crystals and metal-oxide crystals contain the same cation structures indicated that a separate description of the various cation lattices without reference to the anion structure is quite useful.

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The Crystal and Molecular Structure of 9:10-Dihydro-1:2:5:6-Dibenzanthracene

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The structure of 9:10-dihydro-1:2:5:6-dibenzanthracene has been determined by two-dimensional Fourier syntheses. The cell is monoclinic with $a = 9{\cdot}49$, $b = 6{\cdot}77$, $c = 11{\cdot}38$ Å, $\beta = 91° 29'$; 2 molecules ($C_{22}H_{16}$) per unit cell; space group = $P2_1/a$. Atomic coordinates were obtained from F_o and $(F_o - F_c)$ Fourier syntheses on the three principal zones. The molecule is essentially planar (r.m.s. deviation of carbon atoms from mean plane is 0·039 Å); the mean length of the C–C single bond in the central ring is 1·503 Å, the mean bond length of the aromatic rings is 1·401 Å and the mean angle in the aromatic rings is 120° 0'.

Introduction

This compound (Fig. 1) is of interest because it is slightly carcinogenic and is derived from the more strongly carcinogenic parent compound, 1:2:5:6-dibenzanthracene. It is of interest also because of its relation to 9:10-dihydroanthracene. The latter compound was shown by Ferrier & Iball (1954) to have a bent molecule in which two planar halves are inclined to each other at 145°. Beckett & Mulley (1955) subsequently gave some theoretical reasons, based on chemical evidence, why 9:10-disubstituted anthracenes should have bent molecules, and they postulated structures for the *cis-* and *trans-* isomers which can occur when the substituents are different. The present work will show that 9:10-dihydro-1:2:5:6-dibenzanthracene has a *planar* molecule which is not in accord with predictions from normal stereochemical considerations.

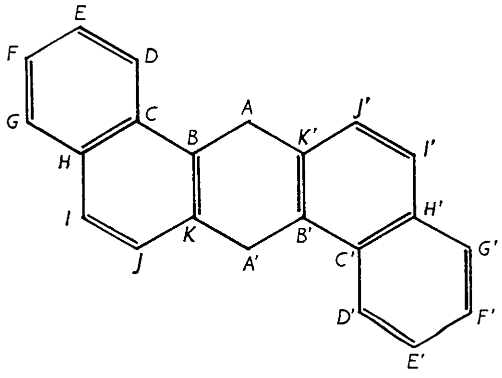

Fig. 1. 9:10-Dihydro-1:2:5:6-dibenzanthracene ($C_{22}H_{16}$).

A preliminary crystallographic study was carried out by Iball (1938), who gave the unit cells and space groups of two crystal forms, both monoclinic. He showed that one form [Form (ii)] had a space group in which the molecules must possess a centre of symmetry, and from this deduced that the molecule must be planar. It is this form which is the subject of the present investigation. The crystals (from a sample kindly provided by Dr J. W. Cook) were the same as were used in the earlier investigation.

Crystal data

The crystals are monoclinic six-sided plates parallel to (001). In the earlier work (Iball, 1938) the unit cell chosen was as follows:

$$a = 9{\cdot}51,\ b = 6{\cdot}77,\ c = 24{\cdot}43\ \text{Å},\ \beta = 111{\cdot}4° .$$

The crystals have negative birefringence with β parallel to b and γ approximately parallel to c. The space group with the above cell is $B2_1/c$, and this centred cell was chosen to conform with the optical directions and also to compare with the similarly shaped cell of the other crystal modification. A primitive cell has however been used in the present work and the axes have been re-determined as follows:

$$a = 9{\cdot}49 \pm 0{\cdot}01,\ b = 6{\cdot}77 \pm 0{\cdot}01,\ c = 11{\cdot}38 \pm 0{\cdot}01\ \text{Å}\ ,\quad \beta = 91{\cdot}5^\circ .$$

The absent spectra are $h0l$ when h is odd and $0k0$ when k is odd. The space group is therefore C_{2h}^5–$P2_1/a$, with two molecules ($C_{22}H_{16}$) per unit cell.

d(obs.) = 1·258, d(calc.) = 1·274 g.cm.$^{-3}$. The volume of the unit cell is 730·4 Å^3. $F(000) = 296$.

Experimental

Equi-inclination Weissenberg photographs were taken with Cu $K\alpha$ radiation about the three principal axes. Intensities were obtained partly by visual estimation and partly by the use of a Hilger non-recording photometer. In the latter case the spots were traversed on the photometer by the light beam and an attempt was made to achieve at least a partial integration of the intensity of the diffraction spot and in this way to compensate for the varying width of spot. The variation of spot width was clearly due to the platy nature of the crystals, and, since it was difficult to prepare specimens which were of uniform thickness, a correction for absorption was made using the method of Albrecht (1939). This correction was generally small as the crystals were small and have a low absorption coefficient for copper radiation.

Determination of the approximate structure

In the space group $P2_1/a$ with two molecules in the unit cell, the molecule must possess a centre of symmetry. If this point of the molecule is placed at the origin of coordinates and if we assume that the molecule is planar the problem is then reduced to one of finding the orientation of the molecular model. This can be done by ordinary trial and error, but with a centrosymmetrical molecule of this type the most systematic 'trial and error' method is to calculate the molecular transform (or use an optical transform if suitable apparatus is available) and then fit the molecular transform to that of the cell as given by the diffraction data (Knott, 1940).

The $h0l$ reflexions were considered first because of the short b axis. The molecular model was constructed with carbon–carbon bonds of 1·41 Å in all the rings. The $00l$ and $h00$ reflexions could be fitted to the molecular transform in several orientations but a few non-axial reflexions such as $(20\bar{1})$ and $(20\bar{2})$, which had large structure factors, indicated the most probable one. The signs of 36 of the largest $h0l$ structure factors were determined from the transform, and by using these and the observed F's a Fourier synthesis was computed. The resulting electron-density map gave only one completely resolved atomic peak (A, Fig. 1) but very reasonable estimates of the coordinates of atoms E and J could be made. Sections were drawn through some of the double peaks, and, with the aid of an assumed shape for a single peak, estimates were made of the coordinates of all the other carbon atoms.

The structural factors for all the observed $h0l$ reflexions were now calculated with McWeeny's (1951) f_C curve and a temperature factor (B) of 3·42 Å^2. The reliability index $R = \Sigma|F_o - F_c| \div \Sigma|F_o|$ was 0·29.

The signs of 67 structure factors were accepted as correct and a further F_o synthesis was carried out. Atoms A, E and J were now completely resolved as single peaks, but the other eight carbon atoms still appeared as four double peaks. The new estimates of the coordinates reduced the value of R to 0·26.

The $0kl$ and $hk0$ zones were now considered, and by making assumptions regarding the lengths of the carbon–carbon bonds, a set of y coordinates was calculated from the projected bond lengths on the $h0l$ electron-density map. The $0kl$ and $hk0$ structure factors were calculated and compared with the observed values. The values of $R(0kl)$ and $R(hk0)$ were 0·27 and 0·28 respectively. From these and the $h0l$ results it was concluded that the carbon atom coordinates were approximately correct.

Refinement of the structure

Since no one projection gave an electron-density map with all atoms resolved the refinement was carried out on all three zones simultaneously, first by suc-

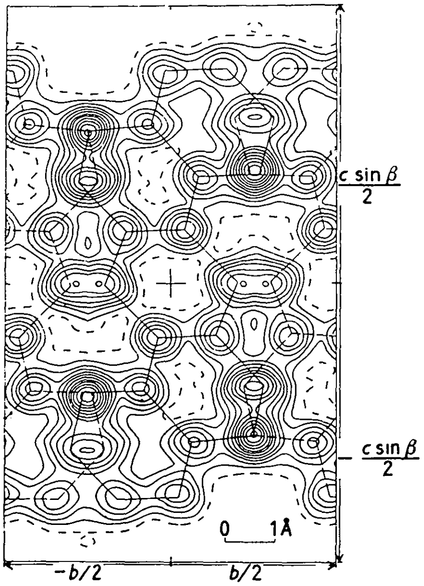

Fig. 2. Electron-density projection perpendicular to a. The contours are at intervals of 1 e.Å^{-2}; the dotted contour is at 2 e.Å^{-2}.

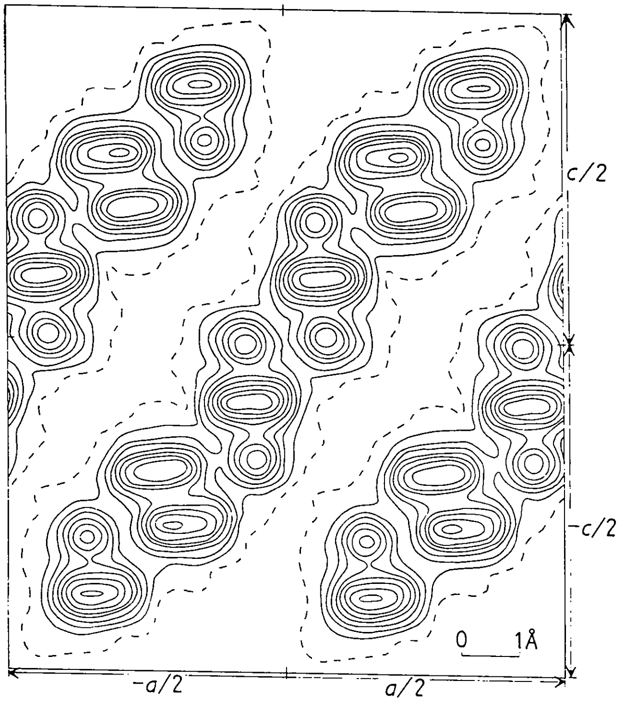

Fig. 3. Electron-density projection perpendicular to *b*. The contours are at intervals of 1 e.Å^{-2}; the dotted contour is at 1 e.Å^{-2}.

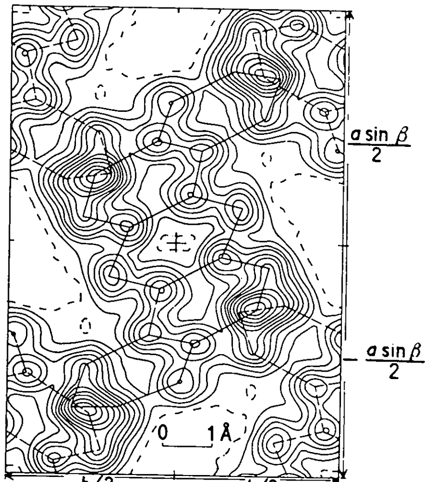

Fig. 4. Electron-density projection perpendicular to *c*. The contours are at intervals of 1 e.Å^{-2}; the dotted contour is at 2 e.Å^{-2}.

cessive F_o syntheses and then by (F_o-F_c) syntheses. When all the signs were considered to be established the final F_o electron-density maps were drawn. They are given in Figs. 2, 3 and 4. The peak positions were determined by the eleven-point semi-analytical method of Burns & Iball (1956). A check on the peak determination was made with the method of Ladell & Katz (1954) and it was found that the results from both methods agreed very well. With the peak positions determined, a correction was applied to each one for the overlapping of neighbouring peaks. As in the case of chrysene (Burns & Iball, 1956), this was done by evaluating the expression

$$\varrho'(r) = \int_0^{s_0} 2\pi s f(s) J_0(2\pi r s) . ds$$

(Cruickshank, 1949), which gives the profile of a single atom, with a given scattering curve $[f(s)]$, and includes the diffraction ripples which appear when the radiation used imposes an artificial limit to the range of diffraction maxima which are observed. By combining two such profiles one then calculates a table of corrections giving the effect on the separation of two *projected* peaks of various true separations of the atomic peaks. In practice it is more convenient to give the correction as a function of the *projected* separation. In the case of some atoms no projection gave a resolved peak and it is difficult to apply the method to these with any confidence. However, the coordinates obtained at this stage compare very favourably with those obtained by the more usual (F_o-F_c) Fourier synthesis refinement. The r.m.s. deviations $(\overline{\Delta x}, \overline{\Delta y}$ and $\overline{\Delta z})$ between the carbon-atom coordinates obtained at this stage and the final coordinates, obtained after repeated (F_o-F_c) syntheses, are $\overline{\Delta x} = 0{\cdot}028$, $\overline{\Delta y} = 0{\cdot}015$, $\overline{\Delta z} = 0{\cdot}009$ Å. $\overline{\Delta x}$ and $\overline{\Delta y}$ include three rather large deviations due to unresolved atoms in the F_o syntheses, and if these are excluded the values of $\overline{\Delta x}$ and $\overline{\Delta y}$ are 0·009 and 0·012 Å respectively. It would seem therefore that for projections where the atomic peaks are resolved the method of correcting

Table 1. *Final coordinates*

Carbon atoms

	x (Å)	*y* (Å)	*z* (Å)
A	0·696	1·339	0·036
B	0·957	0·280	1·088
C	1·874	0·544	2·155
D	2·540	1·782	2·356
E	3·417	2·067	3·398
F	3·536	1·086	4·419
G	2·876	−0·150	4·321
H	2·053	−0·418	3·235
I	1·366	−1·654	3·146
J	0·505	−1·892	2·078
K	0·337	−0·950	1·085

Hydrogen atoms

	x (Å)	*y* (Å)	*z* (Å)
*A*H1	1·587	1·488	0·703
*A*H2	−0·000	2·126	−0·208
*D*H	2·410	2·528	1·598
*E*H	3·943	2·740	3·460
*F*H	4·178	1·295	5·292
*G*H	3·006	−0·895	5·078
*I*H	1·523	−2·400	3·939
*J*H	−0·023	−2·831	2·048

for overlapping (and series termination) with an atomic profile curve gives very good results. (The carbon coordinates given in Table 1 are the means of the results obtained from the $(F_o - F_c)$ syntheses on three zones, and it is interesting to compare the deviations of the values from two zones with the deviations given above. The r.m.s. deviations of (*a*) x coordinates from $h0l$ and $hk0$ zones, (*b*) y coordinates from $0kl$ and $hk0$ zones and (*c*) z coordinates from $h0l$ and $0kl$ zones are (*a*) 0·012, (*b*) 0·014, (*c*) 0·006 Å.) The values of the reliability index R at this stage were as follows:

$$R(0kl) = 0{\cdot}163,\quad R(h0l) = 0{\cdot}163,\quad R(hk0) = 0{\cdot}173\ .$$

The hydrogen atoms were included in the calculations of structure factors by assuming their positions on the basis of a C–H bond of 1·07 Å and normal bond angles. The temperature factors, obtained by plotting $\log_e \Sigma|F_c| \div \Sigma|F_o|$ against $\sin^2\theta$, were $B = 3{\cdot}42$ Å^2 for the $h0l$ zone and $B = 4{\cdot}28$ Å^2 for the $hk0$ and $0kl$ zones.

Three successive $(F_o - F_c)$ syntheses were now computed on each zone. There was no significant change in the reliability indices between the second and third syntheses. The final atomic coordinates are listed in Table 1.

The structure factors of each zone were calculated with the above coordinates, with McWeeny's scattering curves and with the temperature factors given above. They are listed in Table 2, together with the observed values.

The final reliability indices are

$$R(0kl) = 0{\cdot}121;\ R(h0l) = 0{\cdot}156;\ R(hk0) = 0{\cdot}151\ .$$

Table 2. *Observed and calculated structure factors*

0 k ℓ

k ℓ	Fo	Fc	k ℓ	Fo	Fc	k ℓ	Fo	Fc	k ℓ	Fo	Fc	k ℓ	Fo	Fc	k ℓ	Fo	Fc
0 1	35.3	36.1	1 1	3.6	-4.1	2 5	13.8	-11.3	3 9	<1.1	1.4	5 1	<1.1	5.1	6 7	<0.9	-0.5
0 2	52.0	-56.1	1 2	17.8	16.7	2 6	13.5	-10.3	3,10	2.3	3.5	5 2	16.8	-17.4	6 8	4.1	4.1
0 3	16.4	16.4	1 3	3.4	-4.2	2 7	8.0	-7.1	3,11	<1.0	3.2	5 3	5.9	- 6.0	6 9	1.4	0.6
0 4	2.2	-3.3	1 4	13.7	10.6	2 8	4.5	3.9	3,12	2.3	-3.0	5 4	<1.2	1.8	6,10	<0.9	0.1
0 5	11.4	9.1	1 5	6.5	3.2	2 9	<1.2	-1.3	3,13	2.6	-2.5	5 5	<1.2	-0.8	7 1	<1.0	-1.7
0 6	2.6	-1.5	1 6	14.5	-13.6	2,10	1.6	3.6	4 1	1.3	0.5	5 6	1.6	-1.5	7 2	<0.9	-0.2
0 7	3.1	3.4	1 7	3.7	-2.9	2,11	<1.1	-0.6	4 2	11.6	-11.5	5 7	<1.1	-0.9	7 3	<0.9	-1.4
0 8	3.5	-2.3	1 8	1.8	3.1	2,12	<0.9	0.1	4 3	<1.2	1.5	5 8	10.6	9.8	7 4	2.6	-3.6
0 9	9.3	-7.4	1 9	1.7	2.6	2,13	<0.9	0.4	4 4	5.9	7.8	5 9	4.5	3.3	7 5	<0.9	-1.2
0,10	22.5	20.7	1,10	4.7	-5.4	2,14	<0.8	-1.7	4 5	2.7	4.1	5,10	3.6	-3.6	7 6	2.3	2.9
0,11	15.5	13.2	1,11	4.6	-4.7	3 1	2.3	-2.3	4 6	1.4	1.8	5,11	<1.0	1.1	7 7	2.3	1.2
0,12	3.7	-3.4	1,12	3.8	4.3	3 2	13.7	-14.4	4 7	<1.2	1.0	5,12	<0.9	-1.3	7 8	<0.8	-1.2
0,13	<1.0	0.8	1,13	<1.0	1.8	3 3	<1.2	0.1	4 8	<1.1	-0.4	6 1	<1.1	-3.3	8 1	<0.9	-0.7
0,14	<0.9	0.0	1,14	<0.9	-1.1	3 4	8.8	-8.8	4 9	1.9	-1.8	6 2	9.2	9.7	8 2	<0.9	-0.4
2 0	37.3	-37.3	2 1	13.4	-13.8	3 5	2.3	4.2	4,10	<1.0	1.5	6 3	4.7	6.3	8 3	<0.9	-2.2
4 0	15.6	13.8	2 2	16.0	15.4	3 6	3.1	-1.0	4,11	1.7	1.8	6 4	3.9	-6.6	8 4	<0.8	-1.4
6 0	2.6	-2.4	2 3	2.1	-2.1	3 7	<1.2	-3.0	4,12	1.7	-1.7	6 5	<1.0	-0.1	8 5	<0.8	0.4
8 0	0.8	-1.2	2 4	29.3	-28.6	3 8	<1.2	-1.4	4,13	<0.9	-0.7	6 6	<1.0	-1.9	8 6	<0.8	-1.8

h k 0

h k	Fo	Fc	h k	Fo	Fc	h k	Fo	Fc	h k	Fo	Fc	h k	Fo	Fc	h k	Fo	Fc
1 1	28.1	27.3	2 6	4.5	5.4	4 3	9.0	8.5	5 8	1.2	1.9	7 6	0.9	-0.8	9 6	<0.7	1.1
1 2	3.5	-2.0	2 7	3.4	-2.4	4 4	3.8	-1.9	6 1	2.1	-2.9	7 7	1.0	0.9	10,1	8.3	7.0
1 3	2.7	-4.2	2 8	<0.7	0.4	4 5	1.8	-2.6	6 2	1.8	1.7	8 1	7.5	7.7	10,2	8.8	8.4
1 4	0.8	1.4	3 1	4.9	-4.8	4 6	1.9	-3.4	6 3	1.3	-1.2	8 2	6.0	-4.5	10,3	<0.9	-0.7
1 5	<0.8	-0.1	3 2	18.1	-17.5	4 7	1.8	-1.2	6 4	2.7	-2.9	8 3	<0.8	-0.5	10,4	0.9	-0.6
1 6	1.0	2.8	3 3	1.2	-0.7	4 8	1.2	1.2	6 5	1.1	1.9	8 4	<0.8	-0.4	10,5	<0.8	0.2
1 7	<0.8	-1.6	3 4	1.9	1.8	5 1	1.0	-1.3	6 6	<0.9	0.7	8 5	1.1	-0.3	11,1	<0.9	-0.4
1 8	<0.7	0.0	3 5	<0.9	-0.2	5 2	4.9	4.8	6 7	<0.8	-1.4	8 6	<0.7	0.6	11,2	<0.8	0.3
2 1	41.6	48.7	3 6	8.8	-8.6	5 3	8.4	-7.0	7 1	7.9	-6.3	9 1	4.4	2.6	11,3	<0.7	0.1
2 2	21.6	-20.8	3 7	6.6	5.9	5 4	6.6	6.4	7 2	5.3	3.7	9 2	5.7	4.0	11,4	<0.7	-0.8
2 3	23.4	-21.6	3 8	<0.7	-0.5	5 5	6.4	-6.9	7 3	0.8	1.4	9 3	2.8	2.7	12,1	2.4	-2.9
2 4	8.4	-7.9	4 1	3.3	-1.6	5 6	3.8	-4.8	7 4	<0.9	1.0	9 4	1.3	-1.7	12,2	<0.7	-0.5
2 5	1.2	-4.7	4 2	9.2	9.7	5 7	<1.0	-1.2	7 5	2.2	2.6	9 5	<0.8	0.1			

h 0 ℓ

h ℓ	Fo	Fc	h ℓ	Fo	Fc	h ℓ	Fo	Fc	h ℓ	Fo	Fc	h ℓ	Fo	Fc	h ℓ	Fo	Fc
2 0	20.0	-24.1	$2\ \underline{9}$	18.5	15.2	$4\ \underline{6}$	5.7	-3.8	$6\ \underline{3}$	5.7	6.8	$8\ \underline{2}$	4.8	-6.5	$10,\underline{2}$	<1.1	1.9
4 0	12.7	-9.6	$2\ \bar{9}$	3.3	4.4	$4\ \bar{6}$	16.5	15.4	$6\ \bar{3}$	1.8	2.2	$8\ \bar{2}$	<1.3	1.5	$10,\bar{2}$	3.1	5.2
6 0	3.8	-4.0	$2,\underline{10}$	2.0	3.3	$4\ \underline{7}$	4.5	-2.7	$6\ \underline{4}$	5.3	-3.6	$8\ \underline{3}$	2.7	2.7	$10,\underline{3}$	<1.1	-0.4
8 0	1.4	-1.7	$2,\overline{10}$	6.0	-5.4	$4\ \bar{7}$	18.8	-16.6	$6\ \bar{4}$	2.9	-4.6	$8\ \bar{3}$	5.7	4.7	$10,\bar{3}$	1.2	0.3
10,0	2.3	-0.9	$2,\underline{11}$	6.4	7.8	$4\ \underline{8}$	2.3	2.2	$6\ \underline{5}$	3.3	-2.7	$8\ \underline{4}$	4.1	-5.4	$10,\underline{4}$	7.6	-9.3
12,0	4.1	-3.3	$2,\overline{11}$	<1.1	0.6	$4\ \bar{8}$	16.7	-13.9	$6\ \bar{5}$	6.9	-9.5	$8\ \bar{4}$	6.9	-5.3	$10,\bar{4}$	1.3	0.7
$2\ \underline{1}$	22.8	23.9	$2,\underline{12}$	<1.1	-1.5	$4\ \underline{9}$	6.6	7.2	$6\ \underline{6}$	3.3	-0.9	$8\ \underline{5}$	8.0	-8.3	$10,\underline{5}$	<1.0	0.1
$2\ \bar{1}$	62.1	63.9	$2,\overline{12}$	21.2	23.1	$4\ \bar{9}$	<1.2	2.7	$6\ \bar{6}$	5.2	-5.7	$8\ \bar{5}$	11.0	-9.3	$10,\bar{5}$	3.2	3.6
$2\ \underline{2}$	11.9	-13.5	$2,\underline{13}$	<1.1	-2.4	$4,\underline{10}$	<1.1	-1.4	$6\ \underline{7}$	5.5	-4.6	$8\ \underline{6}$	13.0	-12.7	$10,\underline{6}$	3.7	4.3
$2\ \bar{2}$	121.9	-118.1	$2,\overline{13}$	6.7	5.7	$4,\overline{10}$	1.9	-2.6	$6\ \bar{7}$	5.7	7.8	$8\ \bar{6}$	<1.1	-2.3	$10,\bar{6}$	5.5	-6.6
$2\ \underline{3}$	12.6	7.3	$2,\underline{14}$	<1.0	-0.2	$4,\underline{11}$	2.5	-3.4	$6\ \underline{8}$	6.5	-5.5	$8\ \underline{7}$	2.5	2.8	$10,\underline{7}$	<1.2	-0.8
$2\ \bar{3}$	18.0	-15.4	$2,\overline{14}$	4.4	-6.3	$4,\overline{11}$	1.9	2.8	$6\ \bar{8}$	2.6	4.0	$8\ \bar{7}$	<1.1	-0.9	$10,\bar{7}$	4.9	-5.0
$2\ \underline{4}$	20.4	-15.4	$4\ \underline{1}$	3.7	1.5	$4,\underline{12}$	<1.0	0.4	$6\ \underline{9}$	<1.2	0.7	$8\ \underline{8}$	2.7	2.7	$10,\underline{8}$	2.7	2.1
$2\ \bar{4}$	4.4	-0.3	$4\ \bar{1}$	23.3	23.2	$4,\overline{12}$	<1.0	-0.9	$6\ \bar{9}$	11.3	-15.6	$8\ \bar{8}$	<1.1	-2.5	$10,\bar{8}$	<1.0	2.0
$2\ \underline{5}$	25.2	-20.4	$4\ \underline{2}$	18.4	-15.3	$4,\underline{13}$	9.4	-6.9	$6,\underline{10}$	<1.1	0.3	$8\ \underline{9}$	1.4	-2.3	$12,\underline{1}$	<1.0	1.1
$2\ \bar{5}$	1.3	1.1	$4\ \bar{2}$	6.3	3.5	$4,\overline{13}$	<0.9	0.2	$6,\overline{10}$	5.8	-7.2	$8\ \bar{9}$	<1.0	0.3	$12,\bar{1}$	3.0	3.0
$2\ \underline{6}$	13.3	12.7	$4\ \underline{3}$	54.3	-52.0	$4,\underline{14}$			$6,\underline{11}$	5.9	-5.0	$8,\underline{10}$	<1.0	0.3	$12,\underline{2}$	<1.0	-0.2
$2\ \bar{6}$	16.6	-8.9	$4\ \bar{3}$	<1.4	0.3	$4,\overline{14}$	2.7	5.3	$6,\overline{11}$	1.5	1.4	$8,\overline{10}$	<1.0	-0.3	$12,\bar{2}$	7.0	7.2
$2\ \underline{7}$	3.0	-1.0	$4\ \underline{4}$	2.7	5.6	$6\ \underline{1}$	27.8	-29.1	$6,\underline{12}$	5.4	-4.4	$8,\underline{11}$	<0.9	-2.3	$12,\underline{3}$	<1.0	-1.2
$2\ \bar{7}$	2.1	5.2	$4\ \bar{4}$	<1.3	1.3	$6\ \bar{1}$	3.1	1.1	$6,\overline{12}$	<0.9	-1.1	$8,\overline{11}$	2.1	-4.8	$12,\bar{3}$	1.4	1.6
$2\ \underline{8}$	11.3	9.0	$4\ \underline{5}$	16.1	19.4	$6\ 2$	9.4	-11.3	$8\ \underline{1}$	4.6	-6.9	$10,\underline{1}$	<1.1	-0.8			
$2\ \bar{8}$	4.1	-1.9	$4\ \bar{5}$	4.2	4.6	$6\ \bar{2}$	4.5	-2.7	$8\ \bar{1}$	2.8	-5.1	$10,\bar{1}$	<1.1	-2.1			

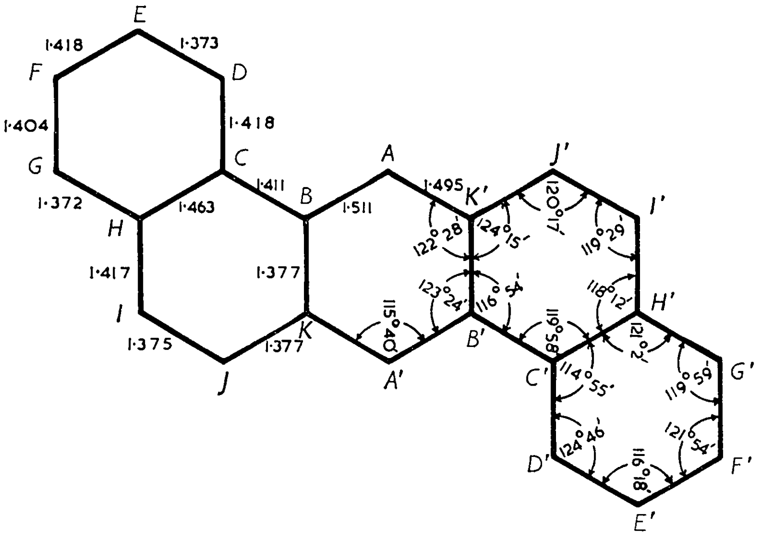

Fig. 5. Bond lengths (in Ångström units) and bond angles.

The standard deviations of the coordinates were estimated by means of Cruickshank's (1949) formulae and are as follows:

$$\sigma(x) = 0{\cdot}0129 \text{ Å}, \quad \sigma(y) = 0{\cdot}0133 \text{ Å}, \quad \sigma(z) = 0{\cdot}0131 \text{ Å} .$$

Discussion of the structure

The mean plane of the molecule was calculated by the least-squares method and its equation is

$$0{\cdot}7678x' - 0{\cdot}3831y - 0{\cdot}5314z' = 0 .$$

(This is with reference to rectangular axes where x' is parallel to a, y is parallel to b, and z' is perpendicular to the plane (001).) The deviations of each carbon atom from the mean plane are as follows:

$A = 0{\cdot}002$, $B = 0{\cdot}045$, $C = 0{\cdot}081$, $D = 0{\cdot}010$,
$E = 0{\cdot}019$, $F = -0{\cdot}059$, $G = -0{\cdot}039$, $H = 0{\cdot}010$,
$I = 0{\cdot}004$, $J = 0{\cdot}004$, $K = 0{\cdot}044$ Å,
(r.m.s. deviation = 0·039 Å).

There is no doubt, therefore, that the molecular is essentially planar. There is no indication of the bending such as exists in 9:10-dihydroanthracene.

The bond lengths and bond angles are given in Table 3 and in Fig. 5. For the aromatic rings the mean bond length is 1·401 Å and the mean angle is 120° 0'.

Table 3. *Bond lengths and bond angles*

	Length (Å)		Length (Å)		Angle		Angle
AB	1·511	*HI*	1·417	*BAK'*	115° 40'	*EFG*	121° 54'
BC	1·411	*IJ*	1·375	*ABK*	123° 42'	*FGH*	119° 52'
CD	1·418	*JK*	1·377	*KBC*	116° 54'	*GHI*	119° 59'
DE	1·373	*AK'*	1·495	*BCH*	119° 58'	*GHC*	121° 2'
EF	1·418	*BK*	1·377	*HCD*	114° 55'	*HIJ*	119° 29'
FG	1·404	*CH*	1·463	*CHI*	118° 21'	*IJK*	120° 17'
GH	1·372			*CDE*	124° 46'	*KJB*	124° 15'
				DEF	116° 18'	*BKA'*	122° 28'

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