520. *Crystal-structure Studies of Polynuclear Hydrocarbons. Part III.*[1] *The α-Modification of Dinaphtho(7′ : 1′-1 : 13)(1″ : 7″-6 : 8)-peropyrene.*

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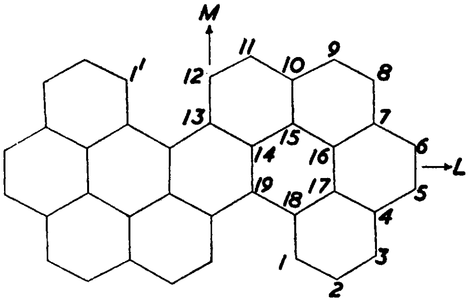
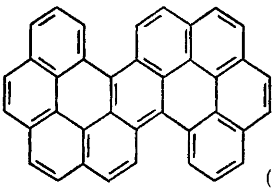
The dinaphthoperopyrene exists in two crystalline modifications. A detailed study of the α-form shows that the unit cell contains four molecules in space group *C*2. Regions of diffuse scattering indicate the presence of a stacking disorder, but in spite of this the molecular dimensions have been determined with considerable precision. In one projection along the short *b* axis (3·855 Å) all the atoms including hydrogen are visible, except on four sites which are randomly occupied. The molecule is distorted so that the distance between the overcrowded carbon atoms is 2·95 Å, but this separation is achieved with little variation of the valency angles from 120°. The strain caused by the molecular distortion is fairly evenly distributed over the molecule, with retention of aromatic character, although there is measurable increase in some bond lengths.

DINAPHTHO(7′ : 1′-1 : 13)(1″ : 7″-6 : 8)PEROPYRENE (I) is obtained along with circumanthracene by treating diperinaphthyleneanthracene with maleic anhydride, and decarboxylating the adduct.[2] The present investigation was undertaken to obtain an accurate account of the geometry of this ring system, and of the molecular dimensions.

FIG. 1. *Regular projection (empirical numbering).*



Severe intramolecular overcrowding with out-of-plane distortion must be expected for this structure, as has already been found in diperinaphthyleneanthracene.[1] Fortunately, a crystal modification of the dinaphthoperopyrene has now been obtained which has one very short axis (3·855 Å) and this has enabled us to carry out a detailed analysis with good resolution of all the atoms in the molecule (Fig. 1). However, the crystal structure exhibits a certain type of disorder, as shown by regions of diffuse scattering in the *X*-ray photographs (Plate 1). This makes it difficult to estimate the absolute accuracy of the bond-length measurements, but the structure-factor agreements are such as to leave no doubt that all the essential features of the structure, including the intramolecular overcrowded distances, have now been determined with considerable precision.


(I)

EXPERIMENTAL

The crystals were obtained by sublimation in a high vacuum. The sublimate consisted mainly of dark red stout hexagonal prisms (which will be called the α-form). There was, however,

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[1] Part II, preceding paper.

[2] Clar, Kelly, Robertson, and Rossmann, *J.*, 1956, 3878.

Plate 1. *Weissenberg photograph of (h0l) showing diffuse rods parallel to a* when l is odd, and thermal diffuse regions.*

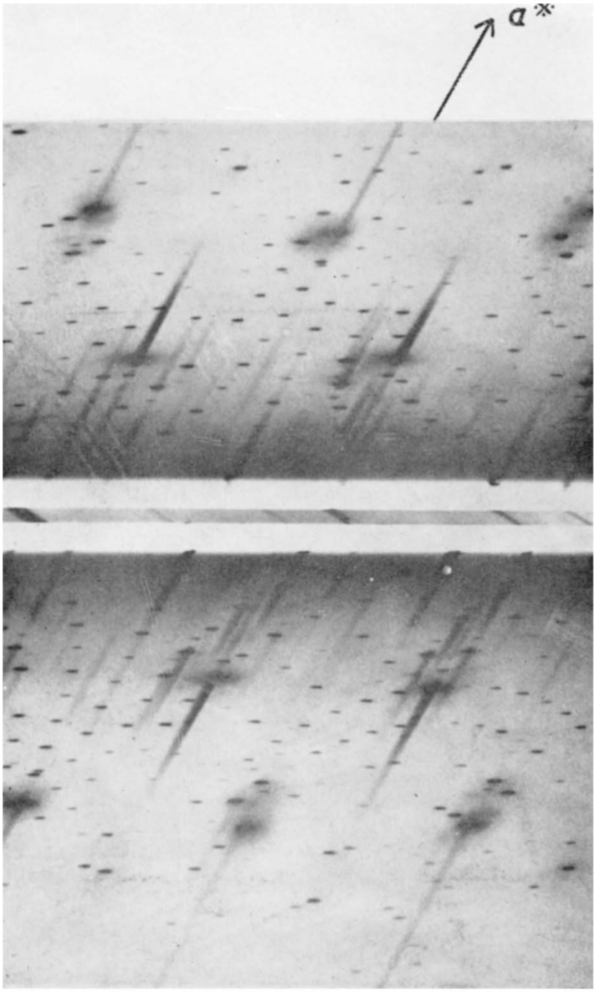

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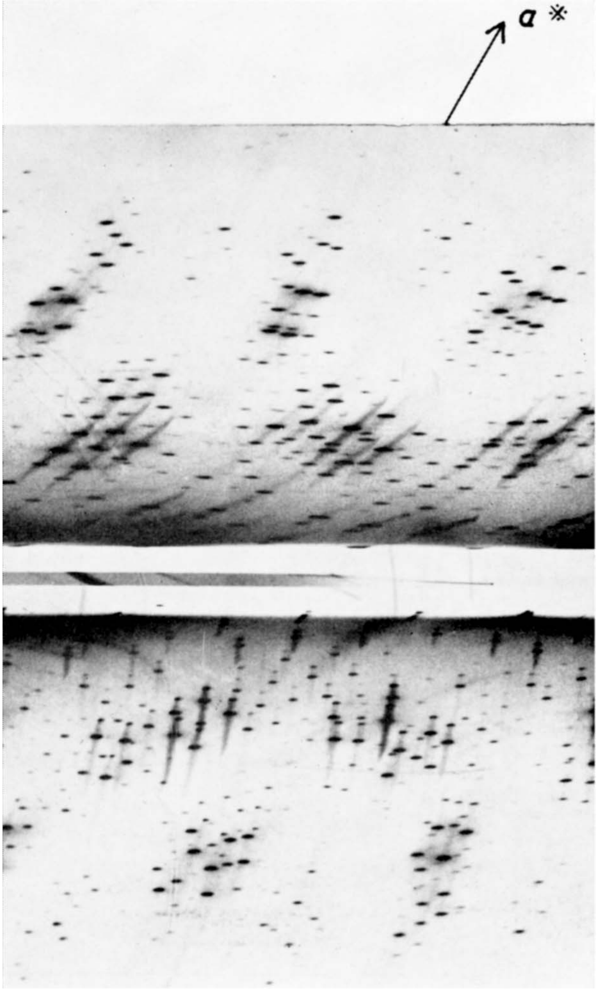
Plate 2. *Equi-inclination Weissenberg photograph of $(h1l)$ showing diffuse rods for all values of l.*



a small quantity of pale red aggregates of very small crystals. One very small single crystal of the pale red (β) form was hand-picked (see following paper).

The α-crystals were elongated prisms with {100}, {001}, and {10$\bar{1}$} faces developed, and had m. p. 340°. Rotation, oscillation, and moving-film photographs showed that the monoclinic unit cell had $a = 30{\cdot}73 \pm 0{\cdot}05$, $b = 3{\cdot}855 \pm 0{\cdot}010$, $c = 19{\cdot}87 \pm 0{\cdot}03$ Å, $\beta = 113{\cdot}0° \pm 0{\cdot}5°$, with a volume of 2167 Å^3. The density, determined by flotation in aqueous potassium iodide solution, was 1·447, in good agreement with the value of 1·446 calculated for four molecules of $C_{38}H_{18}$ per unit cell.

The intensities of all the reflexions observable with Cu-K_α radiation were recorded on moving film exposures for crystals rotating about the *b* and *c* axes, the multiple-film technique[3] being used to correlate strong and weak reflexions. For the crystal rotating about the *b* axis, layers with $k = 0$—3 were recorded, and for the crystal rotating about the *c* axis, layers with $l = 0$—14, the equi-inclination method being used for all non-equatorial layers. The range of intensities measured was about 70,000 : 1, the estimates being made visually. The cross-sections of the crystals, normal to the rotation axes, were 0·25 × 0·18 mm., and 0·53 × 0·44 mm. for the *b*-axis and *c*-axis crystals respectively; errors due to absorption ($\mu = 7{\cdot}65$ cm.$^{-1}$ for $\lambda = 1{\cdot}542$ Å) are negligible, and no corrections were applied.

The values of the structure amplitudes were derived by the usual formulæ for a mosaic crystal; Lorentz and polarisation corrections were applied, together with the rotation factor appropriate to equi-inclination Weissenberg photographs.[4] An approximately absolute scale was derived by Wilson's method[5] and adjusted by correlation with the *F* values of the (*h*0*l*) zone reflexions, calculated from the final co-ordinates.

Although a complete collection of three-dimensional intensity data was made, the present analysis uses only the (*h*0*l*) and (*h*1*l*) structure factors, which are recorded in Tables 4, 5, and 6. As the work proceeded it became clear that a stacking disorder exists in the structure and hence the accuracy with which the atomic co-ordinates can finally be estimated is somewhat doubtful. More detailed refinements with the full three-dimensional data are therefore probably not justified.

In estimating the intensities, those of the Bragg reflexions only were considered, and no estimation was made of the intensity variation in the regions of diffuse scattering (see below).

Space Group: *Diffuse Scattering*.—The only systematically absent spectra are (*hkl*) when $(h + k)$ is odd, so that the space group is C_2^3–$C2$, C_s^3–Cm, or C_{2h}^3–$C2/m$. In the last two space groups, the existence of a mirror plane perpendicular to the *b*-axis requires either the presence of two molecules within one unit translation along *b*, or a mirror plane within the molecule. The first of these alternatives is excluded by the short *b*-axis (3·855 Å), and the second requires that the molecule is planar, and this is unlikely. It may safely be assumed, therefore, that the space group is C_2^3–$C2$.

Further examination of the photographs, however, reveals an interesting series of regions of diffuse scattering. These consist of diffuse rods in reciprocal space parallel to a^*, and passing through the Bragg reflexions, and these rods are present for all values of *k* and *l*, except $k = 0$. In the (*h*0*l*) zone those reflexions with *l* even are all quite sharp, and not joined by diffuse streaks; those with *l* odd are all extremely weak maxima on the diffuse rods parallel to a^*. This is illustrated in Plate 1 which shows a normal-beam Weissenberg photograph of the (*h*0*l*) zone. Note also the thermal diffuse regions surrounding the intense higher order reflexions. Plate 2 shows an equi-inclination Weissenberg photograph of the (*h*1*l*) reflexions, with diffuse rods parallel to a^* for all values of *l*.

The diffraction pattern is typical of an order–disorder structure (Dornberger-Schiff's[6] OD structure) built of layers parallel to the *bc*-plane. Within each layer the molecular arrangement is perfectly ordered, but the sequence of layers is such that there is no true periodicity in the *a* direction. The disorder in the stacking results from the fact that there are two or more energetically equivalent ways in which neighbouring layers can be placed with respect to one another. The diffraction data indicate that there are two sets of layers *A* and *B*, and, since (*h*0*l*) reflexions with $l = 2n$ are all sharp, layer *B* can be made coincident with layer *A* in projection down the *b*-axis simply by translation $\frac{1}{2}c$.

[3] Robertson, *J. Sci. Instr.*, 1943, **20**, 175.
[4] Tunell, *Amer. Mineralogist*, 1939, **24**, 448.
[5] Wilson, *Nature*, 1942, **150**, 152.
[6] Dornberger-Schiff, *Acta Cryst.*, 1956, **9**, 593.

In spite of the fact that the structure is disordered, it might be hoped that all the atoms will be well resolved in projection down the short *b*-axis, and the problem of the complete solution of the structure was approached by considering this projection initially.

Structure Analysis.—Projection on (010). The ($h0l$) zone intensities revealed that, of about 360 independent reflexions with $l = 2n$ which are theoretically observable with Cu-K_α radiation, 260 could be observed (72%); of a similar number of theoretically observable reflexions with l odd, only 20 weak, diffuse reflexions could be observed. The problem of obtaining a trial structure can best be approached by neglecting the l-odd reflexions, so that the projection corresponds to the ($h0l$) projection of space group C_{2h}^{6}–$C2/c$.

Since reflexions with l even are all sharp, there will be obtained in this way a projection of the disordered structure which is a superposition of layers *A* and *B*.

As an initial approximation it may be assumed that the molecule is completely planar, and consists of regular hexagons of side 1·40 Å. Now, the distance between the molecular planes in crystals of large planar aromatic hydrocarbons is about 3·4 Å, equal to the interplanar spacing in graphite. Since this dinaphthoperopyrene is certainly buckled, we might expect a rather larger separation between mean planes drawn through the molecules, and in this case the *b* translation is actually 3·855 Å. It is likely, therefore, that the mean plane through the molecule is almost parallel to (010). This implies that the assumption of a planar molecule will give quite a reasonable trial structure in this projection. The problem of finding the approximate positions of the carbon atoms then reduces to finding the directions of the molecular axes *L* and *M* in a regular projection as indicated in Fig. 1.

The following high-order planes have large structure amplitudes: (24,0,$\bar{2}$), (6,0,12), (8,0,12), (6,0,14), (18,0,$\bar{16}$), (10,0,4), (14,0,$\bar{6}$) and (4,0,$\bar{10}$). If the origin of the projection is taken at the centre of one of the molecules, then it is simple to adjust the orientations of the molecular axes *L* and *M* so that all the atoms lie close to the traces of the above planes. There are six possible molecular orientations, but packing considerations reduce the possibilities to two, which are related by a rotation of 180° about either *L* or *M*. In this projection the two possible orientations differ only in that position 11 may be occupied by an atom or it may be vacant.

Structure factors were calculated for about 90 of the stronger reflexions, McWeeny's scattering curve for carbon with $B = 3{\cdot}5$ Å^2 (determined by Wilson's method [5]) being used. The discrepancy between measured and calculated structure factors was 38·2% for orientation I (atom at position 11), and 44·7% for orientation II (no atom at position 11). A Fourier synthesis was then computed, with about 60 terms, whose signs did not depend on the position of atom 11 and were therefore probably correct. All the carbon atoms were well resolved, except at position 11 where the definition was poor. More accurate parameters for the other atoms were obtained from the Fourier map, and recalculation of the structure factors led to improved agreement between F_o and F_c, but it was not possible to decide between orientations I and II. It was, however, noted that a structure consisting of I and II (1 : 1) gave considerably better agreement than either orientation separately. This structure probably represents superposition of layers *A* and *B*.

Refinement was continued by computing a second F_o synthesis, again with use only of terms whose signs did not depend on the position of atom 11 (215 terms), and choice of new centres. Structure factors were recalculated with the inclusion of a contribution from the hydrogen atoms; hydrogen co-ordinates were assigned on the assumption of C–H bond lengths of 1·0 Å. The process of refinement is outlined in Table 1, in terms of the reliability factor $R = \sum||F_o| - |F_c||/\sum|F_o|$.

The low value of the discrepancy for orientation (I + II) leaves no doubt that this is the true molecular arrangement in the disordered structure. Using the signs of the structure factors calculated from the co-ordinates of the second F_o synthesis, we calculated a third Fourier synthesis (260 terms) [Fig. 2(*a*)]. In this map all the carbon atoms are very well resolved; at position 11 and the position (*O*) obtained from this by rotation about either of the molecular axes *L* or *M* there are peaks corresponding to only one-half of a carbon atom (plus a contribution

TABLE 1. *Refinement process* (R%).

	I	II	I + II
Trial structure	38·2	44·7	—
First F_o synthesis	26·5	29·9	20·3
Second F_o synthesis	20·1	—	11·1

from a peak where two "half-hydrogen atoms" overlap). The best positions of the carbon atoms are shown in Fig. 2(*b*).

All the hydrogen atoms, except those attached to positions 11 and 11′ are reasonably well resolved; those in the overcrowded positions are of course obscured by the half peaks at 11 and 11′.

Finally an $(F_o - F_c)$ synthesis was computed, and ten of the carbon atoms were shifted by small amounts to minimise the slopes at the atomic centres. It is clear that the x and z parameters of the carbon atoms have been determined with considerable precision; since, however, the structure is disordered, each atomic position is the mean of two positions which are extremely close, but nevertheless probably distinct. The complete description of the arrangement of molecules in layers A and B requires consideration of the diffuse as well as the sharp reflexions, and this evidence will now be described.

FIG. 2*a*. FIG. 2*b*.

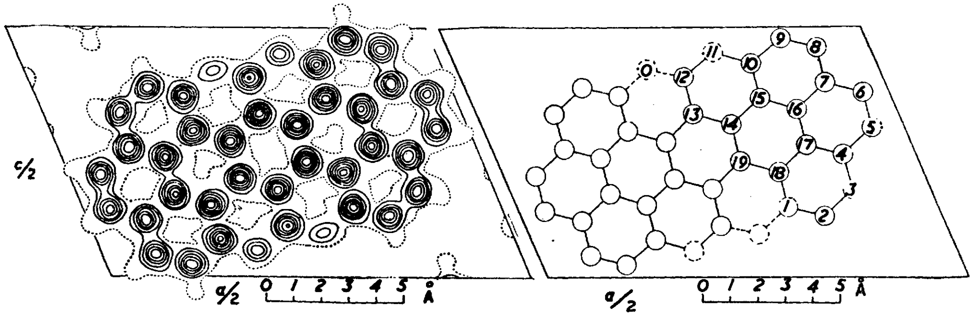
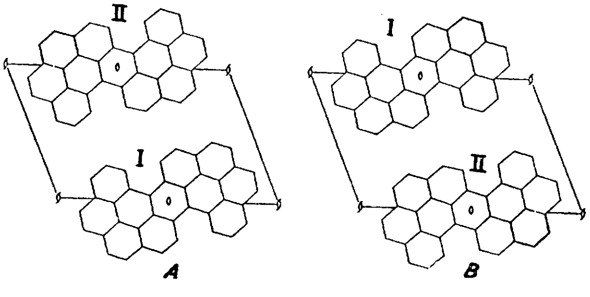


FIG. 2. (*a*) *Final electron density projection on* (010). *Contours at intervals of* 1 eÅ^{-2}, *with the one-electron line broken.*
(*b*) *The positions of the carbon atoms.*

Molecular arrangement in the (010) *projection.* From the results so far obtained about the disordered structure by consideration of the sharp (*h*0*l*) reflexions, each layer, A and B, can be constructed in two possible ways: (*a*) layer A consisting entirely of molecules in orientation I and layer B entirely of molecules in orientation II; (*b*) each layer, A or B, containing molecules in both orientations.

Since, however, the (*h*0*l*) reflexions with *l* even are sharp, layer B can, in projection down *b*, be made identical with layer A by translation $\frac{1}{2}c$, so that the true arrangement of molecules must be (*b*). This requires that each molecule possesses a two-fold axis, coincident with a two-fold axis of the space group, and the arrangement of molecules in the two layers A and B is shown in Fig. 3. The molecular centres are at (0, 0, 0) and (0, *d*, $\frac{1}{2}$), the two molecules are not related by any symmetry element, and the true asymmetric unit consists of half of each molecule. In spite of the fact that space group *C*2 is one of the Sohncke regular point systems, the two molecules, since they are not related, could be optical enantiomorphs.

FIG. 3. *Arrangement of molecules in layers A and B.*



Superposition of the layers gives an accurate account of the intensities of the (*h*0*l*) reflexions with *l* even (sharp reflexions). Values of measured and calculated structure factors are listed in Table 4. An ordered structure consisting of either layer A or layer B would give sharp $(h0l)$ reflexions with l odd, and the structure factors, $F_c(A)$, for this type of crystal may be calculated from the atomic co-ordinates. In a "perfectly disordered" structure, the structure factors, $F_c(AB)$, would be zero. Values of $F_c(A)$ and $F_c(AB)$ are compared with the measured values in Table 5; this comparison reveals that the true structure may be described as a "partially-ordered superlattice," with order extending over only a few unit cells.

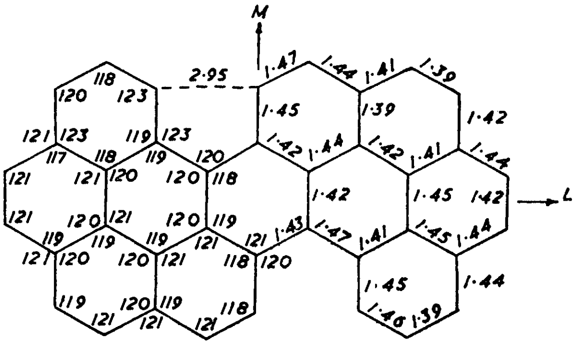
This completes the description of the projection of the structure on (010). A complete description of the molecular geometry and dimensions requires the examination of further data, to determine the third co-ordinates of the atoms.

The y-co-ordinates. No resolution of the individual atoms in the molecule can be expected in projection down the long a or c axes, more especially as the structure is disordered. The problem of finding the y-co-ordinates was therefore approached by considering the $(h1l)$ structure factors.

Approximate y-co-ordinates, found by trial, can be refined by the use of generalised projections. All reflexions are diffuse, so that we cannot hope to obtain perfect agreement between calculated and measured structure amplitudes of the Bragg reflexions.[7] A reasonable measure of agreement might be obtained, however, if we can find an accurate description of layer A alone.

A planar wire model of the molecule was constructed and buckled so that the distance between the overcrowded carbon atoms was 3·0 Å, a value suggested by previous studies.[8]

FIG. 4. *Bond lengths and valency angles in the dinaphthoperopyrene.*



Approximate y-co-ordinates with respect to the centre of the molecule were then determined from this model by projection along the molecular axis M. It now remained to find the positions of the two molecular centres, which are not related by any symmetry element. These two centres lie, one on the two-fold axis at $x = 0$, $z = 0$, the other on the two-fold axis at $x = 0$, $z = \frac{1}{2}$. One molecular centre was taken at (0, 0, 0), and this molecule was arbitrarily buckled in one sense—let us call its configuration D. Then the centre of the second molecule is at $(0, d, \frac{1}{2})$, and its configuration may be D or L. Considering the $(h10)$ and $(h12)$ reflexions, best agreement was obtained with the parameter d taken as $(26/60)b$, and the configuration of the second molecule as L. Structure factors were calculated for about 270 $(h1l)$ reflexions (425 were observed of a possible of about 650 independent reflexions); the discrepancy between measured and calculated values was 29·8%, an encouragingly low value when it is remembered that the structure is disordered and the reflexions diffuse.

In this structure the two molecules have opposite configurations, in spite of the fact that the space group is one of the Sohncke groups. Refinement of the y-parameters proceeded by computing a "difference generalised projection."[9] The shifts in the y-co-ordinates were calculated for all the atoms; these shifts were however applied with caution, since the structure is disordered, and the magnitude of a shift may be the mean of two atomic shifts. Generally, however, the shifts were very reasonable, and recalculation of the structure factors led to

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[7] Harker, Lucht, and Kasper, *Acta Cryst.*, 1950, **3**, 436.
[8] McIntosh, Robertson, and Vand, *J.*, 1954, 1661.
[9] Rossmann and Shearer, *Acta Cryst.*, 1958, **11**, 829.

improved agreement between F_o and F_c. The discrepancy was reduced to 26% over the 425 observed reflexions; values of the measured and calculated structure amplitudes, and the calculated phase constants are listed in Table 6. The agreement between observed and calculated values is not as good as in the ($h0l$) zone, but it is better than might be expected with a disordered structure of this type, and indicates that the y-co-ordinates have been determined with fair accuracy.

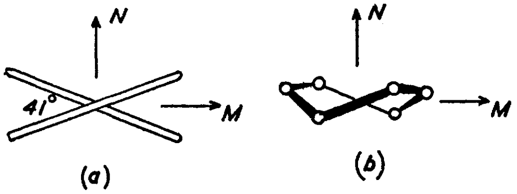


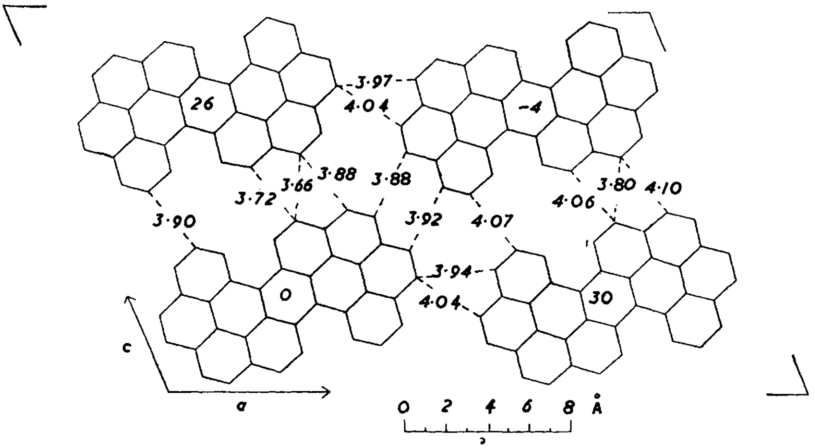
FIG. 5.

(*a*) *Idealised view along molecular axis L showing the mean planes through the outer rings.*

(*b*) *Atoms of the central ring* (*the puckering is exaggerated for clarity*).

Summarising, we see that layer A consists of one molecule situated on the two-fold axis at $x = 0$, $z = 0$, and the centre of this molecule can be chosen as the origin of the space group; a second molecule has its centre at (0, 26/60, $\frac{1}{2}$), and is the optical enantiomorph of the first. The arrangement of molecules in layer B is either identical with that in layer A, or related to it by some symmetry operation such as inversion in a centre of symmetry ($D \longrightarrow L$, $L \longrightarrow D$). However, it does not seem to be possible to describe exactly how A and B are related in the crystal, since, even if the true arrangement were found, perfect agreement between F_o and F_c for the general reflexions could not be obtained, since they are all diffuse. It is unlikely that the agreements found for the ($h1l$) reflexions could be much improved.

FIG. 6. *Intermolecular distances* (Å) (*figures at the centre of each molecule are the y-co-ordinates of the centre in b*/60).



Co-ordinates and molecular dimensions. The final co-ordinates of the carbon atoms are listed in Table 2, expressed as fractions of the unit-cell edges. x and z have been determined from the ($h0l$) zone refinement, and y from the difference-generalised projection, the ($h1l$) zone data being used.

The bond lengths and valency angles in the dinaphthoperopyrene molecule were calculated from these co-ordinates. Two independent values of each bond length and valency angle were obtained (one from each molecule) and the mean values (to the nearest 0·01 Å in bond length and the nearest degree in bond angle) are shown in Fig. 4. The maximum deviation of any individually-determined bond length from the mean value for that bond is 0·027 Å, and the root mean-square deviation for all the bonds is 0·011 Å. The corresponding differences for the valency angles are 1·8° and 0·9°. The average value of the carbon–carbon bond lengths is 1·431 Å.

TABLE 2. *Co-ordinates of the carbon atoms (numbered as in Fig. 1).*

	Molecule I			Molecule II		
Atom	*x*	*y*	*z*	*x*	*y*	*z*
1	0·0735	−0·322	−0·1101	0·1014	0·141	0·6754
2	0·1123	−0·439	−0·1287	0·1484	0·015	0·7253
3	0·1584	−0·372	−0·0770	0·1865	0·071	0·7066
4	0·1648	−0·205	−0·0060	0·1795	0·207	0·6374
5	0·2115	−0·139	0·0472	0·2191	0·301	0·6178
6	0·2191	−0·003	0·1178	0·2115	0·431	0·5472
7	0·1795	0·070	0·1374	0·1648	0·509	0·4940
8	0·1865	0·203	0·2066	0·1584	0·640	0·4230
9	0·1484	0·250	0·2253	0·1123	0·690	0·3713
10	0·1014	0·192	0·1754	0·0735	0·623	0·3899
11	0·0625	0·226	0·1972	0·0256	0·637	0·3359
12	0·0149	0·105	0·1486	−0·0149	0·523	0·3514
13	0·0077	0·005	0·0745	−0·0077	0·426	0·4255
14	0·0470	0·010	0·0534	0·0393	0·443	0·4788
15	0·0940	0·070	0·1060	0·0797	0·510	0·4599
16	0·1326	0·013	0·0845	0·1261	0·450	0·5125
17	0·1261	−0·115	0·0125	0·1326	0·331	0·5845
18	0·0797	−0·155	−0·0401	0·0940	0·297	0·6060
19	0·0393	−0·047	−0·0212	0·0470	0·356	0·5534

TABLE 3. *Deviations of atoms from the mean molecular planes* (Å).

Atom	I	II	Atom	I	II	Atom	I	II	Atom	I	II
1	−0·12	0·00	6	0·03	0·00	11	0·13	−0·26	16	−0·06	0·02
2	0·14	−0·17	7	−0·01	0·03	12	0·34	−0·48	17	−0·08	0·06
3	0·15	−0·18	8	−0·02	0·04	13	0·20	−0·35	18	−0·19	0·17
4	0·02	−0·07	9	0·03	−0·02	14	−0·06	−0·04	19	−0·35	0·24
5	0·04	−0·02	10	0·00	−0·05	15	−0·02	−0·01			

TABLE 4. *Measured and calculated (h0l) structure factors. Sharp reflexions* ($l = 2n$).

hkl	F_o	F_c	*hkl*	F_o	F_c	*hkl*	F_o	F_c	*hkl*	F_o	F_c	*hkl*	F_o	F_c	*hkl*	F_o	F_c
000	—	984	202	48	−46	36,0$\bar{6}$	5	−3	12,08	5	−3	8,0,$\overline{12}$	10	8	12,0,$\overline{16}$	4	6
200	86	85	402	70	72	32,0$\bar{6}$	11	−11	14,08	5	−8	4,0,$\overline{12}$	21	−18	10,0,$\overline{16}$	5	−10
400	111	−112	602	75	−74	30,0$\bar{6}$	17	12	18,08	4	−1	2,0,$\overline{12}$	14	21	6,0,$\overline{16}$	11	−12
600	50	57	802	32	34	26,0$\bar{6}$	16	−19	20,08	47	−48	2,0,12	19	25	2,0,$\overline{16}$	8	−11
800	16	−17	10,02	95	−92	24,0$\bar{6}$	25	−29	22,08	3	−5	4,0,12	5	−10	2,0,16	5	−3
10,00	27	31	12,02	62	−64	22,0$\bar{6}$	9	14	24,08	3	2	6,0,12	75	77	4,0,16	5	−9
12,00	10	11	14,02	18	22	20,0$\bar{6}$	5	−5	26,08	2	−2	8,0,12	83	83	6,0,16	3	−3
14,00	11	10	16,02	21	−21	18,0$\bar{6}$	19	10	38,0,$\overline{10}$	16	−12	10,0,12	8	−19	8,0,16	5	−9
16,00	21	−26	18,02	12	14	14,0$\bar{6}$	198	−196	28,0,$\overline{10}$	12	−7	12,0,12	3	7	10,0,16	12	11
18,00	21	22	20,02	12	−8	12,0$\bar{6}$	47	−49	26,0,$\overline{10}$	12	−9	14,0,12	2	1	12,0,16	5	−9
20,00	14	−12	22,02	15	−17	10,0$\bar{6}$	49	44	22,0,$\overline{10}$	7	4	18,0,12	4	2	16,0,16	16	−17
22,00	16	8	24,02	4	−7	80$\bar{6}$	14	−7	20,0,$\overline{10}$	16	−8	38,0,$\overline{14}$	2	−5	18,0,16	18	−20
24,00	19	10	26,02	5	2	60$\bar{6}$	21	−19	18,0,$\overline{10}$	6	−10	36,0,$\overline{14}$	3	4	24,0,$\overline{18}$	6	9
28,00	15	9	30,02	6	7	40$\bar{6}$	25	21	16,0,$\overline{10}$	25	23	34,0,$\overline{14}$	4	−6	22,0,$\overline{18}$	11	−15
30,00	12	−12	34,02	29	−26	20$\bar{6}$	87	87	14,0,$\overline{10}$	20	18	32,0,$\overline{14}$	3	7	18,0,$\overline{18}$	13	14
32,00	6	7	34,0$\bar{4}$	3	3	206	23	−19	12,0,$\overline{10}$	13	−13	28,0,$\overline{14}$	21	−20	16,0,$\overline{18}$	9	−17
34,00	21	−21	30,0$\bar{4}$	14	11	406	7	7	10,0,$\overline{10}$	21	−22	26,0,$\overline{14}$	5	13	14,0,$\overline{18}$	7	13
36,00	14	−14	28,0$\bar{4}$	25	−28	606	9	7	8,0,$\overline{10}$	18	16	24,0,$\overline{14}$	9	−11	12,0,$\overline{18}$	8	−12
002	164	158	26,0$\bar{4}$	49	45	806	2	2	6,0,$\overline{10}$	7	7	22,0,$\overline{14}$	9	11	8,0,$\overline{18}$	22	−24
004	70	−74	24,0$\bar{4}$	71	69	10,06	5	−1	4,0,$\overline{10}$	192	−181	20,0,$\overline{14}$	5	−1	6,0,$\overline{18}$	31	−34
006	6	3	22,0$\bar{4}$	19	−18	12,06	4	−1	2,0,$\overline{10}$	35	−29	18,0,$\overline{14}$	49	48	2,0,$\overline{18}$	4	−8
008	16	20	20,0$\bar{4}$	20	24	14,06	12	−6	2,0,10	13	−14	16,0,$\overline{14}$	71	67	4,0,18	10	−9
00,10	22	16	18,0$\bar{4}$	24	−23	20,06	27	−30	4,0,10	20	24	14,0,$\overline{14}$	4	−10	32,0,$\overline{20}$	13	−10
00,12	14	−16	14,0$\bar{4}$	41	−39	22,06	28	−27	6,0,10	15	−15	12,0,$\overline{14}$	15	17	30,0,$\overline{20}$	17	−15
00,14	7	16	12,0$\bar{4}$	55	−52	24,06	5	9	8,0,10	16	−16	8,0,$\overline{14}$	3	4	26,0,$\overline{20}$	9	−10
00,18	4	10	10,0$\bar{4}$	27	28	28,06	3	−4	10,0,10	8	−4	6,0,$\overline{14}$	21	15	24,0,$\overline{20}$	7	9
			80$\bar{4}$	72	−68	38,0$\bar{8}$	28	−26	12,0,10	22	20	4,0,$\overline{14}$	14	15	20,0,$\overline{20}$	16	−12
36,0$\bar{2}$	2	−1	60$\bar{4}$	65	66	36,0$\bar{8}$	9	−9	14,0,10	4	−8	2,0,$\overline{14}$	4	−4	18,0,$\overline{20}$	15	−14
34,0$\bar{2}$	3	6	40$\bar{4}$	20	−12	34,0$\bar{8}$	3	4	16,0,10	2	2	2,0,14	15	−17	16,0,$\overline{20}$	3	7
32,0$\bar{2}$	2	−3	20$\bar{4}$	122	−117	32,0$\bar{8}$	4	−3	24,0,10	3	−4	6,0,14	121	124	14,0,$\overline{20}$	3	0
30,0$\bar{2}$	8	8	204	41	34	26,0$\bar{8}$	11	14	26,0,10	4	8	8,0,14	25	23	12,0,$\overline{20}$	4	6
28,0$\bar{2}$	19	−18	404	20	−27	22,0$\bar{8}$	3	−8	38,0,$\overline{12}$	4	6	10,0,14	27	−26	8,0,$\overline{20}$	41	−42
24,0$\bar{2}$	162	155	604	39	39	20,0$\bar{8}$	8	−3	34,0,$\overline{12}$	5	−7	12,0,14	4	4	6,0,$\overline{20}$	15	−15
22,0$\bar{2}$	36	36	804	19	−20	18,0$\bar{8}$	25	29	32,0,$\overline{12}$	9	9	14,0,14	5	−7	4,0,$\overline{20}$	11	12
20,0$\bar{2}$	30	−29	10,04	197	−196	16,0$\bar{8}$	24	−27	28,0,$\overline{12}$	57	−58	18,0,14	5	−6	4,0,20	4	8
18,0$\bar{2}$	20	19	12,04	22	−19	14,0$\bar{8}$	31	−27	26,0,$\overline{12}$	20	−21	36,0,$\overline{16}$	7	9	6,0,20	2	0
16,0$\bar{2}$	12	−6	14,04	36	37	12,0$\bar{8}$	9	5	24,0,$\overline{12}$	7	11	30,0,$\overline{16}$	5	5	30,0,$\overline{22}$	13	−11
14,0$\bar{2}$	19	20	16,04	9	−8	80$\bar{8}$	9	5	20,0.$\overline{12}$	12	9	28,0,$\overline{16}$	5	10	28,0,$\overline{22}$	6	5
12,0$\bar{2}$	10	10	20,04	5	8	60$\bar{8}$	2	3	18,0,$\overline{12}$	6	−8	24,0,$\overline{16}$	7	13	20,0,$\overline{22}$	9	10
10,0$\bar{2}$	29	27	22,04	9	14	40$\bar{8}$	67	−66	16,0,$\overline{12}$	26	−25	22,0,$\overline{16}$	13	−12	2,0,22	14	−14
80$\bar{2}$	28	−30	24,04	5	−3	20$\bar{8}$	81	−78	14,0,$\overline{12}$	7	−15	18,0,$\overline{16}$	138	135	4,0,22	17	−20
60$\bar{2}$	68	62	26,04	4	−4	408	21	−25	12,0,$\overline{12}$	25	26	16,0,$\overline{16}$	51	44	22,0,$\overline{24}$	14	−10
40$\bar{2}$	84	−87	38,0$\bar{6}$	6	−5	808	19	19	10,0,$\overline{12}$	13	−18	14,0,$\overline{16}$	30	−28	20,0,$\overline{24}$	16	−16
20$\bar{2}$	146	141															

The overcrowded non-bonded distances (1 • • • 12) are 2·975 Å and 2·930 Å (mean 2·953 Å).

The molecule has an exact two-fold axis (2), and is propeller-shaped. The strain due to molecular distortion appears to be very evenly distributed over the whole molecule, the three bonds around each carbon atom being nearly coplanar. The carbon atom hybrid orbitals will thus be nearly pure sp^2, and the molecule retains its aromatic character.

The six-membered rings which are furthest from the centre of the molecule ought to show the smallest deviations from a planar structure. The two rings consisting of atoms 4, 5, 6, 7,

TABLE 5.

Measured aud calculated (h0l) structure factors. Diffuse reflexions ($l = 2n + 1$).

hkl	F_o	$F_c(A)$	$F_c(AB)$	*hkl*	F_o	$F_c(A)$	$F_c(AB)$	*hkl*	F_o	$F_c(A)$	$F_c(AB)$	*hkl*	F_o	$F_c(A)$	$F_c(AB)$
$60\bar{1}$	4	17	0	$10,0\bar{3}$	2	12	0	803	5	13	0	$80\bar{7}$	2	17	0
$40\bar{1}$	5	21	0	$80\bar{3}$	4	14	0	12,03	3	−8	0	$60\bar{7}$	5	15	0
401	6	−34	0	203	2	16	0	$10,0\bar{5}$	2	−20	0	207	2	−14	0
601	6	−30	0	403	6	24	0	$80\bar{5}$	5	−25	0	407	2	−11	0
801	5	−18	0	603	5	23	0	$60\bar{5}$	5	−21	0	607	2	−6	0
10,01	5	−5	0												

TABLE 6. *Measured and calculated (h1l) structure factors.*

hk	F_o	$\lvert F_c\rvert$	α(°)	*hkl*	F_o	$\lvert F_c\rvert$	α(°)	*hkl*	F_o	$\lvert F_c\rvert$	α(°)	*hkl*	F_o	$\lvert F_c\rvert$	α(°)
110	41	39	105	912	77	70	53	29,14	2	1	286	$13,1\bar{7}$	61	40	174
310	29	44	212	11,12	29	30	240	31,14	12	10	232	$11,1\bar{7}$	12	8	261
510	41	36	46	13,12	71	56	236	$37,1\bar{5}$	8	6	143	$91\bar{7}$	9	23	119
710	16	18	232	17,12	5	7	13	$35,1\bar{5}$	4	4	332	$71\bar{7}$	24	34	349
910	17	23	70	19,12	14	18	233	$29,1\bar{5}$	4	7	163	$51\bar{7}$	4	14	51
11,10	18	16	60	21,12	4	3	82	$27,1\bar{5}$	4	9	161	$31\bar{7}$	68	83	137
13,10	29	36	232	23,12	7	5	29	$25,1\bar{5}$	52	56	319	$11\bar{7}$	11	13	118
15,10	5	4	22	25,12	10	9	40	$23,1\bar{5}$	4	9	262	117	18	32	342
19,10	4	7	166	29,12	3	4	227	$21,1\bar{5}$	9	18	181	317	7	18	90
21,10	59	50	55	31,12	3	2	330	$19,1\bar{5}$	7	10	227	517	18	29	349
23,10	8	18	43	33,12	9	8	242	$17,1\bar{5}$	7	9	257	717	8	12	57
25,10	50	43	238	$29,1\bar{3}$	13	12	352	$15,1\bar{5}$	48	43	160	917	31	43	126
31,10	4	3	76	$27,1\bar{3}$	9	13	67	$13,1\bar{5}$	102	83	154	13,17	10	18	334
33,10	12	10	48	$25,1\bar{3}$	77	53	348	$11,1\bar{5}$	8	19	260	15,17	4	9	156
35,10	7	6	239	$23,1\bar{3}$	61	45	354	$91\bar{5}$	28	24	190	19,17	16	15	188
$35,1\bar{1}$	20	15	145	$21,1\bar{3}$	5	15	36	$71\bar{5}$	8	18	275	21,17	27	22	172
$29,1\bar{1}$	4	2	307	$19,1\bar{3}$	15	17	352	$51\bar{5}$	7	13	173	25,17	3	6	173
$27,1\bar{1}$	9	8	135	$17,1\bar{3}$	7	9	94	$31\bar{5}$	17	13	117	$35,1\bar{8}$	7	4	243
$25,1\bar{1}$	38	35	336	$15,1\bar{3}$	14	16	334	$11\bar{5}$	21	29	112	$33,1\bar{8}$	3	1	336
$23,1\bar{1}$	76	55	338	$13,1\bar{3}$	60	57	142	115	4	12	96	$29,1\bar{8}$	11	10	225
$21,1\bar{1}$	8	18	100	$11,1\bar{3}$	10	13	342	315	22	23	331	$27,1\bar{8}$	8	10	211
$19,1\bar{1}$	16	20	348	$91\bar{3}$	7	1	65	515	16	22	137	$19,1\bar{8}$	3	5	17
$17,1\bar{1}$	6	18	108	$71\bar{3}$	3	15	266	715	15	19	288	$17,1\bar{8}$	63	43	238
$15,1\bar{1}$	2	16	349	$51\bar{3}$	43	53	171	915	66	40	171	$15,1\bar{8}$	41	36	232
$13,1\bar{1}$	15	9	302	$31\bar{3}$	50	42	188	11,15	45	33	161	$13,1\bar{8}$	72	60	54
$11,1\bar{1}$	16	14	300	$11\bar{3}$	162	213	315	13,15	9	8	334	$11,1\bar{8}$	19	21	68
$91\bar{1}$	25	32	341	113	43	36	210	15,15	4	9	93	$91\bar{8}$	7	15	184
$71\bar{1}$	21	39	105	313	271	55	179	17,15	7	8	1	$71\bar{8}$	4	7	107
$51\bar{1}$	60	71	350	513	21	23	229	21,15	18	24	151	$51\bar{8}$	89	78	51
$31\bar{1}$	44	67	79	713	3	16	225	23,15	6	2	204	$31\bar{8}$	21	16	245
$11\bar{1}$	267	244	345	913	68	56	167	25,15	3	4	341	$11\bar{8}$	92	78	232
111	169	183	345	11,13	97	71	161	$35,1\bar{6}$	13	11	304	118	8	5	330
311	26	29	78	13,13	8	15	253	$33,1\bar{6}$	5	2	0	318	4	3	225
511	31	23	345	15,13	15	12	182	$29,1\bar{6}$	5	4	32	518	13	18	52
711	8	8	48	17,13	4	5	300	$27,1\bar{6}$	19	22	308	718	9	7	29
911	17	11	350	21,13	7	12	118	$25,1\bar{6}$	8	6	276	918	12	7	204
11,11	78	76	142	23,13	8	12	115	$23,1\bar{6}$	6	7	297	11,18	22	21	226
13,11	4	5	339	33,13	11	7	158	$21,1\bar{6}$	6	10	46	13,18	3	4	290
15,11	4	5	268	$29,1\bar{4}$	5	6	187	$19,1\bar{6}$	18	15	217	17,18	12	11	243
17,11	4	10	222	$27,1\bar{4}$	51	43	58	$17,1\bar{6}$	15	19	49	19,18	7	8	246
19,11	11	20	179	$25,1\bar{4}$	38	33	57	$15,1\bar{6}$	9	13	269	23,18	11	10	55
21,11	9	11	227	$23,1\bar{4}$	59	60	232	$13,1\bar{6}$	8	8	325	25,18	2	5	225
23,11	34	39	312	$21,1\bar{4}$	9	15	255	$91\bar{6}$	9	2	289	$37,1\bar{9}$	13	8	181
25,11	6	10	181	$19,1\bar{4}$	6	7	358	$71\bar{6}$	23	11	29	$31,1\bar{9}$	5	9	341
29,11	3	4	217	$17,1\bar{4}$	3	9	207	$51\bar{6}$	30	29	217	$27,1\bar{9}$	15	24	128
33,11	14	9	177	$15,1\bar{4}$	68	55	56	$31\bar{6}$	2	19	186	$25,1\bar{9}$	4	10	111
35,11	15	12	167	$13,1\bar{4}$	17	21	235	$11\bar{6}$	8	19	223	$23,1\bar{9}$	9	17	345
$31,1\bar{2}$	4	4	219	$11,1\bar{4}$	79	75	236	116	9	8	52	$19,1\bar{9}$	10	15	356
$29,1\bar{2}$	11	11	39	$91\bar{4}$	6	11	330	516	7	6	348	$17,1\bar{9}$	9	10	9
$27,1\bar{2}$	15	14	228	$71\bar{4}$	4	8	334	716	65	57	233	$15,1\bar{9}$	40	46	131
$25,1\bar{2}$	8	14	209	$51\bar{4}$	48	36	232	916	17	25	225	$11,1\bar{9}$	17	24	343
$23,1\bar{2}$	22	23	73	$31\bar{4}$	15	45	53	11,16	58	45	58	$91\bar{9}$	10	13	134
$21,1\bar{2}$	6	7	110	$11\bar{4}$	6	15	312	13,16	7	9	76	$51\bar{9}$	62	43	182
$19,1\bar{2}$	8	8	67	114	50	31	20	15,16	4	6	185	$31\bar{9}$	97	65	176
$15,1\bar{2}$	5	13	70	314	2	13	67	19,16	15	24	48	$11\bar{9}$	11	23	229
$13,1\bar{2}$	7	13	56	514	19	24	219	21,16	12	8	247	119	13	23	168
$11,1\bar{2}$	26	29	234	714	10	18	34	23,16	21	16	239	319	5	11	256
$91\bar{2}$	18	9	39	914	39	32	248	$37,1\bar{7}$	22	15	150	519	9	14	178
$71\bar{2}$	8	8	127	11,14	9	18	34	$29,1\bar{7}$	5	8	170	919	12	20	305
$51\bar{2}$	23	27	176	13,14	14	11	45	$23,1\bar{7}$	6	11	142	11,19	3	14	178
$31\bar{2}$	232	236	56	15,14	5	4	213	$21,1\bar{7}$	7	8	315	13,19	3	7	255
$11\bar{2}$	93	111	53	17,14	4	3	84	$19,1\bar{7}$	15	12	150	17,19	6	6	315
112	261	239	235	21,14	6	4	133	$17,1\bar{7}$	10	11	261	19,19	17	18	144
312	17	28	280	23,14	5	11	228	$15,1\bar{7}$	69	42	175	21,19	10	13	143

TABLE 6. (*Continued.*)

hkl	F_o	$\lvert F_c \rvert$	α(°)	*hkl*	F_o	$\lvert F_c \rvert$	α(°)	*hkl*	F_o	$\lvert F_c \rvert$	α(°)	*hkl*	F_o	$\lvert F_c \rvert$	α(°)
27,19	6	1	168	5,1,$\overline{12}$	47	26	232	15,1,$\overline{15}$	14	20	53	17,1,$\overline{18}$	38	37	237
37,1,$\overline{10}$	11	11	51	3,1,$\overline{12}$	54	38	56	13,1,$\overline{15}$	10	20	356	15,1,$\overline{18}$	15	13	252
29,1,$\overline{10}$	19	21	55	1,1,$\overline{12}$	5	5	139	7,1,$\overline{15}$	4	6	300	9,1,$\overline{18}$	13	20	53
25,1,$\overline{10}$	20	28	235	5,1,12	53	61	230	1,1,$\overline{15}$	6	13	135	5,1,$\overline{18}$	14	19	235
19,1,$\overline{10}$	11	6	44	7,1,12	20	14	75	1,1,15	4	10	322	1,1,18	6	9	236
17,1,$\overline{10}$	3	4	245	9,1,12	59	49	58	3,1,15	13	16	141	3,1,18	4	5	207
13,1,$\overline{10}$	17	21	219	29,1,$\overline{13}$	18	17	161	5,1,15	36	26	330	7,1,18	10	8	42
7,1,$\overline{10}$	18	18	250	27,1,$\overline{13}$	19	19	158	7,1,15	35	32	326	31,1,$\overline{19}$	12	12	149
5,1,$\overline{10}$	12	9	281	17,1,$\overline{13}$	56	68	321	9,1,15	8	8	165	23,1,$\overline{19}$	3	6	199
3,1,$\overline{10}$	7	10	275	15,1,$\overline{13}$	15	17	318	17,1,15	13	17	148	21,1,$\overline{19}$	12	16	166
1,1,$\overline{10}$	27	28	47	13,1,$\overline{13}$	9	17	148	31,1,$\overline{16}$	5	6	234	19,1,$\overline{19}$	13	25	309
1,1,10	12	12	218	11,1,$\overline{13}$	8	5	335	27,1,$\overline{16}$	4	5	73	15,1,$\overline{19}$	7	12	170
7,1,10	19	14	260	9,1,$\overline{13}$	4	5	57	23,1,$\overline{16}$	9	8	49	9,1,$\overline{19}$	10	10	178
9,1,10	23	38	50	7,1,$\overline{13}$	19	20	340	21,1,$\overline{16}$	9	3	112	7,1,$\overline{19}$	27	25	159
11,1,10	11	7	75	5,1,$\overline{13}$	18	23	135	19,1,$\overline{16}$	11	11	86	5,1,19	4	11	116
15,1,10	6	6	41	3,1,$\overline{13}$	10	10	343	15,1,$\overline{16}$	15	20	226	33,1,$\overline{20}$	7	9	53
17,1,10	8	13	233	1,1,$\overline{13}$	3	7	45	9,1,$\overline{16}$	3	6	72	29,1,$\overline{20}$	12	12	236
21,1,10	12	13	58	1,1,13	10	13	8	7,1,$\overline{16}$	8	11	54	23,1,$\overline{20}$	8	7	234
29,1,$\overline{11}$	14	13	171	3,1,13	4	14	40	5,1,$\overline{16}$	12	18	236	21,1,$\overline{20}$	3	2	94
27,1,$\overline{11}$	26	23	174	5,1,13	40	36	3	3,1,$\overline{16}$	4	6	256	17,1,$\overline{20}$	5	6	27
25,1,$\overline{11}$	4	10	248	7,1,13	79	60	347	1,1,16	5	10	217	13,1,$\overline{20}$	4	7	216
23,1,$\overline{11}$	4	11	168	9,1,13	9	16	45	3,1,16	34	31	54	9,1,$\overline{20}$	7	11	246
13,1,$\overline{11}$	9	11	190	11,1,13	7	3	323	5,1,16	14	25	47	5,1,$\overline{20}$	7	10	55
11,1,$\overline{11}$	4	12	254	31,1,$\overline{14}$	15	14	234	7,1,16	36	31	239	7,1,20	3	3	248
9,1,$\overline{11}$	12	15	187	29,1,$\overline{14}$	11	14	236	23,1,$\overline{17}$	7	9	337	31,1,$\overline{21}$	17	15	155
7,1,$\overline{11}$	12	14	291	27,1,$\overline{14}$	11	17	55	21,1,$\overline{17}$	9	10	61	15,1,$\overline{21}$	4	8	347
5,1,$\overline{11}$	66	45	151	19,1,$\overline{14}$	59	59	234	19,1,$\overline{17}$	36	28	341	11,1,$\overline{21}$	3	5	331
3,1,$\overline{11}$	47	44	148	15,1,$\overline{14}$	61	66	57	17,1,$\overline{17}$	42	35	334	9,1,$\overline{21}$	5	6	168
1,1,$\overline{11}$	9	4	297	13,1,$\overline{14}$	6	10	100	15,1,$\overline{17}$	5	3	138	7,1,$\overline{21}$	8	10	152
7,1,11	62	76	326	9,1,$\overline{14}$	10	7	63	11,1,$\overline{17}$	5	5	166	3,1,21	10	14	157
9,1,11	22	12	346	1,1,14	4	7	64	7,1,$\overline{17}$	20	30	147	5,1,21	6	6	184
11,1,11	7	11	127	3,1,14	13	10	80	5,1,$\overline{17}$	9	9	155	11,1,$\overline{22}$	9	10	238
13,1,11	7	7	348	5,1,14	27	27	65	1,1,17	5	9	192	9,1,$\overline{22}$	6	12	230
17,1,11	7	11	336	9,1,14	35	26	232	3,1,17	12	15	168	7,1,$\overline{22}$	9	11	62
27,1,$\overline{12}$	3	6	289	15,1,14	5	5	75	5,1,17	10	20	310	5,1,$\overline{22}$	2	2	85
25,1,$\overline{12}$	5	8	34	37,1,$\overline{15}$	12	5	166	15,1,17	6	5	189	1,1,22	3	9	44
21,1,$\overline{12}$	6	2	200	31,1,$\overline{15}$	4	7	337	29,1,$\overline{18}$	4	7	232	21,1,$\overline{23}$	10	13	144
19,1,$\overline{12}$	5	6	0	29,1,$\overline{15}$	10	14	133	27,1,$\overline{18}$	4	2	270	19,1,$\overline{23}$	7	7	159
15,1,$\overline{12}$	17	27	49	23,1,$\overline{15}$	8	8	3	23,1,$\overline{18}$	5	9	215	23,1,$\overline{24}$	7	10	49
13,1,$\overline{12}$	4	4	210	19,1,$\overline{15}$	38	33	356	21,1,$\overline{18}$	39	30	55	19,1,$\overline{24}$	9	11	238
9,1,$\overline{12}$	9	12	36	17,1,$\overline{15}$	82	66	345	19,1,$\overline{18}$	26	24	48	7,1,$\overline{24}$	3	6	223
7,1,$\overline{12}$	45	36	234												

8, 9, 10, 15, 16, 17 are far from the molecular centre, and the mean planes of these atoms in the two molecules (I and II) were found by a least-squares method to be

$$\text{(I)}\quad 0{\cdot}0647\,X' - 0{\cdot}9345\,Y - 0{\cdot}3499\,Z' - 0{\cdot}2826 = 0$$

$$\text{(II)}\quad 0{\cdot}0652\,X' - 0{\cdot}9412\,Y - 0{\cdot}3379\,Z' - 4{\cdot}7697 = 0$$

X', Y, Z' are co-ordinates expressed in Å, and referred to orthogonal axes a', b, c, where a' is perpendicular to b and c. The atoms used to determine the equations all lie close to these planes, but the deviations of the other atoms increase towards the centre of the molecule, as shown in Table 3.

An idealised view of the molecule along the molecular axis L is shown in Fig. 5(*a*), and the shape of the central ring is indicated in Fig. 5(*b*).

All intermolecular distances correspond to normal van der Waals interactions. The distance between any atom and the corresponding atom in the molecule one translation along b is 3·855 Å (the b-axis repeat distance). The mean perpendicular distance between the mean planes through the outer rings [Fig. 5(*a*)] of two molecules related by translation b is 3·62 Å. The shortest lateral contact, within either layer A or layer B, is 3·66 Å. Some of the shorter intermolecular contacts are shown in Fig. 6. Examination of the intermolecular distances projected on (010) shows that there can be no unusually short distances between the molecules of layer A and those of an adjacent layer B, so that the two layers are built into the crystal without any undue strain.

DISCUSSION

It is difficult to estimate the accuracy with which the bond lengths and valency angles have been determined. Cruickshank's formulæ could be applied to the (*h*0*l*) zone data, but this would give a false impression of the accuracy because, although the structure factor agreement is extremely good, each atomic position is really the mean of two extremely close atoms. The close agreement between the independent values of chemically identical bonds (R.M.S. deviation from the mean 0·01 Å) suggests that the molecular dimensions have been determined with considerable precision.

Since the accuracy is rather doubtful, no detailed discussion of bond length variations in the molecule will be attempted, but some general trends may be mentioned. The bonds involving the overcrowded carbon atoms are long, indicating maximum breakdown of aromatic character around these positions. The mean bond length over the whole molecule is 1·43 Å, which is rather greater than the average value for planar aromatic hydrocarbons such as coronene (1·410 Å) or ovalene (1·412 Å). This again suggests that the aromatic character is reduced slightly by the buckling. The bonds 8–9, 15–16, 18–19 increase in that order (1·387 $\longrightarrow$ 1·423 $\longrightarrow$ 1·472 Å), as do similar bonds in benzoperylene[10] and 2 : 3-8 : 9-dibenzocoronene.[11]

The distance between the overcrowded carbons is 2·95 Å. The increase in intramolecular distance compared with a planar model is achieved by buckling the molecular framework, with the strain largely distributed over the whole molecule and with very little departure of the valency angles from the trigonal values. This results in retention of aromatic character in spite of the severe molecular distortion.

The account of the structure which the present analysis has yielded is not quite complete. The positions of all the atoms in each molecule, and the arrangement of molecules in each layer, have been obtained from a consideration of sharp and diffuse reflexions. It has not been possible, however, to describe how the two layers are packed together in the crystal, except that they are related by translation $\frac{1}{2}c$. The data, consisting of the weak diffuse ($h0l$) reflexions with l odd (Table 5), are clearly insufficient for any more complete description. The analysis has, however, established with considerable precision the molecular dimensions and stereochemistry of this large overcrowded molecule.

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[10] White, *J.*, 1948, 1398.
[11] Trotter, *Acta Cryst.*, 1958, **11**, 423.