19. 1. 53 1

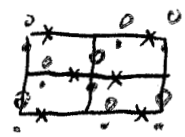
Results of superpositions of 3-dimensional Patterson of crystalline Na DNA

Space group C 2

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

Axial sections

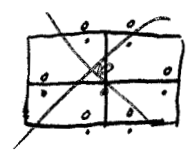
one axial section contains principal maxima (c=0)



the other no important maxima (c = ½)

Peaks at heights 13/30 and 17/30

v strong, also in pseudo-hexagonal array



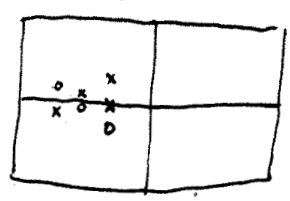
• c=13
o c=17

[N.B. hexagons appear centred, ∴ superposition method is not capable of eliminating central peak. But 1 can't reconcile centring w density
2 would have pseudo-cell of side a ~ b ~ 13 A]

Possible structure having chains along a-c diagonal

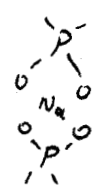
but fibres can't be built this way - unreasonable
∴ search for alternative - gives:-

Figure of 8 structure (in projection). 7 peaks on chain in one cell.



2 pairs of chains / primitive cell
(4 pairs / full cell)
i.e. 56 nucleotides / full cell.

Consistent w density data if
1 ~25% H_2O
2 2 P atoms per peak
i.e. 2 chains "back to back"

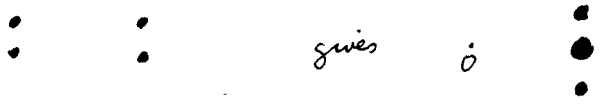


A.K
See later, p45, for rejection of this "atom hair" theory (with 7 pairs in fibre [illegible]

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

Patterson peaks representing Zphosphates

If pairs are all ∥ "orient" & resol" is poor, maxima will give distances between mid-pts of pairs

i.e.  gives

If pairs ⊥ one another, no central overlap

i.e. gives

does this indicate that pairs at c=8 are inclined to other pairs at ½ ∴ 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

Peak at height 0 lies on axis

∴ 2 P atoms attached to similar nucleotides

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

Each chain only) peaks in 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 dimensions)

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

Construction of models

Scale $\frac{1}{2}$" : 1 Å (as in Patterson diagrams)

Backbone chains

PO_4 tetrahedra – wooden balls, tetrahedrally pierced (Fraser) placed in contact.

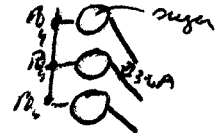
Sugar ring constructed (wire) on Furberg model

Courtaulds models using only phosphates and sugar rings show that it is possible to construct straight-chain model with P–P = 5.7 A, and all sugar rings in identical pos^ns

Pyrimidines for pos^n of least strain, are then inclined at 25–30° to backbone

- this would leave inter-base plane spacing ~ 5.0 A

Base-planes can be tilted on this model to give inter-plane spacing 3.4 A but there is then v little overlap, i.e. v little van der Waals attraction



∴ if P–P distance 5.7 A, not straight chain

– this (among other things) eliminates a-c diagonal structure

Putting Pyrimidine rings ∥ and in full contact we can have 3 phosphates in straight line, at P–P distance ~ 5.7 A

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

⇒ 13 base rings either ⊥ or inclined to chain

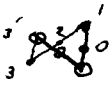
Backbone chain and symmetry at c = 0

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 diad 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  + reasonable angles

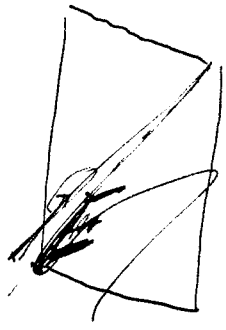
⇒ angle 0–1–2 ~ 100°

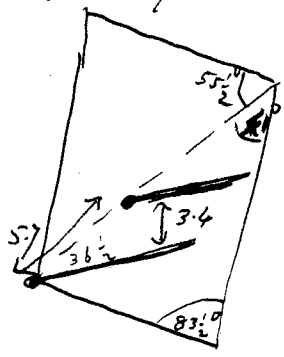
angle 2–3–3′ ~ 110°

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

∴ angles 100 – 110°

Suppose length of pyrimidine nucleotide is in a-c plane
Then for a-c diagonal peak of structure (i.e. peaks 1'-0-1)



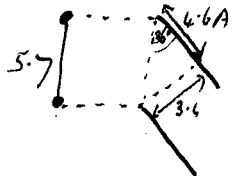


$\sin^{-1}\frac{3.4}{5.7} = 36\frac{1}{2}^\circ$

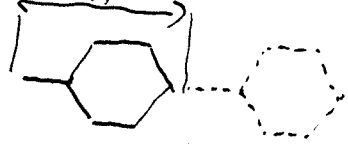
∴ if ~~ba~~ plane of pyrimidine is ⊥ a-c plane, it makes
∠ $36\frac{1}{2}^\circ$ with phosphate chain
and $36\frac{1}{2} + 41 : 77\frac{1}{2}$ with fibre axis

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 and fibre axis

In general, if all P-sugar are equivalent, then $C_1 - C_1' = 5.7$ Å

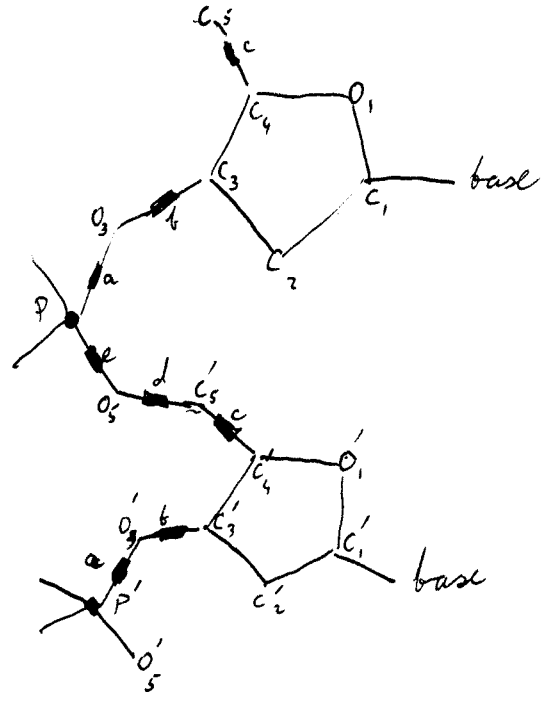


i.e. no overlap of // 4·6Å pyrimidines



∴ sugar rings must be skew to one another,
with ⊥ distance between bonds C_1N and $C_1'N'$ ~ 3·4 Å

- bases then // one another but differently oriented



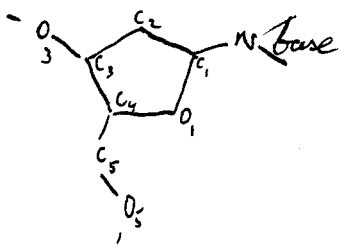
Free rotation of a, b, c, d, e

Wire mode of backbone chain and sugar rings

Scale 1" ≡ 1Å

Sugar ring constructed as in Furberg and Beevers + Cochran

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



All free rotation obtained by making joints with curtain spring

PO_4 tetrahedra

Requirements

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

Observations

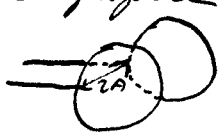
Distance apart of P P' determined by rotations b, c, d, esp. c

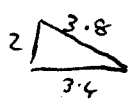
Distance apart of C_2 C_5' ——— ——— a, b, e

(closest approach ~ 1.2")

Fully extended chain gives P – P ~ 6.8 A

If vdw contact @ ~ 3.4 A between bases, since pyrimides are ~ 3A in diameter and of C_1N bonds, seen in projection ⊥ plane of rings, must't be > ~ 2A apart



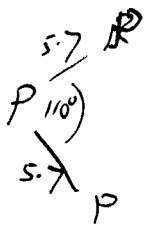


∴ ~~separation~~ distance between N and N' ≯ 3.8 A

It doesn't seem to be possible to put 3 P gps in st. l. w spacing 5.7 A and have C, N bonds in posⁿ for 11 bases at 3.4 A sepⁿ

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

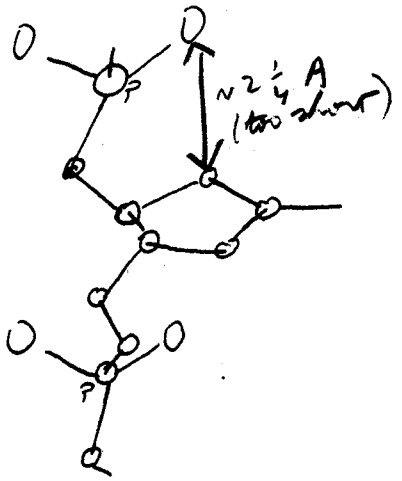
If so, perhaps structure has groups of 2 or 3 bases in 11 contact, and break of contact when chain turns a corner



in this configⁿ it is easy to avoid steric hindrance of sugar rings. Not easy for $P \overset{5.7}{—} P \overset{5.7}{—} P$

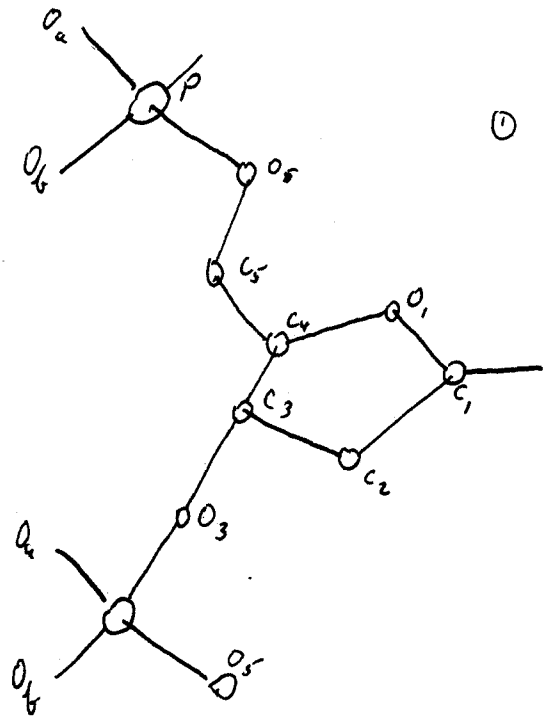
Arrangements of backbone chain with P - P : 5 - 7

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



This leaves ; P<O O directed to one side of sugar ring

2. Sugar rings ~ ∥ P - P — again P<O O to one side



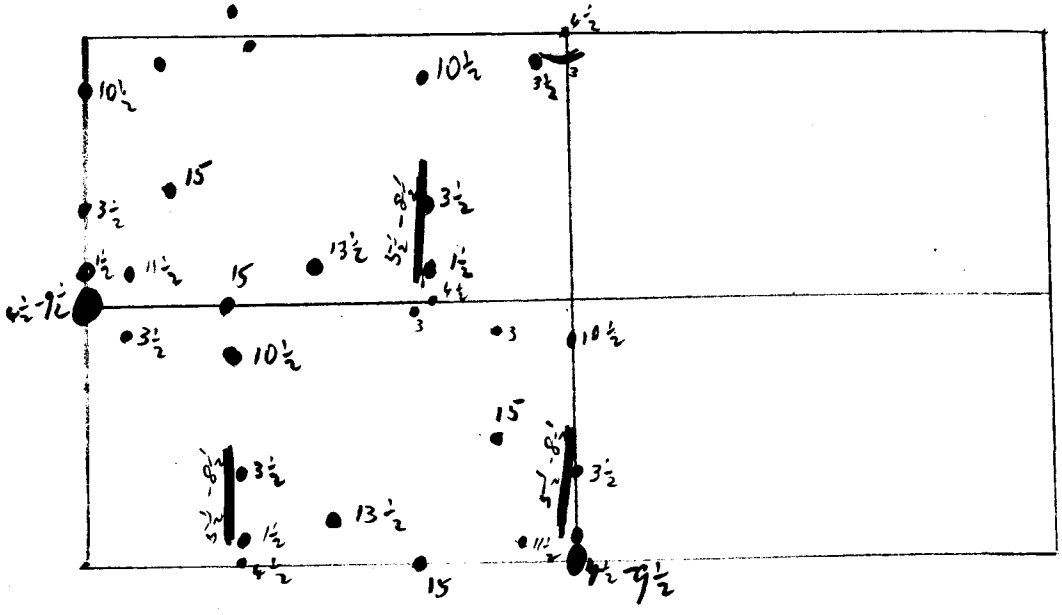
Steric factors

① Make C_5 equidistant from O_3 and O_b

② C_3 tilted away from O_a, but not 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



/ figure of eight A.K.

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, and
Patterson shows that this must be ~ along a - c diagonal
i.e. in same direction as chain
∴ impossible

Superposition

To obtain function which gives members of atom-pairs and not their centres, must take account of fact that V_g is not strictly on axial section but on either side of it

Suppose P - P distance in pair ~ 4.5 A
and corresponds to peak on section 3, a = 5 cms
the axes at $c = 1\frac{1}{2}$, $a = 2\frac{1}{2}$ 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 $\frac{1}{4}$-cell heavy peak, nor does it show poss. alternative form for chain

M2q

Peak at height 13 repeats at $\frac{1}{3}$ b away, ∴ try ~~plac~~ combining M2 and Mq by placing V_q not at height 0 but at height 13

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

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

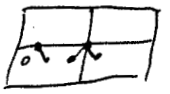
axes are then at height −13 in Mq (and a = 0)
(= 17)

∴ draw Mqc derived from Mq with axes at height 17

and M2B " " M_2 with axis at 0/17

Principal positions of c:2 vectors : Patterson

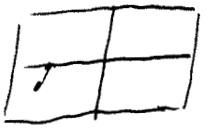
Sections 0 – 2 (twice)



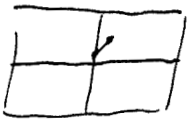
N.B. not at 0

∴ not 11 pairs

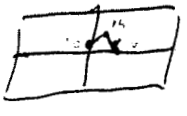
Sections 10 – 12



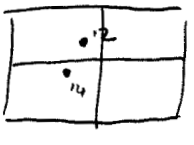
Sections 3 – 5
(or 2 – 4)



Sections 14 – 16



Sections 12 – 14



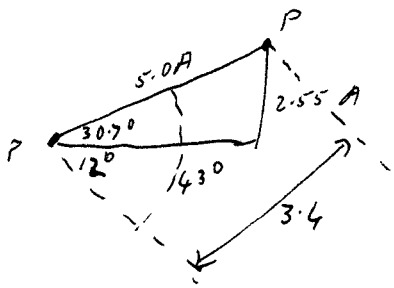
If there are 11 nucleotides per chain

mean inter-P spacing along C-axis is 2.55 Å

If P.P : 5.0 Å

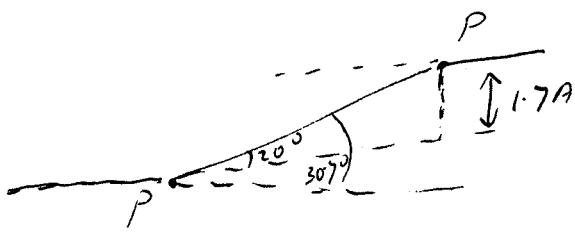
and inter-nucleotide base spacing 3.4 Å

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



but then no contact ∴ bases too small

or if chain is ≠



bases inclined ~ 11° to fibre axis

but only 20° to P-P chain

∴ impossible

Possible steps in chain

Predominant near-origin peaks in P are ~5A

① section 2 peak 122 - strongest of all but c=15
(∴ in general pos^n)

∴ suppose this is important step in chain

also ② step along a-c diagonal (section 3

and ③ section 2, peak 75 (similar to ①, with a-cpt reversed)

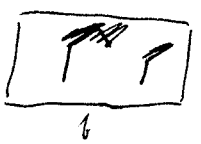
If these are the 3 poss. chain steps, then total number of ②+③ is equal to no. of ①

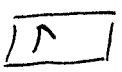
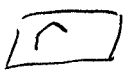
∴ total translation in 'a' = 0

There is no horizontal translation of ~5A

2 consecutive ① can occur (sections 2½ and 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 poorer on 'b' axis than 'a' although 'b' axis is further from main maxima

sim^ly

② can be followed by ③ but not by ①

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

but ③ following ① giving peak c~5, b~$\frac{1}{6}$ which falls in hole

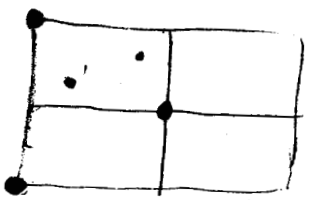
Possible sequences of peaks ① ② or ③

① - ① - ① ② - ② - ② ③ - ③ - ③

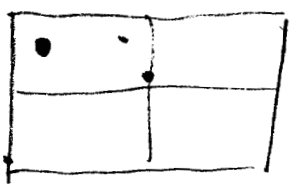
① - ① - ③

M12

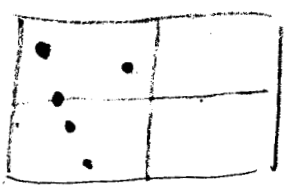
0



1



2



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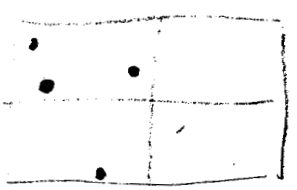


(cont'd from opp.)

This suggests Harker peak c = 6 ~~a = 8.0 cm~~

M 11

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

Possible pos^ns of peaks in -ve regions of Patterson marked in, and ~~mark~~ when they coincide with +ve region of 2nd sheet, they were marked with dotted lines on M 11

M 12

Suppose M11 vector occurs twice consecutively. Then M11 is multiple, 2 structures being related by V_{11}

$\therefore$ M12 is M 11 displaced V_{11} on itself

$a = -5.5$ $b = \cancel{3.3}\ 3.5$

M12 Axes on section 7, with $a \sim -2.0$ cms?

7.2.53

Try M13, using peak at height 4, $a \sim 3.0$ cms $b = 0$ in M11

distance of this peak from peak on section 1 ?

9.2.53

Possible pos^ns of axes in M11

$c = 4$	$a = 3.5$ 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 $\therefore$ gives peak on wrong a-c diag. on section 4
$c = 4\frac{1}{2}$	$a = 0$	gives Harker peaks	$c = 7$ $a = 4.8$ and $c = 11$ $a = -4.8$ } v good

V_{11} gives 2 Harker peaks differing by $c = 4$, $a = -10$ cms

$\therefore$ superposition of a-c section on itself, with displacement $c = 4$, $a = 10$ gives poss. Harker peaks & hence poss. pos^ns of axes

10.2.53

Structure B

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

49c - general trend is as for right continuous helix

(which differs from right discontinuous 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 on each having same z-value, since 2nd chain has opp. signs in ξ & η terms (eq 1-2), & eq^{n} 2 contains only $R^2 = \xi^2 + \eta^2$ & $\tan\psi = \eta/\xi$

13.3.53.

Axes derived from other possible positions of VII' derived from VII

$\frac{1}{2}(a-5$	$\frac{1}{2}(c+2)$	$a-10$	$c+4$	Harker 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	×

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 axis is at $\frac{1}{2}(a-5)$ and $\frac{1}{2}(c+2)$

Observed	$a-10$ (cms)	$c+4$	$\frac{1}{2}(a-5)$	$\frac{1}{2}(c+2)$	
V' good (using dots)	1.4	$4\frac{1}{2}$ +	3.2	$(1\frac{1}{4})$ $1\frac{1}{2}$	~~a = 5.5 ?~~
no V' X	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	11D 1 axis a = 8.0, c = 4
X	23.0	$10\frac{1}{2}$ −	14.0	$(4\frac{1}{4})$ 4	11C try $4\frac{1}{2}$?
V' good but axis better @ 6 ✓	12.8	$13\frac{1}{2}$ −	8.9	$(5\frac{3}{4})$ $5\frac{1}{2}$	M11E no good ∴ origin peaks are lost
V' v good	21.0	$13\frac{1}{2}$ +	15.5	$(5\frac{3}{4})$ 6	
	19.8	20	~~7.4~~ 12.4	9	✓ 11B
		$5\frac{1}{2}$	15.6	$5\frac{1}{2}$	

M911

M9 shows a vector V11 having one end in common with end of V9

∴ put M9 on M11 with origin at a = 2.4 cms b = 6.8

and OM911 is OM9 on 29M11

i.e. axes on M11 at a = 2.4 c = 1
if true axes are M9 axes

M911 blue for axes on M9 axes

M. Wt

~~M~~. primitive unit cell 11.2×10^3

Vol. " " " $12230\ \text{Å}^3$

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

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

$\therefore$ vol. assoc. water $= 12230 - 6620 = 5610\ \text{Å}^3$

$\simeq 45.8\%$ of volume

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

Density of water in Na DNA

Dry density 1.63 gm. vol. .615

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

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

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

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

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 ~~d~~ of mixture 1.52 i.e. vol 1.35 g : $\frac{1.35}{1.52}$ = 0.89 cc

gm. vol. DNA : 0.89 − 0.35 = 0.54

Suppose partial gm. vol. DNA 0.55

d ——— 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 $d = \frac{1.30}{0.85} = 1.53$

a - c diagonal

All Patterson peaks streak along forward a - c diagonal

- this suggest possibility of disorder in direction of diagonal

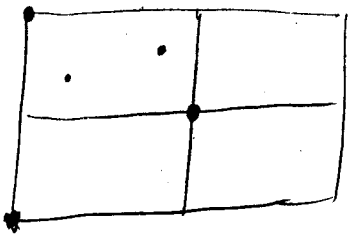
M II C

No good

- Leets 1 – 4 almost nothing

M12 (first 15 sheets only)

0



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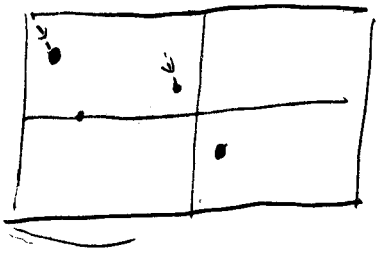

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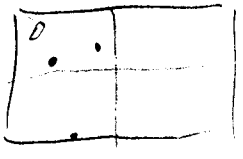

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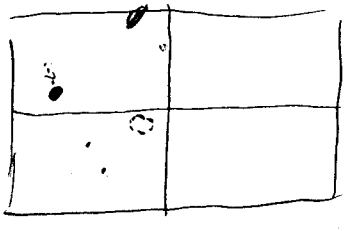

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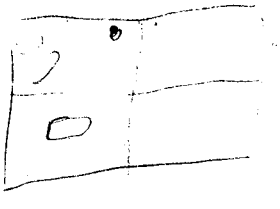

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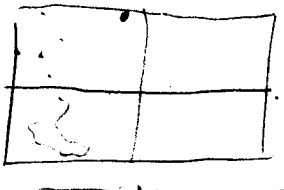

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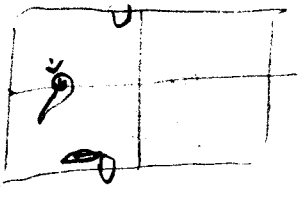

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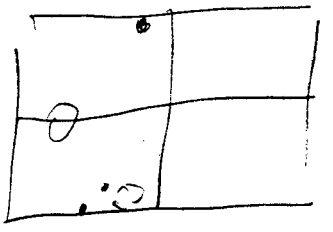

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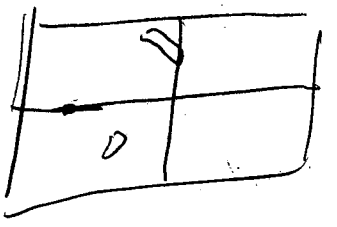

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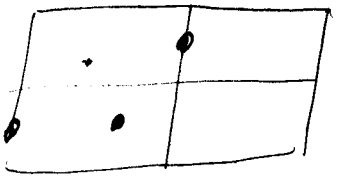

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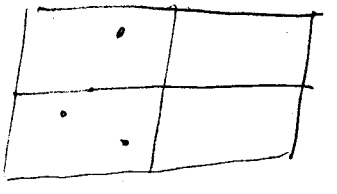

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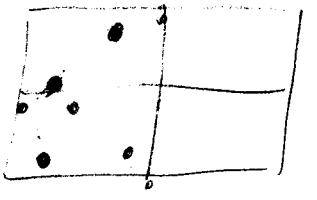

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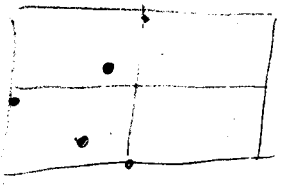

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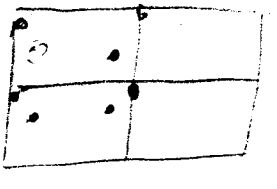

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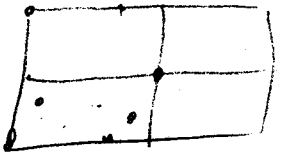
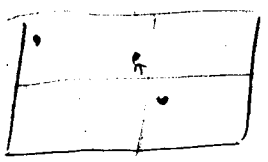


M 4.13.11

O M 13 on 1 M 11, with M 13 reflected across ~~[illegible]~~ B plane
(i.e. turned over short axis

peaks used are 2 on section 0
and 1 on section 28
(marked with red crosses)

0



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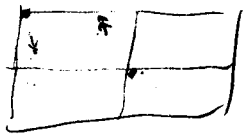

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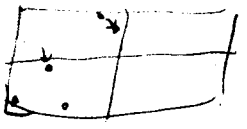

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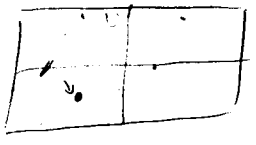

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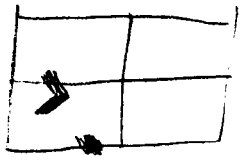


M 13.11

Possible positions of axes

Search for V_{13}', with onset & position. The 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 sects 2/3, 17/18

See preliminary mention of Structure B on 10-2-53 p. 28

23.2.53

Structure B

a.K.

Photograph 51 c

3·4 A arc − 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_{CuKa} = 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	mm on Bernal chart	Conversion factor
20·2	·0625	1° 48′	24·5	·041	·0629	12·6	(·624 ~~·6369~~)
54·7	·1695	4° 49′	9·16	·109	·168	33·6	·614
82 to 100	·254 to ·310	7° 8′ 8° 37′	6·19 to 5·13	·162 ·195	·249 ·300	50·7 61·7	·618 ·617
						mean	·616
120 to ~~152~~ 152	·372 to ·470	10° 12′ 12° 36′	4·34 3·52	·230 ·284	·355 ·438		

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

gives $2\pi R r \simeq$ ~~9·13·4~~ 7·0 for $R = \frac{2\sin\theta}{\lambda} = \frac{1}{d} = \frac{\lambda}{2\pi} = \frac{\cancel{5}\,.27}{\cancel{\lambda}} = \cancel{5}\,.175$

$$\therefore r \simeq \frac{\cancel{13.4}\ 7.0}{2\pi \times .175} = \cancel{12.2}\ 6.36$$

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} : $\left(\frac{5}{34}\right)^2$: .02165

$\therefore \left(\xi/\lambda\right)^2$: .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. in $J_3(x)^2$

or J_5, and $r = 9.4A$, giving ξ/λ : .113

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

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

$\therefore \left(\xi/\lambda\right)^2$: .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

but equation, taking $r = 9.4A$

should have maxima at $\frac{1}{9.4 \times 2\pi}$ (3.83, 7.02, 10.18, 13.32) in ξ/λ

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

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

(in present case, $l = n$)

For equator $I = \left[J_0(2\pi R r_1) + J_0(2\pi R r_2)\right]^2 = J_0^2(2\pi R r_1) + J_0^2(2\pi R r_2) + 2J_0(2\pi R r_1)J_0(2\pi R r_2)$

For n^{th} layer line, $I = FF^* = J_n^2(2\pi R r_1) + J_n^2(2\pi R r_2) + J_n(2\pi R r_1)J_n(2\pi R r_2)\left(e^{in(\phi - 2\pi z/c)} + e^{-in(\phi - 2\pi z/c)}\right)$

$= J_n^2(2\pi R r_1) + J_n^2(2\pi R r_2) + 2J_n(2\pi R r_1)J_n(2\pi R r_2)\cos\left[n(\phi - 2\pi z/c)\right]$

Here terms in $J_n J_n'$ may give <u>negative contribution to intensity</u>

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.

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

$$F_n = e^{in(\psi + \frac{\pi}{2})} \left[J_n(x_1) e^{in\alpha_1} + J_n(x_2) e^{in\alpha_2} + \cdots + J_n(x_\rho) e^{in\alpha_\rho} \right]$$

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

and $x_q = 2\pi R r_q$

and $I = FF^* = \sum_{\rho}^{\rho} J_n^2(x_\rho) + \sum_{\rho \neq q}^{\rho q} J_n(x_\rho) J_n(x_q) \cos[n(\alpha_\rho - \alpha_q)]$

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

$x_1 = x_2$, $\alpha_1 - \alpha_2 = n\pi$

$\therefore$ layer-lines absent for n odd

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

Conclusion

Structure B does not fit right helical theory, even for low layer-lines. ξ-values of first maxima are too small for right-stranded Helix, & even more so for multi-stranded.

Closing radius of helix so that layer-line maxima fit for right-stranded (i.e. $r = 9.4\,A$) gives a bad fit for equator

Outer layer emanating from 3.4 reflection indicates repeat at 3.4 A is a major — i.e. riser represents structure factor of motif figure, which exists only for $c = n \times 3.4$, & figure repeats for 3.4 A not as for helix

ie. J_5 on 5th l.l.
(In R.E.F's terminology, there could still be two chains, unrelated by the symmetry)
See P. 46 A.K.

Structure B if helix, is single-strand helix

since 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 $\xi/\lambda = \cancel{.122}\ .0805$
and 5th ——— ——— $\xi/\lambda = .122$

– these values are reasonable, because max in J_3 and 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 24.5A equator spot

Length of helix of ~~diameter~~ radius 8.5A and 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 that outer helix ($\sim 8.5A$) is heavy part of structure, i.e. P

For radius 10A

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

For radius 9.4A $\quad l^2 = 1156 + 3490 = 4646$ $\quad l = 6.82A$

[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
(c.f. 2A indicated by pos^{n} of P-P peaks = Pattern
d 2.5A " " 11th layer line reflection)

Many kind a.k.

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

∴ single chain has 3.4 Å in c between neighbouring P

∴ structure A has less

There is correct a.K.

Suppose important translation in Patterson is

$$c = \frac{1}{11} \quad b = \pm\frac{1}{11} \quad a = -\frac{2}{11}$$ (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) = does not indicate steps of $\sim\frac{1}{7}$ in c

These reflections due to the bases. R.E.F. missed this. AK.

Structure B

7th layer-line

$2l$: 122 – 138 mm to 2θ : 378 to 427

θ : 10° 21′ to 11° 34′ d : 4·28 to 3·84 A

$\frac{1}{d^2}$: ·0546 to ·0678

$\left(\frac{m}{c}s^2\right)$: $\left(\frac{7}{64}\right)^2$: ·0424 ∴ $\left(\xi/\lambda\right)^2$: ·0122 to ·0254

ξ/λ : ·110 to ·159

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

∴ for $r = 8.5$,

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

for r : 9·4 ξ/λ : ·152

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

7th layer-line should also have max. of same value as 3rd

i.e. ξ/λ : ·039 to ·094

– this is apparently absent

3-chain ~ 2-chain helix?

Chains are not equally spaced, ∴ this would mean n^{th} layer-line contains $\frac{7}{3}n$'s

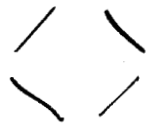
∴ 3-chain helix is highly improbable

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

Also ∵ structure A believed to have 2 chains / unit cell

R.E.F. is not (as) making the correct connection between the A and B. A.K.

N. B.

Outer Patter  emanating from 3·4 spot is not equator

of patter from origin. if it were this would

cross on 5th layer-line

Inner meets on 5th layer-line

$J_{10}(x)$ 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

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 34 A $= \pi \times 100 \times 34 = \frac{10700}{\cancel{11400}}$ A^3

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

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

Since some fairly dry fibres give structure A, 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 $= \frac{7700}{336} = 23$

A form
superposition map

5. 3. 53

M 11

Uses peaks on section 2 which, 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 in b-direction of one relative to other

To find correct pos^n of M11B wrt M11D, look for the 4 origin peaks in each

– these are at heights 8 and 10 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 at 0 on 11B may corresp. height 15 on 11D

∴ ~~rotate through 180°~~ and put 0–7 on 15–22
i.e. on 15–8 upside-down

2) 11B and 11D may give different enantiomorphs

– this corresponds to 0–7 on 0–7 rotated and upside-down

i.e. poss^ns 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 ~~~ -11cms gives good fit for 3-5, quite good for 10~~
- 16.3 3, 5, 8, 10 all fit, and ~~but bad for 8~~ general fit good
∴ Impossible ∵ peaks at 5 not consistent w peaks at 0

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

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

M11D 0-7 on M11B 0-7

M11D at - 15.7cms → good fit for 3, 5, 8, 10 but using v small peaks
general fit good in 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

Presumably during the [illegible] REF was
[illegible] no. ~~[illegible]~~ on the B form. "Rough draft"
dated 17 March 1953

M11 superpositions 18.3.53

~~M11 B and M11 E both have origin peaks of height 8 & 10~~
~~These have different 'a' values, ∴ must relate to different chains~~

~~How can M11 E, 8-15 be fitted to M11 B?~~

M11 B has origin peaks at 8 & 10, M11 E at 5, 7
These have different 'a' values, ∴ either belong to diff. chains
or to diff parts of same chain

A. Diff. chains, same heights

~~M11 E 0-7 on M11 B 8-15 upside-down~~

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

M11 E 0-7 on M11 B 8-15 rotated

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

M11 E 0-7 on M11 B 0-7

a: 1/2 b: −1.0 cms

a: 0 b: −8.2 cms ~~origin~~ 0 peaks good
a: 0 b: +8.8

M11 E 0-7 on M11 B 0-7 rotated and upside-down

Is structure A triclinic?

2-axis can't pass through DNA chain ∵ asymmetric sequence
but superpositions 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 $h\bar{k}l$)
[If structure is triclinic and 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 improbable a) ∵ evidence from enzymatic degradation
b) ∵ prob. imposs. to get 5A equally spaced bases, distanced @ 3.4A

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 streaked along a-c axis

- can this be due to P ... Na in that direction?

- well-resolved ~~beak~~ peak on C:2 suggests 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(r)	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 peak for P-Na distance 3.0A		190.9	190.2	178.4	170.7	175.4	183.9	182.6
Shape of peak for P-Na 2.5A		204.3	214.4	213.0	211.7	208.8	197.3	169.2
Shape of peak 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

$\frac{1}{2}$-peak width of P-P + Na-Na (Patterson) $\sim 1.5 \times 2$ Å

$\therefore$ this is minim dimension.

$\therefore$ Å $\frac{1}{2}$-peak width of P—Na combination must be $\sim 3.0 \times 2$ Å

$\therefore$ this requires P - Na distance ~ 2.0 Å

7.5.53

Attempts to adapt Watson and Crick model to structure A

Modifications introduced

1/ P–P distance decreased from 7·0 A to 5·3 A
(as suggested by peaks on sections 2-3)

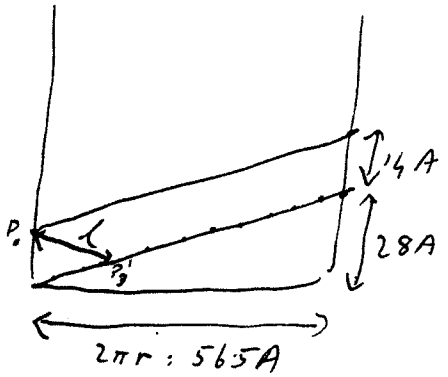
2/ 11 nucleotides per turn instead of 10
(as suggested by meridional peak on 11th layer-line)

3/ 2 chains of helix are equally spaced
(as suggested by pseudo-halving of cell
& 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 in chain

Draw schematically un-wrapped helix



Suppose P_0 P_3' are linked through
atom C_3' of same purine-pyrimidine
complex. Then on W & C model
$P_0 - P_3' = 15·2A$

To obtain length of arc 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 $\frac{5}{22} \times \frac{11}{3} \times 28 = \frac{5}{6} \times 28 = 23·4A$
∴ length of whole turn $= \sqrt{56·5^2 + 23·4^2} = \sqrt{3192 + 548} = \sqrt{3740} = 61·2A$
∴ length of arc $l = \frac{3}{11} \times 61·2 = 16·8A$

8. 5. 53

Length of $P - P'$ bonded through C_3's to same $P_u - P_y$ complex

Crick says 15.2 A

but this is inconsistent w other data of his ~~[illegible]~~ 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 and P on other side

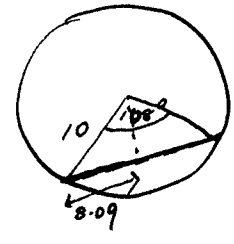
$\therefore PP'$ still ~ 18 A

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

xy cpt of $P_0 P_3'$ is 16.18

z cpt $(15.0 - 3 \times 3.4) = 4.8A$

$\therefore P_0 P_3' = \sqrt{16.18^2 + 4.8^2} = \sqrt{261.8 + 23.0} = 16.8A$



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

$P_0 P_3' \sim 17.6A$

11-residue helix in structure A

Difficulties

Can only have one helix / primitive cell

∴ how account for 13 A vector in C plane?

and how account for pseudo-hexag

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. in structure A is 0·55

In 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 2450 $Å^3$

1 nucleotide + 4 H_2O	415 $Å^3$	giving 59 nucleotides / unit cell
" 5 "	445	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. 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 helices in one direction must be possible, the spacing in other direction being 24·5 Å

but nucleo-protein gives same spacing, 24·5 Å,

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

spacing measured on R & W's published photos

Distances in Å

	① R & W	② Structure B	Ratio ①/②
equatorial	15·4	7·5	2·05
2nd equatorial	21·7	10·3	2·1
3·4 Å reflection	111	57	1·95

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)

∴ $a = 13.1$ Å - impossible for W & C model

or Unit cell contains 2 helices

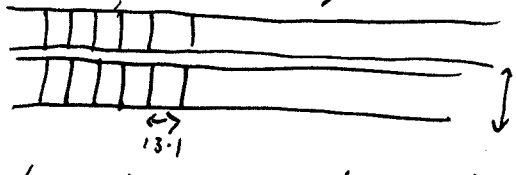
and $a = 26.2$ Å.

This is only slightly distorted from graphite-like structure,

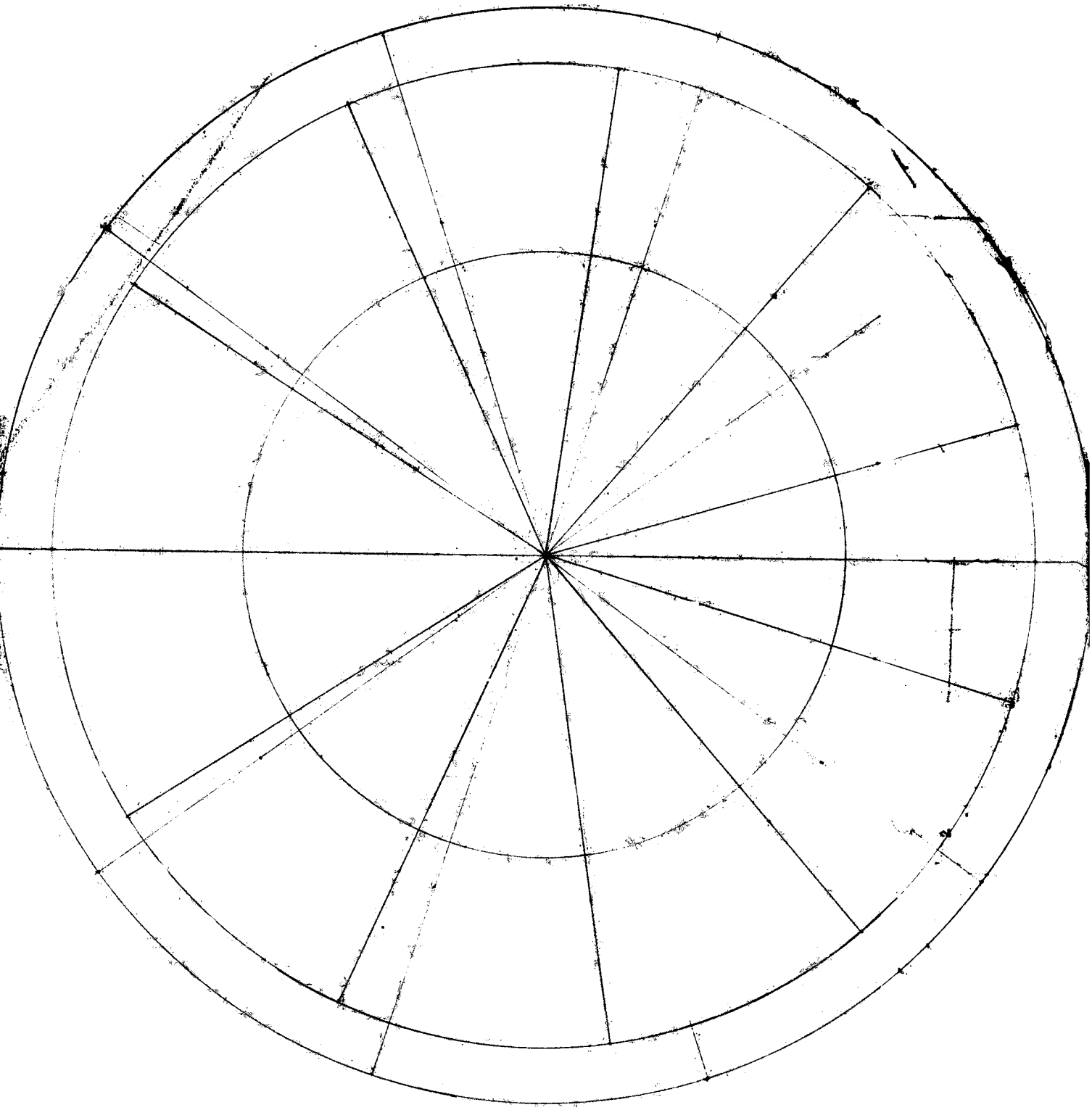
giving inter-helical distance ~ 16 Å

∴ Helices in sheets, with inter-sheet sep^n 24.5 Å and inter-penetrating

giving other dimension $\frac{322}{24.5} = 13.1$ Å



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



1cm = 1Å

W & C modified for structure A

Cylindrical Patterson ~~[illegible]~~ suggests helix of diameter 18A

∴ suppose P_1' on helix of radius 9·0A

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

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

9A 11-residue helix : $18 \sin \frac{32.23°}{2} = 5.07$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. spt of $C_1' - C_1' = 11 \cos 40° = 8.4$A

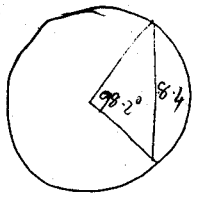
~~∴ C_1' lies on ⊙ of radius 4·2A~~

Suppose P_n and P_n' lie vertically above one another

(∵ 2-height peak suggests this ∴ approx. true)

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

at centre is of length 8·4A



radius : $\frac{4.2}{\sin 49.1°} = 5.55$A $\frac{4.29}{\sin 49.1} : 5.67$A

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

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

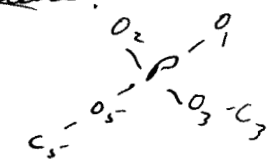
Horizontal spt of $C_1' - C_1'$ is then $5.55 \times 2 \sin \frac{360}{2 \times 11} = 3.12$A

Total $C_1' - C_1'$: $\sqrt{3.12^2 + 2.55^2} = \sqrt{9.73 + 6.53} = \sqrt{16.26} = 4.03$A

Model giving approx right distances & reasonable v d W

C_2 equidistant from O_1, O_5

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



~~Also coplanar with O~~

giving max. v d W distances for $C_2 O_2$ & $C_2 O_5$

$P - O_5 - C_5 - C_4$ ~ planar

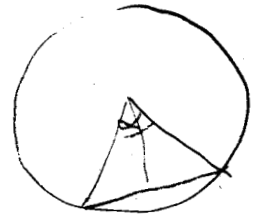
$P - P$ 5.7 Å $C_1' - C_1'$ 4.0 Å

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

Helix of radius 9.0 ~~cm~~ 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



$\alpha = \frac{360}{11} \times n$

x-cpt of vector on cylindrical Patterson

$= 2 \times 9 \sin \frac{360 \times n}{11 \times 2} = 18 \sin 16.35\, n$

$x_1 = 18 \times .2815 = 5.07$

$x_2 = 18 \times .5407 = 9.74$

$x_3 = 18 \times .7559 = 13.60$

$x_4 = 18 \times .9098 = 16.37$

$x_5 = 18 \times .9898 = 17.80$

Distances of atoms from axis i 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
(½)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
6·12	25·8	2·27	·07
4·44	27·9	2·45	·02
4·54	28·5	2·51	$\cdot\overline{05}$
4·55	28·6	2·51	$\cdot\overline{05}$
(½)4·90	30·8	2·71	$(\cdot\overline{15})\cdot\overline{08}$
5·10	32·1	2·82	$\cdot\overline{19}$
5·67	35·6	3·13	~~·20~~ $\cdot\overline{21}$
5·67	35·6	3·13	$\cdot\overline{21}$

Total 21

Intensities in structure A

If one helix per lattice point, then, ~~on equator~~, 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 A

Suppose tilt is about "diad" of complex. Then draw foreshortened complex by reducing distance of each atom from diad by factor ~~sin~~ 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 round 19 Å in structure A

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

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

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

Tilt of bases in structure A

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

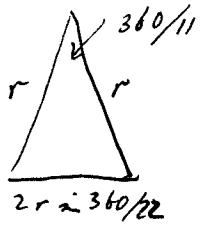
$\therefore$ ~~3~~ 5/3 mean values are 0·56, 0·48, ·44 for these layer-lines

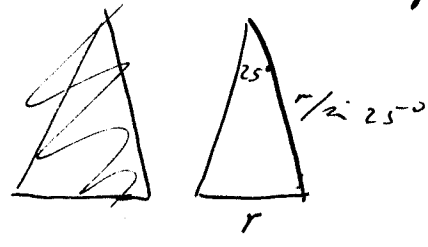
i.e. $\tan^{-1}$ 29°, 26°, 24°

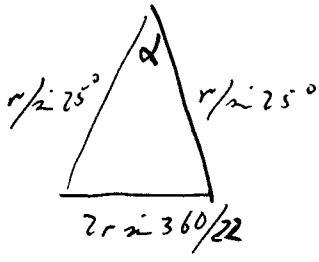
Suppose tilt 25°, find ∠ between planes of neighbouring bases

i.e. ∠ between ⊥'s to planes of bases

These lie on cone of semi-vertical angle 25°





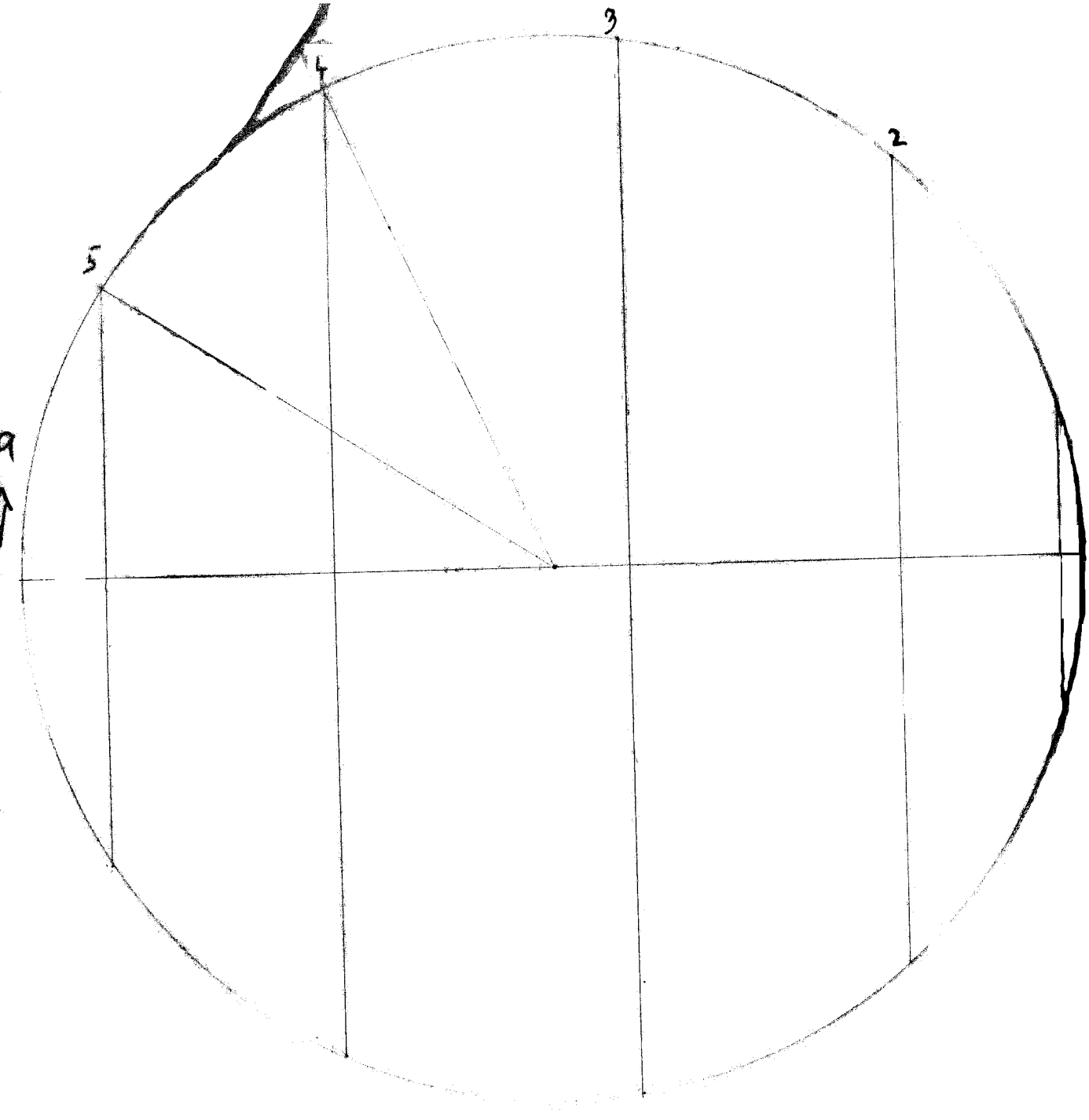


$$\alpha = 2\sin^{-1}\left(\sin\tfrac{360}{22}\sin 25\right)$$

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

$$= 2 \times 6°\,50'$$

$$\simeq 13\tfrac{1}{2}°$$


3
4
2
5

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

'a'		'c'	δ $= \frac{'a'}{22} \times 2.54$	c corrected Å	c section
1. $18 \sin \frac{360}{22}$	$= 18 \sin 16.36^\circ : 18 \times .2818 : 5.07$	c/11	0.6	3.2, 17.2	
2. $18 \sin 360 \times \frac{3}{22}$	$: 18 \sin 49.1^\circ : 18 \times .7559 : 13.6$	3c/11	1.6	9.3, 23.2	
3. $18 \sin 360 \times \frac{5}{22}$	$: 18 \sin 81.85^\circ : 18 \times .9899 : 17.8$	5c/11	2.1	14.9, 0.8	
4. $18 \sin 360 \times \frac{2}{11}$	$: 18 \sin 65.5^\circ : 18 \times .9100 : 16.4$	7c/11	1.9	19.8, 5.8	
5. $18 \sin 360 \times \frac{1}{11}$	$: 18 \sin 32.72^\circ : 18 \times .5404 : 9.74$	9c/11	1.2	24.2, 10.1	

δ is ∵ a-b sections are not ⊥ to fibre axis.

± δ depending on orientation (or hand) of helix

Examination of intra-helical vectors on 3-dimensional shows orient^n & hand to be as indicated opposite, & this gives + δ

Suppose the 2 helices 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 ~~other than P~~ (e.g. N_a)

then there is a similar vector $V_1 - v$

Suppose V_1 has $x = -1$ Å
$y = 0$
$z = 13$ Å (= 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. ~~xyz~~ v ~~section 10, $x = 6$ Å $y = 0$~~
$V_1 - v$ ~~section 4~~

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