Table 6. *Calculated and observed intensities of* $Mg_2B_2O_5$, *artificial*

Intensities estimated visually in the powder photograph (Co $K\alpha$)

hkl	I_o	F_c	*hkl*	I_o	F_c	*hkl*	I_o	F_c
011	*m*	−25	$03\bar{2}$	*s*	−63	$22\bar{2}$	*m*−	22
$01\bar{2}$	*s*	13	$\bar{1}13$	*m*−	−15	221	*w*+	−12
012	*s*	14	113	*s*	52	133	*w*+	−17
$02\bar{2}$	*s*	−35	$\bar{1}14$	*vw*	−1	$\bar{1}41$	*vw*	5
$10\bar{2}$	*s*	59	$\bar{1}23$	*vw*	− 5	204	*vw*	6
102	*vs*	−50	200	*m*+	−44	$23\bar{0}$	*vw*	− 9
013	*vw*	− 3	$2\bar{1}0$	*m*+	−20	026	*m*	−30
$\bar{1}12$	*m*−	−21	$2\bar{1}1$	*m*+	25	231	*vw*	− 1
$10\bar{3}$	*m*−	−10	$20\bar{2}$	*vw*	− 9	$20\bar{7}$	*m*	−24
$\bar{1}21$	*s*	−20	124	*m*−	−15			

the intensities of reflexions observed in the powder photograph of the artificial (triclinic) crystal (Table 6), supporting our statement.

In conclusion the writer wishes to express his sincere thanks to Prof. Ito for suggestion and guidance throughout the work.

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The Structure of Synthetic Polypeptides. I. The Transform of Atoms on a Helix

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The formulæ are given for the Fourier transforms of a number of helical structures; namely, a thin helical wire, a set of identical atoms spaced at regular intervals on a helix, and the general case of a group of atoms repeated by the operation of a non-integer screw. General predictions are made concerning the intensities of the X-ray diffraction pattern of the synthetic polypeptide poly-γ-methyl-L-glutamate, assuming that its structure is based on the α-helix suggested by Pauling & Corey.

1. Introduction

The following calculations were undertaken because of current interest in the structures of certain synthetic polypeptides. The preliminary X-ray data for these polypeptides have been described by Bamford, Hanby & Happey (1951) and their infra-red behaviour by Ambrose & Elliott (1951). Pauling & Corey (1951) have interpreted the structures of the two polypeptides which have so far given the best X-ray diffraction pictures, namely poly-γ-methyl-L-glutamate and poly-γ-benzyl-L-glutamate, in terms of the α-helix described by Pauling, Corey & Branson (1951). In this structure the residues repeat along the helix with a spacing of about 1·5 Å in the chain direction, and Perutz (1951) has found that a strong meridional reflexion of spacing 1·5 Å is given by poly-γ-benzyl-

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L-glutamate. More recently this has also been observed by Bamford, Brown, Elliott, Hanby & Trotter (1952) for poly-γ-methyl-L-glutamate and for a number of other polypeptides. As Perutz (1951) has also found that a 1·5 Å reflexion is given by certain proteins, it is possible that all these substances have basically a common structure. It is therefore important to establish the actual structure beyond doubt for at least one of them.

The other general property of the α-helix is that it repeats exactly only after a number of turns. For poly-γ-methyl-L-glutamate, which has a repeat of 27 Å in the chain direction, Pauling & Corey (1951) have suggested a helix of 18 residues, which goes round five times in 27 Å. The X-ray evidence is consistent with a hexagonal unit cell, with one chain der lattice point, so that all the chains are in identical orientations. The unit cell for poly-γ-benzyl-L-glutamate is only pseudo-hexagonal and has not yet been definitely established.

We have calculated first the transform of a thin helical wire. We have then derived the transform of a set of identical point atoms spaced at regular intervals on a single helix. We have next derived the formulæ for the structure factors for the general case of a group of atoms, with each atom of the group repeated regularly on a helix. From these results we have been able to make certain general predictions, partly of a statistical nature, about the intensities to be expected from a helical structure containing a number of different atoms. We have considered poly-γ-methyl-L-glutamate as a possible example, as it gives the simplest X-ray photograph.

Preliminary accounts of the application of the theory (Cochran & Crick, 1952) and of the experimental data (Bamford *et al.*, 1952) have already been published. The theory was also derived independently and simultaneously by Dr A. R. Stokes (private communication).

2. The transform of a uniform helix

We calculate first the Fourier transform (or continuous structure factor) of a uniform helix (for instance, a wire of infinitesimal thickness) of infinite length, radius r and axial spacing P. If the helix is defined by the equations

$$\left.\begin{aligned} x &= r\cos(2\pi z/P)\,, \\ y &= r\sin(2\pi z/P)\,, \\ z &= z\,, \end{aligned}\right\} \qquad (1)$$

(see Fig. 1), the value of the Fourier transform at a point (ξ, η, ζ) in Fourier (reciprocal) space is given by

$$T(\xi, \eta, \zeta) = \int \exp\left[2\pi i(x\xi+y\eta+z\zeta)\right]dV\,,$$

where dV, is a volume element of the helix. Using (1), and the fact that dV is proportional to dz,

$$T(\xi, \eta, \zeta) = \int_0^P \exp\left[2\pi i\left(r\xi\cos 2\pi\frac{z}{P}+r\eta\sin 2\pi\frac{z}{P}+z\zeta\right)\right]dz\,,$$

apart from unimportant constants of proportionality. This result can be written as

$$T(R, \psi, \zeta) = \int_0^P \exp\left[2\pi i\left\{Rr\cos\left(2\pi\frac{z}{P}-\psi\right)+z\zeta\right\}\right]dz\,, \qquad (2)$$

where $R^2 = \xi^2+\eta^2$ and $\tan\psi = \eta/\xi$.

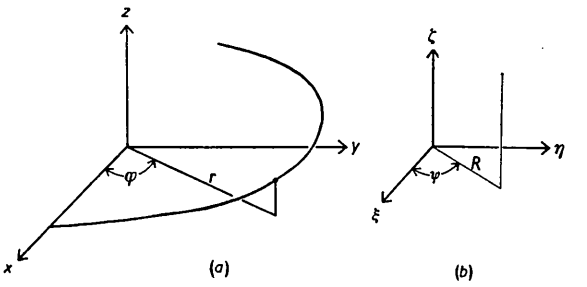

Fig. 1. (*a*) Cartesian (x, y, z) and cylindrical-polar (r, φ, z) coordinates of a point on a helix. (*b*) Corresponding coordinates of a point in reciprocal space.

The integral (2) vanishes unless $\zeta = n/P$, where n is an integer. This corresponds to the fact that the X-ray scattering from a helix which has an exact repeat after a vertical distance P, is confined to layer-lines at heights $\zeta = n/P$ in reciprocal space. Accordingly, we write (2) as

$$T\left(R, \psi, \frac{n}{P}\right) = \int_0^P \exp\left[2\pi i\left\{Rr\cos\left(2\pi\frac{z}{P}-\psi\right)+\frac{nz}{P}\right\}\right]dz\,.$$

This integral may be evaluated by using the identity

$$\int_0^{2\pi} \exp(iX\cos\varphi)\exp(in\varphi)d\varphi = 2\pi i^n J_n(X)\,,$$

taking $X = 2\pi Rr$ and $\varphi = 2\pi z/P$.

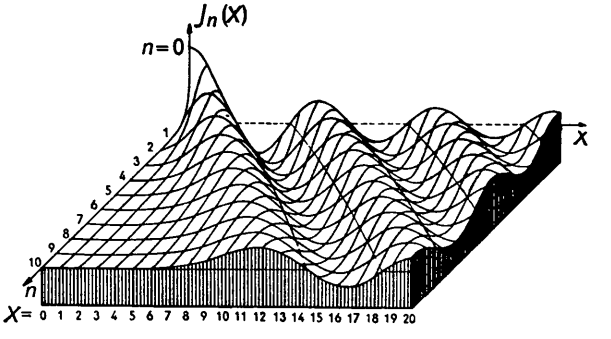

Fig. 2. Illustration of Bessel functions. (Reproduced by kind permission of the publishers from *Tables of Functions* by Jahnke & Emde. New York: Dover Publications.)

Table 1. *Values of n for poly-γ-methyl-L-glutamate*

		← m →											
		−5	−4	−3	−2	−1	0	+1	+2	+3	+4	+5	+6
	−3	—	—	—	—	+3	—	—	—	—	—	—	—
	−2	—	+14	—	—	—	—	−4	—	—	—	—	−22
↑	−1	—	—	—	+7	—	—	—	—	−11	—	—	—
l	0	+18	—	—	—	—	0	—	—	—	—	−18	—
↓	1	—	—	+11	—	—	—	—	−7	—	—	—	—
	2	—	—	—	—	+4	—	—	—	—	−14	—	—
	3	—	+15	—	—	—	—	−3	—	—	—	—	−21
	4	—	—	—	+8	—	—	—	—	−10	—	—	—
	5	+19	—	—	—	—	+1	—	—	—	—	−17	—
	6	—	—	+12	—	—	—	—	−6	—	—	—	—
	7	—	—	—	—	+5	—	—	—	—	−13	—	—
	8	—	+16	—	—	—	—	−2	—	—	—	—	−20
	9	—	—	—	+9	—	—	—	—	−9	—	—	—
	10	+20	—	—	—	—	+2	—	—	—	—	−16	—
	11	—	—	+13	—	—	—	—	−5	—	—	—	—
	12	—	—	—	—	+6	—	—	—	—	−12	—	—
	13	—	+17	—	—	—	—	−1	—	—	—	—	−19
	14	—	—	—	+10	—	—	—	—	−8	—	—	—
	15	+21	—	—	—	—	+3	—	—	—	—	−15	—
	16	—	—	+14	—	—	—	—	−4	—	—	—	—
	17	—	—	—		+7	—	—	—	—	−11	—	—
	18	—	+18	—	—	—	—	0	—	—	—	—	−18
	19	—	—	—	+11	—	—	—	—	−7	—	—	—
	20	+22	—	—	—	—	+4	—	—	—	—	−14	—

The result is

$$T(R, \psi, n/P) = J_n(2\pi Rr) \exp\left[in(\psi+\tfrac{1}{2}\pi)\right], \quad (3)$$

where J_n denotes the nth-order Bessel function.

This gives the amplitude and phase of the X-ray scattering on the nth layer line. The function T has two notable features: (i) $|T| = |J_n(2\pi Rr)|$ is independent of ψ, that is, the modulus of the transform has cylindrical symmetry. (ii) For small values of $2\pi Rr$, $|T|$ decreases rapidly as n increases. This can be seen clearly from the illustration of Bessel functions given in Fig. 2. This figure also enables one to see where the transform will have maxima.

3. The transform of a discontinuous helix

We define a discontinuous helix as a set of points occurring with a vertical spacing p on a continuous helix. X-ray scattering is now imagined to take place from these points only. The scattering from a set of identical atoms in this configuration can be found by multiplying the transform of the set of points by the atomic scattering factor.

Consider a function H which is zero everywhere except on a continuous helix, where it assumes the value unity, and another function K which is zero everywhere except on a set of horizontal planes of spacing p, where it assumes the value unity. The product KH of these two functions is a discontinuous helix. It follows that the transform of KH is the transform of K, convoluted (folded) with that of H. The transform of H was given in the previous section (equation (3)); that of K is easily proved to be zero except on an infinite set of points of spacing $1/p$ along the ζ-axis, where it assumes a value which we may take to be unity. The process of convolution therefore reduces in this case to setting down the transform of the continuous helix with its origin placed at each of the points (0, 0, 0), (0, 0, $+1/p$), (0, 0, $-1/p$), (0, 0, $+2/p$) etc. in turn, and taking the sum (see Fig. 3). The result is the transform of a discontinuous helix, and can be seen to be finite only in planes at height

$$\zeta = n/P + m/p\,, \quad (4)$$

on which it assumes the value $J_n(2\pi Rr)\exp[in(\psi+\frac{1}{2}\pi)]$. Like n, m can assume any integral value, positive or negative. If P/p cannot be expressed as a ratio of

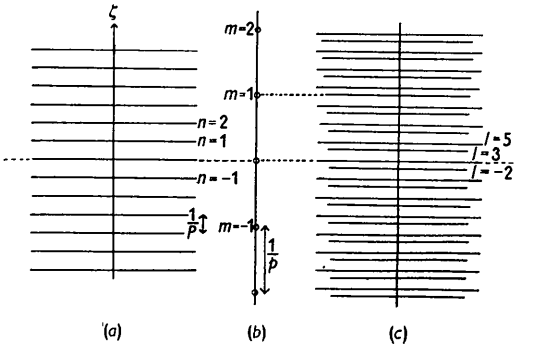

Fig. 3. (*a*) illustrates the fact that the transform of a helix of axial spacing P is finite only in planes at height $\zeta = n/P$, while (*b*) illustrates the fact that the transform of a set of planes of spacing p is finite only at points $(0, 0, \zeta)$ with $\zeta = m/p$. (*c*) is obtained by setting (*a*) down with its origin at height $\zeta = 0$, and again at $\zeta = 1/p$. It is therefore *part* of the transform of a discontinuous helix; the complete transform is obtained by setting (*a*) down with its origin at *every* point $\zeta = m/p$ in turn, and is therefore finite only in planes at height $\zeta = n/P + m/p$.

whole numbers, planes at height $n/P+m/p$, for all values of n and of m, fill the whole of reciprocal space. This case is considered in a later section. If, on the other hand, P/p can be expressed as a ratio of whole numbers, the transform is confined to a set of planes. For example, in the particular case corresponding to poly-γ-methyl-L-glutamate, $P = 5{\cdot}4$ Å, $p = 1{\cdot}5$ Å and $P/p = 18/5$. From (4) we then have

$$\begin{aligned} 5P\zeta &= 5n+18m \\ &= l \text{ (say)} . \end{aligned} \tag{5}$$

The transform is, in this case, confined to layers for which $\zeta = n/P+m/p = l/c$ Å^{-1} with $c = 27$ Å, corresponding, of course, to the fact that the discontinuous helix now has an exact repeat after 27 Å. For any one value of l the transform of the discontinuous helix is now given by

$$F\left(R, \psi, \frac{l}{c}\right) = \sum_n T\left(R, \psi, \frac{n}{P}\right) , \tag{6}$$

the sum being over all values of n which are solutions of (5). For example, when

$$l = 0,\ n = \ldots,\ -36,\ -18,\ 0,\ +18,\ +36,\ \ldots ,$$

and when

$$l = 1,\ n = \ldots,\ -25,\ -7,\ +11,\ +29,\ +47,\ \ldots .$$

The difference between successive values of n is always 18.

In Table 1 we have listed the values of n for values of l between -3 and $+20$, and values of m from -5 to $+6$, for the case of poly-γ-methyl-L-glutamate. This includes all values of n up to 18 for the layer-lines considered.

The same result for the transform of a discontinuous helix which has an exact repeat after a number of turns of the helix have been made, can be obtained by writing down the structure-factor equation in the normal way, and expanding it as a series of Bessel functions. The method we have given is more general, and makes the solution easier to grasp.

As an example of (6) we can take

$$\begin{aligned} F(R, \psi, 0) &= J_0(2\pi Rr)+J_{18}(2\pi Rr) \exp [18i(\psi+\tfrac{1}{2}\pi)] \\ &\quad +J_{-18}(2\pi Rr) \exp [-18i(\psi+\tfrac{1}{2}\pi)]+\ldots \\ &= J_0(2\pi Rr)-2J_{18}(2\pi Rr) \cos 18\psi+\ldots . \end{aligned}$$

The departure from cylindrical symmetry involves only the terms $J_{18}(2\pi Rr)$ etc., which will usually be negligible compared with $J_0(2\pi Rr)$.

Again

$$\begin{aligned} F(R, \psi, 1/27) &= J_{-7}(2\pi Rr) \exp [-7i(\psi+\tfrac{1}{2}\pi)] \\ &\quad +J_{11}(2\pi Rr) \exp [11i(\psi+\tfrac{1}{2}\pi)]+\ldots . \end{aligned}$$

On evaluating $|F|$ in this case, it is found to have an 18-fold axis of symmetry. To the extent that all other terms can be neglected compared with J_7, it has cylindrical symmetry.

Again,

$$\begin{aligned} F(R, \psi, 5/27) &= J_1(2\pi Rr) \exp [i(\psi+\tfrac{1}{2}\pi)] \\ &\quad +J_{-17}(2\pi Rr) \exp [-17i(\psi+\tfrac{1}{2}\pi)] \\ &\quad +J_{19}(2\pi Rr) \exp [19i(\psi+\tfrac{1}{2}\pi)]+\ldots . \end{aligned}$$

Here $|F|$ has almost complete cylindrical symmetry, as only the first term is appreciable, except for $2\pi Rr$ greater than about 15. It can be shown that however many terms are involved, $|F|$ has an 18-fold axis of symmetry over the entire diffraction pattern.

It is of interest to consider what happens if the helix is slightly deformed, so that it repeats exactly only after a larger distance.* For example, suppose the α-helix, instead of having 3·60 residues per turn, had about 3·58, so that the structure repeated after 17 turns containing 61 residues. We can most easily see what happens by fixing attention on a given Bessel function, whose position is defined by n and m.

Now since

$$\zeta = \frac{n}{P}+\frac{m}{p},$$

$$\delta(\zeta) = n\delta\left(\frac{1}{P}\right)+m\delta\left(\frac{1}{p}\right) ,$$

and if $\delta(1/P)$ and $\delta(1/p)$ are small, the Bessel function under consideration will move only a small distance in reciprocal space, especially if n and m are also small. As the true unit cell becomes larger, and the layer lines more closely spaced together, Bessel functions which previously occurred at the same level will now be distributed over different layer lines. As has been stated, if P and p are incommensurable, the transform fills the whole of reciprocal space, but it can do so only by employing Bessel functions of very high order, which in practice can be ignored. The more important Bessel functions of lower order will occur very close to positions given by taking commensurable approximations to P and p. Consideration of the full expressions given in the next section (equation (7)) shows that the values of the terms relevant in practice are only changed infinitesimally. The precision of the determination of P and p is of course limited by experimental error. If the structure were disordered, so that the effective local values of P and p varied, one would expect diffuse layer lines in the region corresponding to the average values of P and p. This appears to be the case for certain of the co-polymers (Bamford *et al.*, 1952).

4. Structure-factor calculation

We shall now consider how numerical calculations can be made when exact coordinates are assumed for all

* The ideas in this section were clarified during discussion with Dr L. Brown.

the atoms in a helical structure. We have to consider how the contributions of a number of sets of atoms on helices of different radii, and which may start off with the first atoms not at $x = r$, $y = 0$, $z = 0$, but at $x = r\cos\varphi$, $y = r\sin\varphi$, $z = z$, are to be combined. The transform of a discontinuous helix, starting with the last-mentioned coordinates, is

$$F \exp\left[i(-n\varphi+2\pi lz/c)\right].$$

This follows from the fact that the displacement of the first point to z in a cell of length c corresponds to a multiplication of the transform by the factor $\exp[2\pi ilz/c]$. The rotation of the helix through an angle φ, to bring the first point to the coordinates given above, results in its transform being rotated in the same direction, and by the same amount. A point then at (R, ψ, ζ) obviously came from $(R, \psi-\varphi, \zeta)$. Hence if a particular term in the series for F had the form $J_n(2\pi Rr)\exp[in(\psi+\frac{1}{2}\pi)]$, it now becomes

$$J_n(2\pi Rr)\exp\left[i(n\psi-n\varphi+\tfrac{1}{2}n\pi+2\pi lz/c)\right]. \quad (7)$$

In poly-γ-methyl-L-glutamate there are ten atoms per residue, and each chain consists of sets of identical atoms occurring at the points of ten different discontinuous helices. It follows that the structure factor F_c of one such unit, for $l = 1$ for example, is given by

$$F_c(R, \psi, 1/c) =$$
$$-\sum_{j=1}^{10} f_j J_7(2\pi Rr_j)\exp\left[i\{-7(\psi+\tfrac{1}{2}\pi)+7\varphi_j+2\pi z_j/c\}\right]+$$
$$\sum_{j=1}^{10} f_j J_{11}(2\pi Rr_j)\exp\left[i\{11(\psi+\tfrac{1}{2}\pi)-11\varphi_j+2\pi z_j/c\}\right]+\ldots.$$

The general expression is

$$F_c(R, \psi, l/c) =$$
$$\sum_n \sum_j f_j J_n(2\pi Rr_j)\exp\left[i\{n(\psi-\varphi_j+\tfrac{1}{2}\pi)+2\pi lz_j/c\}\right]. \quad (8)$$

For the purposes of computation it would be useful to graph the functions

$$C_n = \cos(n\psi)J_n(2\pi Rr),$$
$$S_n = \sin(n\psi)J_n(2\pi Rr).$$

If we write (7) in the form

$$J_n(2\pi Rr)\exp[in(\psi+\varepsilon)], \text{ where } \varepsilon = \tfrac{1}{2}\pi-\varphi+2\pi lz/nc,$$

then (7) becomes $C_n(\psi+\varepsilon)+iS_n(\psi+\varepsilon)$. If, for example, one prepares a contour map of C_n against cylindrical coordinates $(2\pi Rr, \psi)$, one can then place over it a grid whose intersections correspond to the reciprocal-lattice points for the value of r appropriate to a particular set of atoms. By turning this grid to the angle ε (which one has to compute) one can read off $C_n(\psi+\varepsilon)$ for all the reciprocal-lattice points. This process can be repeated for each atom, and the contributions summed; similarly for $S_n(\psi+\varepsilon)$. This is particularly valuable when the phases of the Fourier components are required.

The theory can easily be extended to cover cases where there is more than one chain per lattice point by considering a chain displaced from the origin to the point (x_0, y_0, z_0) and turned about its axis by an angle φ_0. The contribution of this chain to the transform is obtained by multiplying the general expression (7) by a factor

$$\exp\left[2\pi i(hx_0/a+ky_0/b+lz_0/c)\right]\exp\left[-in\varphi_0\right].$$

It is interesting to note that the helix which consists, chemically, of one polypeptide chain, is in fact only one of the possible solutions which are consistent with the general helical arrangement. For example, a discontinuous right-handed helix which has $p=1{\cdot}5$ Å, and makes 5 turns in 27 Å may be regarded as two separate but intertwining left-handed discontinuous helices, each with $p = 3{\cdot}0$ Å and making 4 turns in 27 Å. Such structures will generally not be stereochemically feasible. Conversely, if one has to consider a structure which actually does consist of several chains intertwined, it is convenient for computation to imagine the residues, however they may be connected chemically, to be associated with a single 'primitive' helix, which is chosen as the one for which both the z translation and the angle of rotation between successive residues have the smallest values. All calculations can be made in terms of this one helix, using the theory given above.

5. Application to poly-γ-methyl-L-glutamate

As we have seen, we may imagine the infinite polypeptide chain as made up from a number of sets of atoms, each set consisting of atoms occurring at intervals p on a helix of axial spacing P and radius r. The number of sets of atoms composing one chain will be equal to the number of atoms per residue of the polypeptide; each set will in general occur on a helix of different radius, and if we take one helix as a standard, the others will in general be rotated and translated relative to the first. This helical configuration (defined by P and p) of every set of atoms is in itself enough to enable us to make general predictions about the intensities of the X-ray reflexions to be expected from such a structure—there is no need for detailed assumptions about the exact relative positions of atoms belonging to the same residue to be made. This is a situation which occurs very seldom in X-ray analysis; usually a crystal-structure problem must be solved in detail before anything at all can be said about the atomic arrangement, and conversely only when the structure is known completely can the intensities of the X-ray reflexions be calculated. In this case, the basis of the predictions is that reflexions to which all sets of atoms make only a small contribution will be absent, whereas

reflexions to which a number of sets may contribute are likely to be strong. The contribution of the jth set of atoms is of course the sum over a few values of n of terms of the form (7), so that, if the values of $J_n(2\pi Rr)$ are very small for all values of r which occur in the structure, the corresponding reflexion must be absent. When this quantity is large for many of the values of r which we might expect to be present, the corresponding reflexion is not necessarily strong, as the phase part of the expression (7) may effect a cancellation when the contributions from all sets are summed. On the average, however, such reflexions will be strong.

We assume, therefore, that poly-γ-methyl-L-glutamate is based on the α-helix proposed by Pauling & Corey, so that the structure of one infinite chain can be produced from one residue by the operation of a non-integer screw of 100° and 1·5 Å. We now use the property of Bessel functions, illustrated in Fig. 2, that for small values of the argument $2\pi Rr$, the function $J_n(2\pi Rr)$ is very small when n is large. The greater the value of n, the greater $2\pi Rr$ can be before $J_n(2\pi Rr)$ becomes appreciable. Now, whatever the precise form of the side groups, no atom can lie further than about 8 Å from the axis of the helices if reasonable bond lengths are assumed. For any set of atoms making up the main chain (including the β-carbon atom)—and this accounts for half the total—r is not greater that 3·3 Å, according to Pauling & Corey (1951). The part of the transform covered by the observed diffraction data does not extend beyond $R = 0{\cdot}35$ Å^{-1} ($l \neq 0$), so that in considering the contribution of any set of atoms of the main chain to any reflexion, a value of $2\pi Rr$ greater than 7·2 will not occur. Even when the contributions of atoms of the side groups are considered, $2\pi Rr$ will not exceed 17. The implications of this can be seen by considering the reflexions on the first layer, which are contributed to by Bessel functions of order 7 and 11. For the reflexion $(10\bar{1}1)$, $R = 0{\cdot}097$ Å^{-1}, and $J_7(2\pi Rr)$ is quite negligible for $r < 7$ Å. Only the outermost atoms of the side groups could contribute weakly to this reflexion. A similar calculation shows that the contribution of atoms of the main chain to any reflexions on this layer for which $R < 0{\cdot}35$ Å^{-1} is always very small, although atoms of the side group could make a small contribution. No reflexions are observed experimentally on this layer. Intensities on the second layer depend on $J_4(2\pi Rr)$, so that low-order reflexions are again likely to be weak, and the main contributors to reflexions $(11\bar{2}2)$ and $(20\bar{2}2)$ must be the atoms of the side groups. The third layer involves $J_3(2\pi Rr)$, and we might expect to find some reflexions on it, while on the fourth the intensities depend on $J_8(2\pi Rr)$, so we would expect nothing except possibly at comparatively large values of R. On the other hand, $l = 5$ is contributed to by $J_1(2\pi Rr)$, and many sets of atoms can make large contributions. In short, we can make the general prediction that 'layer lines to which only high-order Bessel functions contribute will be weak or absent, and those to which low-orders contribute will be strong' (Cochran & Crick, 1952). The experimental data of Bamford *et al.* (1952) agree with this prediction in a striking manner, no reflexion appearing on any layer line unless a Bessel function of order 4 or less is involved. In fact the agreement is too good, and suggests that the upper limit to the value of $2\pi Rr$ is more nearly 7 than 17, that is, that the effect of the atoms of the side groups is in some way reduced. This could be due to the side groups having a greater amplitude of thermal vibration, or being more disordered, than the atoms of the main chain. On the other hand, the assumption that the side groups are all equivalent, i.e. that both the main chain and side groups have an 18-fold screw axis, may not be correct. The space group, which is probably $C6_1$, requires only that every *third* side group should be equivalent. If all are equivalent, their relationship to neighbouring parts of their own chain is the same for each, but their relationship to neighbouring parts of adjacent chains falls into three different types. Thus there is no compelling reason for all the side groups to have the same orientation relative to the main chain.

The evidence thus suggests very strongly that the main chain of poly-γ-methyl-L-glutamate is based on the α-helix, or a very similar helix, but it is not possible by this rather general approach to decide whether the side groups also conform strictly to this arrangement.

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