211. *The Crystal and Molecular Structure of Certain Dicarboxylic Acids. Part VI. Sebacic Acid.*

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The crystal structure of sebacic acid has been fully determined by quantitative *X*-ray analysis, and is found to be similar to that of adipic acid. The finer details of the molecular structure are also found to be similar, and there is an indication of certain minor bond-length variations extending over the entire length of the molecule. In the grouping of the molecules in the crystal there is again evidence of a fairly close lateral approach, as well as the usual end-to-end hydrogen bonding through the carboxyl groups. This type of lateral approach appears to be characteristic of the acids of the " even " series. The effect of the hydrogen atoms on the intensities of the *X*-ray reflections is discussed, and it is shown that they make considerable contributions to the structure factors of the large spacing planes. Their presence is also evident on some of the contour maps.

The first three members of the series of normal aliphatic dicarboxylic acids (oxalic, malonic, and succinic) have widely different unit cells and crystal structures. From glutaric acid upwards, however, it has been shown, chiefly by the work of Caspari (*J.*, 1928, 3235; 1929, 2709), that the acids form a well-defined and closely related crystallographic series, composed of two sub-groups, the acids with an even and those with an odd number of carbon atoms in the molecule. The dimensions of the *a* and *b* axes and the angle β are rather similar for both groups, and almost constant for successive members in each group, the chief variant being the *c* axis. The even acids have two centrosymmetric molecules in the unit cell, and the *c* axis gives a measure of the chain length. The odd acids have four molecules in the unit cell, and the length of the *c* axis in this case corresponds to two molecules lying end to end.

In the previous paper (Part V) we have examined the fine structure of adipic acid which may be described as the first normal member of the even series, and have obtained evidence of certain bond-length variations in the saturated chain. To discover whether these effects persist in the higher members of the even series we have now made a similar quantitative *X*-ray investigation of the structure of sebacic acid. Our measurements lead to the rather surprising conclusion that in this saturated chain of ten carbon atoms there are again variations, in the nature of alternate long and slightly shorter bonds, over the entire length of the molecule. It is true that these variations are not much greater than the possible experimental error, but their regularity and their persistence in other members of this series of even acids would seem to be significant.

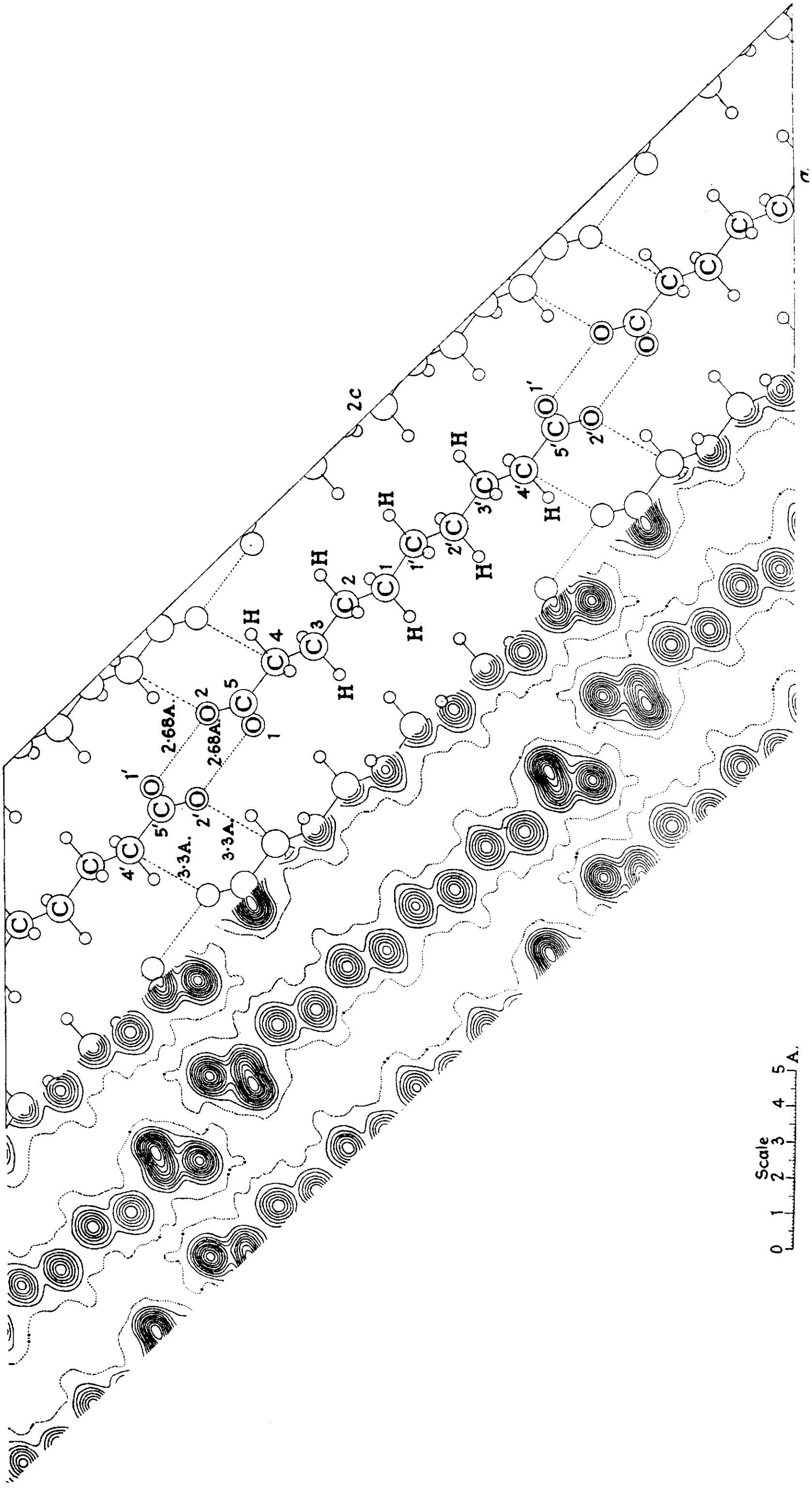
Another point of interest in this analysis concerns the effect of the hydrogen atoms on the intensities of the *X*-ray reflections. These are usually neglected in *X*-ray work, but if as a first approximation we take the scattering power of an atom to be proportional to its atomic number, then hydrogen is responsible for over 16% of the total scattering matter in sebacic acid. At low angles of reflection this effect should be noticeable, and we find that it has in fact a considerable influence on certain reflections, as well as being apparent in the electron-density maps. We make allowance for this effect in our calculations.

Crystal Data.—Sebacic acid, $C_{10}H_{18}O_4$; *M*, 202·2; m. p. 134°; *d*, calc. 1·226, found 1·231. Monoclinic prismatic, $a = 10{\cdot}10 \pm 0{\cdot}03$, $b = 5{\cdot}00 \pm 0{\cdot}01$, $c = 15{\cdot}10 \pm 0{\cdot}05$ A., $\beta = 133{\cdot}8^\circ \pm 0{\cdot}3^\circ$. Absent spectra, ($h0l$) when *h* is odd, ($0k0$) when *k* is odd. Space group $C_{2h}^5(P2_1/a)$. Two molecules per unit cell. Molecular symmetry, centre. Volume of the unit cell, 548 A.^{3}. Absorption coefficient for *X*-rays ($\lambda = 1{\cdot}54$) $\mu = 9{\cdot}08$ cm.$^{-1}$. Total number of electrons per unit cell = F(000) = 220.

The crystals obtained from most solvents are in the form of very thin flakes developed on the (001) face. These are generally unsuitable for *X*-ray work. Slow and careful crystallisation from amyl acetate, however, sometimes yields crystalline fragments which can be cut to give suitable specimens. Crystals so obtained usually show only the (001) and (100) faces, no end faces being identified with certainty. There is marked cleavage on (001) and (100). Further goniometric and optical data are given by Caspari (*loc. cit.*).

Analysis of the Structure.—Probable positions for the molecules in this crystal have been suggested by Caspari (*loc. cit.*) but the work does not lead to the actual determination of any atomic positions. The asymmetric unit in the structure consists of one half molecule. The dimensions of the *a* and *b* axes are almost identical with those of adipic acid (Part V), and it is clear that the molecular arrangement in the two acids is similar, the additional four carbon atoms in the chain of sebacic acid being accommodated by the increased *c* axis. The similarity

FIG. 1.

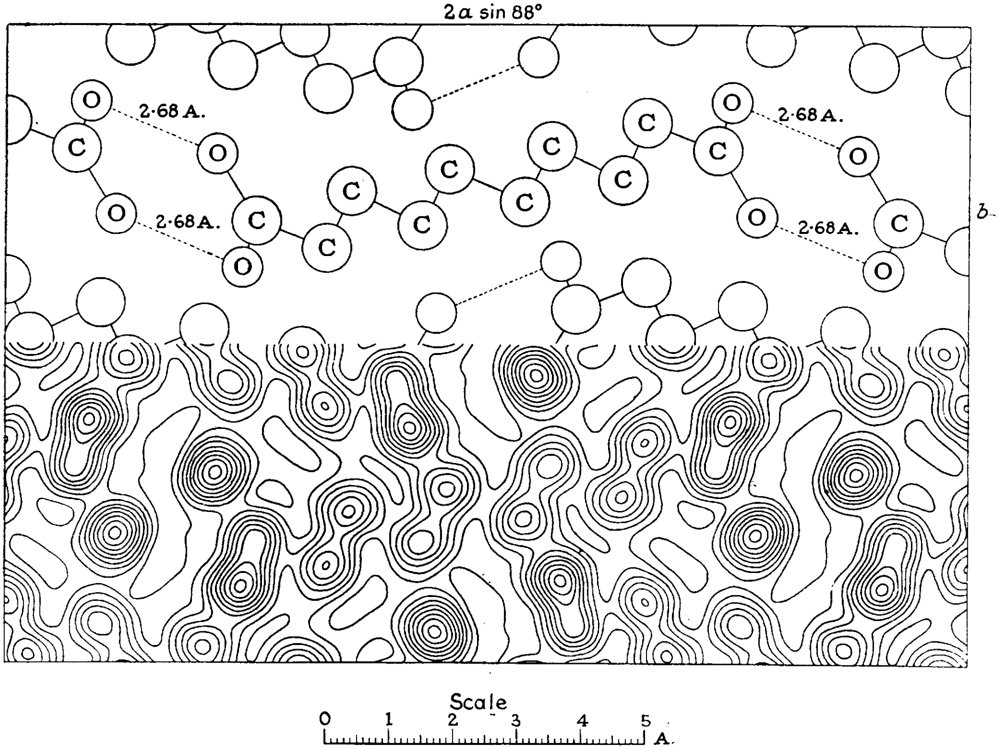


Projection of sebacic acid structure along the b *axis on* (010). *Contour scale: one electron per* A.² *per line, one-electron line dotted.*

of the b axes in the two structures also indicates that the inclination of the molecules to the (010) plane must be approximately the same.

From a consideration of these facts, and an examination of the planes of outstanding intensity, notably the (200), (006), (40$\bar{6}$), (40$\bar{1}\bar{2}$), (20$\bar{6}$), and (20$\bar{1}\bar{2}$) planes, it was possible to find by trial a structure which gave fair agreement between the calculated and measured structure factors. In this structure the whole molecule was assumed to be planar. The co-ordinates were then refined by successive double Fourier syntheses, giving projections of the structure on the (010) plane. The final projection is shown in Fig. 1, and from it accurate values of the x and z co-ordinates of all the atoms except C(5) and O(1) can be obtained.

FIG. 2.



Projection of sebacic acid structure along [101] *axis. Contour scale as in Fig.* 1.

The y co-ordinates were first obtained by trial, and then refined by a further Fourier projection made along the [101] axis using the ($hk\bar{h}$) structure factors. This is shown in Fig. 2. All the atoms are resolved in this case except C(5), the position of which is again uncertain. In this projection the atoms are rather crowded and mutual interference tends to reduce the accuracy. Nevertheless, these two projections together give a fairly precise picture of the complete structure.

Orientation, Co-ordinates, and Dimensions.—The mid points of the seven most central carbon–carbon bonds in the molecule are found to lie very accurately on a straight line, which is accordingly chosen as the principal molecular axis, L. The eight central carbon atoms are also very nearly coplanar ($\pm$0·03 A.), and so the second molecular axis M is chosen in this plane, at right angles to L. The third axis N is perpendicular to L and M. The orientation of the molecule in the crystal can then be expressed by giving the angles (χ, ψ, ω) which these molecular axes make with the crystallographic axes a, b, and c', c' being chosen perpendicular to a and b. These angles are given in Table I.

The co-ordinates of the atoms in the asymmetric crystal unit (half the chemical molecule) are given in Table II, as determined from the final Fourier projections. The figures for atom C(5) are perhaps more in doubt than the others, owing to lack of satisfactory resolution, but the position assigned is fairly well defined by the outer contour levels and cannot be much in doubt. These co-ordinates are referred to the crystallographic axes.

TABLE I.

Orientation of the molecule in the crystal.

χ_L = 50·3°, cos χ_L = 0·6390	χ_M = 63·3°, cos χ_M = 0·4493	χ_N = 51·5°, cos χ_N = 0·6230
ψ_L = 98·2°, cos ψ_L = − 0·1420	ψ_M = 29·9°, cos ψ_M = 0·8668	ψ_N = 118·6°, cos ψ_N = − 0·4780
ω_L = 40·9°, cos ω_L = 0·7560	ω_M = 102·6°, cos ω_M = − 0·2170	ω_N = 128·2°, cos ω_N = − 0·6189

TABLE II.

Co-ordinates. Centre of symmetry as origin.

x, *y*, *z* are referred to the monoclinic crystal axes, and *x′*, *y*, *z′* to the orthogonal axes *a*, *b*, and *c′*.

Atom (cf. Fig. 3).	*x*, A.	*y*, A.	*z*, A.	*x′*, A.	*z′*, A.	$\frac{2\pi x}{a}$.	$\frac{2\pi y}{b}$.	$\frac{2\pi z}{c}$.
C(1)	−0·221	0·270	0·553	0·604	0·399	−7·9°	19·4°	13·2°
C(2)	0·387	−0·630	2·088	1·059	1·507	13·8	−45·4	49·8
C(3)	0·036	−0·094	3·252	2·217	2·346	1·3	− 6·8	77·5
C(4)	0·650	−1·000	4·757	2·646	3·433	23·2	−72·0	113·4
C(5)	0·353	−0·570	5·978	3·789	4·313	12·6	−41·0	142·5
O(1)	−0·501	0·480	5·623	4·396	4·057	−17·9	34·6	134·1
O(2)	1·040	−1·320	7·348	4·050	5·302	37·2	−95·0	175·2

TABLE III.

Co-ordinates referred to molecular axes, L, M, *and* N.

(Origin at centre of symmetry.)

Atom.	*L*, A.	*M*, A.	*N*, A.	Atom.	*L*, A.	*M*, A.	*N*, A.
C(1)	0·649	0·419	0·000	C(5)	5·762	0·272	−0·037
C(2)	1·906	−0·398	0·028	O(1)	5·809	1·510	−0·001
C(3)	3·203	0·406	−0·026	O(2)	6·785	−0·475	−0·128
C(4)	4·427	−0·423	0·002				

TABLE IV.

Molecular dimensions.

C(1′)–C(1) = 1·54 ± 0·02 A.	C(1′)–C(1)–C(2) = 114°
C(1)–C(2) = 1·50 ,,	C(1)–C(2)–C(3) = 115
C(2)–C(3) = 1·53 ,,	C(2)–C(3)–C(4) = 114
C(3)–C(4) = 1·48 ,,	C(3)–C(4)–C(5) = 118
C(4)–C(5) = 1·51 ± 0·03	C(4)–C(5)–O(1) = 120
C(5)–O(1) = 1·24 ± 0·04	C(4)–C(5)–O(2) ≐ 116
C(5)–O(2) = 1·27 ,,	O(1)–C(5)–O(2) = 124

TABLE V.

Intermolecular distances (A.).*

O(1*A*) . . . O(2*C*) = 2·68 ± 0·05	O(2*C*) . . . C(4′*B*) = 3·78 ± 0·05
O(2*A*) . . . O(1*C*) = 2·68 ,,	O(1*A*) . . . C(2*B*) = 3·87 ,,
O(2*C*) . . . C(4*B*) = 3·32 ,,	O(1*A*) . . . C(4*B*) = 3·90 ,,
O(2*A*) . . . O(2*C*) = 3·56 ,,	O(1*A*) . . . C(3*B*) = 3·96 ,,
O(2*C*) . . . O(2*B*) = 3·68 ,,	

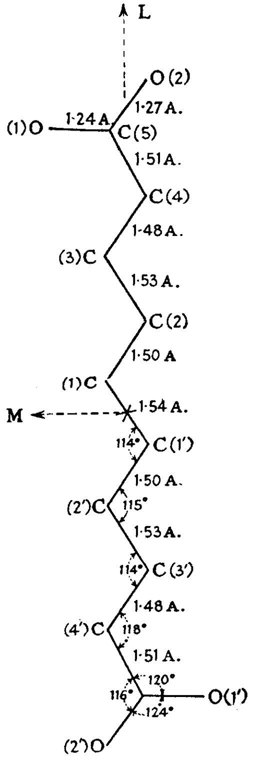
* *A* = standard molecule; *B* = reflected molecule; *C* = molecule one translation along *c* axis.

For many purposes it is convenient to list the co-ordinates of the atoms with reference to the molecular axes, *L*, *M*, and *N*, as defined above. These figures are collected in Table III.

The bond lengths and valency angles within the molecule deduced from these co-ordinates are shown in Fig. 3, and collected in Table IV. The central carbon–carbon bond at the centre of symmetry appears to have the normal length of 1·54 A. After that there is a distinct although slight alternation of long and short bonds extending over the entire length of the molecule. The final bonds connecting to the carboxyl groups, C(4)–C(5), are somewhat uncertain but appear to be slightly longer than the bonds C(3)–C(4) immediately adjacent to them. The structure of the carboxyl group is closely similar to that found in the other acids of the series.

The geometry of the molecule is also very similar to that of the other members of the series, except that in sebacic acid the whole molecule appears to be more strictly planar. The eight central carbon atoms, C(1), C(2), C(3), C(4), C(1′), C(2′), C(3′), and C(4′), probably lie accurately in one plane (±0·03 A.). The plane of the carboxyl group is tilted by approximately 3° from this plane, and the carboxyl-group plane then passes through the centre of symmetry between this molecule and the next molecule along the *c* axis and contains all the atoms of the next adjacent carboxyl group.

FIG. 3.



Dimensions of the sebacic acid molecule.

Intermolecular Distances.—The general pattern of the intermolecular approach distances, which is indicated by the line drawings in Figs. 1 and 2, is remarkably similar to that found in adipic acid (Part V). In particular, the hydrogen bridges between adjacent carboxyl groups are of the same length (2·68 A.). We also find evidence of an unusually short approach distance (3·32 A.) between the carboxyl oxygen atom O(2) and the carbon atom C(4) of the reflected molecule one translation further along the *c* axis. In adipic acid this distance was 3·29 A. The other approach distances are greater than 3·6 A. The values are collected in Table V.

Effect of Hydrogen Atoms on the Intensities of the X-Ray Reflections.—In computing the structure factors for this crystal from the final co-ordinates (see Table VIII), it was noted that the agreement with the measured values for certain large spacing planes remained distinctly poor in spite of careful corrections to the intensities and refinement of the atomic co-ordinates. Further investigation showed that most of these discrepancies could be explained by allowing for the hydrogen atoms, which in sebacic acid account for over 16% of the sum of the atomic numbers.

It is to be expected that hydrogen will make a significant contribution to the total coherent scattering for the low-angle reflections. Atomic scattering curves can be computed, but the allowance for the temperature factor is rather uncertain. In applying the corrections we have accordingly used the following provisional and empirical figures for the hydrogen *f* curve :

sin θ (λ = 1·54) ...	0·0	0·1	0·2	0·3	0·4	0·5	0·6	0·7
f(H)	100	83	58	36	20	8·7	2·9	0

For values of sin θ greater than about 0·4 the corrections are not significant. On the basis of this curve each hydrogen contribution was given a weight of 1 as against a weight of 6 for each carbon and 9 for each oxygen contribution on the empirical carbon–oxygen curve given in the Experimental section.

Co-ordinates were assigned to the hydrogen atoms attached to the carbon chain by assuming a carbon–hydrogen distance of 1·09 A. and a tetrahedral distribution of the valency bonds. The resulting co-ordinates are shown in Table VI.

TABLE VI.

Co-ordinates of hydrogen atoms referred to the monoclinic crystal axes and centre of symmetry as origin.

Atom (cf. Fig. 4).	$\frac{2\pi x}{a}$.	$\frac{2\pi y}{b}$.	$\frac{2\pi z}{c}$.	Atom (cf. Fig. 4).	$\frac{2\pi x}{a}$.	$\frac{2\pi y}{b}$.	$\frac{2\pi z}{c}$.
H(1)	−59°	30°	−9°	H(5)	−50°	3°	55°
H(2)	14	88	26	H(6)	22	61	89
H(3)	− 6	−112	38	H(7)	1	−140	101
H(4)	66	− 55	72	H(8)	75	− 82 .	136

The effect of making corrections for hydrogen on this basis is shown in Table VII, which lists the structure factors for planes with sin θ less than 0·4, and gives the result of the calculation with and without the hydrogen contribution. When the discrepancy is expressed in the usual way as

$$\frac{\Sigma(|\text{F meas.}| - |\text{F calc.}|)}{\Sigma|\text{F meas.}|} \times 100$$

we obtain a figure of 13·8% for the uncorrected F values and only 8·4% for the hydrogen corrected values. The latter figure is very much better than that usually obtained in *X*-ray investigations of organic structures and seems to indicate that the hydrogen correction is generally significant. It will, of course, be especially important in the case of aliphatic compounds where the proportion of hydrogen in the molecule is relatively high.

TABLE VII.

Structure factors for planes with sin θ <0·4 (λ = 1·54 A.) *showing effect of hydrogen.*

hkl.	F, meas.	F, calc. with H.	F, calc. without H.	*hkl.*	F, meas.	F, calc. with H.	F, calc. without H.
200	94·0	+103·0	+99·5	$40\bar{3}$	10·0	+ 11·5	+11·5
400	15·0	+ 19·0	+18·0	$40\bar{4}$	25·0	− 24·0	−25·0
001	33·5	− 34·5	−47·5	$40\bar{5}$	32·5	+ 32·0	+33·5
002	11·0	+ 12·5	+17·0	$40\bar{6}$	59·0	− 54·5	−48·0
003	4·0	+ 4·5	+ 4·5	$40\bar{7}$	10·0	+ 8·5	+11·0
004	9·5	− 9·5	− 9·5	011	28·5	− 30·0	−26·5
005	8·0	+ 7·0	+ 7·0	012	3·0	+ 3·5	+ 2·0
020	2·0	+ 1·5	+ 1·5	013	2·5	− 3·0	− 2·0
203	9·0	+ 9·0	+ 8·5	014	6·5	+ 6·5	+ 6·0
202	2·5	− 2·0	− 2·0	015	7·0	+ 3·0	+ 1·5
201	18·5	− 17·5	−17·5	021	27·0	+ 26·5	+26·0
$20\bar{1}$	11·5	+ 11·5	+ 4·0	022	14·5	− 11·5	−11·5
$20\bar{2}$	3·0	− 4·0	0·0	023	11·5	+ 10·5	+11·5
$20\bar{3}$	13·5	+ 14·0	+15·5	$11\bar{1}$	8·5	+ 8·0	+ 5·0
$20\bar{4}$	23·5	− 24·5	−28·5	$12\bar{1}$	11·0	− 8·5	−12·5
$20\bar{5}$	25·5	+ 22·5	+26·0	$21\bar{2}$	15·5	+ 14·5	+15·0
$20\bar{6}$	19·5	− 19·5	−19·0	$22\bar{2}$	7·0	+ 5·0	+ 7·0
$20\bar{7}$	<0·5	+ 0·5	0·0	$31\bar{3}$	<1·0	0·0	+ 0·5
$40\bar{1}$	26·0	+ 28·0	+29·0	$32\bar{3}$	14·0	+ 15·0	+14·0
$40\bar{2}$	9·0	− 8·0	− 8·0	$41\bar{4}$	8·0	− 8·0	− 7·5

The effect of the hydrogen atoms on the electron-density map is fairly clear in Fig. 1 (see also Fig. 4). After this effect was realised, the co-ordinates assigned to the carbon atoms were varied to see whether the positions assigned might be perturbed by the hydrogens, but within the limits of experimental error this was not found to be the case.

The effect of the hydrogen contribution on planes of large spacing has been noticed before, by Bunn (*Trans. Faraday Soc.*, 1939, **35**, 482) and by Hughes and Lipscomb (*J. Amer. Chem. Soc.*, 1946, **68**, 1970), but this would seem to be the first case in which it has been shown to have a really extensive effect.

EXPERIMENTAL.

X-*Ray Measurements.*—As in the previous investigations in this series, copper *K*-α radiation (λ = 1·54 A.) was used, and the moving-film method was employed to record the intensities.

For the (*h*0*l*) zone the principal crystal specimen, cut from a larger fragment, had cross-section on (010) of 0·30 mm. × 0·11 mm. Relative absorption corrections were not made, as they were found not to be significant for a specimen of this size completely immersed in the *X*-ray beam. To extend the range of intensities, a larger specimen of 1·20 mm. × 0·62 mm. cross-section was used. Combining the results from these specimens, a total of 141 out of a possible 145 reflections were recorded.

For the (*hkh*) zone, a specimen of cross-section 0·55 mm. × 0·45 mm. normal to the rotation axis was used, and for the (0*kl*) zone one of 0·28 mm. × 0·25 mm.

The multiple-film technique (Robertson, *J. Sci. Instr.*, 1943, **20**, 175) was used to correlate the intensities, chiefly by visual estimation, over a total range of about 25,000 to 1. In the different zones, the sets of intensities were correlated by means of their common axial reflections. The usual correction factors were applied, and the structure factors are listed in Table VIII. The absolute scale was obtained by correlation with the values finally calculated from the atomic positions.

Fourier Analysis and Structure Factor Calculations.—The electron-density maps were computed by the usual methods (*idem, ibid.*, 1948, **25**, 28). For the projection on (010) the axial subdivisions were $a/60 = 0{\cdot}168$ A., and $c/60 = 0{\cdot}252$ A. For the normal projection along the [101] axis the subdivisions were $b/30 = 0{\cdot}167$ A. and $a \cos 2{\cdot}1°/60 = 0{\cdot}168$ A.

A plot of the asymmetric crystal unit in the (010) projection is shown in Fig. 4, with the centres finally assigned to the atoms shown in relation to the co-ordinate network. In this diagram the positions of the centres assumed for the hydrogen atoms are also shown.

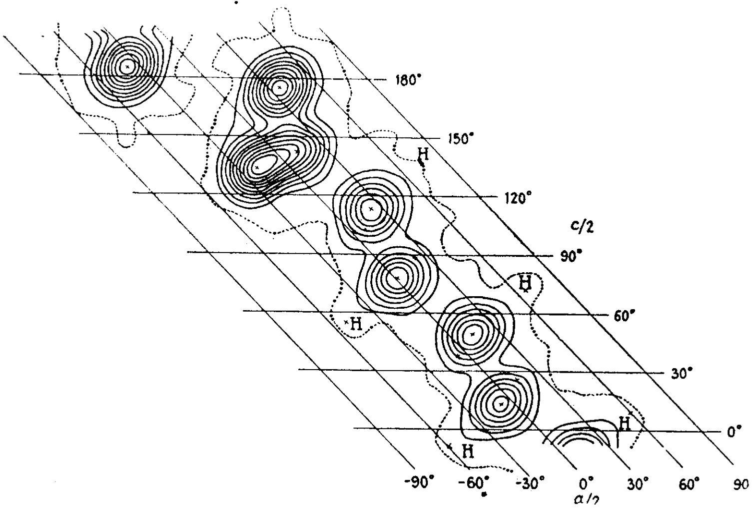
From the final co-ordinates listed in Table II all the structure factors were recalculated and the results are given in Table VIII. The results listed there do not take account of the hydrogen contributions, which are dealt with separately for the large spacing planes in Table VII. For the general calculation of the structure factors the following composite empirical *f*-curve, which appeared to give the best agreement with the observed values, was derived :

sin θ(λ = 1·54)	0·0	0·1	0·2	0·3	0·4	0·5	0·6	0·7	0·8	0·9
$f_{(e)}$	100	85	62	44	33	25	18	13	8·8	5·5

On the basis of this composite curve the contributions of the oxygen atoms were weighted relatively to the carbon contributions in the ratio of 1·5 to 1·0.

The discrepancies finally obtained, expressed as percentages in the usual way, were 16·7% for the $(h0l)$ reflections, 13·2% for the $(hk\bar{h})$ reflection, and 15·7% over all. As has been noted above, these agreements can be very greatly improved for the large spacing planes by taking account of the hydrogen contributions.

FIG. 4.



Asymmetric crystal unit. Centres of atoms marked with crosses.

TABLE VIII.

Measured and calculated values of the structure factor.

hkl.	sin θ (λ = 1·54 A.).	F, meas.	F, calc.
200	0·212	94·0	+99·5
400	0·423	15·5	+18·0
600	0·635	1·0	− 1·5
800	0·846	1·5	− 1·0
001	0·070	33·5	−47·5
002	0·141	11·0	+17·0
003	0·212	4·0	+ 4·5
004	0·282	9·5	− 9·5
005	0·353	8·0	+ 7·0
006	0·423	18·5	+16·5
007	0·494	15·0	−14·0
008	0·564	13·5	+14·0
009	0·635	8·5	− 8·5
0,0,10	0·705	5·0	+ 5·0
0,0,11	0·776	10·0	− 9·5
0,0,12	0·846	5·0	− 5·5
0,0,13	0·917	2·0	+ 1·5
0,0,14	0·987	0·5	0·0
020	0·308	2·0	+ 1·5
040	0·616	<2·5	− 2·0
060	0·924	2·0	− 3·0
2,0,11	0·938	4·0	− 4·5
2,0,10	0·868	1·0	− 0·0
209	0·798	<1·0	− 1·5
208	0·728	4·0	+ 6·0
207	0·659	8·0	−10·0
206	0·588	10·5	+15·5
205	0·521	8·5	+ 8·5
204	0·455	7·5	− 6·5
203	0·388	9·0	+ 8·5
202	0·323	2·5	− 2·0
201	0·263	18·5	−17·5
$20\bar{1}$	0·171	11·5	+ 4·0
$20\bar{2}$	0·154	3·0	− 0·0
$20\bar{3}$	0·168	13·5	+15·5
$20\bar{4}$	0·206	23·5	−28·5
$20\bar{5}$	0·259	25·5	+26·0
$20\bar{6}$	0·319	19·5	−19·0
$20\bar{7}$	0·383	<0·5	0·0
$20\bar{8}$	0·448	9·5	+ 8·0
$20\bar{9}$	0·514	10·5	− 9·0
$2,0,\overline{10}$	0·584	7·0	+ 4·5
$2,0,\overline{11}$	0·653	8·0	− 7·5
$2,0,\overline{12}$	0·720	21·5	−19·5
$2,0,\overline{13}$	0·789	9·5	+ 8·5
$2,0,\overline{14}$	0·858	4·5	− 4·0
$2,0,\overline{15}$	0·928	1·5	+ 1·0
409	0·978	1·5	+ 1·5
408	0·910	1·0	− 0·5
407	0·845	1·0	− 1·0
406	0·780	2·0	+ 4·0
405	0·715	10·0	+11·0
404	0·653	4·0	− 4·0
403	0·589	6·0	+ 8·5
402	0·530	9·5	−11·0
401	0·478	5·0	+ 6·5
$40\bar{1}$	0·380	26·0	+29·0
$40\bar{2}$	0·344	9·0	− 8·0
$40\bar{3}$	0·319	10·0	+11·5
$40\bar{4}$	0·308	25·0	−25·0
$40\bar{5}$	0·314	32·5	+33·5
$40\bar{6}$	0·335	59·0	−48·0
$40\bar{7}$	0·369	10·0	+11·0
$40\bar{8}$	0·410	1·0	+ 0·5
$40\bar{9}$	0·463	7·5	− 7·0
$4,0,\overline{10}$	0·518	7·5	+ 5·5

TABLE VIII.—*continued.*

hkl.	sin θ ($\lambda = 1·54$).	F, meas.	F, calc.
4,0,$\bar{1}\bar{1}$	0·576	6·0	− 4·5
4,0,$\bar{1}\bar{2}$	0·638	36·5	−29·0
4,0,$\bar{1}\bar{3}$	0·698	11·0	+10·5
4,0,$\bar{1}\bar{4}$	0·761	8·0	− 6·0
4,0,$\bar{1}\bar{5}$	0·825	3·0	+ 2·5
4,0,$\bar{1}\bar{6}$	0·893	<1·0	0·0
4,0,$\bar{1}\bar{7}$	0·960	3·0	− 1·0
606	0·979	0·5	+ 0·5
605	0·918	4·0	+ 5·0
604	0·858	2·5	+ 2·0
603	0·795	2·5	+ 1·0
602	0·740	2·0	− 5·0
601	0·688	3·5	+ 6·0
60$\bar{1}$	0·590	14·5	+17·0
60$\bar{2}$	0·549	1·0	+ 1·5
60$\bar{3}$	0·514	4·0	− 4·0
60$\bar{4}$	0·488	2·0	− 2·5
60$\bar{5}$	0·470	11·0	+11·5
60$\bar{6}$	0·463	29·5	−30·0
60$\bar{7}$	0·465	6·0	− 6·0
60$\bar{8}$	0·479	5·0	+ 5·0
60$\bar{9}$	0·503	10·0	−10·0
6,0,$\bar{1}\bar{0}$	0·535	11·5	+11·0
6,0,$\bar{1}\bar{1}$	0·573	10·0	− 9·0
6,0,$\bar{1}\bar{2}$	0·668	22·5	−19·0
6,0,$\bar{1}\bar{3}$	0·686	3·5	− 1·0
6,0,$\bar{1}\bar{4}$	0·719	1·5	− 1·0
6,0,$\bar{1}\bar{5}$	0·773	1·0	+ 0·5
6,0,$\bar{1}\bar{6}$	0·831	2·5	+ 2·0
6,0,$\bar{1}\bar{7}$	0·891	4·5	− 1·5
6,0,$\bar{1}\bar{8}$	0·953	7·0	+ 4·0
803	0·990	2·5	− 1·5
802	0·950	<0·5	+ 0·5
801	0·900	1·0	+ 1·0
80$\bar{1}$	0·803	4·5	+ 4·0
80$\bar{2}$	0·758	2·0	+ 5·5
80$\bar{3}$	0·720	5·5	− 8·5
80$\bar{4}$	0·688	6·0	+ 7·0
80$\bar{5}$	0·660	3·5	− 3·5
80$\bar{6}$	0·636	3·5	− 6·0
80$\bar{7}$	0·623	13·5	−16·5
80$\bar{8}$	0·618	5·0	+ 4·5
80$\bar{9}$	0·618	5·5	− 6·0
8,0,$\bar{1}\bar{0}$	0·628	7·5	+ 9·0
8,0,$\bar{1}\bar{1}$	0·645	9·0	− 9·5
8,0,$\bar{1}\bar{2}$	0·670	3·0	− 3·5
8,0,$\bar{1}\bar{3}$	0·700	11·5	−10·5
8,0,$\bar{1}\bar{4}$	0·738	3·5	+ 2·5
8,0,$\bar{1}\bar{5}$	0·777	1·0	− 0·0
8,0,$\bar{1}\bar{6}$	0·823	1·5	+ 1·5
8,0,$\bar{1}\bar{7}$	0·873	4·0	− 2·5
8,0,$\bar{1}\bar{8}$	0·922	12·5	+ 7·0
8,0,$\bar{1}\bar{9}$	0·978	4·5	− 2·0
10,0,$\bar{2}$	0·970	0·5	+ 1·0
10,0,$\bar{3}$	0·928	1·0	− 2·5
10,0,$\bar{4}$	0·889	2·5	+ 4·0
10,0,$\bar{5}$	0·858	2·5	− 4·0
10,0,$\bar{6}$	0·828	1·5	+ 0·5
10,0,$\bar{7}$	0·806	9·5	−10·5
10,0,$\bar{8}$	0·788	3·0	− 2·5
10,0,$\bar{9}$	0·776	4·5	+ 3·0
10,0,$\bar{1}\bar{0}$	0·770	2·0	+ 0·5
10,0,$\bar{1}\bar{1}$	0·771	1·5	− 2·5
10,0,$\bar{1}\bar{2}$	0·778	1·0	+ 0·5
10,0,$\bar{1}\bar{3}$	0·793	8·0	− 7·5
10,0,$\bar{1}\bar{4}$	0·811	1·0	+ 0·5
10,0,$\bar{1}\bar{5}$	0·835	2·5	+ 2·5
10,0,$\bar{1}\bar{6}$	0·866	3·0	− 4·5
10,0,$\bar{1}\bar{7}$	0·902	1·0	+ 1·0
10,0,$\bar{1}\bar{8}$	0·940	8·0	+ 4·0
10,0,$\bar{1}\bar{9}$	0·983	3·0	+ 0·5
12,0,$\bar{7}$	0·990	2·5	− 2·5
12,0,$\bar{8}$	0·978	2·5	− 3·5
12,0,$\bar{9}$	0·958	4·0	+ 4·0
12,0,$\bar{1}\bar{0}$	0·940	3·0	− 2·5
12,0,$\bar{1}\bar{1}$	0·930	1·5	+ 1·5
12,0,$\bar{1}\bar{2}$	0·925	1·0	− 0·5
12,0,$\bar{1}\bar{3}$	0·925	2·0	− 1·5
12,0,$\bar{1}\bar{4}$	0·930	1·0	− 1·0
12,0,$\bar{1}\bar{5}$	0·941	2·0	+ 2·0
12,0,$\bar{1}\bar{6}$	0·958	2·5	− 2·0
12,0,$\bar{1}\bar{7}$	0·978	2·5	+ 2·0
011	0·170	28·5	−26·5
012	0·209	3·0	+ 2·0
013	0·262	2·5	− 2·0
014	0·321	6·5	+ 6·0
015	0·384	7·0	+ 1·5
016	0·450	16·5	+21·0
017	0·516	7·5	− 7·5
018	0·585	<2·5	+ 2·0
019	0·654	<2·5	+ 1·5
0,1,10	0·721	3·0	− 2·0
0,1,11	0·788	3·0	− 3·0
0,1,12	0·861	6·5	+ 7·0
0,1,13	0·928	3·0	− 2·5
021	0·315	27·0	+26·0
022	0·339	14·5	−11·5
023	0·373	11·5	+11·5
024	0·417	9·0	− 7·5
025	0·468	28·0	+28·0
026	0·523	10·0	−13·0
027	0·581	<2·5	− 2·0
028	0·642	<2·5	− 0·5
029	0·710	<3·0	+ 2·5
0,2,10	0·770	3·0	− 3·5
0,2,11	0·834	<2·5	+ 1·5
0,2,12	0·900	5·0	− 4·5
0,2,13	0·966	<1·5	− 0·0
031	0·467	3·5	+ 4·0
032	0·483	11·5	−12·5
033	0·507	5·0	+ 5·0
034	0·541	10·0	+11·0
035	0·581	2·5	+ 3·0
036	0·626	3·0	+ 4·0
037	0·676	8·0	+ 8·5
038	0·729	4·5	− 3·5
039	0·785	5·0	+ 5·5
0,3,10	0·843	<2·5	− 4·0
0,3,11	0·903	<2·0	+ 2·5
0,3,12	0·964	<1·5	+ 0·5
041	0·619	<2·5	−1·0
042	0·632	2·5	+ 2·5
043	0·651	6·0	− 7·5
044	0·677	13·5	+18·0
045	0·709	5·5	− 6·0
046	0·747	4·5	+ 3·5
047	0·789	5·0	− 5·5
048	0·835	3·5	− 3·5
049	0·885	3·5	+ 2·0
0,4,10	0·936	<2·0	+ 1·5
051	0·773	<2·5	+ 1·5
052	0·782	<2·5	+ 1·5
053	0·798	3·0	+ 4·0
054	0·820	2·5	+ 2·5

TABLE VIII.—*continued.*

hkl.	sin θ ($\lambda = 1\cdot54$).	F, meas.	F, calc.
055	0·846	<2·5	− 2·0
056	0·878	<2·5	+ 1·5
057	0·914	<2·0	− 0·5
058	0·953	2·0	+ 3·0
061	0·926	2·0	+ 2·5
062	0·934	2·5	− 3·0
063	0·947	<1·5	− 0·5
064	0·965	<1·5	+ 0·5
065	0·989	<1·0	− 0·0
$11\bar{1}$	0·189	8·5	+ 5·0
$12\bar{1}$	0·326	11·0	−12·5
$13\bar{1}$	0·474	4·5	+ 4·0
$14\bar{1}$	0·625	2·5	+ 3·5
$15\bar{1}$	0·776	5·0	+ 5·0
$16\bar{1}$	0·930	<1·0	0·0
$21\bar{2}$	0·218	15·5	+15·0
$22\bar{2}$	0·344	7·0	+ 7·0
$23\bar{2}$	0·486	14·5	−14·5
$24\bar{2}$	0·635	5·5	− 6·0
$25\bar{2}$	0·784	4·0	+ 4·5
$26\bar{2}$	0·935	2·5	− 2·5
$31\bar{3}$	0·277	<1·0	+ 0·5
$32\bar{3}$	0·384	14·0	+14·0
$33\bar{3}$	0·515	4·0	− 2·5
$34\bar{3}$	0·657	2·0	+ 2·5
$35\bar{3}$	0·807	3·5	− 3·5
$36\bar{3}$	0·950	3·5	+ 3·5
$41\bar{4}$	0·343	8·0	− 7·5
$42\bar{4}$	0·434	9·0	+ 8·0
$43\bar{4}$	0·559	6·5	− 7·0
$44\bar{4}$	0·687	6·5	+ 5·0
$45\bar{4}$	0·827	3·5	+ 4·5
$46\bar{4}$	0·973	2·0	+ 2·5
$51\bar{5}$	0·413	10·0	+ 9·0
$52\bar{5}$	0·490	10·5	+11·0
$53\bar{5}$	0·600	4·0	+ 6·5
$54\bar{5}$	0·725	8·0	+ 9·0
$55\bar{5}$	0·860	<1·5	− 1·0
$56\bar{5}$	0·999	<0·5	− 1·5
$61\bar{6}$	0·484	9·5	−11·5
$62\bar{6}$	0·553	<1·5	+ 1·5
$63\bar{6}$	0·650	2·0	+ 4·5
$64\bar{6}$	0·768	<1·5	+ 1·5
$65\bar{6}$	0·895	2·0	− 2·0
$71\bar{7}$	0·557	9·0	− 8·5
$72\bar{7}$	0·618	5·5	+ 6·5
$73\bar{7}$	0·708	2·5	− 4·0
$74\bar{7}$	0·815	<1·5	− 1·0
$75\bar{7}$	0·936	<1·0	− 1·0
$81\bar{8}$	0·632	6·5	+ 5·5
$82\bar{8}$	0·685	12·5	−12·5
$83\bar{8}$	0·767	7·5	+ 9·0
$84\bar{8}$	0·867	<1·5	+ 1·0
$85\bar{8}$	0·984	<0·5	− 0·5
$91\bar{9}$	0·705	4·5	+ 3·5
$92\bar{9}$	0·755	7·0	− 6·0
$93\bar{9}$	0·830	3·0	− 1·5
$94\bar{9}$	0·924	<1·0	− 0·5
$10,1,\overline{10}$	0·780	5·0	+ 6·0
$10,2,\overline{10}$	0·824	<1·5	0·0
$10,3,\overline{10}$	0·892	<1·0	+ 1·5
$10,4,\overline{10}$	0·982	<0·5	+ 0·5
$11,1,\overline{11}$	0·855	<1·5	− 1·0
$11,2,\overline{11}$	0·896	<1·0	− 2·0
$11,3,\overline{11}$	0·960	<1·0	− 1·5
$12,1,\overline{12}$	0·930	<1·0	− 0·5
$12,2,\overline{12}$	0·969	<1·0	− 0·5

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