parameters changed appreciably from those used in C because of the inclusion of more data and the different weighting system. The effect was much smaller in the second cycle (changes −0·0015, −0·0000 and 0·0021 Å instead of −0·0016, 0·0008 and 0·0015 Å). Allowing the scale and temperature-factor parameters to change simultaneously with the atomic coordinates here accelerates the refinement while these parameters change appreciably, but the coupling between these parameters and the coordinates would presumably be smaller in another structure composed of more atoms in more general positions.

The standard deviations at the end of the first cycle of this refinement would differ only slightly from those under C′. Neglect of scale and temperature-factor-parameter changes has a smaller effect on the standard deviations than on the atomic positions; in fact, neglecting all off-diagonal elements in the normal equations yields standard deviations differing by less than 10% from the correct values.

The author would like to thank Mr Lincoln Ekstrom for preparing photographs, Mr F. S. Lee for details of his weighting scheme, Dr Truter for informing him of her results before publication, and the Office of Naval Research for financial support.

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Calculated form factors for the 18-residue 5-turn α-helix.*

By Linus Pauling, Robert B. Corey, Harry L. Yakel, Jr.† and Richard E. Marsh, *Gates and Crellin Laboratories of Chemistry, California Institute of Technology, Pasadena, California, U.S.A.*

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Cochran, Crick & Vand (1952) have derived expressions for the evaluation of the Fourier transform of atoms on a helix. With the help of these expressions we have calculated form factors for the equator and first 28 layer lines of the 18-residue 5-turn α-helix.

For atoms arranged in a helical structure, the form factor expression, as derived by Cochran *et al.*, is

$$F_h(R, \psi, l/c) = \sum_n \sum_j f_j J_n(2\pi R r_j) \exp \{i[n(\psi - \varphi_j + \tfrac{1}{2}\pi) + 2\pi l z_j/c]\} ,$$

where R, ψ and l/c are cylindrical coordinates in reciprocal space, r_j, φ_j and z_j are the cylindrical coordinates of atom j in real space, f_j is the atomic form factor, and J_n is the nth-order Bessel function. The summation extends over all values n that satisfy the condition

$$n/P + m/p = l/c ,$$

where P is the pitch of the helix and p is the vertical spacing between equivalent atoms; m and n are integers.

Table 1. *Atomic coordinates for the* 18-*residue* 5-*turn helix (left-handed configuration)*

Atom	r (Å)	φ (°)	z (Å)
C	2·28	0·0	1·48
N	1·57	29·1	0·62
C′	1·61	74·6	1·09
O	1·76	83·5	2·29
βC(1)	3·20	−19·3	0·65
βC(2)	3·44	16·1	2·12

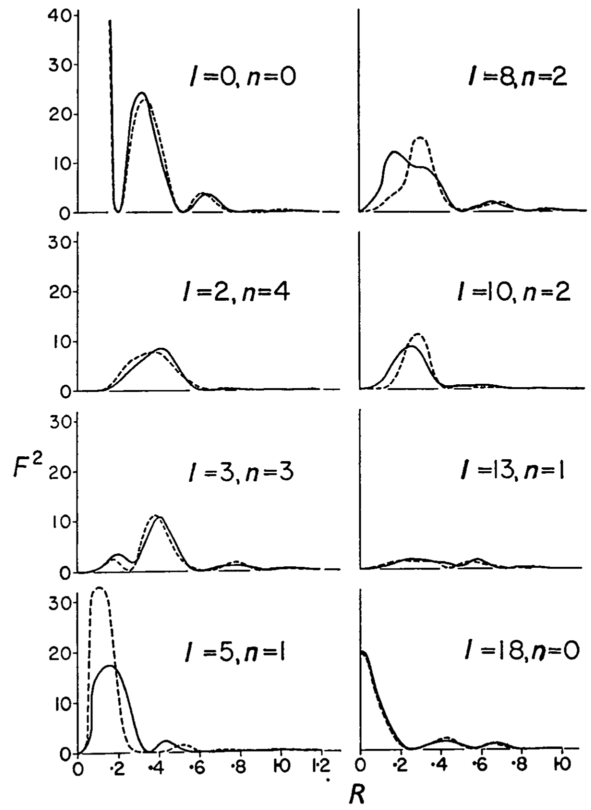

Fig. 1. Plots of F^2 for the most prominent layer lines of the 18-residue 5-turn α-helix. The solid curves are for the β-carbon atom in position 1 (*d* configuration for the left-handed helix) and the dashed curves are for the β-carbon atom in position 2 (*l* configuration for the left-handed helix).

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† Present address: Oak Ridge National Laboratory, Oak Ridge, Tennessee, U. S. A.

Table 2. F^2 *values calculated for the* 18-*residue* 5-*turn* α-*helix*

For each layer line, the top row of figures is for the β-carbon atom in position 1 (*d* configuration for the left-handed helix) and the bottom row of figures is for the β-carbon atom in position 2 (*l* configuration for the left-handed helix).

sin θ/λ →	0	.02	.04	.06	.08	.10	.12	.14	.16	.18	.20	.22	.24	.26	.28	.30	.32	.34	.36	.38	.40	.42	.44	.46	.48	.50	.52	.54	.56	.58	.60
l = 0 n = 0	1089 1089	879 871	514 497	200 187	38.7 35.8	.09 .22	10.31 7.45	22.36 18.07	24.27 22.65	19.65 21.68	12.96 16.29	6.71 8.68	2.06 2.26	.05 .00	.75 1.53	2.64 3.52	3.62 3.59	2.91 2.14	1.42 .77	.33 .16	.00 .02	.06 .00	.12 .01	.13 .07	.14 .22	.18 .40	.22 .44	.22 .27	.13 .07	.02 .00	.01 .06
l = 1 n = 7		.00 .00	.00 .00	.00 .00	.00 .00	.00 .01	.03 .06	.12 .22	.32 .49	.57 .73	.83 .67	1.00 .20	.60 .02	.31 .11	.12 .51	.08 .83	.20 .97	.62 1.16	1.45 1.59	2.48 2.12	3.16 2.42	3.09 2.43	2.31 2.07	1.32 1.44	.57 .76	.15 .25	.01 .04	.11 .22	.08 .14	.11 .22	.19 .25
l = 2 n = −4			.00 .00	.02 .04	.32 .58	1.35 2.32	3.02 4.67	4.66 6.32	5.99 7.05	7.34 7.62	8.37 7.71	8.20 6.74	6.29 4.89	3.53 3.10	1.35 1.80	.28 .81	.03 .19	.09 .08	.21 .24	.30 .30	.26 .20	.14 .12	.05 .08	.06 .03	.07 .01	.04 .03	.01 .05	.00 .03	.01 .01	.01 .02	.02 .03
l = 3 n = 3				.00 .01	.85 .91	2.94 2.38	3.35 1.36	2.05 .30	2.70 3.56	6.50 9.04	9.92 11.12	9.97 8.93	7.02 5.29	3.47 2.58	1.10 1.15	.14 .45	.12 .12	.48 .20	.86 .78	1.10 1.53	1.13 1.73	.89 1.13	.45 .32	.10 .03	.09 .22	.31 .41	.45 .35	.35 .17	.14 .05	.01 .01	.01 .00
l = 4 n = −8					.00 .00	.00 .00	.00 .00	.00 .01	.02 .04	.06 .14	.15 .28	.24 .36	.23 .25	.11 .04	.01 .06	.12 .43	.49 .88	.84 .97	.87 .64	.55 .23	.19 .05	.07 .09	.19 .16	.33 .20	.36 .21	.29 .22	.21 .23	.14 .24	.09 .20	.06 .11	.04 .03
l = 5 n = −1						11.00 31.42	17.37 30.07	15.01 7.91	8.79 1.15	1.92 .21	.06 .07	1.57 .01	2.24 .43	1.33 1.24	.37 1.40	.06 .67	.08 .07	.11 .13	.09 .38	.08 .37	.09 .21	.13 .07	.15 .01	.13 .08	.14 .22	.21 .26	.25 .17	.17 .09	.06 .08	.04 .09	.10 .10
l = 6 n = 6							.00 .00	.01 .01	.11 .22	.47 .85	.96 1.53	1.15 1.59	.91 1.02	.63 .44	.74 .18	1.05 .18	1.14 .39	.88 .70	.50 .84	.26 .69	.22 .53	.28 .51	.47 .48	.26 .30	.11 .09	.04 .03	.11 .09	.21 .12	.21 .11	.11 .07	.02 .03
l = 7 n = −5								.00 .01	.06 .16	.46 .76	.38 1.06	.27 .91	.67 1.12	1.73 1.63	2.58 1.76	2.48 1.62	1.80 1.41	1.23 1.74	.87 1.25	.52 .54	.18 .13	.07 .09	.17 .12	.22 .09	.17 .05	.11 .04	.10 .06	.01 .08	.09 .07	.06 .06	.04 .05
l = 8 n = 2									5.57 1.48	11.73 4.17	9.42 12.74	9.05 14.79	7.41 8.36	3.95 2.68	1.07 .77	.11 .54	.78 .60	1.24 .97	2.05 1.49	1.56 1.85	.91 1.38	.45 .46	.22 .06	.22 .34	.39 .64	.47 .52	.36 .24	.16 .06	.02 .01	.00 .01	.03 .01
l = 9 n = −9										.00 .00	.00 .00	.00 .03	.01 .12	.07 .23	.18 .23	.30 .10	.33 .10	.23 .00	.10 .09	.03 .20	.03 .22	.01 .08	.01 .03	.09 .15	.23 .28	.37 .34	.42 .34	.41 .31	.36 .27	.27 .18	.15 .16
l = 10 n = −2											3.54 .61	8.27 7.90	7.53 10.92	3.14 4.28	.62 .33	.56 .43	.68 .62	.63 .34	.73 .21	.63 .23	.23 .21	.00 .10	.09 .01	.17 .08	.11 .18	.04 .15	.02 .04	.02 .00	.02 .02	.01 .03	.01 .03
l = 11 n = 5												.02 .04	.59 .89	1.64 1.96	1.99 1.79	1.87 1.27	1.88 1.21	1.81 1.52	1.40 1.71	.88 1.32	.40 .57	.12 .15	.04 .11	1.01 .10	.07 .04	.05 .04	.07 .06	.09 .04	.05 .03	.01 .05	.02 .04
l = 12 n = −6													.00 .00	.08 .11	.26 .20	.30 .10	.50 .64	1.21 1.70	1.86 2.03	1.70 1.40	1.03 .69	.50 .33	.27 .21	.18 .24	.12 .27	.08 .20	.06 .09	.04 .11	.04 .02	.05 .02	.05 .01
l = 13 n = 1														1.34 1.42	1.83 1.54	1.39 1.44	1.24 .26	.53 .40	1.02 1.29	1.58 1.23	.94 .74	.14 .40	.05 .17	.27 .18	.34 .33	.23 .31	.10 .17	.04 .04	.05 .00	.05 .04	.04 .07
l = 14 n = 8															.00 .00	.01 .02	.09 .15	.28 .34	.41 .32	.42 .12	.02 .02	.02 .01	.01 .03	.02 .10	.04 .13	.06 .06	.04 .01	.02 .02	.01 .02	.00 .00	.00 .04
l = 15 n = −3																.71 .10	1.05 1.29	.81 1.27	.06 .09	.27 .75	.56 .55	.28 .17	.17 .11	.24 .11	.16 .04	.06 .01	.06 .03	.07 .06	.04 .05	.01 .03	.00 .04
l = 16 n = 4																	.33 .48	.35 .32	.26 .26	.30 .13	.06 .05	.01 .15	.00 .07	.01 .00	.11 .02	.14 .04	.06 .07	.01 .03	.05 .00	.09 .08	.09 .14
l = 17 n = −7																	.00 .00	.01 .02	.15 .12	.52 .16	.70 .19	.59 .73	.49 1.24	.58 1.16	.15 .83	1.06 .59	.93 .51	.54 .50	.20 .37	.04 .15	.00 .02
l = 18 n = 0																		11.80 11.10	.02 .03	1.05 1.13	1.73 2.20	.85 .76	.05 .09	.83 .92	1.17 .89	.49 .32	.03 .03	.07 .02	.18 .11	.17 .18	.11 .18
l = 19 n = 7																			.00 .00	.01 .02	.15 .06	.32 .32	.33 .24	.38 .31	.43 .39	.36 .44	.28 .36	.19 .32	.07 .03	.01 .02	.01 .01
l = 20 n = −4																				.01 .01	.07 .53	.51 .30	2.11 .84	2.06 2.09	1.10 1.96	.38 .60	.05 .01	.05 .16	.28 .33	.50 .34	.44 .26
l = 21 n = 3																					.00 .11	2.61 3.21	4.91 4.33	1.52 1.24	.05 .17	.13 .04	.13 .13	.11 .23	.17 .26	.19 .04	.10 .04
l = 22 n = −8																						.00 .00	.04 .01	.08 .12	.16 .13	.08 .02	.01 .02	.02 .01	.02 .00	.01 .00	.01 .02
l = 23 n = −1																							2.34 2.16	.04 .00	.54 .69	.14 .09	.04 .03	.06 .04	.05 .05	.02 .02	.01 .02
l = 24 n = 6																								.00 .00	.06 .13	.01 .04	.06 .02	.08 .01	.12 .20	.34 .32	.32 .21
l = 25 n = −5																									.03 .05	.41 .32	.23 .13	.24 .20	.35 .50	.32 .43	.20 .23
l = 26 n = 2																										1.53 .97	.43 .84	.09 .07	.07 .10	.32 .17	.17 .11
l = 27 n = 9																											.00 .00	.01 .01	.04 .05	.04 .02	.02 .03
l = 28 n = −2																												1.06 1.11	.34 .37	.00 .04	.12 .06

For the 18-residue 5-turn helix P/p is equal to 18/5, so that $5n+18m = l(5P/c)$. We have chosen a value for p of 1·48 Å; this is close to the value usually observed for the spacing of the prominent meridional reflection that is characteristic of the α-helix. The value of c, the layer-line identity distance, is then 26·64 Å ($= 18p$). For each layer line l, the integer n may assume a family of values; however, in view of the low amplitude of high-order Bessel functions, it is necessary for our purposes to consider only the lowest value of n for each layer line (see Table 1, Cochran *et al.*, 1952). The term $\exp(in\pi/2)$ then becomes only a phase-determining term and may be ignored.

For the 18-residue 5-turn helix, the function F_h is periodic with respect to ψ, repeating every 20°. This is a small enough interval so that we have felt justified in calculating the function at only one value of ψ, viz., at $\psi = 0$. We have made an additional calculation for the zero layer line at $\psi = 10°$; the results of this calculation were insignificantly different from those with $\psi = 0$, and thus confirmed our assumption that $F(R, \psi, l/c)$ can be closely approximated by $F(R, l/c)_{\psi=0}$. It should, however, be emphasized that for helical structures having a symmetry axis of lower order it will probably be necessary to evaluate the form factors at more than one value of ψ.

We have evaluated the expression

$$\sum_j f_j J_n(2\pi R r_j) \exp\,[i(2\pi l z_j/c - n\varphi_j)]$$

for values of l up to 28 (corresponding to $c/l = 0{\cdot}95$ Å) and values of R $(= (4 \sin^2 \theta/\lambda^2 - l^2/c^2)^{\frac{1}{2}})$ up to $\sin \theta/\lambda = 0{\cdot}60$ ($d = 0{\cdot}83$ Å). Atomic coordinates for the atoms included in the calculation are listed in Table 1. These coordinates are very nearly the same as those formulated by Pauling & Corey (1951), and are consistent with a planar peptide group and an N---H $\cdots$ O hydrogen bond with length 2·78 Å. The coordinates as listed correspond to a left-handed helix. Two sets of calculations were carried out, corresponding to the β-carbon atom in position 1 (d configuration for the left-handed helix) and in position 2 (l configuration). The atomic form factors used were those of James & Brindley (1935).

The calculated values of F_h^2 are listed in Table 2. These values are large only for layer lines involving low-order Bessel functions. In Fig. 1 F_h^2 values for these prominent layer lines are plotted against R for easier comparison with diffraction photographs. However, it should be pointed out that no temperature factor has been applied to the calculated values, and they have not been corrected for Lorentz or polarization factors and hence cannot be quantitatively compared with a fiber photograph without the corresponding corrections.

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Book Reviews

Works intended for notice in this column should be sent direct to the Editor (P. P. Ewald, Polytechnic Institute of Brooklyn, 99 Livingston Street, Brooklyn 2, N.Y., U.S.A.). As far as practicable books will be reviewed in a country different from that of publication.

Report of the Conference on Defects in Crystalline Solids. Pp. 429 with many figs. and plates. London: The Physical Society. 1955. Price 40*s*.

This work is the report of a conference held in Bristol in July 1954. It consists of 47 papers besides a small number of discussion remarks.

Imperfections of the crystalline lattice have a profound influence on many physical properties of solids. Emphasis has been given today mainly to research on those properties which allow discrimination between different kinds of lattice faults. Since imperfections are often coupled to each other, the task of unravelling the structure of imperfect solids remains formidable.

It seems that modern magnetic resonance techniques are especially suited to distinguish between lattice imperfections. More than 90 pages, about one-fourth of the space of the volume, are devoted to resonance experiments. Several papers show that paramagnetic resonance in insulators and semiconductors gives detailed information on impurity states and colour centres. Experiments are dealt with by Kittel which furnish direct evidence of the charge distribution around F-centres. The contribution of nuclear magnetic resonance experiments to the study of crystal imperfections is most impressive. Bloembergen gives a systematic survey of the information which nuclear magnetic resonance can furnish on various imperfections such as dislocations, vacancies and interstitials, foreign atoms, electrons and holes etc. The influence of magnetic dipole-interaction and of quadrupole effects is dealt with separately. The energy levels of nuclei with quadrupole moments are affected by the inhomogeneity of the local electric field. Therefore it becomes possible to measure, for instance, the variations of the stress field in the immediate surroundings of an impurity atom. The measurement of more conventional quantities can be extended and refined. The narrowing of the line width which occurs when the spin phase-memory time of a rigid lattice is of the order of the mean time which a nucleus spends at a given site leads to an elegant and consistent determination of the constants of self diffusion for the alkali metals (Slichter). The association of impurity atoms and vacancies to which they give rise is also reflected in the nuclear resonance line width (Cohen & Reif). The same phenomenon is dealt with in more conventional careful experiments (Haven) and has been treated theoretically (Lidiard).

A set of papers deals with the effect of different lattice faults on the optical and electrical properties of nonmetals both experimentally and theoretically. The lattice faults in part of this work have been introduced by high-energy particle and γ ray irradiation.

It is remarkable that no fewer than nine papers deal with the physical effect of radiation disarrangement. This kind of experiment is often rather complicated by the simultaneous occurrence of different lattice imperfections and also of 'radiation anneal'. Its scientific interest lies in the special kinds of imperfection produced, such as 'thermal spikes', and in the considerable deviations from equilibrium which can be reached. The volume contains a review article on radiation disarrangement by Koehler & Seitz.

Among other interesting work on diffusion, attention must be directed to Turnbull's paper on precipitation, which shows that several precipitation processes are many orders of magnitude too rapid to be accounted for by volume diffusion. Diffusion short circuits must then be rate-controlling. In the case of cellular precipitation the