.

∴ Tension per 100 sq A° = $\frac{10}{\pi \cdot 25 \cdot 10^{-6}} \cdot \frac{10^{-16}}{1} = \frac{10^4}{\pi \cdot 25 \cdot 10^{10}}$ ≈ 10^{-7} grams wt per 100 sq A°

If molecules are close packed as in Structure A. Then have 2 molecules occupying 22 × 40 sq A°. ie 880 sq. A°. Now the Tension produced across each molecule is 1.63 grams wt. ∴ This is equivalent to a load of 3.26 grams wt per 880 sq A°. In a fibre of 10μ consisting only of Crystallites Xsection = $\frac{\pi \cdot 25 \cdot 10^{-6}}{10^{-16}}$ sq A° = $\frac{\pi \cdot 25 \cdot 10^{+10}}{880}$ units of 880 sq A°

∴ load on fibre comparable to load in Centrifuge = $\frac{\pi \cdot 10^{10}}{8 \cdot 8 \cdot 4} \cdot 3.26$ grams wt.

ie = $2.91 \cdot 10^6$ Kilograms.

= $2.91 \cdot 10^9$ grams wt

[60] is BLANK

FOLLOWED BY 2
OTHER BLANKS AND
ONE TORN OUT SHEET.
ORDER OF NOTEBOOK
THEN REVERSED, I.E. STARTS
FROM OTHER END OF BOOK

100 bonds

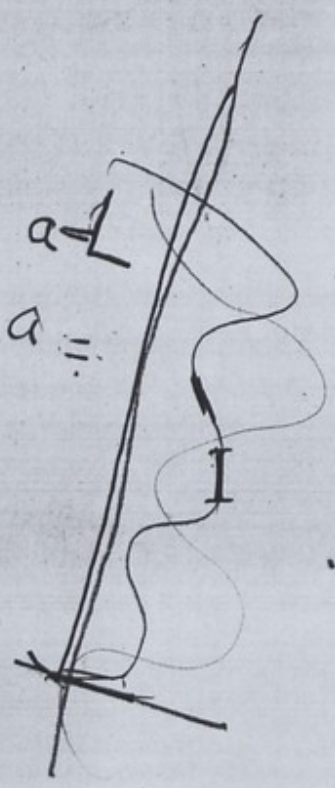
5 | 4 | 20

5 H₃ 4 H₂ 20 H₁.

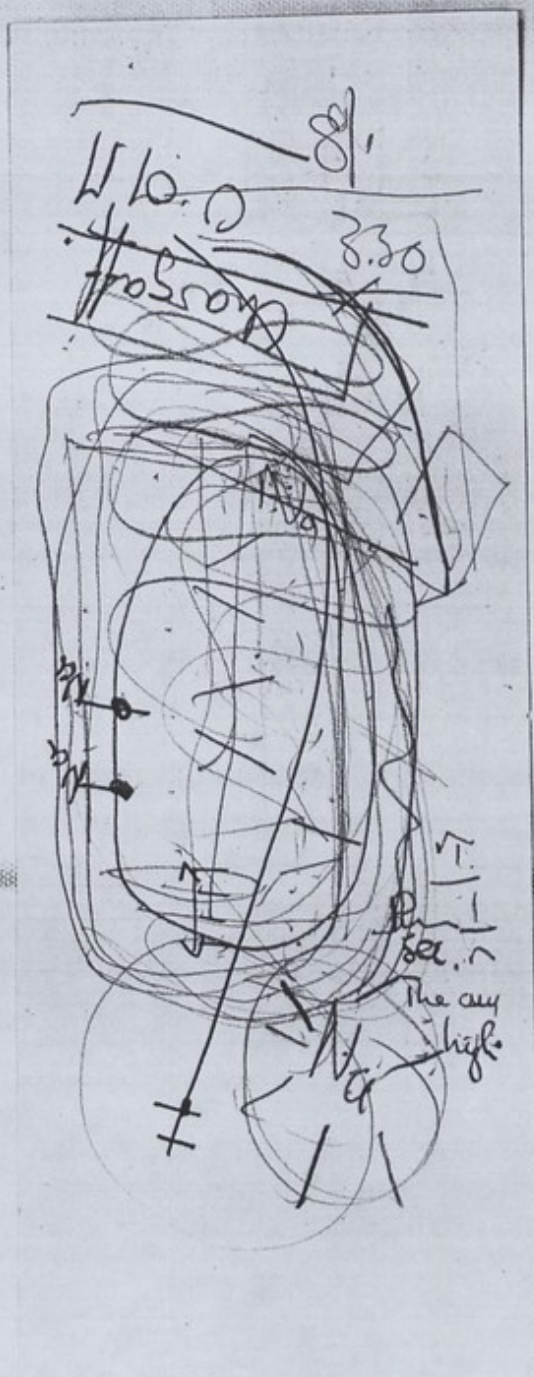
H = 1 bond.

20 H.

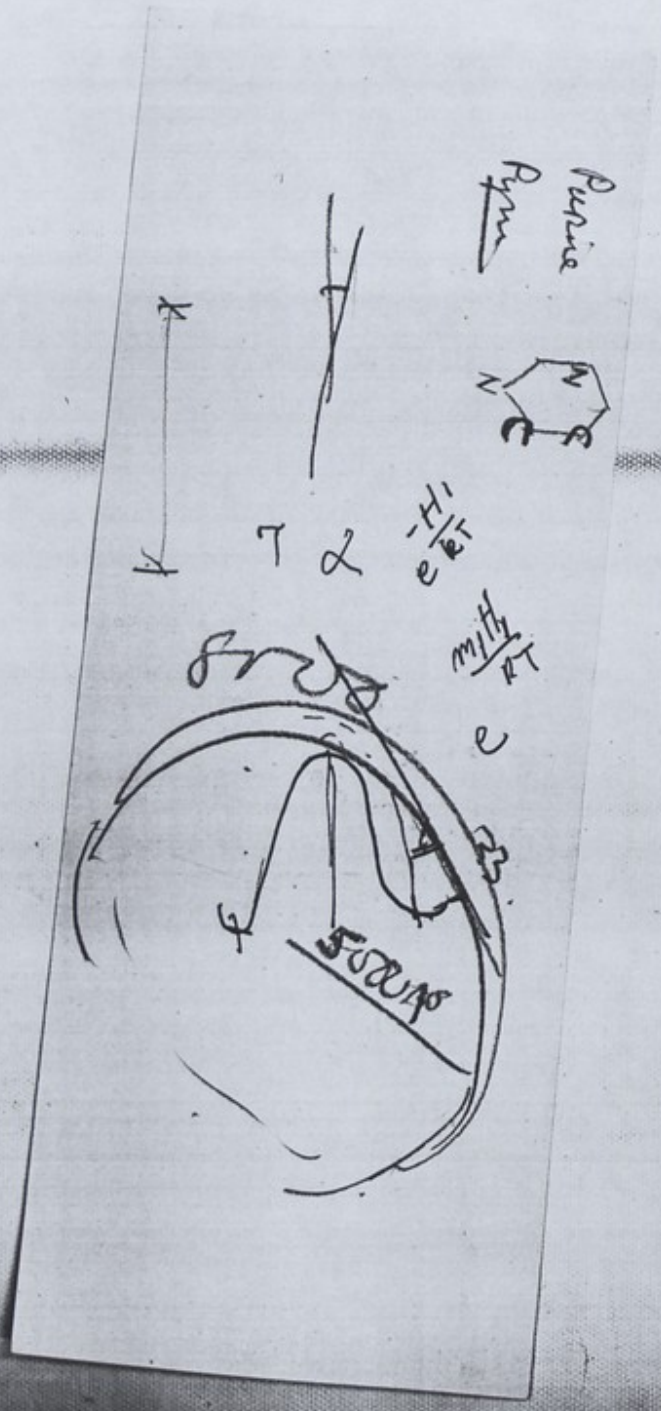
20 H₁



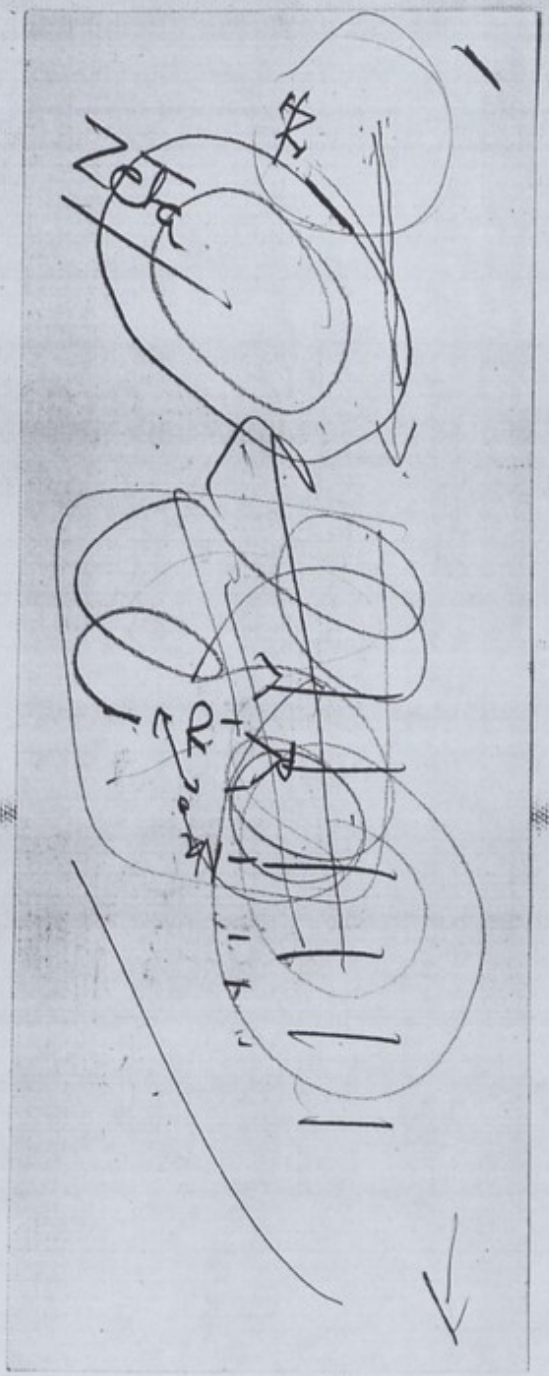
"A"
SIDE TWO?
AFTER [p. 59]



"A"
SIDE 1.
LAID IN
R.F. NOTEBOOK
AFTER [p.59]

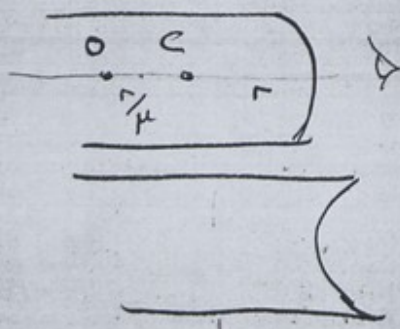


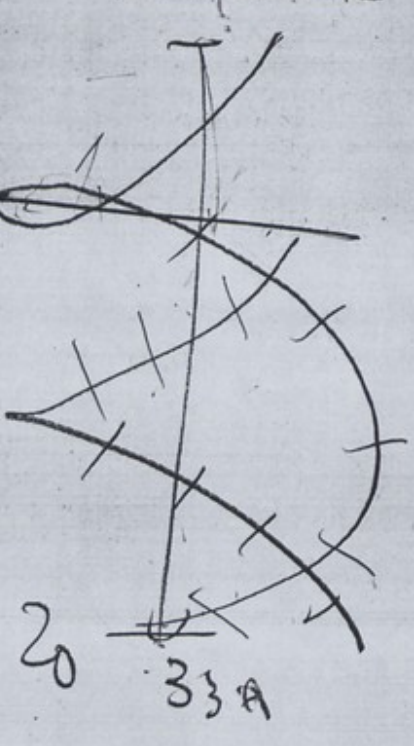
"B"
SIDE a
LOAD IN AFTER
[p 59]



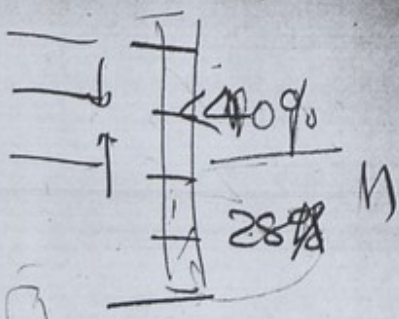
"B"
SIDE B
LAID IN
AFTER p 59

2 hours 30 mins/question.
4 questions.





20 33⅓



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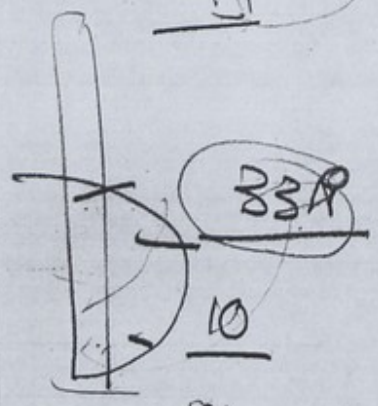
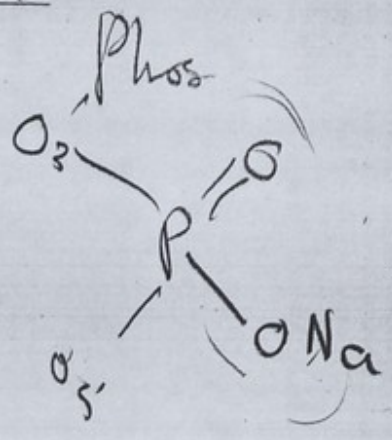


10



"C" "D"

LAID IN AFTER [p 59]
VERSOS ARE BLANK

PASTEDOWN
FLYLEAF
BLANK

Stiwtels Math Crystal Physics

I

Strain defined by τ_{11} τ_{22} τ_{33} τ_{23} τ_{31} τ_{12} - the components of a symmetrical 2nd order tensor.

Which can be written τ_1 τ_2 τ_3 τ_4 τ_5 τ_6.

Stress defined similarly as σ_{11} σ_{22} σ_{33} σ_{23} σ_{31} σ_{12}.

The components of τ are linear functions of σ. ie $\therefore \tau_i = \sum_k S_{ik} \sigma_k$

S_{ik} = elastic modulus.

$i, k = 1, \ldots 6$.

This is fourth order tensor, with 21 compts.

A triclinic crystal will - have all 21 S_{ik} values independently existing.

With higher symmetry this no: is diminished.

Consider a Diade Axis: direction x_3. (Rotation of 180° about this axis) (brings lattice into self coincidence)

Now each tensor is represented by a matrix,

$$\begin{vmatrix} \times & \times & 0 \\ \times & \times & 0 \\ 0 & 0 & \times \end{vmatrix}$$

still has matrix case the components with a $\times$ remaining constant & the 0 will change sign.

Therefore unless τ_i changes sign when σ_k changes sign then (ie $i = k$ & same sign) S_{ik} vanishes.

Hence

$$\left.\begin{matrix} S_{14} & S_{15} \\ S_{24} & S_{25} \\ S_{34} & S_{35} \\ S_{46} & S_{56} \end{matrix}\right\} = 0 \qquad S_{44}\ S_{55} \qquad S_{45}$$

$$\underset{\sim}{S} = \begin{vmatrix} S_{11} & S_{12} & S_{13} & 0 & 0 & S_{16} \\ & S_{22} & S_{23} & 0 & 0 & S_{26} \\ & & S_{33} & 0 & 0 & S_{36} \\ & & & S_{44} & S_{45} & 0 \\ & & & & S_{55} & 0 \\ & & & & & S_{66} \end{vmatrix}$$

Reflect across diagonal: symmetrical tensor.

This matrix now only has 13 compts.

Consider now Orthorhombic Crystal : 3 diode axes. X_1 X_2 X_3.

Now we get

$$\underset{\approx}{S} = \begin{vmatrix} S_{11} & S_{12} & S_{13} & & & \\ & S_{22} & S_{23} & & & \\ & & S_{33} & & & \\ & & & S_{44} & & \\ & & & & S_{55} & \\ & & & & & S_{66} \end{vmatrix}$$

only 9 components left.

Tetragonal System 1 + 2 axes are equivalents everything will reduce to

6 comps. S_{11} S_{12} S_{13} S_{33} S_{44} S_{66}.

Cubic 3 comps. $\therefore S_{11} = S_{33}$ $S_{12} = S_{13}$ $S_{44} = S_{66}$

$S_{11} = 1/$ Young's Modulus. E.

$-\frac{S_{12}}{S_{11}}$ = Poisson's Ratio. S

Lattice Energy Depends on arrgt of atoms. Change in arrgt every time.

The arrgt for min. latt energy is the one that atoms chose. for any given deformation. Can calc. how potential energy varies.

Meas. of Elastic Moduli

1/ To Measure a particular S_{ik}. Apply small stress & observe particular strain. Or vice-versa.

These values very small. Use interferometric technique.

2/ Dynamic methods are better. eg. Oscillation of cantilever to find E.

Stationary Waves set up in 3 dimensional block. Get various normal modes of vibration. These can be calc. theoretically. They are very high frequency. Ultra-sonic region.

Electric Properties of Crystals

III

Put isotropic subs. in field of strength $\underline{E}$. It will become polarized. The extent of this can be described by a vector $\underline{P}$. Can find relation twix $\underline{P}$ & $\underline{E}$. In isotropic subs.

$$\underline{P} = K \cdot \underline{E}$$

$K \equiv$ dielectric susceptibility.

$[J_0(x)]^2 = \frac{1+\sin 2x}{\pi x}$

RECTO OF SHEET LAID IN BETWEEN II AND III

$x = 39.\ 2x = 78°.\ \frac{78}{\pi} = 24.83$

$\therefore 2x = 24.\pi + 149°$

$\therefore \sin 2x = \sin 31° = 0.5145$

$\therefore J_0(x)^2 = \frac{1.5145}{\pi \cdot 39} = .01235$

$= .111$

$x = 38.7.\ 2x = 77.4.\ \frac{77.4}{\pi} = 24.(65)$ $J_0(x)^2 = \frac{1.707}{\pi \cdot 38.7}$

$2x = -1 + 115°$ $\sin 2x = \sin 65 = 0.707$ $= .01406$

$J_0(38.7) = .118$ $1.906/\pi 38.7 = .0177$

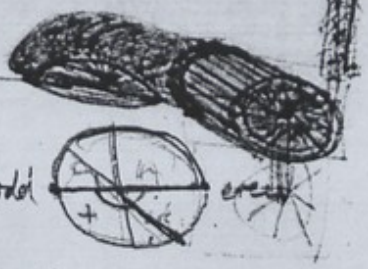
24 65 117° ... 63°. $\frac{1.883}{\pi 38.7} = .0155$

$\frac{1244}{}$

$x = 34.\ 2x = 68.\ \frac{68}{\pi} = 21.64$ $\sin 65° = 0.906$

$2x = -1 + 115°.\ \sin 2x = 65$ $J_0(31) = \frac{1.906}{\pi 34} = .1785$

1336



$1 + \sin 2x = \pi x$

$J_0(x) = \frac{\cos x + \sin x}{\sqrt{\pi x}}$

odd even

$x = 34$. Then $\frac{34}{\pi} = 15.82$ $x° = 15.180° + 147\frac{1}{2}°$ complement $= 32\frac{1}{2}°$

$\therefore \cos +\ \sin -ve.\ \therefore J_0(x) = 0.537$

$\cos x = 0.843$ .306

$\cos(\alpha+\beta) = \cos\alpha\cos\beta$ $\sin\alpha\sin\beta$

$\cos\beta$ — $147\frac{1}{2}$

$\cos(180 - 32\frac{1}{2})$

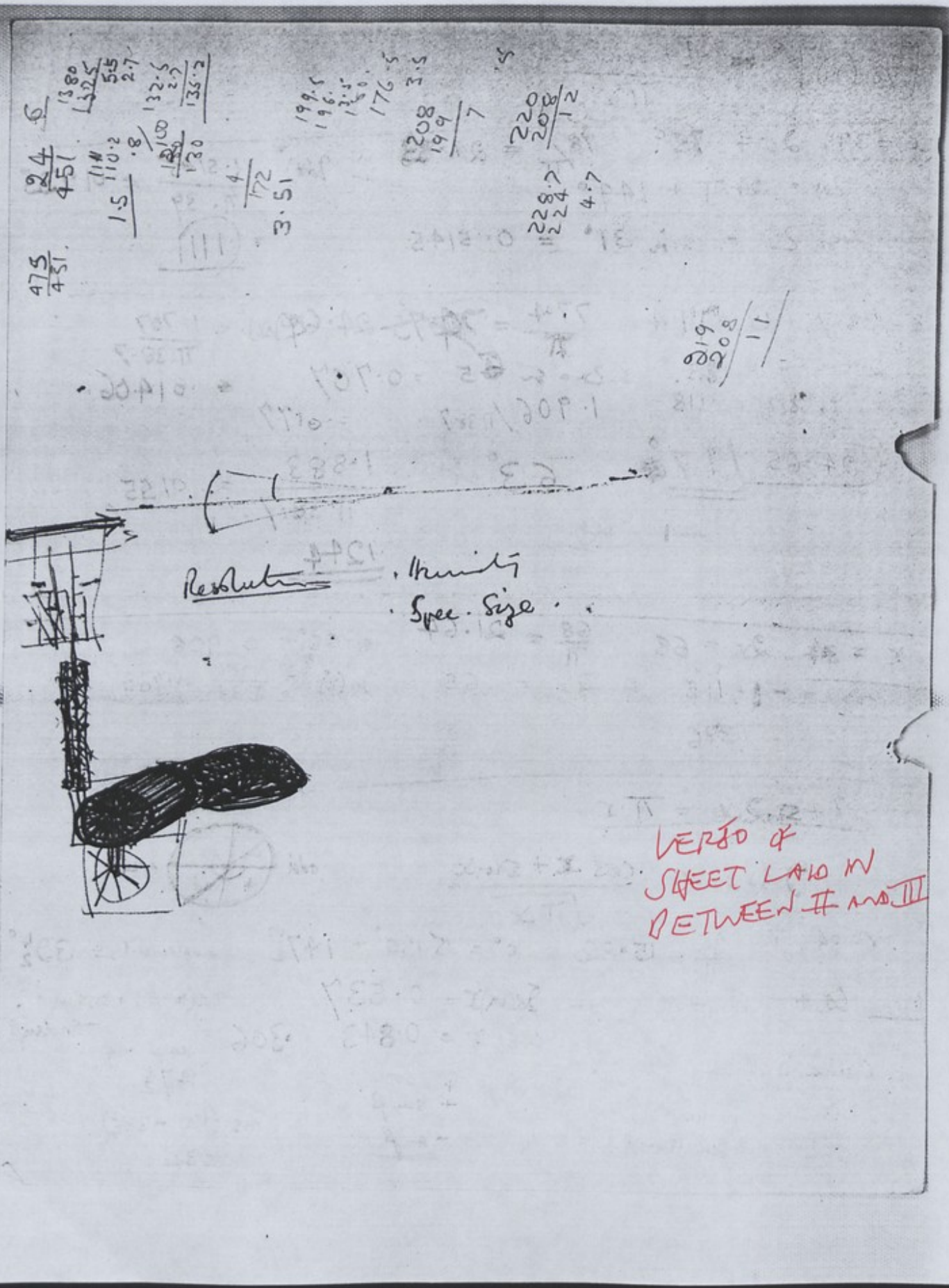
$\cos 32\frac{1}{2}$.

$\therefore$ Cosine is during +ve.

$\sin(\alpha+\beta) = \sin\alpha\cos\beta + \cos\alpha\sin\beta$

$\sin(180+\beta) = + \sin\beta$

$\sin(180-\beta) = -\sin\beta$



VERSO OF SHEET LAID IN BETWEEN II AND III

Bernal 8th Feb. Discharge effect on clearing mica in vacuo. K ions hit glass which fluoresces.

II

Cleaves easiest down the K 12 co-ord sheet. By weathering take out K. → Clay. Bentonites. take in layers of water water between Potass. sheets wet in mica structure.

(Kaolin from felspar.)

Normal clay has silica tetrahedron — silicate thk. 7°A.

Sheet clays, say 20 A° thick ∞1000 wide.

large hexagonal lattice of felspar. Reproduced industrially

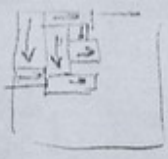
Put charge on lattice eg -ve charge happy for +ve ions.

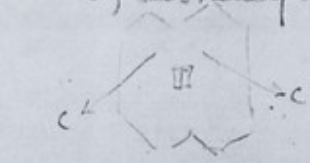
Zeolite. Large holes. Collect Carbonates.

Sub. opaque ∴ optic axes of crystallites are randomly arranged. ie Birefringence high. so cannot be "optically" clear.

Twinned crystals will also be opaque (same reason)

either a) domains b) secondary growth on twins.





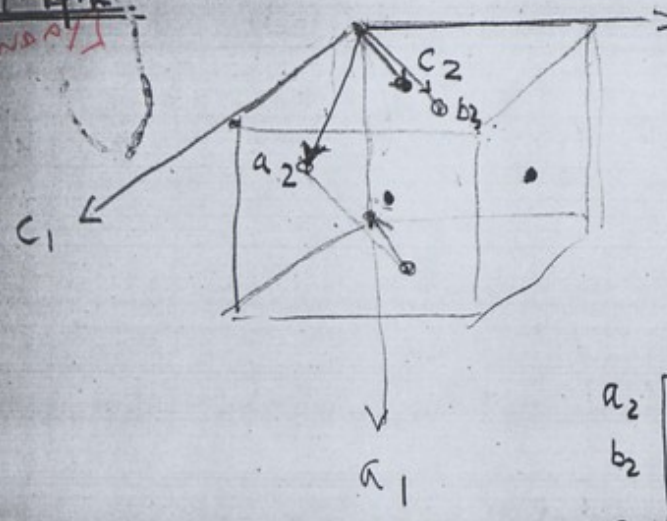
High sym. breaks down, tendancy to twinning & pseudo-structure.

Ref Bragg Structure of Minerals.

Eq. 19+b

[MONDAY]

V



$a_2 = \frac{1}{2}a_1 + \frac{1}{2}c_1$

$b_2 = \frac{1}{2}a_1 + \frac{1}{2}b_1$

$c_2 = \frac{1}{2}b_1 + \frac{1}{2}c_1$

a_2	$\frac{1}{2}$	0	$\frac{1}{2}$
b_2	$\frac{1}{2}$	$\frac{1}{2}$	0
c_2	0	$\frac{1}{2}$	$\frac{1}{2}$

Face centered Cube

transformed to ~~side~~ primitive cube.

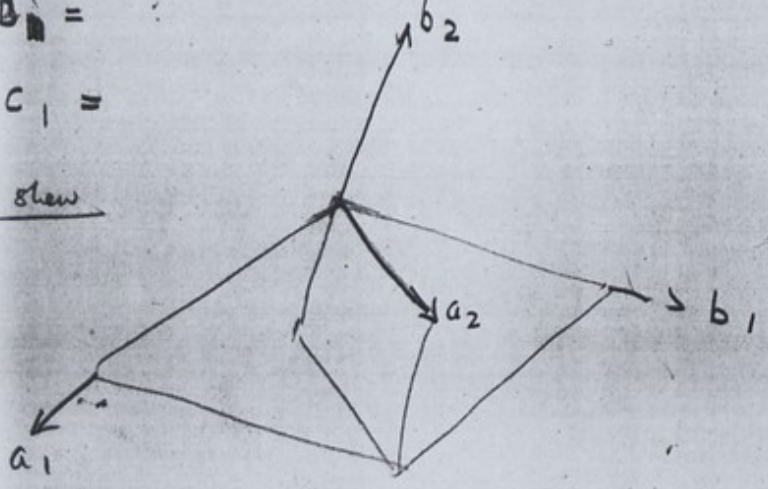
$a_1 = +a_2 + b_2 \blacksquare c_2$

~~$+2b_2 = 2c_2$~~

$b_1 =$

$c_1 =$

Show



c axis same.

Large cell = 3x Small Cell.

VI

General transformation Numonics

(Monday Feb 25th)

	h_1	k_1	l_1	
	a_1	b_1	c_1	
h_2 a_2	S_{11}	S_{12}	S_{13}	a_2^* u_2 x_2
k_2 b_2	S_{21}	S_{22}	S_{23}	b_2^* v_2 y_2
l_2 c_2	S_{31}	S_{32}	S_{33}	c_2^* w_2 z_2
	a_1^*	b_1^*	c_1^*	
	u_1	v_1	w_1	
	x_1	y_1	z_1	

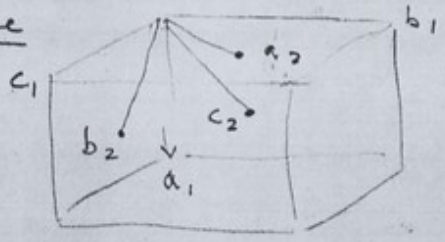
Read left to right for a_2 in terms of a_1

For a_1^* in terms of a_2^* read top to bottom

NB > Relations derived for face-centered cube apply to any face centered lattice.

@ If here chose axes incorrectly, ie do not obey right hand rule on evaluation of determinant get -ve result.

Face Centered Cube



$$a_2 = \begin{pmatrix} 0 & \frac{1}{2} & \frac{1}{2} \\ \frac{1}{2} & 0 & \frac{1}{2} \\ \frac{1}{2} & \frac{1}{2} & 0 \end{pmatrix}$$

$$\begin{pmatrix} -1 & 1 & 1 \\ 1 & -1 & 1 \\ 1 & 1 & -1 \end{pmatrix}$$

$$h_1 = -h_2 + k_2 + l_2$$
$$k_1 = h_2 - k_2 + l_2$$
$$l_2 = h_2 + k_2 - l_2$$

$$\begin{cases} h_1 + k_1 = 2l_2 = 2n \\ k_1 + l_1 = 2n \\ l_1 + h_1 = 2n \end{cases}$$

So can get conditions for absent spectra by expressing $h\,k\,l$ in terms of Primitive Unit.

VII

Rhombohedron. Face Centered.

Co-ords

000	$\frac{1}{4}\ \frac{1}{4}\ \frac{1}{4}$
$0\ \frac{1}{2}\ \frac{1}{2}$	$\frac{1}{4}\ \frac{3}{4}\ \frac{3}{4}$
$\frac{1}{2}\ 0\ \frac{1}{2}$	$\frac{3}{4}\ \frac{1}{4}\ \frac{3}{4}$
$\frac{1}{2}\ \frac{1}{2}\ 0$	$\frac{3}{4}\ \frac{3}{4}\ \frac{1}{4}$.

$$\begin{array}{|ccc|c} -1 & 1 & 1 & x_1 \\ 1 & -1 & 1 & y_1 \\ 1 & 1 & 1 & z_1 \\ \hline x_2 & y_2 & z_2 & \end{array}$$

$$x_2 = -x_1 + y_1 + z_1$$
$$y_2 = x_1 - y_1 + z_1$$
$$z_2 = x_1 + y_1 - z_1$$

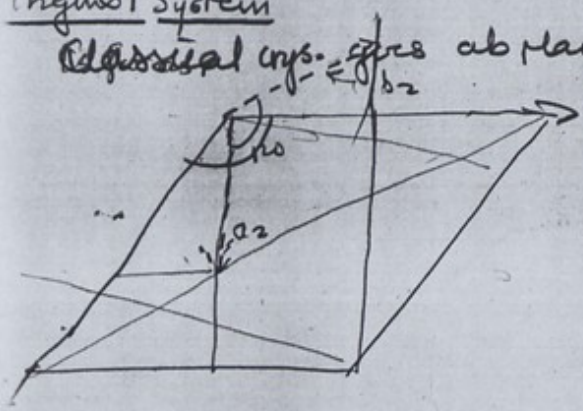
This gives co-ords of Primitive Cell. 000 ; $\frac{1}{4}\frac{1}{4}\frac{1}{4}$
100 ;
010 ;
001 ;

points differing by an integer in Units of corner of cell.

So in terms of Rhombohedral lattice only have 2 atoms/unit cell instead of eight. Coords 000, $\frac{1}{4}\frac{1}{4}\frac{1}{4}$

Trigonal System

Hexagonal axes. ab planes ∥ to axis



3 fm
3 m 1

Now $a_2 = \frac{2}{3}a_1 + \frac{1}{3}b_1$

$b_2 = -\frac{1}{3}a_1 + \frac{1}{3}b_1$

$c_2 = c_1$

$a_1 = a_2 - b_2$

Now $b_1 = a_2 + 2b_2$

$c_1 = c_2$

1

Theorem.

h_1 a_1' h_2 a_2'

$$\begin{array}{|ccc|} \frac{2}{3} & \frac{1}{3} & 0 \\ \frac{1}{3} & \frac{2}{3} & 0 \\ 0 & 0 & 1 \end{array}$$

a_2' b_1' x_1

&

$$\begin{array}{|ccc|} 1 & -1 & 0 \\ 1 & 2 & 0 \\ 0 & 0 & 1 \end{array}$$

$\therefore h_1 = h_2 - k_2$

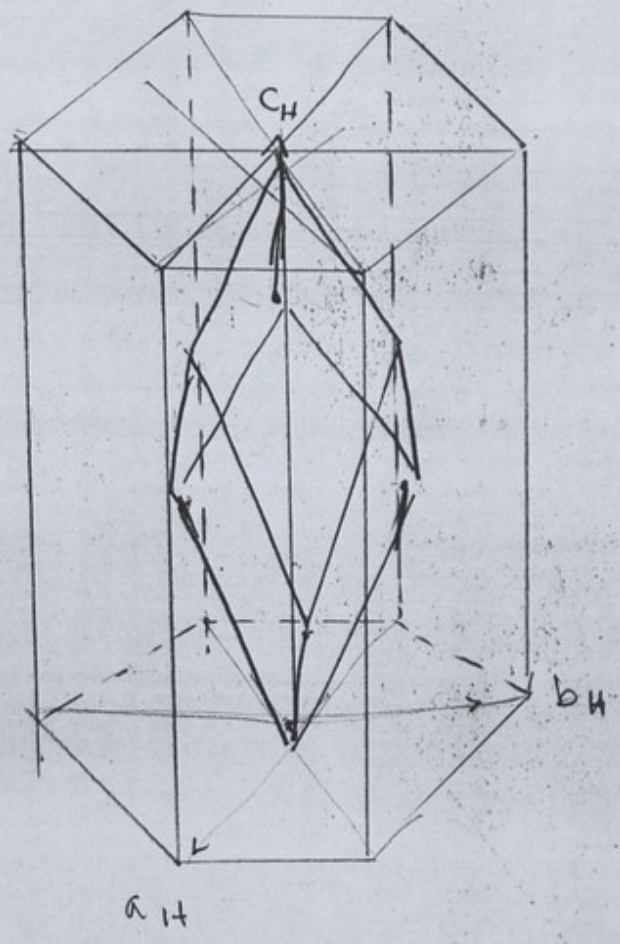
$k_1 = h_2 + 2k_2$

$l_1 = l_2$

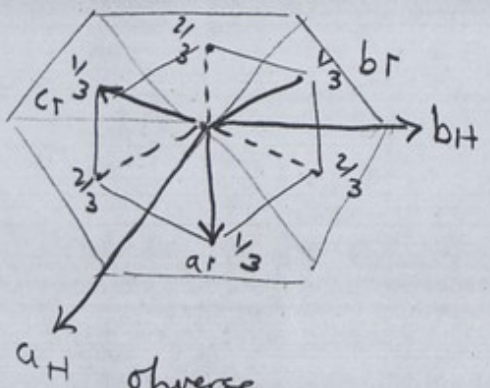
Now $h_1 - k_2 = 3n$

If find only planes are reflecting when $h_1 - k_2 = 3n$ then have taken to large a cell.

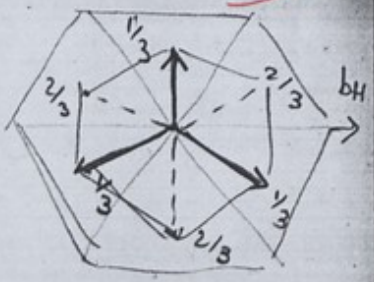
VIII



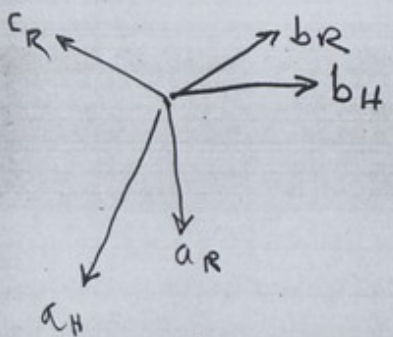
IX



Obverse position.



Reverse position



$$a_H = a_R - b_R$$

$$b_{1H} = b_R - c_R$$

$$c_{1H} = a_R + b_R + c_R$$

	h_R	k_R	l_R
h_H	1	−1	0
k_H	0	1	−1
l_H	1	1	1

So $h_H = h_R - k_R$

$k_H = k_R - l_R$

$l_H = h_R + k_R + l_R$

$(-h + k + l)_H = 3k_R = 3n$.

So if find for hkl planes for hexagonal unit give $3n$ for $(-h + k + l)$ then true unit is rhombahedral.

Worksout Reverse case.

XII

Jeffries Monday 25th. Feb.

1, Finished off his method of setting NB Read his paper in Acta.

2, Method of Wiese & Lonsdale. J. Sci. Insts. 1948-213.

We obtain values of arc corrections, but without knowing which arcs they apply to.

$$\tan\gamma = x_1/2\sqrt{2}r \qquad \tan\beta = x_2/2\sqrt{2}r.$$

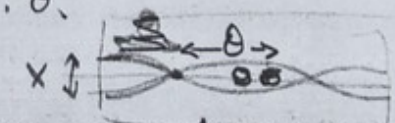
$$\tan\delta - \tan i_1 = \frac{1}{4r}(x_2 \sim x_1)$$

Hence find which arc needs > corr^{n} & apply the > correction.

Find the > arc by looking at shape of layer lines of the arc. photo.

The cross-arcs on the equator. is caused by the line about which rep. lattice was tilted. θ.

O is centre.



If $\theta = 45$. Then require equal arc corrections.

For $\theta < 45°$ The bottom arc requires more correction.

For $\theta > 45$ " Top arc " " .

Check. Measure X. = $x.^{\circ}$ of $R = 57.3$ mm.
in mm's

For correction the arc // to beam direction

Now wish to know direction to apply them. ⊥ to _ at centre

Just look at film and move arc ⊥ to beam to bring trace down horizontal.

For arc // to beam look [ ] trace of abs edge of photo.

Summary

1,

2, One arc // to X-ray beam in middle of arc.

3, Meas. x_1 & x_2 at $\theta = 45$.

Ruth Mach 1st
Magnetic Props

$\underline{H}$ $\underline{M}$ . . $\underline{M} = K \underline{H}$ [magnetic susceptibility $\equiv K$] XIII

$\underline{B}$ magnetic induction. $\underline{B} = \underline{H} + 4\pi \underline{M}$

H = Field
M = Magnetisation along Field strength in Material. $= \underline{H}(1 + 4\pi K)$

Isotropic Substances

$1 + 4\pi K \equiv \chi$. Magnetic Permeability.

$\therefore \underline{B} = \chi \underline{H}$

This exactly // to for with dielectric properties. But electric permeativity always positive & > 1. ($\underline{1} + 4\pi K$) But ~~K~~ can be $\gtrless 0$.

If ~~K~~ > 0. Paramagnetic. If ~~K~~ < 0. Diamagnetic.

" $\chi > 1$. " $\chi < 1$ "

Also here K varying with H. ie Ferromagnetic.

Anisotropic Substances.

Here we expect Magnetisation & Magnetic Field to be in different directions. ie $\underline{M}$ & $\underline{H}$ generally $\neq //$.

But that generally $\underline{M}$ is some linear function of $\underline{H}$. ie $\underline{M} = \underline{\underline{K}}\, \underline{H}$ where $\underline{\underline{K}}$ indicates some tensor. This indicates H_1, H_2 & H_3 are respectively linear functions of H_1, H_2 & H_3.

Can be shown $\underline{\underline{K}}$ is a symmetrical Tensor described by 6 compts. Can ∴ chose set of co-ords such that ~~K~~ diagonal terms vanish. ie Using "preferential co-ords" have :-

$M_1 = K_1 H_1$. $M_2 = K_2 H_2$ $M_3 = K_3 H_3$.

So here 3 orthogonal Magnetic Axes. (ie M & H // along each axis)

(Can construct magnetic ellipsoid. Semi-axes numerically $\propto \equiv KH$)

NB K usually very small. ie Magnetic Behaviour generally can be disregarded. Not so with dielectric properties.

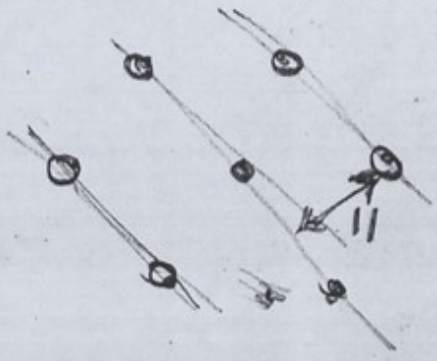
To measure K. Staff in Form of thin rod. Do magnetometer expt. but direction of axes in rod must be known.

The magnetic polarization is typical of that of Impurity of molecular crystals towards highly.

? 1) Why order so much better at rt ∠s to fibre length.
α. myosin — β myosin.

XIV

α. shows 11 A° at rt ∠s to fibre length. This is as ∴ is 11 A° is not the distance twixt chains but the crystallographic plane separation. Probably Hexagonally packed.



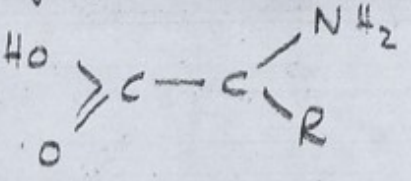
Collagen Group:

Rings in chain shorten 5·2 down to 4. A°.

NB Super contracted state of α myosin. Stretch in hot water, release & it curls up showing about 44° & not 5·2 A° repeat.

NBB Can't have Protein Crystal without Mother liquors. The two are in Thermodynamic equilibrium.

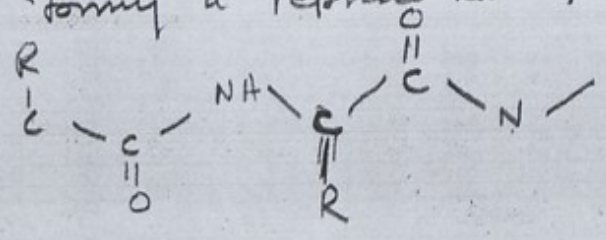
Dec March 1st Proteins Crystallographic View-Point :-

a) Polymers of amino acids. 

replaced by chains of suitable length + Benzene ring + Sulphur atom..

b) 23 amino acids.

c) Polymerised by OH of one group linking on NH_2 group of the next. Forming a Peptide Link?



Simple proteins of one type of R are made chemically - ie Synthetic polypeptides.

d) Amphoteric Properties.

e) Pyt. & Valie Border Photo. Get broadening at 4-5 A°. 1926-27. Astbury on Wool. Fibres.

f) Bernal & Crowfoot. 1932. Took photo of Wet Crystal.

g) Hb's from different species crystallise in diff forms. eg Rat Horse & Human.

h) Order in wet crystalline goes down to 2A°. (Why breaks up on drying?)-

i) Get $\frac{V \times \rho}{1.66}$ = Cell. M.Wt: But even though know Space Group can't be sure of n. The no. of units for chains per cell. eg P21. has two positions so could be 2 chains/cell.

j) Hb. Monoclinic. β changes with hydration. Not gradually but in discrete stages. Reversible. But not always able

XVI BLANK

verse from completely dried state. ∴ of denaturation
protein. In native protein have polypeptide chains in
state. On denat. chains extend to β.

XVII.

Cell of Hβ is C2. Monoclinic. 4 general positions. But
nly 2 mols/unit cell. This means they must lie on a
-fold axis & can split 'em.

)xh on insulin shows. water goes in structure around
olecules & not it into 'em. ∴ get good dried pulvers &
et same Pattern from (ratio's of vectors / intervals) wet & dry.

XVIII

BLANK

Mon March 4th.

1) Attach glass fibre to end of lead wire. Better for [illegible] & changing orientation of crystal.

2) Tabulate runs.

Reflection No	ξ	Index	Intensity

XIX

Calcite $Z = 2$. (ie no: of molecules). $a = 6.361$. $\alpha = 46° 7'$

Rhombohedral cell.

C. $0, 0, 0$; $\frac{1}{2}\frac{1}{2}\frac{1}{2}$ Ca $\pm \left|\frac{1}{4}\frac{1}{4}\frac{1}{4}\right|$ Oxygens $\frac{1}{4}\frac{\bar{1}}{4}0$, $0\frac{1}{4}\frac{\bar{1}}{4}$, $\frac{\bar{1}}{4}0\frac{1}{4}$.

$\frac{1}{4}\frac{3}{4}\frac{1}{2}$, $\frac{1}{2}\frac{1}{4}\frac{3}{4}$, $\frac{3}{4}\frac{1}{2}\frac{1}{4}$

Transformation. Rhombs - Hexagonal.

	a_H	b_H	c_H		
a_r	$\frac{2}{3}$	$\frac{\bar{1}}{3}$	$\frac{\bar{1}}{3}$	x_r	$x_h = \frac{2}{3}x_r - \frac{1}{3}y_r - \frac{1}{3}z_r$
b_r	$\frac{\bar{1}}{3}$	$\frac{1}{3}$	$\frac{\bar{1}}{3}$	y_r	$y_h = \frac{1}{3}x_r + \frac{1}{3}y_r - \frac{2}{3}z_r$.
c_r	$-\frac{1}{3}$	$-\frac{2}{3}$	$\frac{1}{3}$	z_r	$z_h = \frac{1}{3}(x_r + y_r + z_r)$
	x_h	y_h	z_h		

Hexagonal cell positions of C, Ca & Oxys. are :-

C. $0, 0, 0$, ; $0, 0, \frac{1}{2}$ Ca. $\pm \left|0\ 0\ \frac{1}{4}\right|$ Oxygens. $\frac{1}{4}\ 0$ [illegible]; $0\ \frac{1}{4}\ 0$; [illegible]

$\frac{\bar{1}}{4}\ 0\ \frac{1}{2}$; $0\ \frac{\bar{1}}{4}\ \frac{1}{2}$; $\frac{1}{4}\ \frac{1}{4}\ \frac{1}{2}$

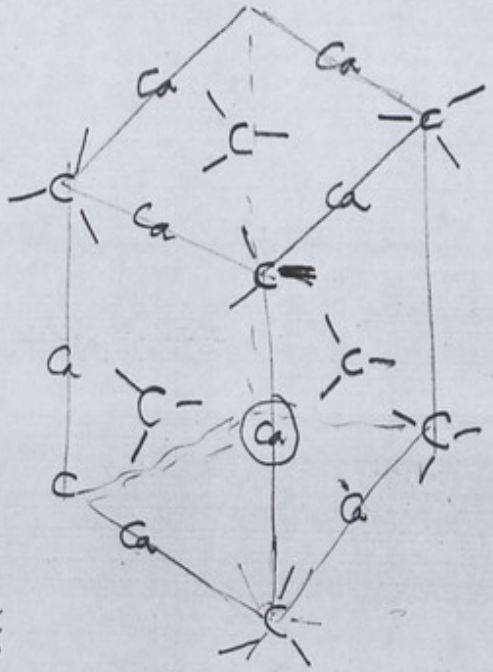
NB If had $x_r y_r z_r$ as $\frac{3}{4}\ \frac{1}{4}\ 0$.

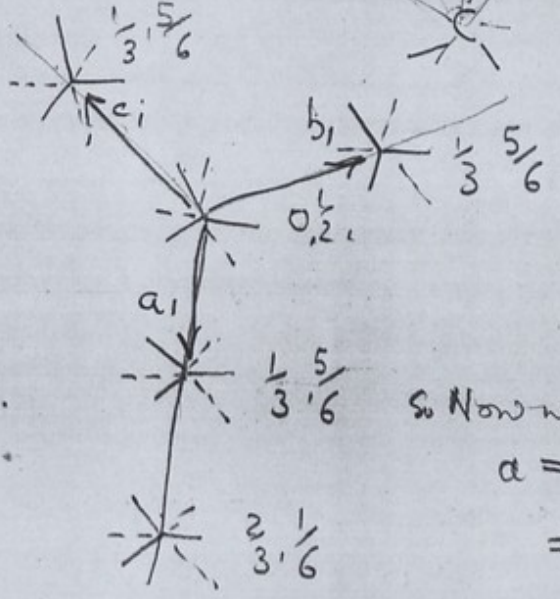
[illegible] $0\ 0\ \frac{\bar{1}}{12}$, $\frac{1}{3}\ \frac{1}{3}$. Remember in we have to add

000, $\frac{2}{3}\ \frac{1}{3}\ \frac{1}{3}$, $\frac{1}{3}\ \frac{2}{3}\ \frac{2}{3}$ to all coords. ∴ have now 6 molecules in Unit Hexagonal cell.

Compare Calcite with NaCl.

XX





a_1, b_1, c_1 smallest unit cell.

a_1 ends up $\frac{1}{3}$ above the ringed Ca, i.e. into next cell to next similar Carbon. The Ca itself is $\frac{1}{2}$ up.

So Now we have

$$a = \frac{1}{4}A + \frac{1}{4}(A+B+C)$$
$$= \frac{1}{2}A + \frac{1}{4}B + \frac{1}{4}C$$

$$b = \frac{1}{4}A + \frac{1}{2}B + \frac{1}{4}C \qquad c = \frac{1}{4}A + \frac{1}{4}B + \frac{1}{2}C.$$

in terms of Rock Salt structure. Which necessitates axes of two units of the rhombohedron drawn top of page i.e. 8 such cells of Rock Salt like Calcite

Get Transformation Matrix.

	A	B	C
a	1/2	1/4	1/4
b	1/4	1/2	1/4
c	1/4	1/4	1/2

	h	k	l	
	a	b	c	
HA	3	$\bar{T}$	$\bar{1}$	X
KB	$\bar{T}$	3	$\bar{T}$	Y
LC	$\bar{T}$	$\bar{1}$	3	Z

The carbons in the Rock Salt like structure have co-ordinates ;-

$|0,0,0,\ 0\tfrac{1}{2}\tfrac{1}{2},\ \tfrac{1}{2}0\tfrac{1}{2},\ \tfrac{1}{2}\tfrac{1}{2}0|$ + 000, $\tfrac{1}{2}\tfrac{1}{2}\tfrac{1}{2}$

$0\tfrac{1}{4}\tfrac{1}{4},\ \tfrac{1}{4}0\tfrac{1}{4},\ \tfrac{1}{4}\tfrac{1}{4}0$

$0\tfrac{3}{4}\tfrac{1}{4}\ \tfrac{1}{4}0\tfrac{3}{4},\ \tfrac{3}{4}\tfrac{1}{4}0.$

Giving $x = 3X - Y - Z$
$y = -X + 3Y - Z$
$z = -X - Y + 3Z.$

Hence $|000,\ \tfrac{1}{2}\tfrac{1}{2}\tfrac{1}{2}|$ $\bar{\tfrac{1}{2}}\tfrac{1}{2}\tfrac{1}{2}$.

Similarly all other points are same as $\bar{1}\bar{1}0$ but in another cell.

Now $H = 3h - k - l$ If multl H by 2 and add up
$K = -h + 3k - l.$
$L = -h - k + 3l$

$2H + K + L = 4h = 4n$
$H + 2K + L = 4n.$
$H + K + 2L = 4n$

Similarly $H + k = 2n$. etc Giving conditions for reflection.

Aragonite

$a = 4{\cdot}94$ $b = 7{\cdot}94$ $c = 5{\cdot}72.$ $Z = 4$ (orthorhombic)

General Oxygen Positions. (Equal-Item)

$xyz;\ \tfrac{1}{2}+x, \bar{y}, \bar{z}+\tfrac{1}{2};\ \bar{x}, \bar{y}+\tfrac{1}{2}, z+\tfrac{1}{2},$
$\bar{x}yz;\ \tfrac{1}{2}-x\ \bar{y}\ \bar{z}+\tfrac{1}{2}\ \ \bar{x}, \bar{y}+\tfrac{1}{2}\ z+\tfrac{1}{2}$
$\tfrac{1}{2}+x, \tfrac{1}{2}+y\ \bar{z}$
$\tfrac{1}{2}-x, \tfrac{1}{2}+y\ \bar{z}$

Where $x = {\cdot}228$
$y = {\cdot}322$
$z = \tfrac{1}{6}$

Point Space Group

xyz & $\bar{x}yz$ related by $0yz$ plane.

xyz & $x, \tfrac{1}{2}-y, \tfrac{1}{2}+z$ ---------- Glide plane $c/2$ at $x\ \tfrac{1}{4}\ z$ $\therefore$ m

xyz & $\tfrac{1}{2}+x, \tfrac{1}{2}+y, \bar{z}$ ------ Glide plane a or b / 2 at $xy0$ $\therefore$ m c n

We only have 8 points & not as an Orthorhombic ~~P~~ C lattice in P.

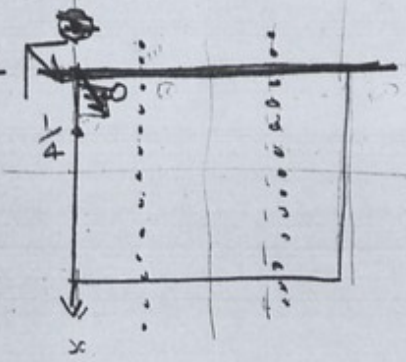
XII a Pmcn - but not in International Tables.

Corresponding one is Pnma. common one.

To transform from Pmcn to Pnma we must change

$x \to y \quad y \to z, \; z \to x$.

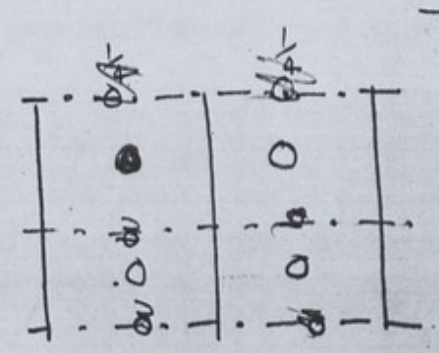
Pmcn



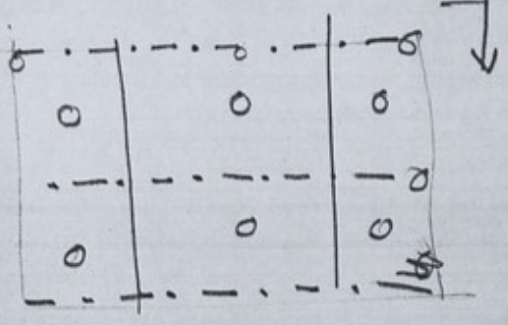
The centrosymmetrical point to xyz is $\frac{1}{2}-x, \bar{y}, \bar{z}+\frac{1}{2}$.

ie $\frac{1}{4}\,0\,\frac{1}{4}$ is Centre of Symmetry.

Pnma



Hence $\frac{1}{4}\,\frac{1}{4}\,0$ is Centre of Symmetry



Pnma with origin transformed to centre of symmetry.

ie glide n. 0yz giving co-ords. $x\,y\,z \;\; \bar{x}, \frac{1}{2}+y, \frac{1}{2}+z$

plane m $x\,\frac{1}{4}\,z$ " $x\,y\,z \;\; x, \frac{1}{2}-y, z$

glide a $x\,y\,0$ $x\,y\,z \;\; \frac{1}{2}+x, y, \bar{z}$

add all co-ords of this lattice must be ;-

i.e. Operate on 1st line with plane at $x\ \frac{1}{4}\ z$. query further point $\bar{x}, \bar{y}\ \frac{1}{2}+z$.

Now go 1st line, glide $x\ 0\ ;-\ \frac{1}{2}-x, \frac{1}{2}+y$

Glide n. $\frac{1}{4}\ y\ z$, $x\ y\ z$. $\frac{1}{2}-x\ \frac{1}{2}+y\ \frac{1}{2}+z$ ~ ①

Plane m $x\ \frac{1}{4}\ z$ $x\ \frac{1}{2}-y\ z$ ~ ⑤

glide a $x\ y\ \frac{1}{4}$. $\frac{1}{2}+x\ y\ \frac{1}{2}-z$ ~ ②

operate on ① with m. $\frac{1}{2}-x, \bar{y}, \frac{1}{2}+z$.

∴ ① with a, $\bar{x}\ y+\frac{1}{2}, \bar{z}$ Plus $\bar{x}\bar{y}\bar{z}$.

$\frac{1}{2}+x\ \frac{1}{2}-y\ z$

~~$\frac{1}{2}-x\ \bar{y}\ \frac{1}{2}+z$~~

~~$\bar{x}, \frac{1}{2}+y, \frac{1}{2}-z$~~

Substitute in these values, $x = \frac{1}{6}$, $y = \cdot 228$ $z = \cdot 322$.

Network Work and Structure Factor.

Prob. write down co-ords of equivalent points

add cosines i.e. $A = \sum \cos 2\pi(hx+ky+lz)$

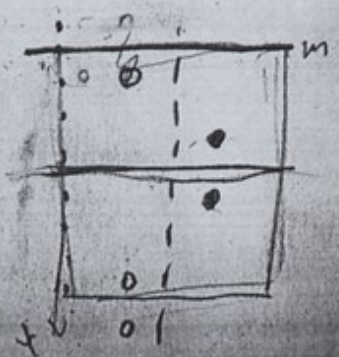
& sines $B = \sum \sin 2\pi$ etc.

Get A + B in simplest forms.

$F = \sqrt{A^2+B^2}$

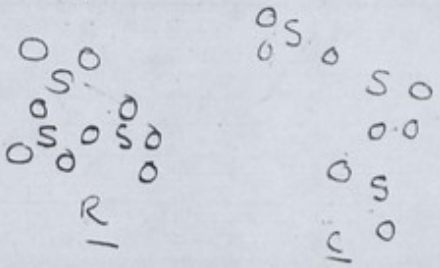
xyz $\bar{x}y\bar{z}$, $x\ \frac{1}{2}, \bar{y}, z+\frac{1}{2}$.

$\frac{1}{2}-x, \bar{y}, \frac{1}{2}+z$.

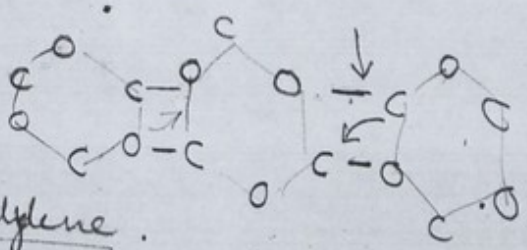


Same SO_3. Form chain polymer or ring polymer.

XXIV



Similarly



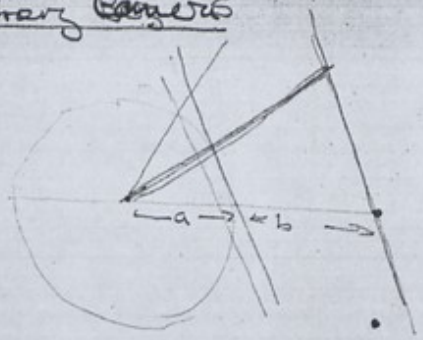
Trioxymethylene.

Irradiate with UV → get polyoxymethylene.

Jeffries Weissenberg Cameras

XXV

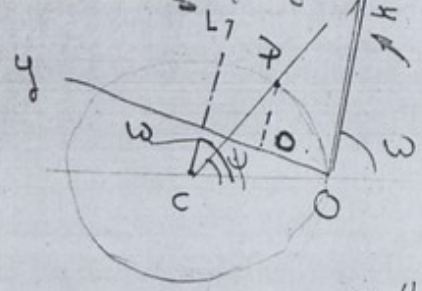
1 Procession Camera.



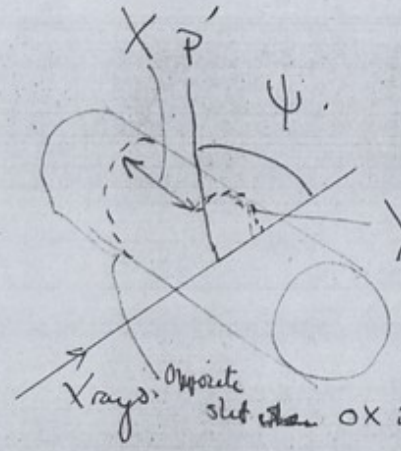
a/b kept constant and film follows the recip. lattice in & out of the sphere of reflection

keeping magnification constant.

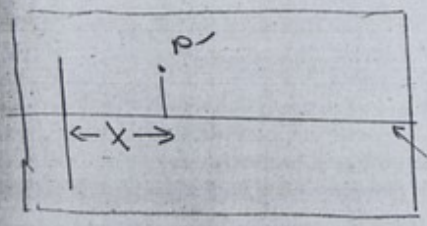
2 Weissenberg. (Straight)



CL // OX.



then OX is along beam.



$$\therefore \quad PD = CP\cos(\omega-\psi) - OC\cos\omega.$$

Now for zero layer line $OC = 1. = CP$. ie $PD = \cos(\omega-\psi) - \cos\omega$.

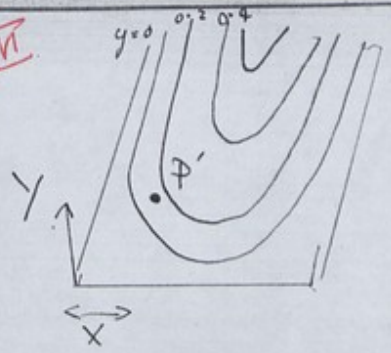
$$y = OD = \cos\omega\cdot\sin\omega - CP\cdot\sin(\omega-\psi) = \sin\omega - \sin(\omega-\psi)$$

$$\psi = Y/R \qquad X = C\omega. \quad \therefore x = \cos\left(\frac{X}{C} - \frac{Y}{R}\right) - \cos\frac{X}{C}.$$

$$\& \; y = \sin\left(\frac{X}{C}\right) - \sin\left(\frac{X}{C} - \frac{Y}{R}\right)$$

ie Measure up X, Y from photograph & then calculate x & y the reciprocal lattice co-ords. They can also be got straight from photographs by means of a chart (of Bessel Charts).

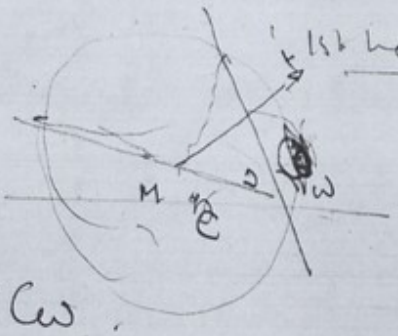
XXII



Weissenberg Chart

Curves give y value right away.
y contours up to y = 1·8.

Take another chart at right Δs to other use get Δ values.



$$\psi = \frac{Y}{R} = 2\theta$$

$$X = Cw.$$

$$\upsilon = \frac{\pi}{2} + \theta - \phi$$

$$x = \cos\left(\frac{X}{C} - \frac{Y}{R}\right) - \cos\frac{X}{C}$$

$$= C\left(\frac{\pi}{2} + \frac{Y}{2R} - \phi\right) 2R.$$

$$y = \frac{2}{C} R X - \left(\frac{\pi}{2} - \phi\right)$$

$$Y = AX + B.$$

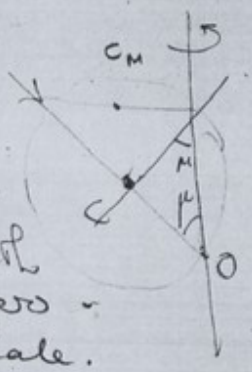
Now $C_{11} = \sqrt{1 - \zeta_n^2}$.

Equivalents

1 No blind region.

2 Straight lines on Photographs

3 Use same chart for nth layer nett as for zero - Merely altered scale.



NB Precession & D'Hong & Berman Cameras give undistorted Reciprocal Lattice.

... = Ref Manual

Update Space Group application in Fourier Analysis

$$\rho(XYZ) = \frac{1}{V} \sum_{-H_1}^{H} \sum_{-K_1}^{K} \sum_{-L_1}^{L} \left| F(hkl) \right| \times \cos\left[2\pi (hX + kY + lZ) - \alpha(hkl) \right]$$

(electron density at any point X Y Z)

Problem To express this in suitable manner for summation. ie how thing changes for different values of hkl.

Point UVW in reciprocal space. $P(UVW) = \frac{1}{V^2} \sum_{-\infty}^{+\infty} \sum_{-\infty}^{+\infty} \sum_{-\infty}^{+\infty} \left| F(hkl) \right|^2 \times \cos 2\pi (hU + kV + lW)$.

So this only changes with F. Y we have

$$\left| F(hkl) \right|^2 = A'^2 + B'^2$$

$$\alpha(hkl) = \tan^{-1} B'/A'$$

Where $A' = \sum_r f_r \cos 2\pi (hx_r + ky_r + lz_r)$

(sum over all atoms r) f_r = Scattering Factor

$$B' = \sum_r f_r \sin 2\pi (hx_r + ky_r + lz_r).$$

Consider case $Pmn2_1$ (Simple Orthorhombic Lattice)

10 sets of equiv. points are. xyz, $\bar{x}\bar{y}z$. $\frac{1}{2}+x, \bar{y}, \frac{1}{2}+z$ $\frac{1}{2}-x, \bar{y}, \frac{1}{2}+z$

Now $A' = f_a A_a + f_b A_b + f_c A_c \ldots\ldots$

Where A_a is sum of cosines of equivalent points of scattering factors f_a.

$$A_a = 4 \cos 2\pi hx \cos 2\pi \left(ky - \frac{h+l}{4} \right) \cos 2\pi \left(lz + \frac{h+l}{4} \right)$$

So $B_a = 4 \cos 2\pi hx \cdot \cos 2\pi \left(ky - \frac{h+l}{4} \right) \sin 2\pi \left(lz + \frac{h+l}{4} \right)$

XXVIII

Consider now all planes for $h+l=2n$.

Then $\frac{2\pi}{4}.2n$ becomes $n\pi$. ie $ky - n\pi$ or $ky + n\pi$.

But which ever way it changes both signs giving a positive value

So $A = 4\cos 2\pi hx . \cos 2\pi . ky . \cos 2\pi lz$

$B = 4\cos 2\pi . hx . \cos 2\pi . ky . \sin 2\pi . lz .$ } $h+l = 2n$

$h+l = 2n+1.$

$A = -4\cos 2\pi hx . \sin 2\pi ky . \sin 2\pi lz$

$B = 4\cos 2\pi hx . \sin 2\pi ky . \cos 2\pi lz .$

Now to consider what happen if change sign of h or k or l.

Now $|F(hkl)|^2 = \sqrt{A'^2 + B'^2}$ so won't be effected by change of sign. Only value change can have an effect.

But A + B do not change value when they change sign

So $|F(hkl)| = |F(\bar{h}\bar{k}\bar{l})| = |F(hk\bar{l})$

$= |F(\bar{h}kl)|$

$= F(h\bar{k}l)|$

(NB with Monoclinic this would'nt be true .. But Orthorhombic sufficiently high symetry 'does give change of value' ↓ change of sign in h or k or l),

Consider $h+l=2n$ $\alpha(hkl) = \tan B'/A'$. [Consider the effect of $A \& \bar{B}$

Now if change sign of B. get $\alpha(\bar{h}\bar{k}\bar{l}) = -\alpha(hkl)$.

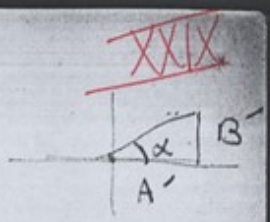
Sign of cosine doesn't change with $-\theta$. So change of sign of h or K won't affect sign of A or B. But l will

$\alpha(\bar{h}kl) = \alpha(hkl) = \alpha(h\bar{k}l)$. But $\alpha(hk\bar{l}) = -\alpha(hkl)$

XXIX

$h+k=2n+1$

$$\alpha(\bar{h}\bar{k}\bar{l}) = -\alpha(hkl)$$
$$\alpha(\bar{h}kl) = \alpha(hkl)$$
$$\alpha(h\bar{k}l) = \pi + \alpha(hkl)$$
$$\alpha(hk\bar{l}) = \pi - \alpha(hkl).$$



Now consider what happens when these values go into formula for $\rho(XYZ)$ the electron density. More simple to consider $P(UVW)$ first.

General Term $= \frac{1}{V^2} \sum_{-\infty}^{\infty} \sum_{-\infty}^{\infty} \sum_{-\infty}^{\infty} |F(hkl)|^2 \cos 2\pi(hU+kV+lW)$

(i.e. one in which no value is zero. But only the values of hkl separated from −ve "+ve")

$+|F(\bar{h}\bar{k}\bar{l})|^2 \cos 2\pi(-hU-kV-lW)$

$+|F(\bar{h}kl)|^2 \cos 2\pi(-hU+kV+lW) \quad +|F(h\bar{k}l)|^2 \cos 2\pi(hU-kV+lW)$

$F(h\bar{k}l)$ etc $\quad + \bar{h}k\bar{l}$

$F(hk\bar{l})$ " $\quad + \bar{h}\bar{k}l$

Now Fs are identical. So we can write,

$$\text{General Term} = \frac{1}{V^2} \sum\sum\sum |F(hkl)|^2 \cdot$$
$$\{\cos 2\pi(hU+kV+lW) + \cos 2\pi(hV-kV$$

$$= \frac{8}{V^2} \cdot \sum_{1}^{\infty} \sum_{1}^{\infty} \sum_{1}^{\infty} |F(hkl)|^2 \cos 2\pi hU \cos 2\pi kV \cos 2\pi lW.$$

This simple for Pattersons because here same F for all hkl's.

XXX

Electron Density

General Ten = $\frac{1}{V}\sum^{h}\sum^{k}\sum^{l} |F(hkl)| \cos\left[2\pi\left[(hX+kY+lZ) - \alpha(hkl)\right]\right.$

$+ |F(\bar{h}k\bar{l})| \cos\left[2\pi\left(\bar{h}X - kY - lZ\right) - \alpha(\bar{h}k\bar{l})\right] + \text{etc.}$

substitution $\pm\alpha(hkl)$

Now cos unchanged if Θ sign changed. So we have

General Ten = $\frac{2}{V}\sum^{h}\sum^{k}\sum^{l} |F(hkl)| \cos\left[2\pi(hX+kY+lZ) - \alpha(hkl)\right]$

$+ |F(\bar{h}kl)| \cos\left[2\pi(-hX+kY+lZ) - \alpha(\bar{h}kl)\right]$

$+ |F(h\bar{k}l)| \cos\left[2\pi(hX-kY+lZ) - \alpha(h\bar{k}l)\right]$

$+ |F(hk\bar{l})| \cos\left[2\pi(hX+kY-lZ) - \alpha(hk\bar{l})\right]$

The 2 outside accounts for all pairs, i.e. $\bar{h}k\bar{l}$ $\bar{h}\bar{k}l$ etc.

Gen T = $\frac{2}{V}\sum^{h}\sum^{k}\sum^{l} |F(hkl)| \{$ cosines as above $\}$.

Now ~~F(hkl)~~ What happens for $h+l = 2n$ & $h+l = 2n+1$.

i.e. Gen T. = $\frac{2}{V}\left\{ \sum\sum\sum |F(hkl)| \left(\begin{array}{l} \text{for } h+l=2n \\ \text{cosines etc. as above} \\ \text{except for } +\alpha(hk\bar{l}) \\ \text{in last one.} \end{array} \right) \right.$

$+ \sum^{h}\sum^{k}\sum^{l} |F(hkl)| \left(\begin{array}{l} \text{for } h+l=2n+1. \\ \text{Cosine here are changed. 1st two} \\ \text{stay the same} \quad \text{second two go to} \end{array} \right.$

$\cos\left[2\pi(hX-kY+lZ) - (\pi+\alpha(hkl)\right]$

$\cos\left[2\pi(hX+kY-lZ) - (\pi-\alpha(hkl)\right]$

XXXI

$$\text{Gen Te} = \frac{8}{V}\left\{ \sum_h \sum_k \sum_l |F(hkl)| \cos 2\pi hX \cos 2\pi kY \cdot \cos[2\pi lZ - \alpha(hkl)] + \sum_h \sum_k \sum_l |F(hkl)| \cos 2\pi hX \sin 2\pi kY \sin[2\pi lZ - \alpha(hkl)] \right.$$

NB XYZ are not co-ords of atoms but points in the cell

Eg (h00.) To find value of $\alpha(h00)$.

h even. will not change sign whatever $h^{\pm}$

h odd. same for $\bar{h}$ or h.

$\therefore \alpha(h00) = \tan^{-1} B/A = 0$ [~~$4\cos 2\pi h$~~ $\because \sin 0 = 0$]

But for h even. $\tan\alpha = 0/A$ so 0 or π.

for h odd $\tan\alpha = 0/0$ i.e. $\alpha = 0$.

$\therefore \alpha = 0$ or π.

$\therefore$ F(h00) is either +ve or −ve.

$\therefore$ Gen Ten. $\frac{2}{V} \sum_h F(h00) \cos 2\pi hX$. only for even values.

(0k0). Value of $\alpha(0k0)$.

k even. $A = 4\cos 2\pi ky$. $\therefore \tan\alpha = 0/A$ i.e. $\alpha = 0$ or π

$B = 0$.

~~k odd~~ $A = 0$ if $4\cos 2\pi ky$ comes out positive $\alpha = 0$

if −ve. $\alpha = \pi$.

(00l). l even. $A = 4\cos 2\pi lz$ $\therefore B/A = \tan 2\pi lz$ || Must not cancel like this

$B = 4\sin 2\pi lz$ $\alpha = 2\pi lz$ ∴

Must remember $A = f_a A_a + f_b A_b$ etc.

l odd. $A = 0$. $\alpha = 0$.

$B = 0$

$\therefore \frac{2}{V} \sum_l^2 |F(00l)| \cos[2\pi lZ - \alpha(00l)]$ for even l's only.

(0kl) XXXII

l even. $A = 4\cos 2\pi ky \cos 2\pi lz$
$B = 4\cos 2\pi ky \sin 2\pi lz$

$\therefore$ B/A must be worked out & get $\alpha(0kl)$ even

l odd $A = -4\sin 2\pi ky \cdot \sin 2\pi lz$
$B = 4\sin 2\pi ky \cdot \cos 2\pi lz$

B/A must be worked out & get $\alpha(0kl)$ value for k odd.

$$\left.\begin{aligned} \alpha(0\bar{k}\bar{l}) &= -\alpha(0kl) = \alpha(0k\bar{l}) \\ \alpha(0\bar{k}l) &= \alpha(0kl) \end{aligned}\right\} \text{ l even}$$

A projection of OKL would then only need 4 terms in general expr.

$$\left.\begin{aligned} \alpha(0\bar{k}\bar{l}) &= -\alpha(0kl) \\ \alpha(0\bar{k}l) &= \pi + \alpha(0kl) \\ \alpha(0k\bar{l}) &= \pi - \alpha(0kl) \end{aligned}\right\} \text{ l odd}$$

$$\text{Gn Ten} = \frac{4}{V}\left\{\sum_{k}\sum_{l}^{l\text{even}} |F(0kl)| \cos 2\pi kY \cos\left[2\pi lz - \alpha(0kl)\right] - \sum\sum^{l\text{odd}} |F(0kl)| \sin 2\pi kY \sin\left[2\pi lz - \alpha(0kl)\right]\right\}$$

NB $CaCO_3$. Ca & C's occupy special positions
O's general positions.

So when sum $B' = f_{Ca}B_{Ca} + f_C B_C + f_O B_O$

Hon sum B_{Ca} ors only special positions & B_O ors all posns.

LAID IN BETWEEN ~~XXXII~~ AND XXXIII

UNIVERSITY OF LONDON KING'S COLLEGE

BIOPHYSICS COLLOQUIUM

The following Colloquium will be given in Room 27C on Wednesday, April 22nd, 1953, at 4.30 p.m.

H.G. Davies: The Use of Interference Microscopy to Determine Dry Weight in Living Cells and as a Quantitative Cytochemical and Morphological Method.

February 18th 1963

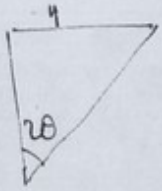
J.T. RANDALL
Head of Department

VE250 87

"BIOPHYSICS COLLOQUIUM" SHEET

2d

$\frac{y}{R} = \tan 2\theta \cdot R$



$\frac{y}{2} = R \sin 2\theta$.

$6.8 \sin\theta = 1.539$.

$\sin\theta = \frac{1.539}{6.8} = 0.226$.

(h0l) $h+l$ even. $A = 4\cos 2\pi hx \cdot \cos 2\pi lz$

$B = 4\cos 2\pi hx \sin 2\pi lz$.

$h+l$ odd $A = 0 = B$.

This is what you expect from $P_{m}n_{2_1}$ because $\int n$.

So get finally.

$$\frac{4}{V}\left\{ \sum_{h}^{} \sum_{l}^{h+l=2n} |F(h0l)| \cos 2\pi hx \cos[2\pi lz - \alpha(h0l)] \right.$$

(hk0) $A = 4$ etc h even. | h odd. $A=0$. $B = 4$ etc.

$B = 0$

$\alpha = 0$ or π. according to sign of A. | $\alpha = \pi/2$ or $3\pi/2$ according to sign of B.

$$\delta\tau = \frac{4}{V}\left\{ \sum_{h}^{h=2n} \sum_{k}^{} F(hk0) \cos 2\pi hx \cos 2\pi ky \right.$$

$$- \sum_{h}^{h=2n+1} \sum_{k}^{} F(hk0) \cos 2\pi hx \sin 2\pi ky$$

Now substitute in these formula. Special points with symmetry m.

i.e. $0yz$ & $\frac{1}{2}\,\bar{y}\,\frac{1}{2}+z$.

Next Term. Mondays. Magnetism & Neutron Diffraction. Beb at UC. in Chemistry Theatre. ~~2nd Thurs~~ 30th April. 6pm.

Jeffries 30th. A. 61. Weissenberg

XXXIV Crystal lattice (with spots weighted of reflection intensities) will have same symmetry.

Any symmetry in zero plane won't be picked up in other layers.
" " ⊥ " " will " " " " " "

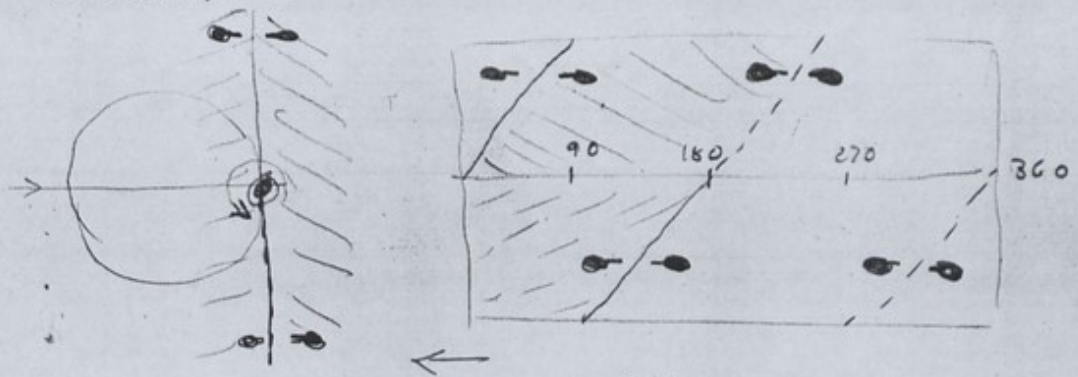
Symmetry in a layer can be expressed by;-

1) Rotors. (rotation axis) 2, 3, 4 & 6 fold.

2) Lines of Symmetry. . | . This caused either by ↑ two fold axes in plane or a | mirror plane ⊥ to layer.

NB A 2fold rotor is either a equivalent of sym. in plane or a two fold axis ⊥ to plane.

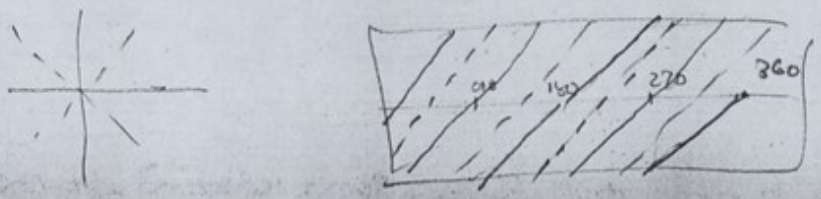
Consider a ~~plane~~ with (~~only one point~~ it) no symmetry at all.
Take one point



← Direction motion of film.

Angulodistance in rep. is linear distance on film.

With a 4fld axis we have lines of symmetry at 45°. This gives added difficult in recognising full symmetry axes.



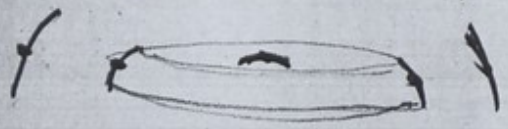
Fibre Photographs NB Rep. of Powder photo is a set of concentric spheres.

Perfect fibre - set of crystallites all aligned in fibre axis ~~but with~~ all possible orientations around that axis.

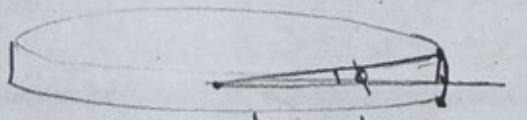
∴ The Rep is a series of circles, one for each crystallite point with different distances from fibre axis.

Alternatively one can regard fibre as a single rotating crystal.

In practical fibres. Range of movement of crystallites away from fibre axis. ie Rep. oscillates thro' angle of disorientation as it is rotating. So annulus of a sphere instead of circle;-



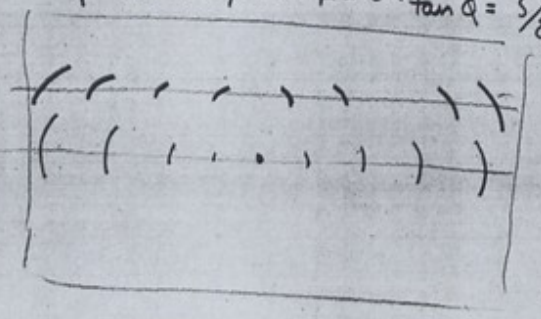
Exception is points on axis of fibre. These become caps of a sphere in disorientation.



NB Further out from fibre axis the larger the annulus for a given angle of disorientation ϕ

(? How are these arcs related to Measurement

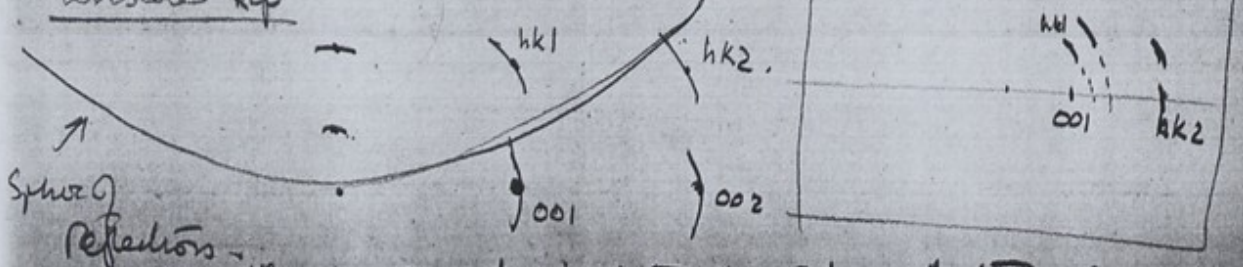
Measure zero layer line $\frac{1}{2}$ angle ϕ given angle by ζ and ξ values of end of arc. $\tan\phi = \zeta/\xi$.



NB fact of it being a fibre usually means it has monoclinic symmetry.

How to find true position of first layer line difficult, due to arc's. To identify this. Put fibre horizontal & take series of oscillation photos.

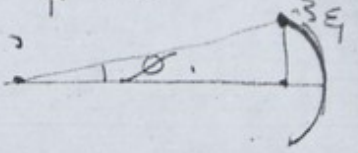
Consider Rep



NB 001 annulus just touches sphere reflection. So short sharp line. 002 misses hk2 sphere. Then oscillate. Get more as

~~XXXII~~ Longer ~~wk~~ l down onto zero layer line. Then get value of ~~distan~~ 2x accurately. Same for all other points

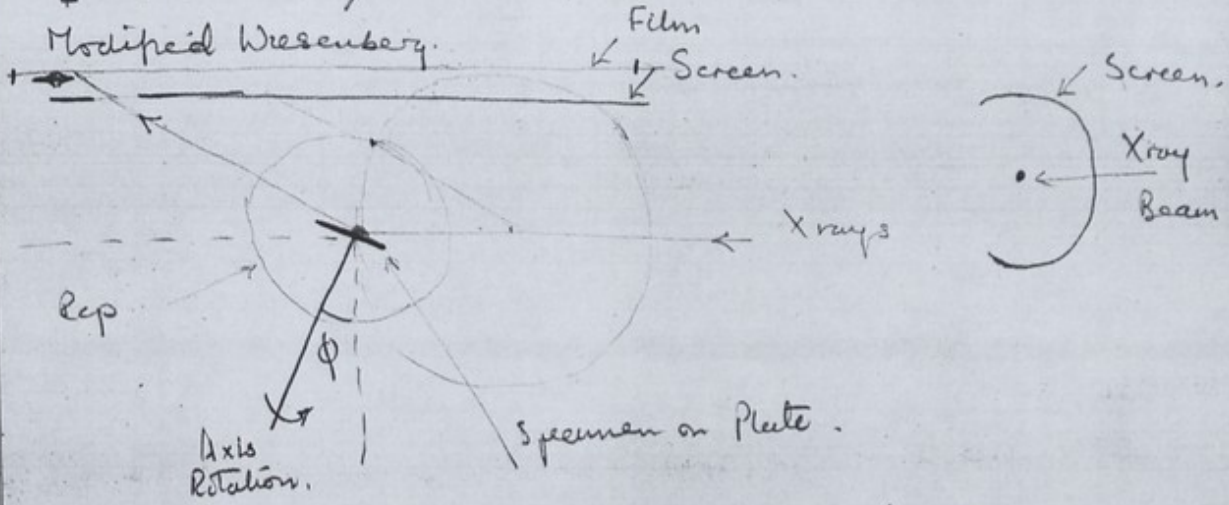
NB ϕ obtained from measuring ends of arcs on median or equator should remain constant.



Delphis Monday 7 May.

Preferred Orientation

Ref. Wooster. J. Sci. Insts. 25 129. 1948.



Any performed revolution is ~~cap~~ on the rep. lattice sphere

Miss Lonsdale 3rd Term First Lecture Magnetism

XXVII

Couple. $G = mHl\sin\theta$.

If $H = 1$. $G = ml$ provided $\theta = 90°$

$ml \equiv M$. The Magnetic Moment.

Coulomb's law m_1 ——r—— m_2 $F \propto \frac{m_1 m_2}{r^2}$. $F = \frac{1}{\mu}\frac{m_1 m_2}{r^2}$.

Hence definition of Unit magnetic pole. Placed at dist. 1 cm. from an equal pole in a non-magnetic medium. experiences repulsion $F = 1$ dyne.

Dimensions of m from this definition $[m] = \mu^{\frac{1}{2}} \cdot L^{3/2} \cdot M^{\frac{1}{2}} \cdot T^{-1}$.

C.G.S. E.M.U.

Field Strength

Defined from $H = \frac{m}{r^2}$ ie Force in dynes at distance r. from m.

So Unit H. Field is force in dynes exp. by unit pole placed at that point

Hence $[H] = \mu^{-\frac{1}{2}} \cdot L^{-\frac{1}{2}} \cdot M^{\frac{1}{2}} \cdot T^{-1}$.

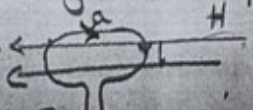
Magnetic Moment Max. couple that can be exerted on the magnet in a uniform field of unit intensity. ie $ml \equiv M$ dyne cms/oersted

Intensity of Magnetisation (I) M per unit vol. or pole strength/unit area

Current i in circle of wire radius r. Field at centre $= \frac{2\pi i}{r}$

Field only axis of a solenoid, n turns/cm. $4\pi n i$.

Force on conductor length l by H $\perp$ to l. $F = Hidl$.

Max couple on circuit  would be $Hil\,a = H.i \times$ Area Coil.

ie Magnetic Moment of any circuit = $i \times$ Area of Magnetic Shell.

Magnetic Induction B. In Isotropic med. No. of lines of force crossing unit area $\perp$ to field. (Flux density). Units Gauss

Magnetic Flux Area × Field Strength within the material Units Maxwell's.

∴ Flux density may be expressed in gauss or Maxwells/sq cm.

Now the result

$$B = H + 4\pi I \quad \text{in a medium}$$

Permeability $F = \frac{M_1 M_2}{\mu d^2}$. or from Gauss's law $B = \mu H$.

NB Cannot prove experimentally that the two values of μ are the same.

$B = \mu H$. in a field. $I = kH$ for any medium.

where $k \equiv$ Susceptibility. VOLUME SUSCEP.

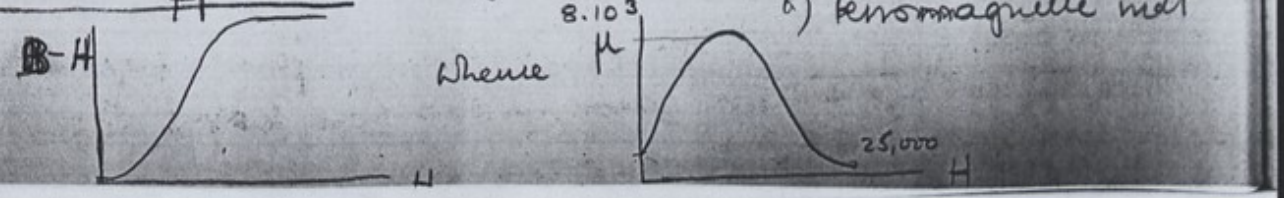
Whence $B/H = 1 + 4\pi I/H$ ie $\mu = 1 + 4\pi k$.

Mass Susp. $\chi = \frac{k}{\rho}$ ρ = density.

ATOMIC Susp Mass susp. per gram-atom.

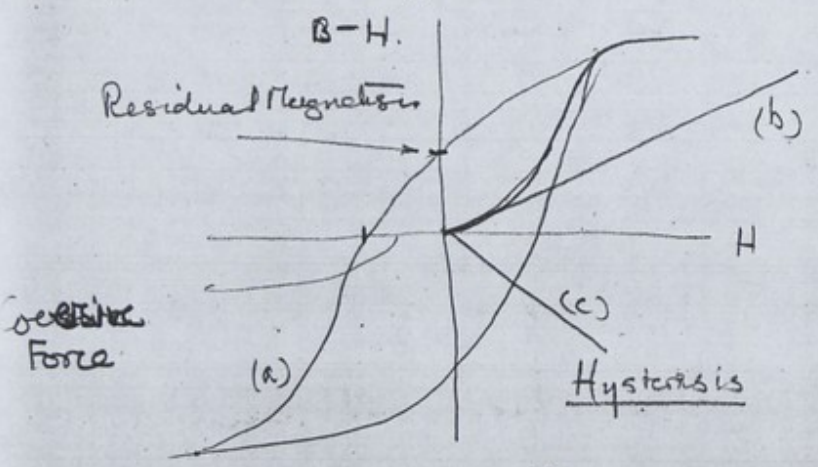
A = atomic wt in grams. $\chi_A = \chi A = k$. Atomic Volume

Variation of μ with H Magnetisation curves.



a) Ferromagnetic mat

NB $B = H + 4\pi I$. So that after certain value of H, I must decrease to keep B constant? Surely I reaches saturation also. ~~To some~~
Therefore Plot $B - H$ against H.



(a) Soft Iron.
(b) Paramagnetic.
(c) Diamagnetic

For a Ferromag. $B \gg H$.
hence $\mu \gg 1$. eg Single cry. Iron.
$\mu \rightarrow 10^6$.

The suscep. large and +ve. Depends on H & temp. T. (in complicated way).

Saturation Intensity, achieved at low fields. $\rightarrow >$ as T loss.
Induced mag. does not all disappear when field removed. Therefore these subs. have characteristic hysteresis curves.

As temp. raised get fairly abrupt discontinuity in magnetism (it drops to low value) and also pretty sharp discontinuity in physical props eg spec. ht.
This temp. termed Curie Point. θ_f.
Get Ferromagnetism changing to paramagnetism.

Anti Ferromagnetics Abrupt changes in physical props at θ_f but don't have ferromagnetic props below θ_f.

XL

Isotropic Paramag. will, if free, a) Move from weaker to stronger part of a non-uniform field.

(b) Set its max length in direction of field at that point

NB Putting a magnetic material ~~creates non~~ in uniform field creates non uniform field

$B > H$. $\therefore \mu > 1$. I adds to the field H & K is +ve. Except in very large fields at very low temps K is independent of H but varies with temp. according to Curie-Weiss law. $\chi_m = \text{const}/T - \theta$

χ_M = Mol susep. ($\simeq 10^{-4}$ cgs emu).

T = abs. temp. θ = chara. of substance.

Isotropic Diamagnetic

a) Moves stronger – weaker part of field }
b) Set max length $\perp$ to field. }

c) remain stationary in a uniform field. Since magnetism so low doesn't create non-uniform field

$B < H$. $\mu < 1$. Since $B = H + 4\pi I$. I must oppose H & K is –ve. For a "perfect diamag" $\mu = 0$. $k = 1/4\pi$. For normal dia's K independ. of H and of temp. & of change of state. Many exceptions to this rule. $k \simeq -10^{-6}$ cgs emu.

Explanation of all mag. props. lies in electronic structure imposed field acts or retards electrons in orbits.

all electron produce a mag. field. (& current).
Neighbouring atoms perturb each other structure.
In some atoms with incomplete shells, if electrons have spin get an incomplete shell ≡ to a magnetic.
Atom now unbalanced so may be regarded as a permanent magnet.

If here spins balanced in absence of a field. Stuff is Diamagnetic. No resultant magnetic moment in atom.
On imposed field will unbalance spin

In single crystal have different χ in different directions so refer to Three Principle directions. $\bar{\chi} = \frac{\chi_1 + \chi_2 + \chi_3}{3}$
and get Ellipsoid of Susceptibility as in Refractive Index.

Langevin & Larmor developed theory showing that

$$\chi_A = -\frac{Ne^2}{6mc^2} \sum_n r^2$$

$$= -2.83\,10^{10} \sum_n r^2$$

r = Radius Electronic Orbit
N = Avogadro's No:

This supposes Spherical Symetry of atom.

$\overline{\pi r^2}$ = Projected electron orbit. (Mean Value).

So by measuring χ_A can get a value for $\overline{\pi r^2}$ ie to average radius of atom.

Electron Diffraction 3rd May 1930 Wave Mechs. Free Electrons.
G.P. Thompson.

XLII Refs Trans. Faraday Soc. Vol. 31 P 1051. 1935.
Finch, Quarrell, Wilman.

Fast Electron Diff. (Slow speeds require more elaborate techniques)
30 - 60 KV.
Debroglie Wavelength. $\lambda = h/mv = 1/20$ th A°.
Differences twix X & Elect. a) λ
b) less penetration of beam.

1937 G.I Finch & Wilman. Ergeb. d. exakten Naturwiss.
IG 353. 1

1939 Thompson & W Cochrane. "Theory & Practice of Elec. Diff
Macmillan 1939.

1944 Von Laue. Materiewellen und ihre Interferenzen.
(Identical 2nd edition '48) Published Berlin.

1948 Science Progress - Jan. pl. 1948. Finch & Wilman.
Discussion of Electron Microscopy & Electron Diffraction
relative fields of information.

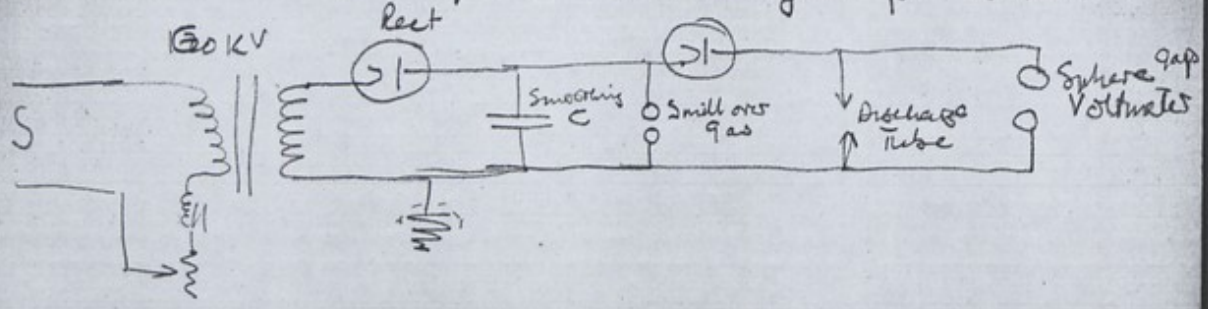
1949 Research. Vol 2. 352. Wilman.

Apparatus Electron Diff. Camera

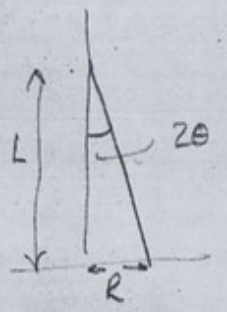
50 cms Spec. to Fluorescent screen. Normal Work.
25 cms - 20 cm Spec. - Fl. Sc. for Single Crystal where
want wide range on screen.

Anode Diaph. 1/10 mm. diameter in Nickel Foil. Should be
as small as convenient. 1/10 mm. small as possible for
general purposes.
Cold Cathode Gas Discharge 1 micramp beam current.
Apply const. current & have const. leak.

Above 70 KV. necessary to use Hot Cathode.
160 KV has been achieved by Wilman. Designed for 200KV.



Relation twix λ & radius R. of Ring diff :—



$\sin\theta = n\lambda/2d$ since λ so small θ is $\simeq 1^\circ$.

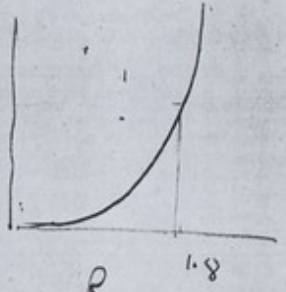
$R = L\tan 2\theta \simeq L.2\theta$. $\because \theta$ small.

ie $R = \lambda L/d$. ie $d = \lambda L/R$.

When L = 50 cm & R = 1·8cm. gives correction $\simeq$ 1 in 1,000

Small correction for outer rings. $d = \lambda L/R(1-\delta)$

Crystals generally small. So accuracy of ring definition not high enough to warrant correction.



1 Mica sheets 100A° thick ⊥ to beam gives you 2 dimensional grating.

2 With thicker sheet. Get pattern like newtons rings. 2 dimensional pattern in middle clearly, on rest of plate pattern limited by hard zones.

3 With a thicker crystal plate get series of black & white lines over plate. Pick out pairs & use seperation to get R.

Kikuchi lines.

1B $\delta = \frac{3}{8}\left(\frac{R}{L}\right)^2 - \frac{31}{128}\left(\frac{R}{L}\right)^4 + \ldots$

Jeffries. 2. XLIV May 7th. Meas. of Intensities

a) Comparative only b) Absolute scale

Large specimen easily dealt with, compare reflex. with standard crystal of another area. Need to know volume & therefore need rho.

Gases & liquids Ref. Randal. Liquids some grain

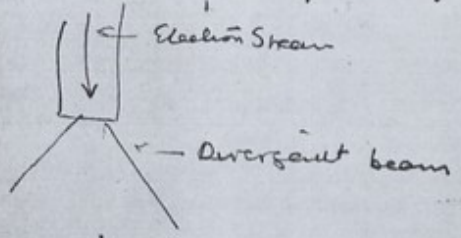
Small crystal causes each point in rep. space to be little volumes. This gives broadened powder line.

Shape in rep. opp to that in ③

Thermal Vibrations

Divergent Beams

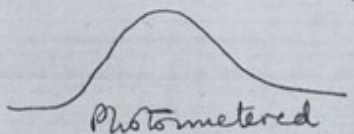
Get beam by Taking Knup's Mask & melted foil underneath



Disorder & Randomness

Disorder usually: layers shift along. Mixed crystal.

Causes distortion or modification of rep. Unsymmetrical volumes around lattice points



Next Monday week.

Thurs May? Monday. XLV

Paramagnetism. $\mu > 1$, independent of H. from 1 → 1.001.
Na, K. O. Rare Earths, + Fe's above Curie Point.

Occurs when electrons are unbalanced giving results

Quantum no: n
Orbital moment L Angular momentum $= h/2\pi$.
Spin moment S. " " $S = 1/2$
U resultant moment $L \vee S$ " " $(L+S)$ to $(L-S)$.

This U, causes resultant magnetic moment, permitting it to set in $(2J+1)$ diff positions in field. This tendency to line up in field direction is opposed by 1) Thermal motion 2) field in crystal due to crystallisation.

If ~~field is~~ crystal anisotropic may get anisotropic paramagnetism.

Atomic mag. moms. meas. in Bohr magnetons. $\left(\frac{he}{4\pi m}\right)\mu$.
Got by expressing electron in terms of current equiv. & multiplying by effective atomic area.

Magnetic moment $\frac{1}{2}$ for spin moment while for Orbital, but result U. not necc integer.

Some para obey Curie law. $\chi = \frac{C}{T}$. others the Curie-Weiss law $\chi = \frac{C}{T-\theta}$ ← nearly Curie Temp.

~~Ferromagnetism~~ Incomplete inner shell in atom with either Spin or Orbital moment. To find which meas. Gyromagnetic ratio.

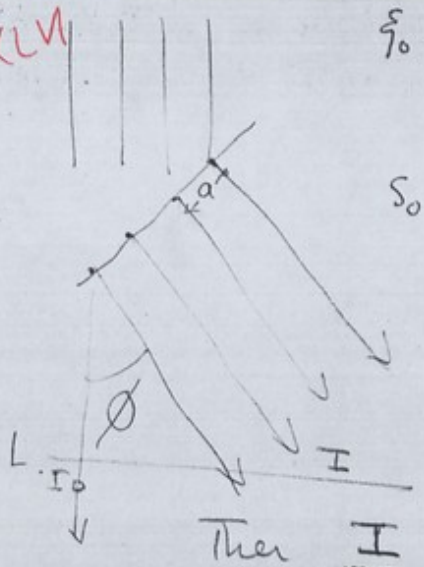
Ang. mtm / mag. mnt. $= \frac{2m}{e}$ if due to orbital
$= \frac{m}{e}$ if due to spin unbalanced

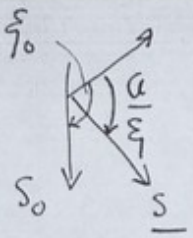
If both spin & orbital get something betw.

Now $\chi_1\ \chi_2\ \chi_3$ the three principle directions of susceptibility.
Mean $= \bar{\chi} = \frac{\chi_1 + \chi_2 + \chi_3}{3}$. Depends on structure and texture.

Consider White Tin. tetragonal. metallic. If now decrease

XLVI





Path Difference

$$\underline{a}(\underline{S} - \underline{S_0}) = h\lambda$$

h some integer.

Phase difference δ given by

$$\frac{2\pi}{\lambda}(h\lambda) = \underline{2\pi h}$$

Let ψ be scattering power of each lattice point

Then $$\frac{I}{I_0} = \frac{\psi^2}{R^2} \cdot \frac{\sin^2 M_1 h\pi}{\sin^2 h\pi}.$$

M_1 is no. of lattice points along row.

$$a(\cos\xi - \cos\xi_0) = h\lambda.$$

Tuesdays: Booth 10. Advanced tech. in X-ray. Organic Structure Analysis.
(Tomlin)
Not much help after.

Refs. 1 Beevers Lipson. 1934. Phil Mag. 17 855.
2 " " 1936 Nature. Lond. 137 825.
3 " " 1936. Proc Phys. Soc. 48 772.

Patterson + Tunell. 1942 Am. Mineralogist 27 655.
How to handle sub lattices.

Tin stays each state is diamagnetic. when yet grey non-metallic tin
Thus shows that paramag. due to conducting electrons. In this case
then, no temperature dependence.

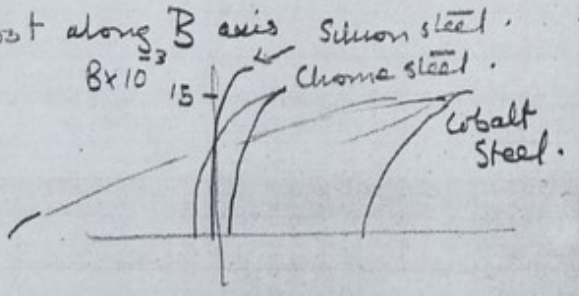
XLVII

Progress in Physics 4 368. 1938. K. Lonsdale. Isotropy

Ferromagnetism Fe Co Ni, and by Alloys with rough. Elements.
and alloys such as Heusler alloys eg Cu_2MnAl.
Gallenium Ga. Fe_3O_4. SnMn. Pb-Cr. (20-50% Cr).
all show hysteresis. NB B.H = Magnetic Energy. imp. for performance of magnet.

Carbon steel easily demag. Small remanence
Compressed oxides. Fe_3O_4 perm. mag. large remanance.
(powder)
+ Co Fe_2O_4

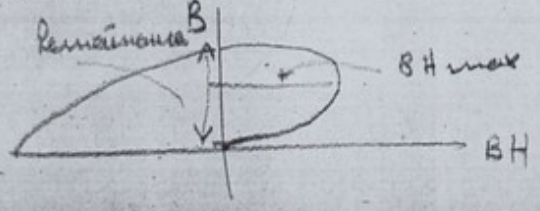
Silicon steel has hysteresis loop almost along B axis



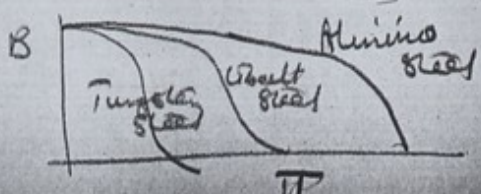
Chrome steel like carbon steel
Cobalt steel like comp. powder.
Ferro-mag. material with
High remanance is Hard.
Low " Soft.
ie Soft. Material has high μ. low hysteresis
" Hard " " lower μ high " .

Soft magnets are usually unstrained materials. Hard stuff got by putting in impurities or creating a high strain. & has B.H a high maximum value.

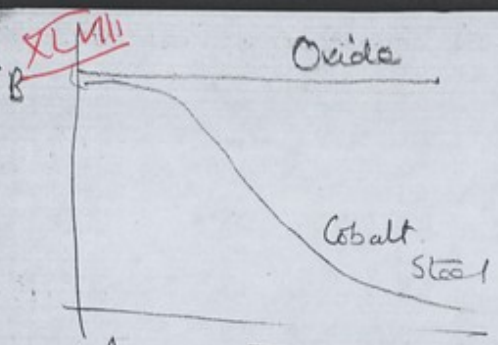
NB Remanance B



Temp dependence

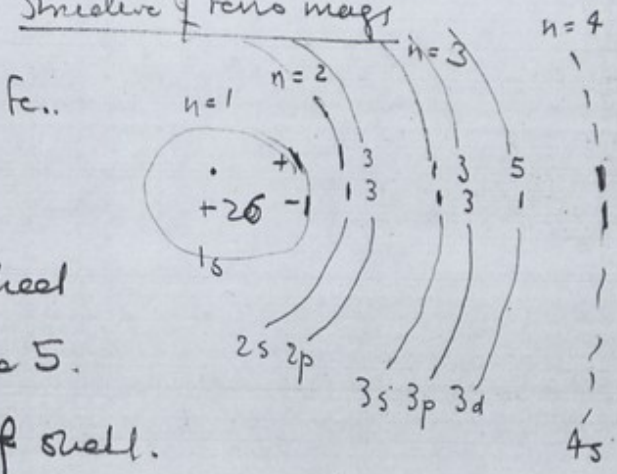


XLMII



Carbon reduces permeability.
Silicon steel has high μ because it causes carbon to crystallise out.

Structure of Ferro mags



So the unbalanced spin moment occurs in 3d shell

Co. has 7. Iron 6, Chrom 5.

Gd. has unbalanced spin in 4f shell.

But must also have periodic atomic dist. ~~tax~~ crystalline state.

D = distance betw atoms.

r = radius of energy shell in which spins uncompensated

D/r should lie within certain limits

	Ti	Co	Mn	Fe.
D/r :	2·24	2·36	2·94	3·20

Strain can cause the D/r to come into this range.

Weiss says that in Ferro. solids a field exists which lines up the elementary atomic magnet. Can evaluate it by

a) Thermal energy at Curie point ($\equiv$ to lining up force)

KT_c so $\mu_B H_{mf} \simeq KT_c$

H_{mf} = molecular field
μ_B due to single electron.

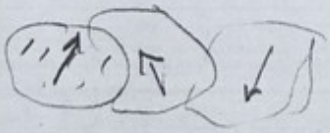
~~Then~~ find $H_{mf} \sim 10^7$ oersted.

Field on any one magnet due to neighbouring magnet, if they all
~ μ_B moment get $H \sim 10^3$ oersteds. XLIX.
Shows that the field lining up spins is not the inter molecular
field, but some exchange, quantum force.

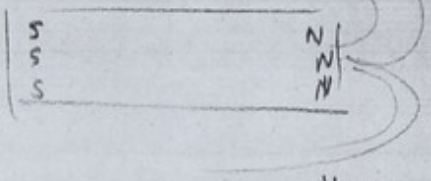
In unmagnetised material Domains exist. with randomly orientated
resultant moments.

Switch on field and

a) Domains in right direction grow.
b) Others turn into field

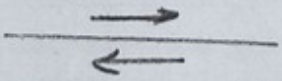


Magnetic Energy 3 kinds. ⊥ Magnetostatic (Large)
due to lines of force outside the crystal.

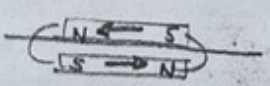


2 Domain wall Energy.

Region on each side
of wall oppositely magnetised.



eg.

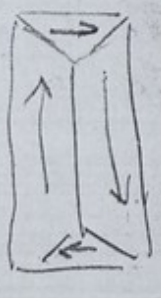


1) Less
2) increasing

So magnetostatic energy decreased & domain wall energy increased.

3 Magnetostriction Energy. If mag. free to do so, it will lengthen along direction of magnetisation. But can't in crystal.

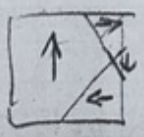
Crystal breaks up into lots of these regions. Then 2) = 3)



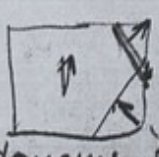
1) gone (closed system)
2) Small
3) large.

Magnetisation

Non magnetic
(∵ closed system



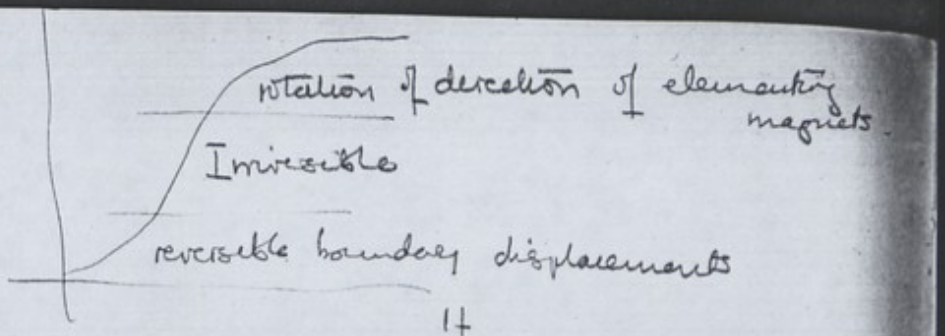
H Favoured one grows.



H

Other domains turn.

If polycrystal are

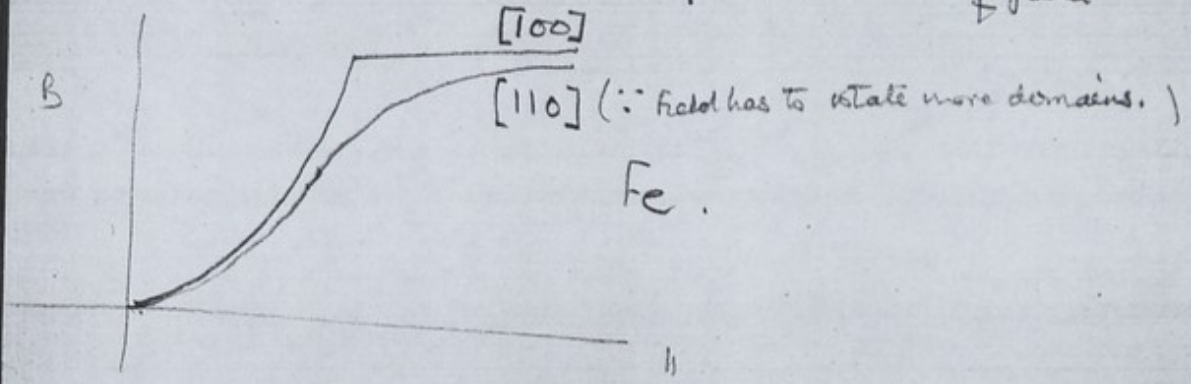


With anisotropic crystal (all ferros are) then some directions are said to be those of "easy magnetisation".

eg Fe. easy mag. along cube directions [100]

Ni. " " " [111] direction.

Get diff. curve B – H. depending on direction of field



In general Work reqired to mag. crystal in any direction is $W = K_0 + K_1 \sum a_1^2 a_2^2 + K_2 \sum a_1^2 a_2^2 a_3^2$

= Work required to magnetise unit volume to saturation, in any direction!

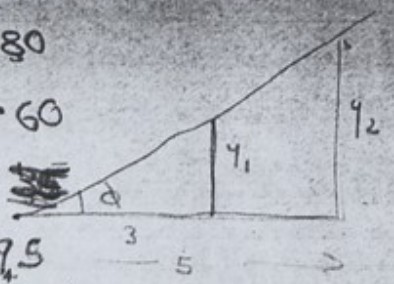
a_1 = Direction cosines of field
a_2 = relative to directions
a_3 = of easy magnetisation

K_0 is resident mag. along [100]

K_1 & K_2 are 1st & 2nd anisotropy consts.

NB W shows anisotropy in cubic crystal.

	tan ψ	r. tan ψ = y mm.	
$\psi_1 = 3^\circ\ 13'$	= 0.05600	1.680	2.80
$\psi_2 = 6^\circ\ 26'$	= .112	3.36	5.60
$\psi_3 = 9^\circ\ 41'$	= .17063	5.1189	8.5315
$\psi_4 = 12^\circ\ 57'$	= .22995	6.8985	11.495
$\psi_5 = 16^\circ\ 16'$	= .29177	8.7521	14.585
$\psi_6 = 19^\circ\ 38'$	= .35674	10.7022	17.835
$\psi_7 = 23^\circ\ 5'$	= .42620	12.786	21.310
$\psi_8 = 26^\circ\ 37'$	= .50112	15.0336	25.055



$\frac{y_2}{y_1} = \frac{5}{3}$

LAID IN BETWEEN L + LI

Wilman Thursday Ilford "Special Rapid". Not too contrasty so can get on the fainter rings. (Glass).

I

Alternative form of $d = \lambda/R(1-\delta)$. is $\frac{\lambda L}{R}(1+\delta')$.

$$\delta' = \frac{3}{8}\left(\frac{R}{L}\right)^2 - \frac{13}{128}\left(\frac{R}{L}\right)^4 +$$

Remember d from this formula includes the order number n. ie $d = \frac{d_{hkl}}{n}$

Intensities $\frac{I}{I_0} \sim \frac{S^2 p}{d^2}$ S = Structure Factor.

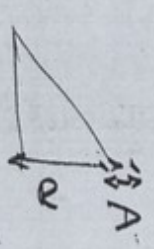
Use Elec. Diff. for intensifications.

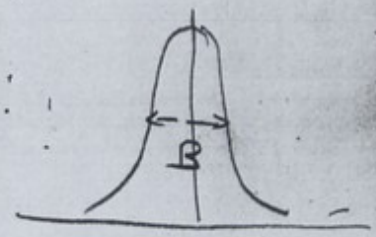
Large crystals with sharp rings may have altered Intensities due to crystal shape.

Mixture Relative Intensities from materials depends on crystal size. Those with small crystals will show up strongly. Those large will not.

For large crystaline mats. compress to pellet with smooth surface use grazing incidence.

Ring Breadth & Particle Size





$\therefore B = 0.9\frac{\lambda}{t\cos\theta}$ for X rays.

Here $t\cos\theta \to 1$. So $B \to 0.9\frac{\lambda L}{t}$

Where t = Thickness in direction of beam.

If $B = 0.1$ cms. $t \sim 25 A^\circ$.

Single Crystals

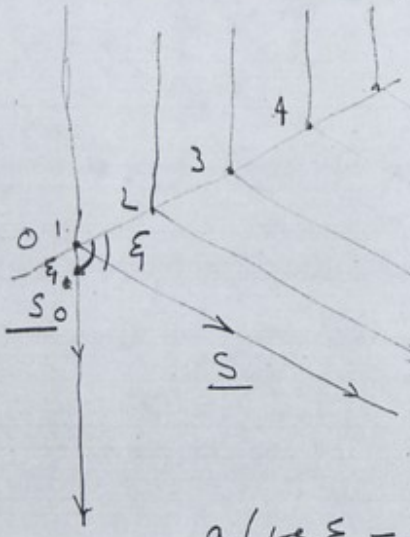
Interpretation made in three ways;-

1/ Laue Zones
2/ Reciprocal lattice (Ewald sphere)
3/ Bragg-Reflections.

1/ The unit of diffraction can be taken as one lattice row. This is then modified by presence of other rows.

Consider one lattice row, period a. & diffraction in one direction,

[1]



S_0 = Unit vector incident beam

S = " " diffracted "

Path Difference = $\underline{a}\underline{s} - \underline{a}\underline{s}_0$

$= \underline{a}(\underline{s} - \underline{s}_0) = h\lambda$

h an integer, for reinforcement of diffracted beam.

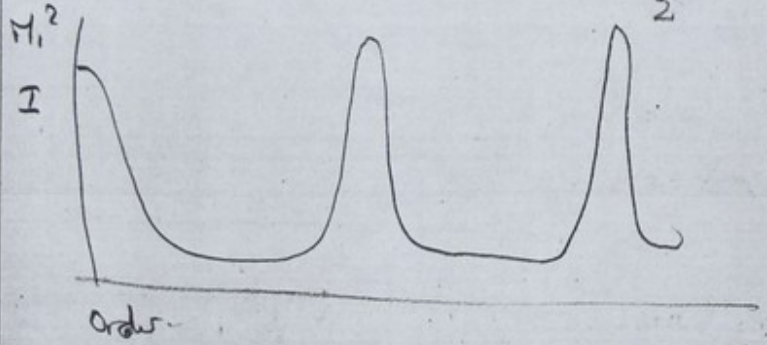
$$a(\cos\xi - \cos\xi_0) = h\lambda$$

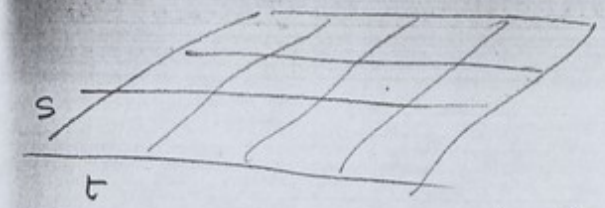
Cone of diffraction, semiangle ξ. termed Laue Cone. Intersection on plate, Laue Zone.

Now 1st ray has amplitude $y_1 = \psi_1 A \cos\omega t$

$$y_n = \psi A \cos(\omega t + M_1 - \delta)$$

Total Resultant $Y = \frac{\psi}{R} \cdot \frac{\sin\frac{M_1\delta}{2}}{\delta^2 \frac{\delta}{2}} = \frac{\psi^2}{R}\left(\frac{\delta^2 M_1 h\lambda}{\delta^2 h\lambda T}\right)$





$$\frac{I}{I_0} = \frac{\Phi^2}{R^2} \frac{\sin^2 \pi_1 k}{r} \frac{\sin^2 \pi_2 k}{\sin^2 \pi k} \cdot \frac{\sin^2 \pi_3 k}{\sin^2 \pi k}$$

Crystals have to be limited in one direction for our known $\underline{a}\ \underline{b}\ \underline{c}$ $\underline{a}.(\underline{s}+\underline{s}_0 = h\lambda$

III

$$\underline{a}(\underline{s}-\underline{s}_0) = h\lambda$$
$$\underline{b}(\underline{s}-\underline{s}_0) = k\lambda$$
$$\underline{c}(\underline{s}-\underline{s}_0) = l\lambda.$$

$$\underline{r} = (\underline{r}\,\underline{a})\underline{a}^2 + (\underline{r}\,\underline{b})\underline{b}^2 + (\underline{r}\,\underline{c})\underline{c}^2$$

$$\underline{s}-\underline{s}_0 = (\underline{s}-\underline{s}_0\ \underline{a})\underline{a}^* + \ldots$$

$$= (h\underline{a}^* + k\underline{b}^* + l\underline{c}^*)\lambda.$$

$$\frac{\underline{s}-\underline{s}'_0}{\lambda} = h\underline{a}^* + k\underline{b}^* + l\underline{c}^*$$

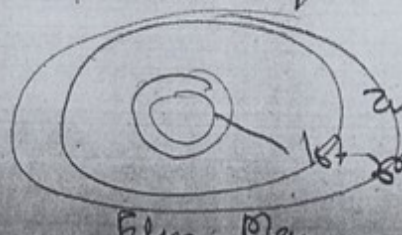
Get extension of rep. points along c^*. a length $\propto \frac{1}{M_3}$.

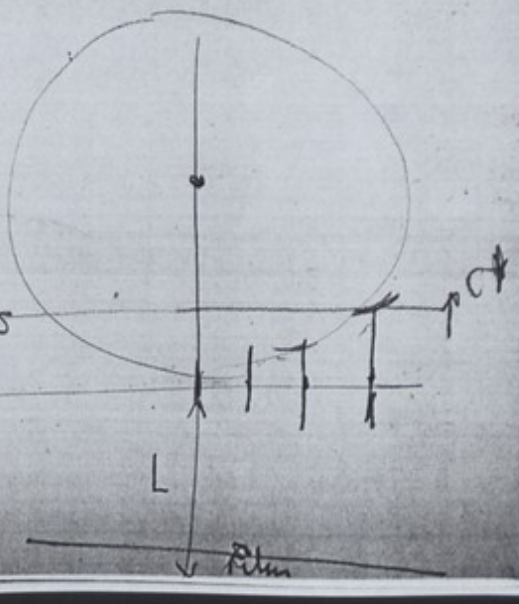
60 kV electrons give $\frac{1}{20}$th $A^0\lambda$.

∴ Radius of reflecting sphere is 20 A^0

So cuts in points near straight thro' beam

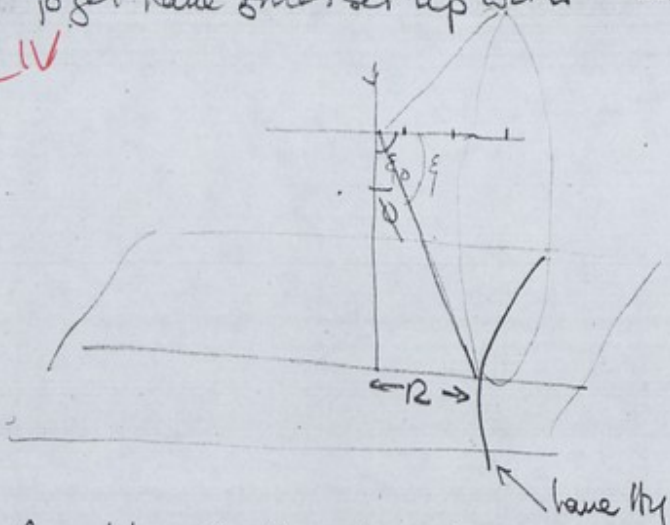
So pattern on plate is undistorted near centre of ~~Ewald~~ plate.





To get Laue zones set up with lattice row // to Primary beam.

LIV



$\xi_0 = 90°$

$\phi = (90 - \xi)$

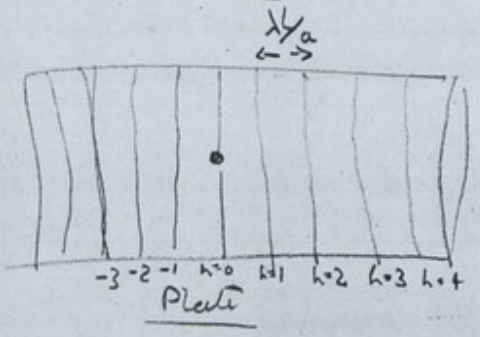
$a(\cos\xi - \cos\xi_0) = h\lambda$

Becomes $a \sin\phi = h\lambda$.

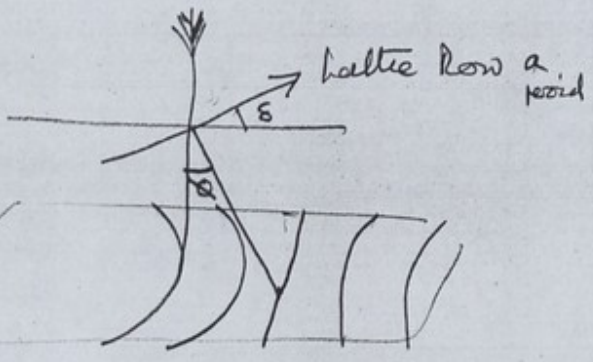
$R = L\tan\phi$. Now when h is small ϕ is small. So that

$R = h\lambda L / a$

This means successive Laue zones should be successive almost straight lines.



This is with Primary Beam along a lattice row.

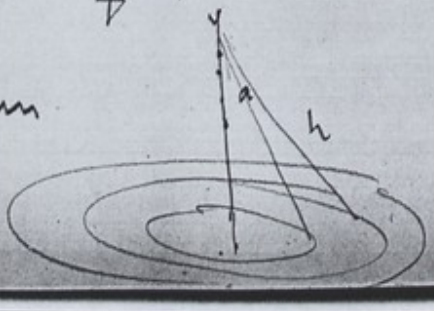


Incline lattice row δ to beam. get $R = \lambda L / a\cos\delta$

as δ small just get projection of a, i.e. $a\cos\delta$.

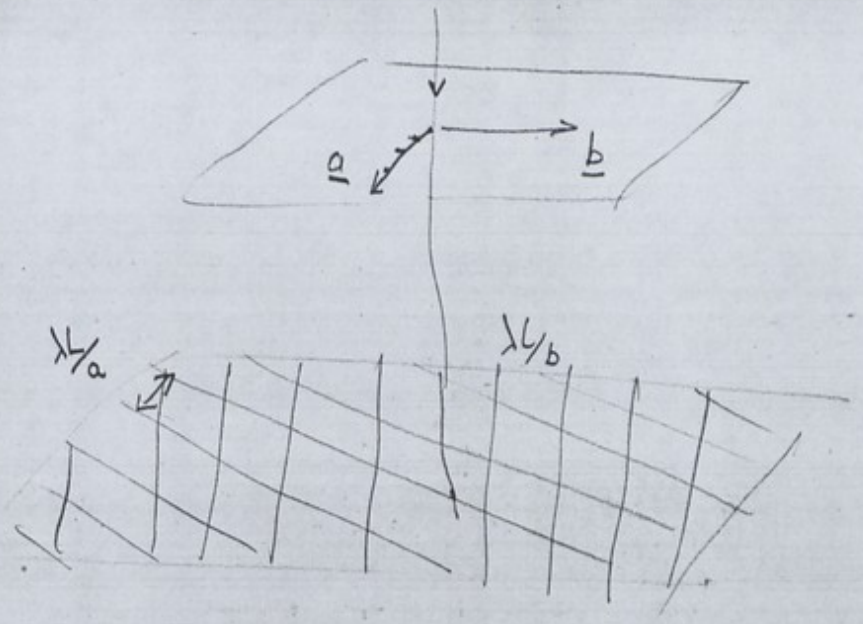
With rep lattice row // to beam

$R = L\sqrt{2h\lambda / a}$.



If a two dimensional matt get product of two linear rep. was

LV



Surface Investigation

Grazing incidence. Get broad bands zones if surface rough, & so show up plenty of spots from two dimensional If smooth no or few spots.

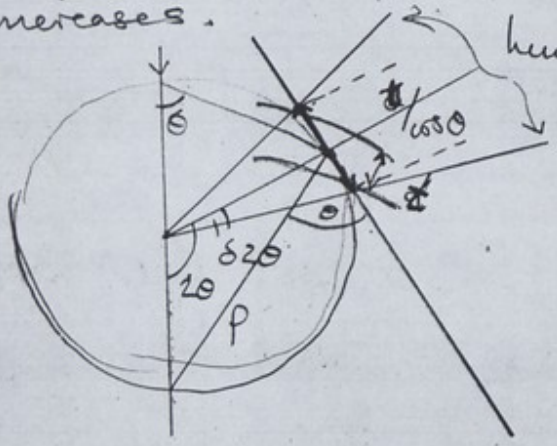
22 May. Tuesday. 6pm. Imp. College. (next door to Imp Chem)

Jeffries Monday 21st May:-

Distortion in Powder Photography.

Effect of small size:- gives same effect for 1st ---nth order. Think of it as causing thin sphere of the sphere of reflection to broaden out into a shell. But the thicknesses of shells near in & far out all same.

Whereas:- Distortion, strain etc causes these successive shells to increase in thickness ie 1st — nth order, broading increases.



Thus if reflection due to broadening of RCP point (ie the thin powder sphere has gone into a shell thickness d).

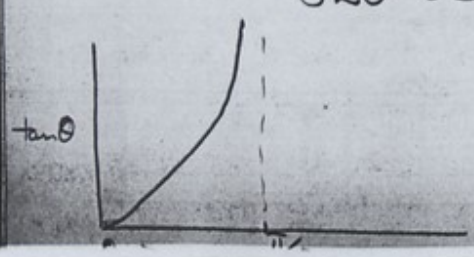
As see from diagram $\therefore \rho = 2\sin\theta$. & $\delta 2\theta = \frac{d}{\cos\theta}$.

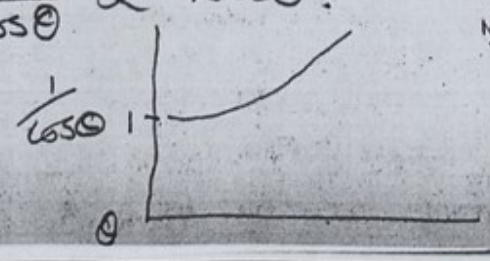
For small crystal size:- t constant.

$\therefore$ Line broadening. $(\equiv \delta 2\theta) \propto \frac{1}{\cos\theta}$.

For Strain:- t increases with ρ. $t \propto \rho \propto 2\sin\theta$

Whence $\delta 2\theta \propto \frac{2\sin\theta}{\cos\theta} \propto \tan\theta$.





NB The rate of increase of $\frac{1}{\cos\theta} < \tan\theta$.

LVII

cedure

ria Single crystal of suitable size.

cedure 1 Study on microscope and look for a likely crystal.

a) Polarized light. Straight extinctions. (ie uniform extinction)

b) If rocky crystal, immerse in liquid of same average refractive index which will tend to cut out refraction effects.

c) Good faces d) Size about ≏ 1/4 mm. cube.

a) Interference figures to find out if uniaxial or biaxial

) If biaxial & no faces mount with axis along extinction direction.

) If faces present plot results of goniometry on a stereogram.

3 Mount on a fibre (glass), with chosen direction along the fibre.

4 If suspect a perfect crystal, dip it in liquid air.

Set the crystal with a major reciprocal lattice plane ⊥ to rotation axis.

a) If optical faces set by light reflections.

(b) By a layer line method. (Weiss & Coal)

NB Stick crystal onto glass fibre & fibre onto lead wire. Then orient by bending lead wire.

c) Use single reflections. (Jeffries)

6 Rotation photographs about 3 axes.

7 Laue rec. photo to establish lattice symmetry to take in the

8 Oscillation photos about one axis to take in the necessary extinctions of the Rep lattice and/or Unnecessary plots of the layer ⊥ to an axis + in either case photos about another axis to obtain missing reflections.

VIII

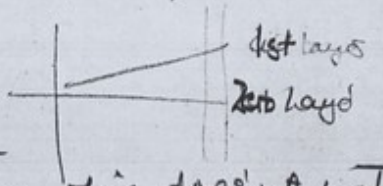
4. Indexing the Photographs → Estimate Intensity Correlate Photo's.
~~estabon~~ unit cell dimensions

1. Correct intensities :- a) ~~Hooft~~

b) Absorption. (NB Monoclinic has unique axis.)

c) Geometrical + polarization The reflections at low + high θ's are enhanced. Lorentz.

d) Obliquity factor. ~~Cox~~ Shaw.



2nd layer goes thro more emulsion than 1st layer. If restrict to one layer then this doesn't matter

e Primary + secondary extinctions (Mosaic effects etc)

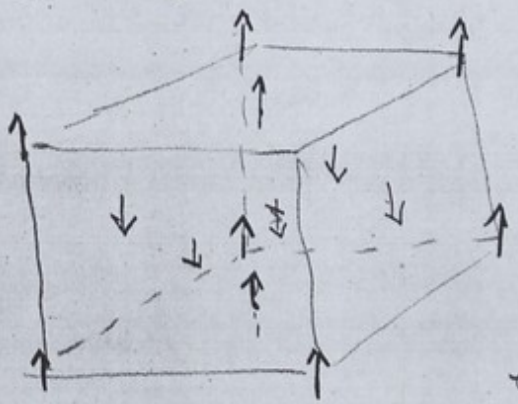
1st May Monday Mrs Lonsdale

4X

Crystal of pyrotite eg $Fe_{1-x}S$. hexagonal with enormous anisotropy

15, 7500, 150,000 oersted are the fields necessary to saturate ⊥ to field & least one // to c axis. This property used to make powerful magnets. Condense metal in bar along direction of easy magnetisation

If particle $< 10^{-6}$ cm it can be one domain. Therefore need to turn dipoles themselves. So no initial part to curve as domain turn. Require very high field. So can use permanent magnets of oxides which will be unaffected by alternating field, (until it gets very high to affect the dipoles) can get single crystals domains much larger than the average 10 cm.



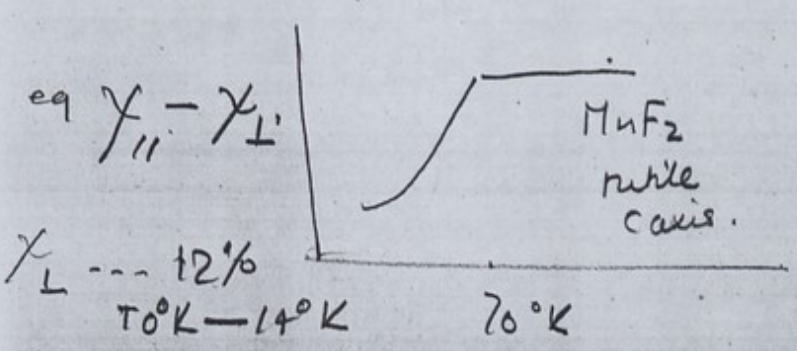
↑ Indicates spin direction

Face-Centered Cubic lattice

↓ A

↑ B Sub-lattices.

This type of affairs used to explain ferrolike behaviour at certain temps of paramagnetics.



$\chi_{//}$ ---- 12% at 0°K.

Paramags:-

MnO MnS MnSe

FeO

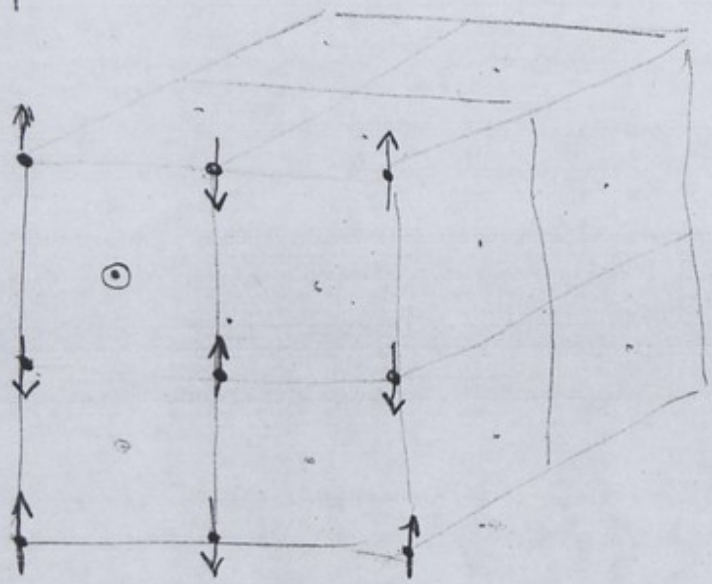
NiO

CoO.

Rooksby (QEC) showed that do get change in pattern with temperature. 20°C −70°C −180°C

Roothsby:- FeO (really $Fe_{1-x}O$ ∴ always deficiency in ions).
Change is greater the less value of x. ie More perfect the lattice the > the antiferromagnetic change.

Cu



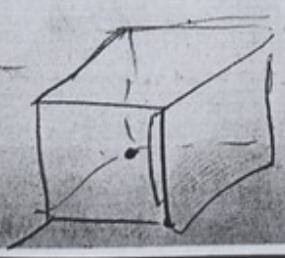
• M_n
○ Oxygen

Neutron diffraction can distinguish between spin directions, // & anti-//. This shows in case of MnO, proved also that Magnetic cell 2× chemical cell in each direction.

Face centered cell gives positions 000, $0\frac{1}{2}\frac{1}{2}$, $\frac{1}{2}0\frac{1}{2}$ $\frac{1}{2}\frac{1}{2}0$ +

Position	Spin		
000	↑	Structure proposed by Shull from Neutron Diffraction.	Néel [001] ↑ [00$\bar{1}$] ↓
$00\frac{1}{2}$	↓		
$\frac{1}{4}\frac{1}{4}\frac{1}{4}$	↑		
$\frac{1}{4}\frac{1}{4}\frac{1}{2}$	↓		
$\frac{1}{4}0\frac{1}{4}$	↑		
$\frac{1}{4}0\frac{3}{4}$	↓		
$\frac{1}{2}\frac{1}{4}\frac{1}{4}$	↑		← [1$\bar{0}$0]
$\frac{1}{2}\frac{1}{4}\frac{3}{4}$	↓		→ [$\bar{1}$00]

Structure proposed on theoretical grounds only. Neutron diffraction can't decide between them



Part of Néel's idea is have four sub-lattices of spins in different directions in each one but paired // & anti // as before. Would give same effect. LXI

Suggestion is that only get anti-magnetism where have Oxygen or Sulphur as an intermediary.

$CrTe$. Chromium telenide is ferromagnetic

$MnTe$. antiferro-

Explanation. In Cr^{++} 3d shell < half-filled

Mn^{++} " " > " " .

If electron goes in to Cr. will have // spin.

" " " " Mn ∴ shell > ½ filled will have more weakly anti // spin.

Fe_3O_4 Magnetite. (Spinel structure $^{++}A\,B_2^{+++}O_4^{--}$ a) (dordant T_i)

Random spinels $B(AB)O_4$ b)

a) A tetrahedrally surrounded

b) B octa " "

If take stuff with formula $M\,Fe_2^{+++}\,O_4$ & can be $MO.Fe_2O_3$

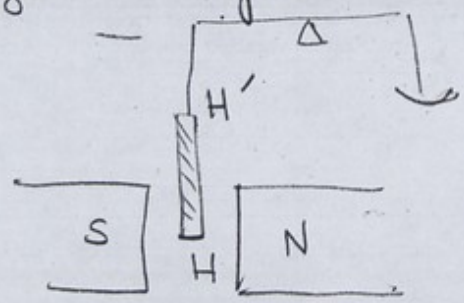
where M stands for some metal. If M = Zn Cd ordinary paramagnetic (χ doesn't change with temp.) If M = Mn Fe Co Ni Pb Mg all ferro-mags but not as strong as they should be. Due to fact that they have a nett quantity of unbalanced spin. These called Ferrimagnetics.

NB Can polarize beams of neutrons using Fe_3O_4, & Shull (USA) has made polarizing microscope using

Fe_3O_4 as polarizer & analyser.

LXII

Susceptibility



Gouy's Method

Gives Average ψ

Suscept. of powder K. Balance force by weights.

" " medium K_0 force $= \frac{1}{2}(K-K_0)A(H^2-H'^2) = mg.$

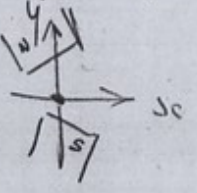
A = area of block. H high H' as small as possible.

Where m = weight required for balance.

Calibrate apparatus with standard material.

Faraday's Method

Using varying field. Can be got by inclined pole-pieces & suspend stuff in fluid & observe



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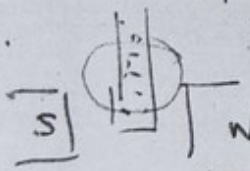
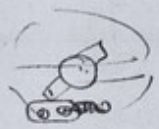




~~If Para or Dia~~

Then suspend in solution of opposite ψ. When $\psi_{solute} = \psi_{solid}$ no movement

$$f = \frac{1}{2}(K-K_0)V\frac{\partial H_y^2}{\partial x}$$

V = volume of Particle

This gives susceptibility along y direction.

$SrBr_2 + xH_2O$ get density right. Diamag.

$NiCl_2 + yH_2O$ " " " Para mags.

so act as mixed with variable density & variable ψ.

May 28th. Monday

Perfect Diamagnetic ($K = \frac{1}{4\pi}$.)

Diamagnetic. $\mu = i\pi r^2$ $\quad i = -\frac{e\omega}{2\pi}$ $\quad e$ = electronic charge (e.m.u).

$\Delta\omega = H\frac{e}{2\pi}$ (ω = ang velocity of electron in orbit)

$\Delta\mu = \pi r^2\left(\frac{-e\Delta\omega}{2\pi}\right) = -e^2/4m\, Hr^2$.

$\chi_A = \frac{N\Delta\mu}{H} = -\frac{Ne^2}{4m}\sum \overline{r^2}$ $\quad \overline{r^2} = x^2+y^2$ (Projected orbit). $\pi\overline{r^2}$

$= \frac{-Ne^2}{6m}\sum \overline{r^2} = -2.83\,10^{0}\sum \overline{r^2}$. $\quad \overline{r^2} = x^2+y^2+z^2$

So if know atomic radii can calc. the susceptibility. True also for paramag. atoms & ferro.

Calc values; etc

	H_e	N_e	A	K_r	X_e	$\times 10^{-6}$
Tab values	1.9	6.75	19.54	28.0	42.4	
e. .. 2		2.8	2.8888	(28−18.8)	(2.8−18.18.8)	
(Previous calculations)	1.68	5.07	16.67	29.33	44.78.	

The following obs. & calc values all scaled to that of helium

Assuming χ's additive.

Calc. χ for atom core & valency electrons seperately. Valency electrons have largest effect ($\overline{r}$ larger) Can then calc atomic radius. Observe χ and subtract theoretical χ for core & target

	Calc	Obs
Li^+	0.7	(0.7)
Na^+	3.7	6.1
K^+	18.1	14.6
Rb^+	27.0	22.0
Cs^+	37.1	35.1
F^-	7.2	9.4
Cl^-	22.9	24.2
Br^-	30.7	34.5

Calc. value of χ for valency, hence atomic radius. Agrees with X ray obs.

Can also find out if atomic radius varies with chem. comb. χ for ion in crystal different, slightly, from that in free state.

SOLUTIONS

Wiedemann's Law If have solutions, conc c.

CXIV

$c_s = \frac{m}{m+M}$ Then $(M+m)\chi_{solution} = m\chi_{solute} + M\chi_{w.}$

$\therefore \chi_{solution} = c_s\chi_s + (1-c_s)\chi_{water}$ (χ = mass susceptibility)

Can ∴ calc. χ solution if know conc. & χ solute.

Pascal's law Mol. susceptibility χ_M of a compound $A_\alpha B_\beta C_\gamma \ldots$ given by

$$\chi_M = \Sigma \alpha\chi_A + \lambda.$$

Where $\alpha, \beta, \gamma \ldots$ are no. of atoms of suscept. $\chi_A \chi_B \chi_C \ldots$

& λ is a constitutive correction constant. (depends on no. of bonds)

Can ∴ find χ for groups. eg Hexane & next highest differ by CH_2 so sub. χ's & get χ for CH_2.

Measurement of χ absolute difficult. Generally calc. from Pascals law.

For $-\overset{|}{C}=\overset{|}{C}-$ $\lambda = +5.5$. If however add atomic susceptibility find must add this constant

For $-C \equiv C-$ $\lambda = +0.8$.

Polymers $\psi_p = n\psi_M + (n-1)\lambda$ - where λ = correction constant for one bond.

ψ_M = susb. for single group).

$\therefore$ Mass $\chi = \dfrac{n\chi_M + (n-1)\lambda}{M}$ M = mol. wt of single group.

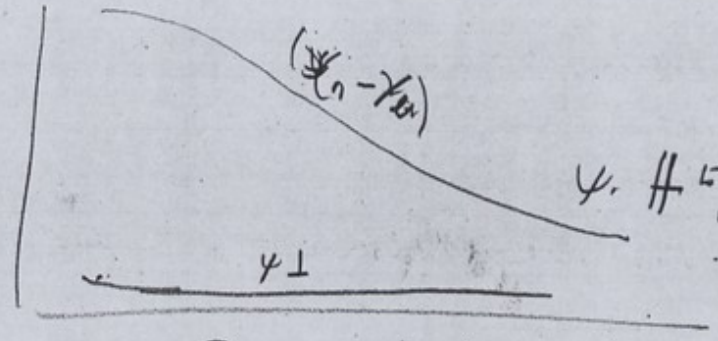
(plot - Mass ψ against n. Get hyperbola. Can follow extent of polymerisation this way.

Consider $K_4[Fe(CN)_6]$ 4- CN, mole charges & giving 26 + 6 + 4 = 36.

For $K_3^+(Fe(CN)_6)^{3-}$ dsp^2.

Most metals have small pos. ...

Graphite



Therefore large electron orbits in basal planes of graphite.

$r = 10\,A^\circ$.

Both planes made of conjugated double bonds large values of anisotropy. So ψ depends on molecules & by ...

If undelivered please return to :—
UNIVERSITY OF LONDON
SENATE HOUSE, MALET STREET,
LONDON WC1E 7HU

FRANKLIN Notebooks

PROF. WILKINS.

(DNA HISTORY)

(4 notebooks ?)

A' Sep. 51 ⇒ Mar 52
[9-15 Nov 51 all weighing]

B' Mar 52 ⇒ oct 52

C' 19 Jan 53 ⇒ 27 July 53

nothing
14.10.52 –

from
A.R. Stokes, Esq., Ph.D.,
King's College, Dept. of Physics,
Strand,
LONDON, WC2R 2LS.

RD

BY H.

B[1] Mar April 52 → Oct 52

No mention of dead axis in this?

2½ weeks before the Death of Helix meeting.

March. much trouble with salt in April. Tilting expts.

(July 18 Death of Helix announced to Stokes)

July 2 Failed to try concl help on oriented sheets? cyl. Pat. Tried 13.5 A diam

Much. Trouble with Salt confined to Sept in long series of photos

N.B. no mention of 11th l.l. reflection.

or measurements on good B pattern other than l.l. spacing 34 A° which was made (same time?) as photo?

July 7. revising lattice 17 A to $\beta = 93°$.??

Fuller et al $97 \pm 0.4°$

2.5.52 (apparently?) first mention of 33–34 A°. Was that the first time it was measured?? yes?

P. 7 Helix

2.5.52

"if there is a helix"

crypt to wet.

Use predominant equat. reflection ~ doubled (but of course they do not correspond)

18.4.52 — July 15. → Oct trouble with salt causing → 14.10.52 (Film 78) failure not to give A.

MHFW's notes. June 76.

March - April 1952

spray of salt accumulator on fibre where H_2 exits through collimator

2.99

. Long series of microphotographs at 75% RH (not preserved) in Lindemann tube. Trial short-exposure films were generally good ✓

specimen subsequently went non-crystalline during long exposure. Twice drying at room T over P_2O_5 in attempt to improve photograph apparently spoilt specimen. Specimen non-crystalline at 75% was never re-converted to crystalline ✓

Tilting camera

Series of tilting photographs ✓ minor adjustments to camera.

All specimen silk thick fibres (40–70μ) 75% RH

18.4.52 75% Ni filter

(45) 3 films. Exposure unknown (3–7 days, ∴ 6 exts)
Single fibre ~40μ
→ good photo, showing some double orientation N.B

(T0) specimen previously X-talline, now gives "wet" diagram (49) see below
(2 films, ~3 days)

(T1) Single fibre, ~50μ. 16 hrs
Tilt ~14° (edge set to 61)

(T2) Chromium 21 hrs, thin V filter
Tilt as above

(T3) As T2. 2 films
On 18/21.4.52. 6 p.m. (Friday)
Still running Sat., filament turned on before Mon. 21st
Developed 21.4.52 3 p.m. Dirty centre.
Specimen deteriorating → "wet" ∴ changed

(46) As (45), but Cr and V filter
Exposure as for T3 – result blank films

(T4) Exposure 16 hrs, 1 film, no filter Tilt ~18°
→ "wet" diagram v well oriented. Dirty centre
∴ specimen transferred to Unicam ?

T4 specimen was dried 4 hrs over P_2O_5 ∴ this apparently destroyed x-talinity ∴ New specimen not dried

(T5) New specimen. Beam centred ~~vertically~~
Tilt ~18°. Lead pinhole removed from tube. No filter
X specimen moved. V dirty centre ∴ replace pinhole

(47) As (46). On 7 p.m. 21.4.52
Exposure to 26.4.52 10 a.m. ~~10 a.m. 22.4.52~~
Result – X-tal diffraction pattern of foreign body + diffuse ring
Specimen has "necked" over collimator hole → ~⅔ diameter of needle

(T6) Black paper over film ∴ dirty centre blacked
due to soft radiation scattered from glass collimator
– shadow of DNA fibre (~50μ) appears sharply
on dirty centre. Specimen as ∴ T5, no filter
Exposure 3 days. Weak x-talline diagram ∴

26.4.52 Copper target replaced

(48) 3 rolled fibres (for double orientation) viewed edge on, Industrial G film,
no filter, exposure 16 hrs
→ mainly wet photo, v strong exposure
– no trace of X-tals shown by (47) although
collimator had not been cleaned meanwhile
∴ X-tals were discharge product of DNA fibre

Filament life ~ 250 hrs

Filament

? See above p. 2

(49) Specimen from TO (which gave good "wet" photo) re-exposed at 75% RH. 2 films, Ni
29.4.52 11 a.m. – night of May 1-2 (filament burned out)
i.e. exposure 33 – 44 hrs
NB Film B back to front. V good "wet" photo
New filament

(50) Drilled fibre, 75%, no filter, Industrial Cu
2.5.52 3.20 pm – 5.00
⇒ wet photograph, mod. well oriented
∴ put specimen & dry over P_2O_5

(51) Specimen as (49) with holder centred over collimator so as to include both 3.4 Å arcs

51c measured on FON 53

2.5.52 7.30 p.m. – 6.5.52 5 a.m. with interruption of 32 hrs i.e. 62 hrs

(50) Sticks = outer pair of diagram ( ))) are v strong and differently shaped from normal "wet" diagram, big more rounded. Is this an effect due to double orientation of e.g. elliptical blocks?

(47)

$2\ell = 2 \times 14.2$ cm $= 2D$ 5

Shows rings of spots. D Diameter, measured
Assume specimen-film distance 14.2 mm

2(l-a)	Style	tan 2θ	θ	d	log d
1.65	m	.581	15°5′	4.38	.641
1.89	v w	.665	16°48′	3.95	.597
2.13	m	.750	18°26′	3.671	.5575
2.29	w	.806	19°26′	3.43	.535
2.63	s	.926	22°24′	3.13	.495
2.70	w	.951	21°47′	3.08	.489
3.14	s	1.106	23°56′	2.82	.450

Also four diffuse rings at 8–9 Å

Cell prob. too small to be phosphate

Wyckoff gives $AgPO_3$ cubic, a = 6.00
KH_2PO_4 tetrag. a = 7.43, c = 6.97
$(NH_4)H_2PO_4$ " 7.53 7.54
Li_3PO_4 orthorhombic 4.86, 6.10, c = 6.07

$NaHCO_3$ a = 7.51, b = 9.70, c = 3.53, β = 93° 19′
NH_4HCO_3 7.29 10.79 8.76

ref to helix ↓

(49) 49B

Rough measurements on projection drawing (2.5.52) (tapping layer-lines with straight)

Layer-line spacings, mm :— (: 2z)

14·8, 30·5, 46, —, 79, —, —, 131

Suppose specimen-film distance = 14·4 mm

3·4 Å meridional are here $2z = 164$ mm, $\theta = 13°4'$, $\tan 2\theta = \cdot 491$

$\tan 2\theta = \frac{2z}{2 \times 167}$

$\therefore$ Specimen-film distance for projection : $\frac{166}{2} \times \frac{1}{\cdot 491} = 167$ mm

$\therefore \tan 2\theta$ for layer-lines = $\frac{2z}{2 \times 167} = \frac{2z}{334}$

= ·043, ·094, ·1378, —, ·2365, —, —, ·392, —, ·506

θ = 1°16', 2°37', 3°55', —, 6°34', —, —, 10°42', —, 13°29'

d = 34·8, 16·8, 11·3, —, 6·64, —, —, 4·14

Multiplying by 1, 2, 3, —, 5, —, —, 8, 9, 10 gives :—

34·8, 33·6, 33·9, 33·2, 33·2, 33·2

$\therefore$ layer-line spacing : 33 – 34 Å

3·4 are ~ corresponds to 10th layer-line

(if helix is non-integral no. turns per turn, 3·4 are not necessarily lie on a layer-line) ✓

if there is a helix

Equator strong doublet at 20·8, 23·2 mm

On above approx (using 3·4 cm) this gives 24·6 Å, 22·1 Å

This suggests co-existence of 2 phases differing only by 1 molecular layer of water separating chain units

Some erratic effect in humidity? (we never observed this in much later work MW)

Taking mean pos^n of 1st doublet and centre of diffuse equatorial spot gives 23·3 Å, 13·8 Å, 9·3 Å, 5·42 Å

~~They do not fit hexag. close-packing~~

this fact, together with the 3·4 are lying on a layer-line suggests that there is an integral no. (or nigh fractional no.) of residues per turn of helix (if there is a helix) even in the "wet" state.

In passing from "crystalline" to "wet" the predominant strong equatorial spacing is approximately doubled, & the fibre-axis period is extended by ~ 25%

(77 Å → 34 Å)

do not correspond! Odd confusion?

(Lengthening of fibre?)

There is a weak equat^l at longer spacing on 2 patterns

(52) A 51, with Na_2CO_3
on 6.5.52 6 p.m.

51A

Running a projection and taking meridional arc to be 3.5
gives equatorial zenith 26.3 and 9.93 (week of 4 days)

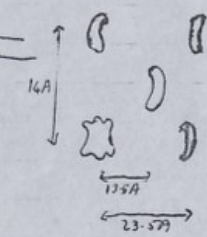
2 July 52

2.7.52

according to Klug she failed to try to fit the correct helix.

Notes on first cylindrical Patterson

General form

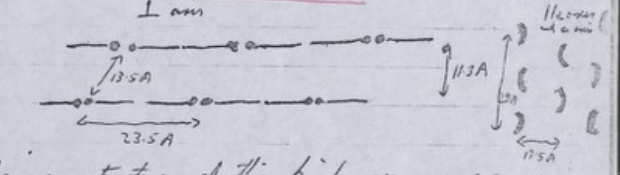


There is no indication of an helix of diameter 11A.
The vertical banana-shaped peaks fits curve calc. for helix of diameter 13.5A having 2 turns / unit cell
If a helix there is only one strand
(2-strand helix would give ⊗)
If a helix, it is v far from continuous uniform density. Has obey transf for x 6-7 A.
Helix does not explain vertical short vector ~ 4A (this is superimposed on peak at origin, so represents true distance of > 4A). But if there is a flat banana-like unit in structure, with banana axis ∥ fibre axis this vector is explained.

Cylindrical Patterson should give unit cell. Projection of a and b axes on plane ⊥ fibre axis being ~ 13.5 and 23.5 A. } differs little from 60°
~~If bananas are flat & vertical, not helical, this explains why there are 23.5A arcs but ~~ ~~they are~~
i.e. trabeculae all ~ ½ size of previously considered primitive cell of monoclinic face-centred lattice.

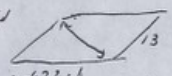
Again, the dimensions of this cell make a helical structure impossible - if helices of 13.5A diameter there is the wrong space - the long spacing filled.

Suggests rather a double sheet structure



Also a structure of this kind seems necessary to explain double orientation in diagram 45. Effect poss. due to preferential orientation of sheets w.r.t. surface of fibre, and not all of fibre in beam (though nearly all of fibre was in beam)

July 7th

Pattern max. at $x \sim 13A$, $z \sim 7A$ can not be ...
point
∴ call 

would have a lattice vect...
with both x and z values intermediate between t...
of the 2 vectors observed. No trace of this.
∴ Pattern was extended to 46A
this shows a large peak at $x \sim 35A$, $z \sim 7$
i.e. it is to the peak at 23A as is the 13A peak to the ...
∴ this is not a lattice point
It seems probable that both lattice vectors are
~~included~~ contained in the 23A peak. Because the ...
form might be due to one peak on x-axis and
one slightly off and nearer origin. This would give
$\beta \sim 93°$, which seems reasonable for measuring
There is no lattice peak between 24A and,
at the nearest, 36A. ∴ the cell is strongly
centrosymmetrical

15 July

July 15th

by Petti. [illegible] near. // [illegible] between 4-5 ft
and N 14 E

· Fire is in narrow straight chain of high density // axis.
: o high-density regions or discrete regions, not columns
Cyg between x = 6 & x = 10

14 Aug → 1 Sep

14.8.52

(60) Fair fibre of Sigiera 10 node circuits (~120μ) covering ½ of 80μ aperture, to look for double orientation due to edge effect
14.8.52 12.15 p.m. – 15.8.52 10.45
fibre grey. Trace of double orientation ?

(61) Sigiera (2), fibre ~15μ Free white Xtalline
15.8.52 11.45 – 18.8.52 9.45
→ wet diagram (v weak)

(62) Sigiera (3). Pulling properties resemble (1) rather than (2). Fibre ~5-0μ
18.8.52 4 p.m. – 19.8.52 3.30 p.m.
→ Xtalline photograph (poor)

(63) 19.8.52 6 p.m. – 25.8.52 11 a.m.
As (60), same fibre, covering ~⅓ hole
no double orientation

(64) Fibre Sigiera (1) ~40μ, 75% RH
25.8.52 12 p.m. – 26.8.52 6 p.m.
Good photograph, but with strong trace of xtalline impurity – withdrawn thicker

(65) Fibre used in (60) and (63) replaced. 75% RH
26.8.52 7 p.m. – 27.8.52 3 p.m. – 20 hrs

(66) As above, using $Ca(NO_3)_2$ sat.
27.8.52 4 p.m. – 28.8.52 2 p.m. – 22
→ similar to (65 but with one xtalline impurity

(67) As above, using $CaCl_2$ (in jar: flasks sintered bubblers) stood over calc. chlor.
28.8.52 6.30 p.m. – 29.8.52 3 p.m.

(68) Over $Ca(NO_3)_2$ 3.30 p.m. 29.8.52
29.8.52 Exposed 5 p.m. – 30.8.52 12 p.m. – 19
→ photograph similar to 67

(69) Over P_2O_5 in hydrogen, 12.30 p.m. 30.8.52
1.30 p.m. on → 31.8.52 8 a.m.
Fibre fogged ✗ repeat

(70) As (69)
1.9.52 10.30 a.m. – 2.9.52 2 p.m.
again fogged (1 strong line)
– this due to acid vapour?

(71) Repeat as (70). On 2.9.52 4 p.m. → 3.9.52 4.30
fogged again
- must be : wet vapour. Why ?

(72) $NaClO_3$
3.9.52. 4.45 in camera
Exposed 6.15 - dry 2.15 4.9.52

(73) Na_2CO_3
4.9.52 5.30 in camera
Exposed 6.30 — 5.9.52 2.30
→ X-tallin photo A

(74) Wetted by standing ~10 minutes over dil. sol $NaClO_3$
→ length change, moved off collimator hole
then exposed it in till came back over hole &
exposed to Na_2CO_3 in camera 4 p.m. 5.9.52
Exposed 5 p.m. - 6.9.52 11 a.m.
Fibre too flimsy - too wet

fibres close to hole in collimator stays in B at 75% r.h

from Sigma (3)

(75) New fibre, ~100 μ, light blue very close to collimator hole (~0.2 mm fibre exposed)
In camera, with Na_2CO_3 1 p.m. 6.9.52
Exposed 3 p.m. — 8.9.52 10 a.m.
→ wet photo with trace of crystallin

(76) Same fibre as (75), with $NaClO_3$ 11 a.m.
exposed 11.40 — 3.30
→ "wet" photo
∴ genuine drag third over P_2O_5 before exposing to $NaClO_3$

(77) 9.9.52 exposed 1.20 — (?)
→ wet photograph

could not get it back to B from

(78) 14.10.52 New fibre, 60-70 μ. Over $NaClO_3$
Crystal 45 m. —

(A) Sep 51 → Mar 52

Could be 2 notebooks 9-15 Nov 51 ish all weighing for water content of DNA

10 oct selected fibres good extinction

Swelling experiments
20.12.51. 'non-pulling' Segner dna (i.e not normally used for X-ray) rapidly doubled diam at 92% r.h. + at 100% after 2 hrs increased by about 10 times!

Sept. 1951 → Dec 51 – 3 Mar 52

Segner N.A., bundle of fibres, selected dumped over sat. $KClO_3$ & straightened & slightly extended.
Micro camera. Fluorescent screen. No filter

1. 1st small specimen, over $KClO_3$. 2 hrs 10 m
2. New specimen 10 m
   pack v. wet, drop of water in camera
3. Same, dried, over sat. $KClO_3$
4. stretched ~ 50% of its length, over $KClO_3$
5. Same specimen, over sat. NH_4Cl, 15 m

19.9.51 3 p.m. in camera, N_2 flow started. Sat. NH_4Cl in camera
New filament
20.9.51 Exposure 2.15 – 5.45

80%

6. 20.9.51 6.30.p.m Some specimen in camera, over Na_2CO_3 in camera 2 in H_2 flow
21.9.51 exposure 3½ hours
~~22.9.51 Exposed 4 hrs~~ 92%

7. As 6. 21.9.51 6 p.m. H_2 flow, Na_2CO_3
~~24.9.51~~ 6 exposed 5 hrs
Specimen was stuck ~ 0%

~~8~~ 7 ~~23.9.51 12 p.m. $NaNO_2$ equil. @ 78%~~
~~24.9.51 5 p.m. H_2 flow, Na_2CO_3~~
26.9.51 Exposed 3 hrs (3–6 p.m.)

~~8 26.9.51 2 p.m. over $NH_4Cl + KNO_3$~~

~~Na_2CO_3 92%~~

end of Sept.

8. 27.9.51
5 p.m. over sat $CaNO_3$ → equil @ 51%
5.30 – 6.00 (49–53%)
1.10.51 11.30 – 5.00
(6 hrs)

9. Specimen built up from ~ 30-35 Silver fibres, stuck together by keeping wet. ?!

1.10.51 6 p.m. over H_2, sat NH_4Cl
2.10.51 10.15 – 12.30

10. 2.10.51 over Na_2CO_3 (92%)
1 hr to equilibrate, 4 hrs exposure
– sample moved: it was wet

10 Oct

Strange experiment using NH_4Cl. volatile salt? MW

10.10.51

Single fibre of Sigrer DNA, fairly thick, part selected as giving better extinction than most thick fibres. though not perfect

Micro camera

100μ collimator (fibre diameter ≈ ¼ collimator diameter)

Ni filter

Specimen stretched over collimator using holder, then under set, glued to collimator on either side of hole

0.26 m.a. 36–38 KV

2 p.m. H_2 through sat. NH_4Cl through camera, sat. NH_4Cl in camera

2.30 p.m. tube on

12.10.51

11 a.m.

NH_4Cl solⁿ found in camera (specimen unharmed)

Fibres developed ∠ no good

(10) A B & C

12.10.51
Some specimen & cond^n, repeat
2 p.m. camera set up w H_2 & NH_4Cl sat.
8 p.m. tube on (Filament 69 hrs)
13.10.51 4 p.m. Filament burnt out
15.10.51 11.30 a.m. tube on (New Filament)
filament burnt out during night of 16-17, &
not developed

17.10.51 tube in position, pulling, flattening
Tube cleaned, new filament
→ new lighter flame (to light with)
5 p.m. tube on

18.10.51 5½ Same again, during night
Tube cleaned, new filament 4 p.m.
19.10.51 Stopped for 6 hrs to renew brass cap
20.10.51 H_2 stopper blown off during night. Stopped 7 hrs
21.10.51 ✓
22.10.51 Filament burned out during night.
Renewed & target cleaned. Started 2 p.m.
23.10.51 2 p.m. ✓✓ - developed

25 hrs
31-43
2-15
53-77
24

Total exposure 135 — 184 hours

end of Oct Chargaff?? Yugoslav

23.10.51 Yougoslav carbon (3) 2.30 – 5.30

(11) β Coli 6 p.m. (NH_4Cl, filter)

24.10.51 12 p.m. stopped (18 hrs)

(12) 24.10.51 4 p.m. embryo rat tail collagen

H_2 through sat. $Ca(NO_3)_2$, not in camera

exposed 1 hr

25.10.51 10.30 – 1.00

3.30 – 10.00 } 10 hrs

3 films, tail specimen ∴ distance ~ 1

Equatorial arc 3.8 mm

$\tan 2\theta = \frac{1.9}{13.5} = .14$ $\theta = 4° 0'$

$d = 11.0$ A

Diffuse ring 8 to 13 mm

$\tan 2\theta = .30$ to $.48$ $\theta = 8° 21'$ to $12° 48'$

$d = 5.3$ to 3.5 A

Meridional arc 17 mm

$\tan 2\theta = .63$ $\theta = 16° 6'$

$d = 2.8$ A

30.10.57

Oct 30

Pin-hole photographs on Ehrenberg tube

Pinhole size - 5 divisions on micrometer scale
$= \frac{5}{80} = .0625$ mm

Distance pin-hole → tube cross ~ 1.15" = 29 mm

Distance " → film 12", 20" and 29"
i.e. 305, 510 and 740 mm

Size of image. @ 29" 1.5 → 2.3 mm × 3.2 → 5.5 mm
" 20" 1.0 → 1.6 mm × 2.3 → 3.7 mm

∴ penumbra @ 29" $\frac{0.5}{2} \times \frac{2.3}{2} = 0.4 \times 1.15$ mm

" " 20" $\frac{0.6}{2} \times \frac{1.4}{2} = 0.3 \times 0.7$ mm

∴ focal size (given by 29" image) $= \frac{1.15}{29} \times 0.4 \times \frac{1.15}{29} \times 1.15$
$= .016 \times .046$ mm²

Decembrium Glass Tube

cath. int. diam. 15·55 mm

Length 70 mm

(13)

2 Nov

2.11.51

Bundle of Sigma fibres (prepared Sept. 51) in micro-camera on Decembrium tube. Stopped to collimator near hole w. narrow 0·1 mm Al strips.

Ni filter 2½ ma., 37 KV, bias

$NaClO_3$ sol^n, H_2 ∠ in camera

11.00 a.m. camera set up, H_2 over

11.45 tube on

5.45 Off } 6 hours

(13a) As above, with Na_2CO_3 sol^n (92%)

2.11.51 6.30 p.m. specimen in camera, H_2 flow

7 p.m. tube on

3.11.51 Filament burnt out during night

5.11.51 Transferred to Chemistry tube

11.45 tube on

Good diam., 2·4 angs through filament (ult. protonema ~ 1 cm thick)

5.45 Off

→ "wet" photo

5 → 9 Nov-51
10

(15) As above

5.11.51 6.30 over H_2, $NaClO_3$

6.11.57 4.00 - 9.45 } 10½ hrs

7.11.57 10.45 - 3.30 }

→ 'crystalline'

(16) 7.11.51 4.00 over $Ca(NO_3)_2$, H_2

6.00 on

8.11.57 Switched off during night

on 11.30 - 3.00

→ 'crystalline'

(17) As (16). 5.11.51 6.00 on 9.11.51 10.00 off

Specimen broken – no photo

(18) 9.11.51 Same specimen, pared down with Al strips one end basic

10.30 over $CaCl_2$, H_2

11.45 - 3.00 (filament burned ~ 3pm)

10.11.51 New filament

10.30 on (switched off some time between 12.30 & 1.30 & on again 1.30)

3.00 off

Filament life 33.45 hrs

(19) As above

P_2O_5 in camera H_2 through 98% H_2SO_4

10.11.57 H_2 3.30 p.m.

12.11.57 10.45 on } 7¼ hrs

6.00 "

P_2O_5 in camera got v wet. film blackened probably ∴ acid vapour

(20) As above

after H_2 through 98% H_2SO_4, over KOH on P_2O_5

P_2O_5 in camera

13.11.57 4 p.m. H_2 through camera

5.45 tube on "

Specimen moved } 22 hrs

14.11.57 4 p.m. — 15.11.57 12 noon

(21) As above Na_2CO_3

15.11.57 12.45 in camera, H_2 'drying plate'

5.30 on } 22 hrs

16.11.57 9.30 "

Filament 55 hrs so far

French rat DNA?

(22)

H_2 about 16.11.57 4.30 over Na_2CO_3 "dry" photo
6.30 on } 19½ hrs ∴ good resolution
17.11.57 2.00 off }

(23) 17.11.57 4 p.m. over $K_2Cr_2O_7$ (99%) ∴ wet
8.11.57 12.00 specimen has visibly wetted
18.11.57 12.~~15~~ ∴ camera over Na_2CO_3
12.55 on } 22½ hrs. Hydrogen flow stopped during night
19.11.57 11.15 off } "dry" photo

(24) Specimen wetted by standing over $K_2Cr_2O_7$, then
over Na_2CO_3 ∴ camera 4 days during exposure
30 hrs

French rats

(25) French rats, specimen A. Bundle of fibres
straight from tube placed over 100μ collimator
26.11.57 3.30 ∴ camera over $NaClO_3$
27.11.57 5.00 on } 17½ hrs Top film, fine grain
28.11.57 10.30 off } 2nd film, monocoarse
(liquid got into camera at start)

19½
22½
30
·7½
89½

Filament 145 hrs
so far

Odd idea ↘ 6 Dec

DNA fibres suspended in alcohol - water - alkali mixtures

6.12.51 6 p.m. Bundle of fibres, as received (Signer non-polling)

1. Wt bottle + suspended fibre 64.4 g
   " " + alcohol 75.4 g
   " " " + water 76.1 g
   + ~ 0.01 g KOH

8.12.51 + more water ~ 72.7 g
nearly dissolved
(a little left clinging to upper fibre

---

2. Fibre bundle tied w fine Cu wire, suspended in 70% alcohol
   → v highly swollen gel
   added little alcohol (~ 5%)
   - still v swollen gel
   added ~ 0.03 g solid KOH (to ~ 18 cc liquid)
   fibre bundle immediately shrinks & transparent gel becomes opaque — Violent treatment!
   Shrunk to ~ ⅓ length (in ~ 10 mins)
   Removed from liquid shown it to be still gelatinous
   - left to stand - liquid

10 Dec

10.12.57 10 a.m.

K-specimen apparently unchanged. (Sol yellow, prob.: smell from Cu wire)

Specimen removed, and gelatinous piece of length ~ 3 in. stretched to fibre 30 - 70 μ, ~ 2 cm long

- stretching v easy and smooth → +ve fibre

∴ reject

3. Rej 3 p.m. bundle of fibres suspended in 10 c.c 70% + 10 c.c 80% alcohol.

3.35 still opaque (but gelatinous). Transferred to 70% alcohol

5.30 Added 0.05 gm KOH

- specimen broke

4. Added fibre bundle, room dry, to KOH-alcohol - untouched for 3. Shrinkage observed as in 2.

Pulled out to +ve fibre

N.B. These +ve fibres when smeared or when pulled ± ∴ for fibres always remain +ve

fibres in alcohol solutions

11.12.57 Repeated above expts omitting KOH, to see if alcohol alone affects stretching properties. → Gels/threads now behaving as normal material. Not easy to pull to thick fibres as after KOH treatment, & not → rope at any stage

Sound to thin fibres + slats → always readily −ve

13.12.51 Bundle of ~ 20-30 Sigiura pulled fibres tied together with fine Cu wire & suspended in sat. KCl − H_2O − alcohol mixture 11 a.m.
- mixture made up to give extensive swelling
3.30 p.m. put to wash in 70% alcohol
Stretched & broke

Now specimen 20-30 fibres put in KCl − H_2O − alcohol ~5.30 p.m.
14.12.57 11 a.m. put to wash in 70% alcohol
5 p.m. dried over P_2O_5
17 Dec. 12.57 11 a.m. in camera

KOH ?!

13 Dec.

(26) 6 fibres (+ve) of KOH-treated DNA in adapted Guinier camera (specimen over lead guard-hole on Hilger plate of new micro-camera) No filter. 75% humidity ($NaClO_3$)
12.12.57 7 p.m. on. 11 p.m. still on
13.12.57 10 a.m. off during night. Switched on
5 p.m. developed → black film
Repeat with slits more closed (weather good)
6 p.m. → 11 a.m. (14.12.57) (17 hrs)

(27) Bundle of KCl-treated Sigiura fibres
17/12.57 11.30 in camera over H_2, sat. $NaClO_3$ (75%)
(adapted Guinier camera, specimen on brass plate with guard-hole)
12.00 On
~~Dec. 15~~

diam swelling of Signer fibres (non-pulling)
2× at 92% rh !
10× in water (almost)

11–25 Dec
→ 31 Dec 51

20.12.51

Swelling of fibres

Fibres of "non-pulling" Signer DNA, swelling observed under microscope

① Small fibre ~ 0.6 scale divisions (i.e. 8 μ) at narrowest but mounted point
enclosed in 92% humidity (sat. Na_2CO_3)
Rapid swelling → ~ 2× diameter - well-united part rather less
?

② Fibre of marginal quality, finest at best part ~ 8 μ,
Enclosed by water
Rapid swelling → ~ 2× diameter
then slow
after 2 hours, diameter increased ~ × 10 .
length increase small (straight stretched fibre, with ends fixed
→ only slightly wavy)

Small drops of condensed water visible everywhere except
immediately on outer side of fibre (showing that even
for 10-fold linear swelling reduction of VP is appreciable)

11.12.51 → 28.12.51

2 attempts to photograph single fibres ~ 10 μ after
heating one, one exposure 2 weeks; one 1 week
→ very poor intensity, much 'impurity' as only
discarded DNA (need new "non-pulling" Signer specimen)

(28)

27.12.51 Single fibre of old Signer DNA after 3 weeks
over P_2O_5 (pulls v well) ~~0.001~~ 0.001" Al over ½ film 3 films
Cookeh? Baked over-night at > 50° (6 p.m. - 10 a.m.)
28.12.51 5 p.m. in camera, H_2, $NaClO_3$
6.00 tube on (new filament)
29.12.51 12 noon beam v weak
31.12.51 10 a.m. beam invisible. Developed
→ wet photograph
specimen baked over overnight before next photograph

(29) 67% RH 3 films
Poor resolution

(30) As (29) 68% RH 1 film
still poor resolution

Jan 52

(31) 7.1.52
~70% RH, new fibre ~ 40μ
Beam down tube, chromium target, no filter
on 7.30 p.m.
8.1.52 2.30 off. Blank film
- fibre moved: not stuck directly on collimator

(photo under-exposed, & resolution on equator v poor)

(32) 22.1.52
Bundle of ~10 fibres of Signer DNA 2
Micro-camera, Ni.
Specimen dried 3 hrs over P_2O_5. Then @ 75% RH
22.1.52 6 p.m. → 23.1.52 10 a.m.
wet diagram

(33) 24.1.52 6 p.m. → 25.1.52 10.30 a.m.
3 20-40μ fibres Signer DNA 2. Dried 50°
no filter, 73% RH
→ wet diagram (with badly fogged centre)?

7 Jan 52
→ 24 "

25.1.52 → 1.2.52 Series of photographs with Signer DNA 1 and 2, humidities 60-80%, always → "wet" photo
is this: specimens were heated in air? (40-60°C)

(34) as above, Signer 1, no filter, 65% RH
→ "wet" photo 1.2.52. 16 hrs

(35) New specimen dried room T over P_2O_5 ~ fifty 6 fibres
→ "wet" photo 2.2.52 16 hrs

(36) 3.2.52 4 30μ fibres
New Signer DNA ~ fifty. 74% RH
3.2.52 2 p.m. → 5.2.52 11 a.m.
→ "wet" photo

(37) New filament
Bundle of Signer DNA fibres, wetted & stretched to ~ 2× length
No $CaCl_2$ tube, no hygrometer (use "silica gel"); No filter
5.2.52 2.30 → 6.2.52 10 a.m.
→ "xtalline" photo, v weak exposure & poor resolution

10.55 specimen on camera & oven at 50°C till 2.30

7 Feb 52
→ 3 Mar

38 Specimen as above: after 4½ hrs @ 50°. Ni filter
7.2.52 3.00 – 8.2.52, 3:00 — 24 hrs
→ "crystalline", apparently better oriented. Absolutely lightly better but still poor. ⊥ to elevated ~ 80°
In oven 3.30, exposed 3 days – forgot

38 ~6 Sigma 1 fibres // but converging
~½mm in depth from surface of collimator. Ni. $NiCl_2$
12.2.52 9.30 on
→ photo showing some well-oriented — strong amorphous ring. Specimen entered 1/st +ve fibre – presumably +ve fibre gave amorphous ring

39 2 fibres Sigma ② ~20–30μ ⌐8⌐ strong
no filter, 75% RH
18.2.52 3 p.m. on. 19.2.52 10 a.m. off
→ "wet" type photo ∨ trace of fine spots on equator

40 4 Sigma ① fibres, 18–30μ. Dried 6 hrs over P_2O_5
Ni, 75% RH
20.2.52 5.30 → ? (tube off during night – probably very faint)
→ ∨ weak "fibre", orientation apparently good, resolution doubtful

41 Same specimen, reset w 3 fibres ∠ smaller hole Ni
21.2.52 11.00 on } 48 hrs
23.2.52 11.00 off
→ ∨ good, even good, resolution moderate.
Repeat longer exposure

42 New filament (filter not burned), about longest Ni. 3 fibres
23.2.52 1.00 on
26.2.52 off for 1 hr to clean target } 116 hrs
28.2.52 10.00 off

43 This is odd after such long exposure to salts. Is this evidence for hysteresis + after drying?
Same specimen, 92% RH
(test for 1h over 92% showed fibres dried more)
28.2.52 12.00 on.
29.2.52 2.30 a.m. off (H_2O_4 ff) } 14½ hrs
→ X-talline

44 Same specimen but now only 3 fibres (farthest East)
29.2.52 5 p.m. on
10.30 p.m. filament burned out
1.3.52 12.30 p.m. on. 3.3.52 12 a.m. off
3.3.52 11 a.m. on

This may be 2nd Notebook for weighing data.

Weighing

9 => 15 XI 51

Adsorption of water by DNA

4 specimens (3 French arcuous nets / Signer fibre-pulling) in weighing bottles in vacuum dessicator.

Save dates in earlier part for X ray pattern

9. 11. 51 4 p.m. Weighing bottles and specimens (in specimen tubes) evacuated over P_2O_5

10. 11. 51 1.30 p.m. Bottles weighed empty + DNA

12. 11. 51 11 a.m. re-weighed 5 p.m. re-weighed 5.30 evacuated over sat. KOH

13. 11. 51 10.15 weighed 5 p.m. re-weighed 5.30 p.m. over sat. $CaCl_2$

14. 11. 51 10.30 a.m. Humidity 40% (hygrometer-correction) weighed, then left over sat. $CaCl_2$ not evacuated

5 p.m. 39% re-weighed

5.30 p.m. over $Ca(NO_3)_2$

15. 11. 51 11.45 77%

2.30 re-weighed 76.5%

2.45 over sat. $NaNO_2$

6.30 71% weighed

Specimen	S	F	C	B
Weighing bottle	1	2	3	4
Wt bottle	8·3959	8·0798	9·5953	7·9100
Bottle + specimen	8·4318	8·1291	9·7185	7·9425
13/11/51				
Specimen 13/11/51	0·0359	·0293	0·1232	0·0325
12.11.51 11 a.m.	8·4289	8·1288	9·7173	7·9425
" 5 p.m.	8·4291	8·1287	9·7175	7·9421
Specimen	0·0331	·0289	0·1221	0·0323
13.11.51 10 a.m.	8·4314	8·1303	9·7216	7·9443
" 5 p.m.	8·4313	8·1303	9·7215	7·9442
Wt H_2O	·0023	·0016	·0041	·0019
	7%	5·5%	3·4%	5·9%
14.11.51 10.30	8·4341	8·1321	9·7256	7·9470
5 p.m.	8·4341	8·1321	9·7254	7·9470
Wt H_2O 13/11/51	·0051	·0034	·0080	·0047
	15·4%	11·9%	6·6%	14·6%
15.11.51 11.45	8·4428	8·1372	9·7377	7·9555
Wt H_2O 7%	·0138	·0086	·0203	·0132
	41·7%	29·8%	16·6%	40·8%
2.30	8·4425	8·1370	9·7376	7·9552

	S	F	C	B
	1	2	3	4
13.11.51 6.30 p.m.	8·4413	8·1363	9·7362	7·9541
H_2O (mean) 7%	0·0025	0·0076	0·0188	0·0118
	37·8%	21·2%	15·4%	36·6%
14.11.51 10.15	8·4416	8·1363	9·7360	7·9573
" 3 p.m.	8·4428	8·1372	9·7375	7·9552
7·8% H_2O	·0138	·0080	·0203	·0132
	41·7%	25·8%	16·9%	40·8%
" 5.45	—	8·1380	9·7388	7·9564
Wt H_2O		·0023	·0214	·0141
8%		32·2%	17·5%	43%
17.11.51 2.45	—	8·1476	9·7614	7·9691
Wt H_2O		·0189	·0440	·0320
9%		65·4%	36·0%	83·0%
18.11.51 12.30	—	8·1502	9·7749	7·9740
Wt H_2O		·0215	·0575	·0317
9·8%		74·5%	47·1%	98·2%
19.11.51 10.15	—	8·1457	9·7743	7·9690
Wt H_2O 8%		·0170	·0569	·0267
		58·9%	46·6%	82·7%

16.11.51 10.15 weighed 71%
10.45 over sat. NH_4Cl
3 g.m. 78.5 - weighed
gives the results as $NaNO_2$
3.45 g.m. over Na_2CO_3
5.45 weighed 87%
17.11.51 2.45 96% weighed
3.00 over $K_2Cr_2O_7$
18.11.51 12.30 98% weighed
12.45 over sat. KCl
19.11.51 10.15 87.5% weighed
10.30 over sat. $NaClO_3$
2.15 76.5 - weighed
20.11.51 10.30 76.5% weighed
" 3.30 74.5% "
" 3.45 over $NaNO_2$
" 7.00 weighed (forgot hygrometer. Shd be 71%)
over $CaCl_2$.
21.11.51 10.30 40.5% weighed
" 3 g.m. over sat KOH
22.11.51 10.30 weighed
23.11.51 11.30 "
" 11.45 evacuated over P_2O_5 26.11.51 11.30 weighed

	S	F	C	B
	1	2	3	4
Dry wt	0.0331	0.0289	0.1221	0.0323
" + bottle	8.4290	8.1287	9.7174	7.9423
19.11.51 2.25	8.4427	8.1423	9.7306	7.9651
76.5%				
20.11.51 10.30	8.4447	8.1398	9.7629	7.9580
" 3.30	8.4441	8.1391	9.7610	7.9569
H_2O, 10.30 76.5%	.0157	.0111	.0455	.0157
	47.5	38.4%	37.3	48.6%
20.11.51 7.00	8.4425	8.1379	9.7577	7.9552
71% (1)	.0135	.0092	.0403	.0129
	40.8%	31.8%	33.0%	40.0%
21.11.51 10.30	8.4374	8.1347	9.7318	7.9503
40.5%	.0084	.0060	.0144	.0080
	25.4%	20.9%	11.8%	24.8%
22.10.51 10.30	8.4328	8.1317	9.7236	7.9455
23.10.51 10.30	8.4327	8.1317	9.7236	7.9455
	.0038	.0030	.0062	.0032
	11.5%	10.4%	5.1%	9.9%
26.11.51 11.30	8.4289	8.1285	9.7175	7.9418

4.12.57	4.30	74.5%	- weighed
	4.40	over H_2SO_4, wetter	
	6.50	82.5%	- weighed
	7.00	over P_2O_5	
5.12.57	10.30	over H_2SO_4	
	2.00	79%	- weighed
	6.00	83.5%	- weighed
6.12.57	11.00	over sat. KCl	Exp. 65%
8.12.57	4.15	87.5%	- weighed
	5.00	over P_2O_5	

		S	F	C	D
		1	2	3	4
		0.0331	0.0289	0.1221	0.0323
		8.4290	8.1287	9.7174	7.9423
4.12.57	4.30	8.4384	8.1353	9.7300	7.9573
	74.5%	0.0094	0.0066	0.0126	0.0090
		28.4%	22.8%	10.3%	27.9%
4.12.57	6.50	8.4396	—	—	7.9526
		32.0%			32.5%
8.12.57	2.00	79% 8.4371	8.1345	9.7285	7.9499
		24.5%			23.5%
	6.00	83.5% 8.4411	8.1372	9.7335	7.9541
		36.9%			36.5%
8.12.57	4.45	87.5% 8.4675	8.1410	9.7518	7.9599

Adsorption of water by DNA at 25°

8-10 Jan 52

Weighing bottle ① Sigmer batch ② not pre-heated
② " " pre-heated ~~4 hrs~~ 75° over P_2O_5
③ as ②
④ Fresh rats B, treated as ② and ③

Specimens cooled overnight over P_2O_5 and
weighed 10.30 a.m. ~~3.1.52~~ 4.1.52
11.10 in thermostat 26° over sat. KOH
2.45 weighed. 2.55 Replaced in thermostat
6.15 re-weighed
6.30 ~~in~~ over 25° over H_2SO_4 - H_2O
7.1.52 10 a.m. to dry (< 2%) in charged H_2SO_4 sat
7.15 18 % RH weighed
7.30 put over water H_2SO_4
8.1.52 10.30 a.m. RH 42 % weighed
2.30 put over water H_2SO_4
9.1.52 10.30 a.m. 67 % - weighed
11.30 put over water H_2SO_4
7.0 75 % - weighed - over water H_2SO_4

10.1.52 3.00 78 % - weighed Left for 10 days over same sol^n

Dry wt DNA		·0920	·0614	·0318
	1	2	3	4
Bottle only	7·3623	8·0998	9·5953	7·9100
4.1.52 10.30 Bottle + specimen	~~—~~ (7.46?)	8·1918	9·6567	7·9418
4.1.52 2.45	7·4797	8·1962	9·6596	7·9435
" 6.15	7·4763	8·1973	9·6604	7·9439
Wt H_2O		·0055	·0037	·0021
% H_2O		6·0%	6·0%	6·6%
7.1.52 7.15	7·4698	8·1972	9·6601	7·9437
Wt H_2O	·0096	·0054	·0034	·0019
% H_2O 18%		5·9%	5·5%	6·0%
8.1.52 10.30	7·4740	8·2005	9·6625	7·9449
Wt H_2O	·0138	·0097	·0058	·0031
% H_2O 42%		9·5%	9·4%	9·7%
9.1.52 10.30	7·4829	8·2095	9·6688	7·9487
Wt H_2O	·0227	·0177	·0121	·0069
% H_2O 67%		19·3%	19·7%	21·7%
9.1.52 7.00	7·4858	8·2119	9·6707	7·9502
75%	·0256	0·0201	0·0140	0·0084
		21·9%	22·8%	26·4%
10.1.52 3.00	7·4942	8·2195	9·6759	7·9533
Wt H_2O	·0340	0·0277	~~0·0208~~ 0·0192	0·0115
% H_2O 78%		~~30·1%~~ 30·1%	~~31·3%~~ 31·3%	~~36·2%~~ 36·2%

→ 18 Feb 52

22.1.52 5 p.m. 78.5% (still in 23c, since 10.1.52)
23.1.52 10.30 a.m. 85%
25.1.52 6 p.m. 86%

30.1.52 4.30 p.m. 85.5% left to dry over P_2O_5
12.2.52 10 a.m. weighed. Over H_2SO_4 ~ 40%
14.2.52 3 p.m. 39.5%

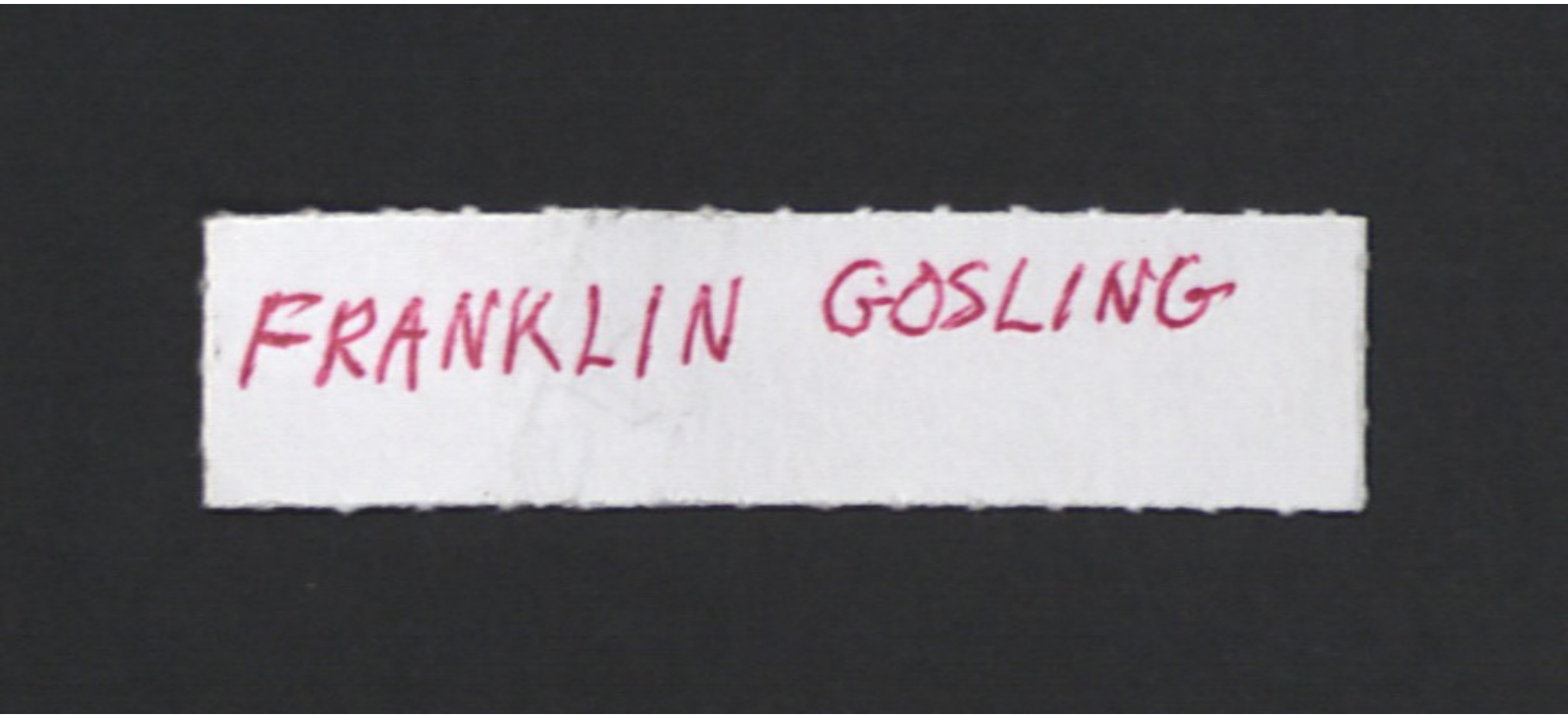
18.2.52 5.30 p.m. 40% weighed
added little water

Dry wt	0979	·0920	·0714	·0318
	1	2	3	4
initial + bag & wt	7.4602	8.1918	9.6527	7.9418
		8.1905	9.6557	7.9412
22.1.52. 5 p.m. 78.5%	7.4990 ~~7.4796~~	8.2257	9.6796	7.9540
$1/3 H_2O$ 78.5%	·0388	·0331	·0229	·0122
% H_2O	39.1%	36.9%	37.3%	38.4%
23.1.52 10.30 a.m.	~~7.50~~ 7.5042	8.2304	9.6832	7.9564
85%	·0440	·0386	·0265	·0146
% H_2O	45.0%	42.0%	43.2%	45.9%
25.1.52 6 p.m.	7.5083	8.2344	9.6859	7.9575
86%	·0482	·0426	·0292	·0156
% H_2O	49.2%	46.3%	47.5%	49.0%
30.1.52 4.30	7.5080	8.2343	9.6856	7.9571
% H_2O 85.5%				
12.2.52 10 a.m.	7.4602	8.1905	9.6557	7.9412
14.2.52 3 p.m.	7.4721	8.2011	9.6630	7.9455
18.2.52 5.30	7.4720	8.2010	9.6628	7.9453
Wt H_2O	·0118	·0105	·0071	·0041
% H_2O 40%	11.9%	11.4%	11.1%	12.9%

→ 29 Feb 52

20.2.52	6.30	47.5%	weighed. H_2O added
21.2.52	11 a.m.	66.5%	weighed. replaced
23.2.52	5 p.m.	66%	weighed. Added little H_2O
25.2.52	2.30	73.5%	re-placed
27.2.52	11.30	74%-	weighed. Added 10 drops water
28.2.52	2.30	76%+	weighed & replaced
29.2.52	12.00	75%	weighed (W) & replaced
1.2.52	4.30	76%	weighed added 8 drops, replaced
4.2.52	5.30	78%	weighed

		1	2	3	4
	Bottle stopper	7.4602	8.1905	9.6557	7.9412
20.2.52	6.30	7.6734	8.2023	9.6626	7.9456
	W+H₂O	.0132	.0118	.0079	.0044
	47.5%	13.5%	13.0%	13.1%	14.1%
21.2.52	11.30	7.4821	8.2086	9.6882	7.9483
23.2.52	5.30	7.4811	8.2094	9.6884	7.9484
	W+H₂O	.0209	.0189	.0127	.0072
	66%	21.4%	21.8%	21.0%	23.1%
25.2.52		7.8354	8.2134	9.6715	7.9503
27.2.52		7.4858	8.2138	9.6717	7.9506
	W+H₂O	.0256	.0233	.0160	.0094
	74%	26.1%	25.7%	26.5%	30.1%
1.2.52	4.30	7.4875	8.2154	9.6729	7.9514
		~~7.4885~~	~~8.2164~~	~~9.6735~~	7.9520
4.2.52	5.30	7.4885	8.2164	9.6735	7.9514
		~~7.4885~~			
4.2.52	5.30	7.4921	8.2144	9.6753	7.9530


FRANKLIN GOSLING

Check for missing page?

24 Feb!

V. brief entry on 10.2.53. 120 with much crossed out MW

48

See [illegible] Structure B on 2-2-53

A.K.

23.2.53

13 days after the 2 sentences about NB 49 C possibly indicating a helix. MW

Structure B

Photograph 51 C

3·4 A are − 158·5 mm on projection

∴ 158·5 = 2R tan 2θ where R is effective specimen-film distance for projection

For d = 3·40 A, θ (calc) = 13° 4′ tan 2θ = 0·491

$$R = \frac{158.5}{2 \times 0.491} = 161.4 \text{ mm} \qquad 2R = 322.8$$

Equator mm	tan 2θ	θ	d (Å)	1/d	λ/d	on Bragg chart	Correction factor
20·2	·0625	1° 48′	24·5	·041	·0629	12·6	(·624 ~~·630~~)
54·7	·1695	4° 49′	9·16	·109	·168	33·6	·614
82	·254	7° 8′	6·19	·162	·249	50·7	·618
~~to~~ 100	to ·310	8° 37′	~~to~~ 5·13	·195	·300	61·7	·617
						mean	·619
120	·372	10° 12′	4·34	·230	·355		
~~to~~ ~~152~~ 152	to ·470	12° 36′	3·52	·284	·438		

These equatorial maxima do not correspond to maxima ∝ $J_0^2(x)$,

which are approximately at 0, a, 2a, 3a

min. $\bar{J}_0(x)$ for x	3·83 10·18
max. $\bar{J}_0(x)$ for x	7·02 13·32

Best first coarse 1st max. is missing (9·16 A reflexion is v weak)

The max. at $\frac{\lambda}{d}$ = ·27, ~~·405~~ ·391, and ·149 ·27

gives $2\pi R r \simeq$ ~~7·34~~ 7·0 for $R = \frac{2\pi\theta}{\lambda}$, $\frac{1}{d} = \frac{\lambda}{2\pi}$ ~~·27~~ ·175

$\therefore r \simeq \frac{7.0}{2\pi \times .175}$ = ~~12~~ 6·36

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5th layer line

1st diffuse spot

$2l$: 88 to 100 mm $\tan 2\theta$: .2725 to .310 θ 7°37′ to 8°37′

d: 5.80 to 5.10 $\frac{1}{d^2}$: .0298 to .0385

$c^2/4^2 J_2^2$: $\left(\frac{3}{34}\right)^2$: .02165

$\therefore \left(\frac{\xi}{\lambda}\right)^2$: .0082 to .0169 ξ/λ : .0905 to .130

ξ : .139 to .200

1st max. for $J_5^2(x)$ has $x \sim 6.5$

$\therefore$ if r : 6.36A, $R = \xi/\lambda = \frac{6.5}{2\pi \times 6.36}$: .163

- fits better with max. $\doteq J_3(x)^2$.

or J_5, at r : 9.4A, giving ξ/λ : .113 which agrees with measurement MW

MW

3rd layer line

1st streak of spots

$2l$: 49 to 65 mm $\tan 2\theta$: .152 to .201 θ : 4°19′ to 5°41′

d: 10.24 to 7.76 $\frac{1}{d^2}$: .00953 to .01665

$\frac{11}{c^{*2}}$: $\left(\frac{3}{34}\right)^2$: .00780

$\therefore \left(\frac{\xi}{\lambda}\right)^2$: .00153 to .00885, ξ/λ : .0391 to .0940

1st max. for $J_3^2(x)$ has $x \sim 4.2$

$\therefore R = \xi/\lambda = \frac{4.2}{2\pi \times 6.36}$: .105

for r: 9.4A $R = \xi/\lambda$: .071 reasonable fit MW

MW

but equator, taking r: 9.4A

MW

Trying to fit one value of r only

should have maxima at $\frac{1}{9.4 \times 2\pi}$ (3.83, 7.02, 10.18, 13.32) $\doteq \xi/\lambda$

i.e. at .065, .119, .172, .226 and zero at 2.40 " and zero at .0406

or ξ : .100, .183, .265, .348

and zero at ξ : .0625 i.e. exactly on observed strong peak

Hence bad fit

MW

Step in right direction – adding J_n for different values of r.

MH

2 helices of different radius for single case of whole number of residues per turn.

Following Cochran Crick & Vand (Acta Cryst. 5 581, 1952)
term $J_n(2\pi Rr)e^{in(\psi+\frac{1}{2}\pi)}$ becomes $J_n(2\pi Rr)e^{i(n\psi-n\phi+\frac{1}{2}\pi+2\pi lz/c)}$
(in present case, $l=n$)

For equator $I=\left[J_0(2\pi Rr_1)+J_0(2\pi Rr_2)\right]^2 = J_0^2(2\pi Rr_1)+J_0^2(2\pi Rr_2)+2J_0(2\pi Rr_1)J_0(2\pi Rr_2)$

For n^{th} layer line, $I=FF^* = J_n^2(2\pi Rr_1)+J_n^2(2\pi Rr_2)+J_n(2\pi Rr_1)J_n(2\pi Rr_2)\left(e^{in(\phi-2\pi z/c)}+e^{-in(\phi-2\pi z/c)}\right)$

$= J_n^2(2\pi Rr_1)+J_n^2(2\pi Rr_2)+2J_n(2\pi Rr_1)J_n(2\pi Rr_2)\cos\left[n(\phi-2\pi z/c)\right]$

Here terms in $J_n J_n'$ may give negative contribution to intensity

but on any layer-line, moving out from the meridian, when the first maxim appears in a J_n contribution (i.e. for the J_n term corresponding to longest value of r) there is no negative term in I, since all other J_n terms are small & +ve

∴ even for complex helical structures, first maxima should give maxim diameter.

roughly correct but really not right. it assumes that nucleotide is radial (all in same plane) & maybe she did not realise it was an assumption MH

On equator, first max. (in J_0^2), excluding central max, neither -ve J_0, ∴ max. diameter can't necessarily be got from equator

In general

$$F_n = e^{in(\psi + \frac{\pi}{2})}\left[J_n(x_1)e^{in\alpha_1} + J_n(x_2)e^{in\alpha_2} + \cdots + J_n(x_p)e^{in\alpha_p}\right]$$

where $\alpha_q = \phi_q - 2\pi z_q/c$

& $x_q = 2\pi R r_q$

$$\therefore I = FF^* = \sum_p^p J_n^2(x_p) + \sum_{p \neq q}^{pq} J_n(x_p) J_n(x_q) \cos[(\alpha_p - \alpha_q)]$$

& same argument applies

i.e. first max. give outside radius

but later max. & equatorial non-central max. complicated

2-strand helix with pairs of groups at opp. ends of diameter

~~$J_n(x_p) - J_n(x_q)$~~ $x_1 = x_2$, $\alpha_1 - \alpha_2 = n\pi$ ~~n~~ yes

died along fibre axis? MW

$\therefore$ layer-lines absent for n odd

& $I = 4J_n^2(x)$ for n even

page number?

(42)

Conclusion

Structure B does not fit right helical theory, even for low layer-lines. S-values of first maxima are too small for right-stranded helix, & even more so for multi-stranded. i.e. we would have Jn on nth l.l. for n strands equally spaced.

Closing radius of helix so that layer-line maximum for four right-stranded (i.e. r = 9·4 Å) gives v bad fit for equator (OK but one should not worry too much because of simplifying assumptions MW)

Outer stage meeting from 3·4 reflection indicates repeat at 3·4 Å is v important — i.e. view  represents structure factor of whole figure, which exists only for c = n λ 3·4, & figure repeats for 3·4 Å spot as for helix

For r = 9·4 Å
She seems to take lack of agreement between 3rd & 5th l.l. with equator to rule out 'single helix' model
Over hasty rejection
MW.

Note underlining of if ! MW

(In R.E.F's terminology, these could still be "type of form", modelled on the 2-strand ones) QK!

Structure B if helix is single-strand helix

i.e. 2-strand, fitting 5th layer-line max. to $J_{10}(x)$, and require $r \sim 17A$ which is much too big

Suppose ~~diameter~~ radius of outer helix 8·5 A

This gives 3rd layer-line max. at $\xi/\lambda = .0805$

at 5th ——— ——— $\xi/\lambda = .122$

– these values are reasonable, because max $\doteq J_3$ / J_5 is near outer edge of peak

For equator, we then have max. at $\xi/\lambda = .072, .132, .190, .250$

and zero for $\xi/\lambda = .045$

– this still has zero rather near the 2nd 5A equator spot

Length of helix of diameter radius 8·5A pitch 34A

$l^2 = 34^2 + (8.5 \times 2\pi)^2 = 1156 + 2850 = 4006$

$l = 63.3$

∴ distance between atoms on 8·5A radius helix $= \frac{63.3}{10}$

$= 6.3A$

Intensity of inner \ / compared with rest of photograph suggests the outer helix (≈8·5A) is heavy part of structure, i.e. P

~~good argument~~ This is not our argument about radial nucleotide MW

For radius 10A

$l^2 = 1156 + 3950 = 5106$ $l = 7.15A$

For radius 9·4A $l^2 = 1156 + 3690 = 4666$ $l = 6.82A$

A + B similar!
MW

[If right-hand helix as above is basis of structure B, the structure A is probably similar, with P-P distance along fibre axis < 3·4 A, probably 2-2·5A

similar with respect to P-P dist
MW

(c.f. 2A indicated by pos" of P-P peaks – Pattern d 2·5A " " 11th layer line reflection)

a.k.

Now with radius 8·5 A she seems to feel discrepancy of 3rd & 5th with equator less serious & is prepared to consider the model evidently 'similar' does not mean that A is helical see Klug
MW

24.2.53 5

NB only Second day on B. MW

Single-strand helix for structure B rules out atom-pairs for structure A (with 7 pairs in fibre period)

∴ single strand has 3.4 A ± c between neighbouring P

∴ structure A has less

This is correct A.K.

If Suppose important translation in Patterson is

$c = \frac{1}{11}$ $b = \pm\frac{1}{11}$ $a = -\frac{2}{11}$ (corresp. approx. to Patterson peak)

Then important reflections are those for which

$$h\left(-\frac{2}{11}\right) + k\left(\pm\frac{1}{11}\right) + l\cdot\frac{1}{11} = 1$$

$$-2h \pm k + l = 11$$

$$-2h \pm k = 11 - l$$

i.e. on 11th layer-line and expect only 0, 0, 11

and mass of reflections on layer-lines 6, 7, 8, without (001) ⇒ does not indicate steps of $\sim\frac{1}{7}$ ± c

First reflection lines from bases. Less by 1/7 than FET missed this. G.K. A.K.

← That seems extraordinary. Klug says she missed the bases. MW
MW ➡ octq2

Structure B

7th layer-line

2ℓ : 122 – 138 mm to 2θ : .378 to .427

θ : 10° 21′ to 11° 34′ d : ~~3.69~~ 4.28 to 3.84 Å

$\frac{1}{d^2}$: .0546 to ~~.0377~~ .0678

$\left(\frac{\ell}{c^*z}\right)$: $\left(\frac{37}{34}\right)^2\left(\frac{7}{54}\right)$: .0424 ∴ $(\xi/\lambda)^2$: .0122 to .0254

ξ/λ : .110 to .159

I^r max. for $J_7(x)$ has $x \sim 9.0$

∴ for $r \sim 8.5$,

$R = \xi/\lambda = \frac{9}{2\pi \times 8.5}$: .168

for $r = 9.4$ ξ/λ : .152

N.B. Here we expect observed max. to be displaced outwards ∴ Lorentz etc

9

> 7th layer-line shd also have max. of same value as 3rd

i.e. ξ/λ : .039 to .094

– this ∴ apparently absent

3-chain or 2-chain helix?

Chains are not equally spaced, ∴ this wd mean n^th layer-line contains 3Zn ✓

∴ 3-chain helix is highly improbable (~~could be possible if suitably spaced~~)

∴ chains wd be non-equivalent (2 chains ~~cannot~~ cd be equivalent)

Also ∴ structure A believed to have 2 chains /unit cell [symmetry or other evidence MW

i.e. B has 2 chains because A has 2 chains.

by density B must be 2 or 3. MW

R.F. was at last making the correct correction A Y

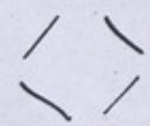
At last

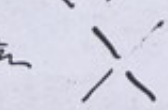
why missing? was it because of spottiness or l.c.? MW

Structure B, 51 c

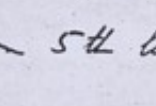
Layer. Line	1st max ξ/λ obs	ξ/λ for r: 9.4	ξ/λ for r: 8.0	ξ/λ for r. 85
0	0.041 ~~0.905 – 0.130~~	.065 zero ∞ .0406	.076 zero 0.048	zero 0.045
1				
2	MW			
3	0.391 – 0.940	0.071	.083	.0805
5	0.905 – 0.130	0.113	.133	.0122

next page is 5 May MW
This is last B discussion.

N. B.
Outer Patter  emanating from 3.4 spot is not equat

1 patter  from origin. if it were they would cross on 5th layer-line

OK
(or is it confused?)
MW

Inner  meets on 5th layer-line OK.

$J_{10}(x)$ has first max. for $x \sim 11.8 = 2\pi Rr$

Observed max. on equator, $R = .162$ to $.195$

$\therefore r = 11.6$ to 9.6 OK

Here observed max. is displaced inwards $\therefore$ 3rd max. of J_0 for $r = 9.4$A has $R = .172$

Density

Volume of cylinder radius 10A, height 34A $= \pi \times 100 \times 34 = \cancel{34000}$ 10700 A^3

Vol. dry nucleotide (density 1.63) = 336 A^3

$\therefore$ no. nucleotides / cylinder $= \frac{10700}{336} = 32$

need to ignore low water content B patterns! M

Since some fairly dry fibres give structure B, density of cylinder is prob. near density of dry Na DNA, water lying mainly outside cylinder.

$\therefore$ this suggests 3 chains

but not easy to reconcile w structure A

For helix of radius 8.5A Vol. cylinder $= \pi \times 8.5^2 \times 34 \simeq 7700$ A^3

no. nucleotides $= \frac{7700}{336} = 23$

NB Check for missing pages

R4 Feb 1

v. brief entry on 10.2.53. with much crossed out MW

48

23.2.53

Structure B

Photograph 51 C

13 days after the 2 Sinclairs about NB 49 C possibly indicating a helix. MW

3·4 A are − 158·5 mm on projection

∴ 158·5 = 2R tan 2θ where R is effective specimen-film distance for projection

For d = 3·40 A, θ (Cu Kα) = 13° 4′ tan 2θ = 0·491

$$R = \frac{158.5}{2 \times 0.491} = 161.4 \text{ mm} \qquad 2R = 322.8$$

Equator mm	tan 2θ	θ	d (Å)	1/d	λ/d	on Orval chart	Conversion factor
20·2	·0625	1° 48′	24·5	·041	0629	12·6	(·624)
54·7	·1695	4° 49′	9·16	·109	·168	33·6	·614
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to 100	to ·310	8° 37′	to 5·13	·195	·300	61·7	·617
						mean	·616
120	·372	10° 12′	4·34	·230	·355		
to 152	to ·470	12° 36′	3·52	·284	·438		

These equatorial maxima do not correspond to maxima ∝ $J_0^2(x)$,

which are approximately at 0, a, 2a, 3a

min. $J_0(x)$ for x	3·83 10·18
max. $J_0(x)$ for x	7·02 13·32

Best fit, assume 1st max. is missing (9·16 A reflexion is v weak)

Then max. at $\frac{\lambda}{d}$ = ·27, ~~·405~~ ·391, and ·149 ·27

since $2\pi R r \triangleq 7.0$ for $R = \frac{2\pi\theta}{\lambda}$, $\frac{1}{d} = \frac{\lambda}{2\pi} \cdot$ ~~·274~~ ·175

$$\therefore r \triangleq \frac{7.0}{2\pi \times 175} = 6.36$$

page 2
39

5th layer line

1st diffuse spot

$2l$: 88 to 100 mm $\tan 2\theta$: .2725 to .310 θ 7°37' to 8°37'

d : 5.80 to 5.10 $\frac{1}{d^2}$: .0298 to .0385

$c^{*2} \frac{L^2}{c^{*2}}$: $\left(\frac{5}{34}\right)^2$: .02165

$\therefore \left(\frac{\xi}{\lambda}\right)^2$: .0082 to .0169 $\frac{\xi}{\lambda}$: .0905 to .130

ξ : .139 to .200

1st max. for $J_5^2(x)$ has $x \sim 6.5$

$\therefore$ if r : 6.36A, $R = \frac{\xi}{\lambda}$: $\frac{6.5}{2\pi \times 6.36}$: .163

- fits better with max. ÷ $J_3(x)^2$

or J_5, and r : 9.41, giving $\frac{\xi}{\lambda}$: .113 which agrees with measurement MW

3rd layer line MW

1st break of spots

$2l$: 49 to 65 mm $\tan 2\theta$: .152 to .201 θ : 4°19' to 5°41'

d : 10.24 to 7.76 $\frac{1}{d^2}$: .00953 to .01665

$\frac{11}{c^{*2}}$: $\left(\frac{3}{34}\right)^2$: .00780

$\therefore \left(\frac{\xi}{\lambda}\right)^2$: .00153 to .00885 $\frac{\xi}{\lambda}$: .0391 to .0940

1st max. for $J_3^2(x)$ has $x \sim 4.2$

$\therefore R = \frac{\xi}{\lambda}$: $\frac{4.2}{2\pi \times 6.36}$: .105

for r : 9.6A $R = \frac{\xi}{\lambda}$: .071 reasonable fit MW

but equator, taking r : 9.6A MW

MW

trying to fit one value of r only

should have maxima at $\frac{1}{9.6 \times 2\pi}$ (3.83, 7.02, 10.18, 13.32) ÷ $\frac{\xi}{\lambda}$

i.e. at .065, .119, .172, .226 — zero at 2.40 — zero at .0406

or ξ : .100, .183, .265, .348

— zero at ξ : .0625 i.e. exactly on observed strong peak

hence bad fit MW

Step in right direction – adding J_n for different values of r.

MW

2 Helices of different radius for simple case of whole number of residues per turn.

Following Cochran Crick & Vand (Acta Cryst. 5 581, 1952)
term $J_n(2\pi Rr)e^{in(\psi+\frac{1}{2}\pi)}$ becomes $J_n(2\pi Rr)e^{i(n\psi - n\phi + \frac{1}{2}\pi + 2\pi l z/c)}$
(in present case, $l = n$)

For equator $I = \left[J_0(2\pi Rr_1) + J_0(2\pi Rr_2)\right]^2 = J_0^2(2\pi Rr_1) + J_0^2(2\pi Rr_2) + 2J_0(2\pi Rr_1)J_0(2\pi Rr_2)$

for n^{th} layer line, $I = FF^* = J_n^2(2\pi Rr_1) + J_n^2(2\pi Rr_2) + J_n(2\pi Rr_1)J_n(2\pi Rr_2)\left(e^{in(\phi - 2\pi z^*/c)} + e^{-in(\phi - 2\pi z/c)}\right)$

$= J_n^2(2\pi Rr_1) + J_n^2(2\pi Rr_2) + 2J_n(2\pi Rr_1)J_n(2\pi Rr_2)\cos\left[n(\phi - 2\pi z/c)\right]$

Here terms in $J_n J_n'$ may give negative contribution to intensity

but on any layer-line, moving out from the meridian, when the first maxim appears in a J_n contribution (i.e. for the J_r term corresponding to largest value of r) there is no negative term in I, since all other J_n terms are small & +ve

∴ even for complex helical structures, first maxima should give maxim diameter.

roughly correct but really not right. it assumes that nucleotide is radial (all in same plane) & maybe she did not realise it was an assumption MW

On equator, first max. (in J_0^2), excluding central max, neither -ve J_0, ∴ max. diameter can't necessarily be got from equator

In general

$$F_n = e^{in(\psi + \frac{\pi}{2})}\left[J_n(x_1)e^{in\alpha_1} + J_n(x_2)e^{in\alpha_2} + \cdots + J_n(x_p)e^{in\alpha_r}\right]$$

where $\alpha_q = \phi_q - 2\pi z_q/c$

& $x_q = 2\pi R r_q$

$$\therefore I = FF^* = \sum_{0}^{p} J_n^2(x_p) + \sum_{p \neq q}^{pq} J_n(x_p)\, J_n(x_q)\cos[(\alpha_p - \alpha_q)]$$

& same argument applies

i.e. first max. give outside radius

but later max. & equatorial non-central max. complicated

<u>2-strand helix</u> with pairs of groups at opp. ends of diameter

$x_1 = x_2$, $\alpha_1 - \alpha_2 = n\pi$

∴ layer-lines absent for n odd ← yes — died along fibre axis? MW

& $I = 4J_n^2(x)$ for n even

ipa? number?

42

Conclusion

Structure B does not fit single helical theory, even for low layer-lines. ξ-values of first maxima are too small for single-stranded helix, & even more so for multi-stranded. i.e. we would have Jn on 1st l.l. for n.s strands equally spaced.

Closing radius of helix so that layer-line maximum for for single-strand (i.e. r = 9·4 A) gives v bad fit for equator (OK but one should not worry too much because one is simplifying MW)

Outer shape / \ \ / meaning for 3·4 reflection indicates repeat at 3·4 A is v important — i.e. over \/ /\ segments structure factor of motif figure, which exists only for c = n × 3·4, & figure repeats for 3·4 n not as for helix

For r = 9·4 A
She seems to take lack of agreement between 3rd & 5th l.l. with equator to rule out 'single helix' model
Over hasty rejection
MW.

Note underlined of if ! MW

Structure B if helix is right-hand helix

ie 2-strand, hitting 5th layer-line max. at $J_{10}(x)$, not require $r \sim 17A$ which is much too big

Suppose ~~diameter~~ radius of outer helix 8·5 A

This gives 3rd layer-line max. at $\xi/\lambda = .0805$

at 5th ——— ——— $\xi/\lambda = .122$

– these values are reasonable, because max $\simeq J_3$ — J_5 is near outer edge of peak

For equator, we then have max. at $\xi/\lambda = .072, .132, .190, .250$

not 1 zero for $\xi/\lambda = .045$

– this still has zero rather near the 2·5 A equator spot

Length of helix of ~~diameter~~ radius 8·5 A pitch 34 A

$l^2 = 34^2 + (8.5 \times 2\pi)^2 = 1156 + 2850 = 4006$

$l = 63.3$

∴ distance between atoms on 8·5 A radius helix $= \frac{63.3}{10}$

$= 6.3 A$

Intensity of inner \ / compared with rest of photograph suggests ~~good agreement~~ the outer helix ($\sim 8.5 A$) is heavy part of structure, i.e. P

This is not our argument about radial nucleotide MW

For radius 10 A

$l^2 = 1156 + 3950 = 5106$ $\quad l = 7.15 A$

For radius 9·4 A $l^2 = 1156 + 3690 = 4666$ $\quad l = 6.82 A$

A + B similar! MW

If single-strand helix as above is basis of structure B, the structure A is probably similar, with P-P distance along fibre axis < 3.4 A, probably 2-2.5A

similar with respect to P-P dist MW

(c.f. 2A indicated by posn of P-P peaks – Pattern d 2.5A " " 11th layer line reflection)

Now with radius 8.5 A she seems to feel discrepancy of 3rd & 5th with equator less serious & is prepared to consider the model.

evidently 'similar' does not mean that A is helical see Klug MW

24.2.53

NB only Second day on B MW

Single-strand helix for structure B rules out atom-pair theory for structure A (with 7 pairs in fibre period)

∴ single strand has 3.4 A ≈ c between neighbouring P

∴ structure A has less

This is correct A.K.

If Suppose important translation in Patterson is

$c = \frac{1}{11}$ $b = \pm\frac{1}{11}$ $a = -\frac{2}{11}$ (corresp. approx. to Patterson peak)

Then important reflections are those for which

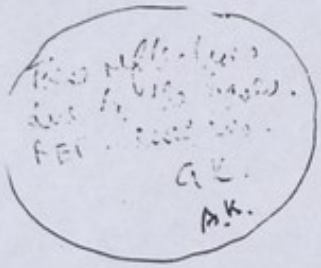
$$h\left(-\frac{2}{11}\right) + k.\left(\pm\frac{1}{11}\right) + l.\frac{1}{11} = 1$$

$$-2h \pm k + l = 11$$

$$-2h \pm k = 11 - l$$

i.e. on 11th layer-line and expect only 0,0,11

and mass of reflections on layer-lines 6, 7, 8, without (00l)'s does not indicate steps of $\sim\frac{1}{5} \approx c$



← That seems extraordinary. Klug says she missed the bases. MW
MW ~~to~~ octgr

Structure B

7th layer-line

2ℓ : 12.2 – 13.8 mm $\quad \therefore 2\theta$: .378 to .427

θ : 10° 21′ to 11° 34′ $\quad d$: ~~3.91~~ 4.28 to 3.84 Å

$\frac{1}{d^2}$: .0546 to ~~.0377~~ .0678

$\left(\frac{S_{11}}{C^{*2}}\right)$: $\left(\frac{\frac{7}{34}}{\frac{3}{34}}\right)^2 \frac{7}{84}$: .0424 $\quad \therefore \left(\frac{\xi}{\lambda}\right)^2$: .0122 to .0254

ξ/λ : .110 to .159

1st max. for $J_7(x)$ has $x \sim 9.0$

$\therefore$ for $r \sim 8.5$,

$R = \xi/\lambda = \frac{9}{2\pi \times 8.5}$: .168

for $r = 9.4$ ξ/λ : .152

N.B. Here we expect observed max. to be displaced outwards : Lorentz etc

8th layer-line must also have max. of same value as 3rd

i.e. ξ/λ : .039 to .094

– this is apparently absent

3-chain or 2-chain helix?

Chains are not equally spaced, $\therefore$ this 3rd max. 8th layer-line contains 3 2s ✓

$\therefore$ 3-chain helix is highly improbable (~~could be possible if suitably spaced~~)

$\Rightarrow \therefore$ chains must be non-equivalent (2 chains ~~change~~ to be equivalent)

Also : structure A believed to have 2 chains / unit cell (symmetry or other evidence MW)

i.e. B has 2 chains because A has 2 chains.

Any density B must be 2 or 3.

MW

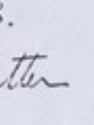
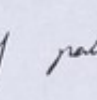
~~M.F.T. would [illegible]~~ At least [illegible] A ?

why missing? was it because of spottiness or l.l.
MW

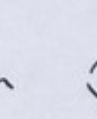
Structure B, 51 c

Layer. Line	I$_{max}$ ξ/λ obs	ξ/λ for r:9.4	ξ/λ for r:8.0	ξ/λ for r. 85
0	0.041 ~~0.905 – 0.130~~	.065 zero ∅ .0406	.076 zero ∅ 0.048	zero 0.045
1				
2	MW			
3	0.391 – 0.940	0.071	.083	.0805
5	0.905 – 0.130	0.113	.133	.0122

next page is 5 MAY MW
This is last B discussion.

N. B.
Outer Pattern  extending from 3·4 just is not equat
1 pattern  from origin. if it were this would
cross on 5th layer-line

OK.
(or is it confused?)
MW

Inner  meets on 5th layer-line OK.

$J_{10}(x)$ has first max. for $x \sim 11.8 = 2\pi R r$

Observed max. on equator, $R = .162$ & $.195$

$\therefore r = 11.6$ & 9.6 OK

Here observed max. is displaced inwards $\therefore$ 3rd max. of J_0 for $r = 9.6$A has $R = .172$

Density

Volume of cylinder radius 10A length 34 A $= \pi \times 100 \times 34 = 10700$ A^3

Vol. dry nucleotide (density 1·63) = 336 A^3

$\therefore$ no. nucleotides / cylinder $= \frac{10700}{336} = 32$

need to ignore low water content B patterns! M

Since some fairly dry fibres give structure B, density of cylinder is prob. near density of dry Na DNA. water lying mainly outside cylinder.

$\therefore$ this suggests 3 chains

but not easy to reconcile w structure A

for helix of radius 8·5A Vol. cylinder $= \pi \times 8.5^2 \times 34 \simeq 7700$ A^3

no. nucleotides $= \frac{7700}{336} = 23$

NB check for completeness

24 Feb!

v. brief entry on 10.2.53. [illegible] with much crossed out MW

48

23.2.53

13 days after the 2 sentences about NB 49 c possibly indicating a helix. MW

Structure B

Photograph 51 c

3·4 A are − 158·5 mm on projection

∴ 158·5 : 2R tan 2θ where R is effective specimen-film distance for projection

For d : 3·40 A, θ (calc) : 13° 4′ tan 2θ : 0·491

$$R = \frac{158.5}{2 \times 0.491} = 161.4 \text{ mm} \qquad 2R = 322.8$$

Equator mm	tan 2θ	θ	d (Å)	1/d	λ/d	on Optical chart	Correction factor
20·2	·0625	1° 48′	24·5	·041	·0629	12·6	(·624)
54·7	·1695	4° 49′	9·16	·109	·168	33·6	·614
82 to 100	·254 to ·310	7° 8′ to 8° 37′	6·19 to 5·13	·162 to ·195	·249 to ·300	50·7 to 61·7	·618 to ·617
						mean	·616
120 to 152	·372 to ·470	10° 12′ to 12° 36′	4·34 to 3·52	·230 to ·284	·355 to ·438		

These equatorial maxima do not correspond to maxima ∼ $J_0^2(x)$,

which are approximately at 0, a, 2a, 3a

min. $J_0(x)$ for x	3·83 10·18
max. $J_0(x)$ for x	7·02 13·32

Best fit, as 1st max. is missing (9·16 A reflexion is v weak)

The max. at $\frac{\lambda}{d}$: ·27, ~~·405~~ ·391, and ·149 ·27

given $2\pi R r \simeq 7.0$ for $R = \frac{2}{\lambda}\theta$, $\frac{1}{d} = \frac{\lambda}{2\pi} \cdot$ ~~·175~~ ·175

$$\therefore r \simeq \frac{7.0}{2\pi \times 175} = 6.36$$

page 2. 39

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5th layer line

1st diffuse spot

$2l$: 88 to 100 mm $\tan 2\theta$: .2725 to .310, θ : 7°37′ to 8°37′

d : 5.80 to 5.10 $\frac{1}{d^2}$: .0298 to .0385

$c^2 \frac{l^2}{4^2}$: $\left(\frac{3}{34}\right)^2$: .02165

$\therefore \left(\frac{\xi}{\lambda}\right)^2$: .0082 to .0169 $\frac{\xi}{\lambda}$: .0905 to .130

ξ : .139 to .200

1st max. for $J_5^2(x)$ has $x \sim 6.5$

$\therefore$ if r : 6.36A, $R = \frac{\xi}{\lambda}$: $\frac{6.5}{2\pi \times 6.36}$: .163

- fits better with max. ~ $J_3(x)^2$

or J_5, and r : 9.4A, giving $\frac{\xi}{\lambda}$: .113 which agrees with measurement MW

3rd layer line

1st streak of spots

$2l$: 49 to 65 mm $\tan 2\theta$: .152 to .201 θ : 4°19′ to 5°41′

d : 10.24 to 7.76 $\frac{1}{d^2}$: .00953 to .01665

$\frac{4}{c^2} \frac{l^2}{c^2}$: $\left(\frac{3}{34}\right)^2$: .00780

$\therefore \left(\frac{\xi}{\lambda}\right)^2$: .00153 to .00885, $\frac{\xi}{\lambda}$: .0391 to .0940

1st max. for $J_3^2(x)$ has $x \sim 4.2$

$\therefore R = \frac{\xi}{\lambda}$: $\frac{4.2}{2\pi \times 6.36}$: .105

for r : 9.4A $R = \frac{\xi}{\lambda}$: .071 reasonable fit MW

but equator, taking r : 9.4A MW

Trying to fit one value of r only MW

should have maxima at $\frac{1}{9.4 \times 2\pi}$ (3.83, 7.02, 10.18, 13.32) ~ $\frac{\xi}{\lambda}$

i.e. at .065, .119, .172, .226 and zero at 2.40 ... and zero at .0406

or ξ : .100, .183, .265, .348

and zero at ξ : .0625 i.e. exactly on observed strong peak

Hence bad fit MW

Step in right direction – adding J_n for different values of r.
MW

2 helices of different radius for simple case of whole number of residues per turn.

Following Cochran Crick & Vand (Acta Cryst. 5 581, 1952)
term $J_n(2\pi Rr)e^{in(\psi+\frac{1}{2}\pi)}$ becomes $J_n(2\pi Rr)e^{i(n\psi-n\phi+\frac{n}{2}\pi+2\pi lz/c)}$
(in present case, $l=n$)

For equator $I=\left[J_0(2\pi Rr_1)+J_0(2\pi Rr_2)\right]^2 = J_0^2(2\pi Rr_1)+J_0^2(2\pi Rr_2)+2J_0(2\pi Rr_1)J_0(2\pi Rr_2)$

For n^{th} layer line, $I=FF^* = J_n^2(2\pi Rr_1)+J_n^2(2\pi Rr_2)+J_n(2\pi Rr_1)J_n(2\pi Rr_2)\left(e^{in(\phi-2\pi z/c)}+e^{-in(\phi-2\pi z/c)}\right)$

$= J_n^2(2\pi Rr_1)+J_n^2(2\pi Rr_2)+2J_n(2\pi Rr_1)J_n(2\pi Rr_2)\cos\left[n(\phi-2\pi z/c)\right]$

Here terms in $J_n J_n'$ may give negative contribution to intensity

but on any layer-line, moving out from the meridian, when the first maxim appears in a J_n contribution (i.e. for the J_r term corresponding to longest value of r) there is no negative term in I, since all other J_n terms are small & +ve

∴ even for complex helical structures, first maxima should give maxim diameter; roughly correct but really not right, it assumes that nucleotide is radial (all in same pl
maybe she did not realise it was an assumpt
MW

On equator, first max. (in J_0^2), excluding central max, neither -ve J_0, ∴ max. diameter can't necessarily be got from equator

In general

$$F_n = e^{in(\psi + \frac{\pi}{2})} \left[J_n(x_1) e^{in\alpha_1} + J_n(x_2) e^{in\alpha_2} + \cdots + J_n(x_p) e^{in\alpha_r} \right]$$

where $\alpha_q = \phi_q - 2\pi z_q / c$

and $x_q = 2\pi R r_q$

and $I = FF^* = \sum_{p}^{p} J_n^2(x_p) + \sum_{p \neq q}^{pq} J_n(x_p) J_n(x_q) \cos[(\alpha_p - \alpha_q)]$

and same argument applies

i.e. first max. give outside radius

but later max. and equatorial non-central max. complicated

2-strand helix with pairs of groups at opp. ends of diameter

~~$J_n(x)$~~ $x_1 = x_2$, $\alpha_1 - \alpha_2 = n\pi$

∴ layer-lines absent for n odd ✓ yes

and $I = 4 J_n^2(x)$ for n even

died along fibre axis?
MW

page number?

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Conclusion

Structure B does not fit single helical theory, even for low layer-lines. S-values of first maxima are too small for single-stranded helix, & even more so for multi-stranded. i.e. we would have Jn on nth l.l. for n strands equally spaced.

Closing radius of helix so that layer-line maximum for fit single-strand (i.e. r = 9.4 Å) gives v bad fit for equator (OK but one should not worry too much because one is simplifying MW

Outer shape / \ \ / meeting from 3.4 reflection indicates repeat at 3.4 Å is v important — i.e. over \/ /\ repeated structure

factor of much figure, which exists only for c. n × 3.4, —

figure repeats for 3.4 Å spot as for helix

For r = 9.4 Å

She seems to take lack of agreement between 3rd & 5th l.l. with equator to rule out 'single helix' model

Over hasty rejection

MW.

Note underlining of if ! MW

(ie ~5 on [illegible] (In R.E.F's terminology Aline could still be two chains, unstacked (as in alpha) or stacked (as in beta) See P. 46) QK! 3

Structure B if helix is triple-strand helix

viz 2-strand, fitting 5th layer-line max. to $J_{10}(x)$, not requiring $r \sim 17A$ which is much too big

Suppose ~~diameter~~ radius of outer helix 8·5 A

This gives 3rd layer-line max. at $\xi/\lambda = .0805$

at 5th ——— ——— $\xi/\lambda = .122$

– these values are reasonable, because max $\doteq J_3$ — J_5 i.e. near outer edge of peak

For equator, we then have max. at $\xi/\lambda = .072, .132, .190, .250$

and 1 zero for $\xi/\lambda = .045$

– this still has zero rather near the 2½·5 A equator spot

Length of helix of diameter radius 8·5A pitch 34A

$l^2 = 34^2 + (8.5 \times 2\pi)^2 = 1156 + 2850 = 4006$

$l = 63.3$

∴ distance between atoms on 8·5A radius helix $= \frac{63.3}{10}$

$= 6.3A$

Intensity of inner \ / compared with rest of photograph suggests ~~good agreement~~ This is not our argument about radial nucleotide MW

that outer helix (~8·5A) is heavy part of structure, i.e. P

For radius 10A

$l^2 = 1156 + 3950 = 5106$ $\quad l = 7.15A$

For radius 9·4A $l^2 = 1156 + 3690 = 4666$ $\quad l = 6.82A$

A + B similar!
MW

[If right-hand helix as above is basis of structure B, the structure A is probably similar, with P–P distance along fibre axis < 3.4 A, probably 2 – 2·5A

similar with respect to P–P dist.
MW

(c.f. 2A indicated by posn of P-P peaks – Pattern d 2·5A " " 11th layer line reflection)

a.k

Now with radius 8·5 A she seems to feel discrepancy of 3rd & 5th with equator less serious & is disposed to consider the model evidently 'similar' does not mean that A is helical see Klug
MW

24.2.53 5

NB only Second day on B MW

Single-strand helix for structure B rules out atom-pairs for structure A (with 7 pairs in fibre period)

∴ single strand has 3.4 A ≃ c between neighbouring P

∴ structure A has less

This is correct A.K.

∴ Suppose important translation in Patterson is

$c = \frac{1}{11}$ $b = \pm\frac{1}{11}$ $a = -\frac{2}{11}$ (corresp. approx. to Patterson peak)

Then important reflections are those for which

$$h\left(-\frac{2}{11}\right) + k.\left(\pm\frac{1}{11}\right) + l.\frac{1}{11} = 1$$

$$-2h \pm k + l = 11$$

$$-2h \pm k = 11 - l$$

i.e. on 11th layer-line and expect only 0,0,11

and mass of reflections on layer-lines 6, 7, 8, without (001)'s does not indicate steps of $\sim\frac{1}{5} \simeq c$

This reflection was very faint. does not mean FET missed it. AK. A.K.

← That seems extraordinary. Klug says she missed the bases, MW ~~MW~~ octgr

Structure B

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θ : 10° 21′ to 11° 34′ d : ~~3.691~~ 4.28 to 3.84 Å

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$\left(\frac{|F|^2}{C}\right)$: $\left(\frac{P_3}{P_4}\right)^2 \left(\frac{J_7}{B_4}\right)^2$: .0424 $\therefore \left(\frac{\xi}{\lambda}\right)^2$: .0122 to .0254

ξ/λ : .110 to .159

I.e. max. for $J_7(x)$ has $x \sim 9.0$

$\therefore$ for $r \sim 8.5$,

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for r : 9.4 ξ/λ : .152

N.B. Here we expect observed max. to be displaced inwards : Lorentz etc

N9

) th layer-line shd also have max. of same value as 3rd

i.e. ξ_1/λ : .039 to .094

– this : apparently absent

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Chains are not equally spaced, : this wd mean ~ th layer-line contains 3 2s ✓

∴ 3-chain helix is highly improbable (~~could be possible if suitably spaced~~)

∴ chains wd be non-equivalent (2 chains ~~cleavage~~ wd be equivalent)

Also : structure A believed to have 2 chains / unit cell (symmetry or other evidence MW

i.e. B has 2 chains because A has 2 chains.

by density B must be 2 or 3.

MW

R.F.I. would look making the correct correlation A Y.

At least

why missing? was it because of spottiness or l.l.'. MW

Structure B, 51 c

Layer. Line	I$_{max}$ sinθ/λ obs	sinθ/λ for r: 9.4	sinθ/λ for r: 8.0	sinθ/λ for r: 85
0	0.041 ~~0.905 – 0.130~~	.065 zero ~ .0406	.076 zero 0.048	zero 0.045
1				
2	→ MW			
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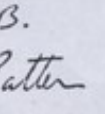
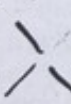
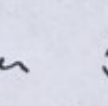
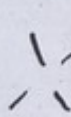
next page is 5 May MW
This is last B discussion.

N.B.
Outer Pattern  emanating from 3.4 spot is not equal
to pattern  from origin. If it were they would
cross on 5th layer-line OK.
(or is it confused?)
HW

Inner  meets  on 5th layer-line OK.

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Here observed max. is displaced inwards $\therefore$ 3rd max. of J_0 for $r = 9.6$ A has $R = .172$

Density

Volume of cylinder radius 10A, height 34 A $= \pi \times 100 \times 34 = 10700$ ~~21400~~ A^3

Vol. dry nucleotide (density 1.63) = 336 A^3

$\therefore$ no. nucleotides / cylinder : $\frac{10700}{336} = 32$

need to ignore low water content B patterns! M

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For helix of radius 8.5A Vol. cylinder $= \pi \times 8.5^2 \times 34 \simeq 7700\ A^3$

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FRANKLIN
B Felicia

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BRISTOL 24.2.99

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RF

notebook 53 All 1953

(with my note 99 MW)

all this seems clearly before seeing DH.
(but the 17 Mar Typescript seems uncertain).

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