195. *The Crystal Structure of the Monoclinic Modification of* 1 : 2-5 : 6-*Dibenzanthracene. A Quantitative X-Ray Investigation.*

By J. MONTEATH ROBERTSON and J. G. WHITE.

The crystal and molecular structure of the monoclinic modification of 1 : 2-5 : 6-dibenzanthracene has been determined, and the co-ordinates of all the carbon atoms are given. The space group is $P2_1$, and the molecule does not display any crystallographic symmetry. The final results, however, indicate a planar structure with the molecular symmetry required by the chemical formula. All the bond lengths have been evaluated and agree well with those obtained from a study of the orthorhombic modification, already described. When the most reliable bond-length measurements are selected from these two independent crystal-structure determinations, excellent agreement is obtained with the theoretical calculations of Vroelant and Daudel.

Two distinct crystalline modifications of 1 : 2-5 : 6-dibenzanthracene are known. The orthorhombic form, first described by Krishnan and Banerjee [1] and by Iball,[2] has been analysed in detail by the present authors.[3] The unit cell contains four centro-symmetric molecules in the space group Pcab (D_{2h}^{15}), and in the best projection of the structure 18 of the 22 carbon atoms in the molecule were separately resolved, yielding measurements of 18 of the 26 carbon–carbon bond lengths.

Only preliminary data have so far been recorded [4] for the second, monoclinic, form. We have now completed the analysis of this modification, and the results are of interest in completing the bond-length data for this hydrocarbon and in providing one of the few examples of polymorphous organic crystal structures where reasonably accurate values of the atomic co-ordinates are known for both modifications. The monoclinic form is of low symmetry, with two crystallographically asymmetric molecules in the space group $P2_1$ (C_2^2). With 22 carbon atoms in the asymmetric crystal unit the analysis is thus considerably more complex than for the orthorhombic form. But the final results yield a clear projection of the molecule, with 18 of the 22 carbon atoms resolved (Fig. 1). By assuming a centre of symmetry in the molecule (as demanded by the chemical structure but not required crystallographically) co-ordinates can be assigned to the unresolved atoms

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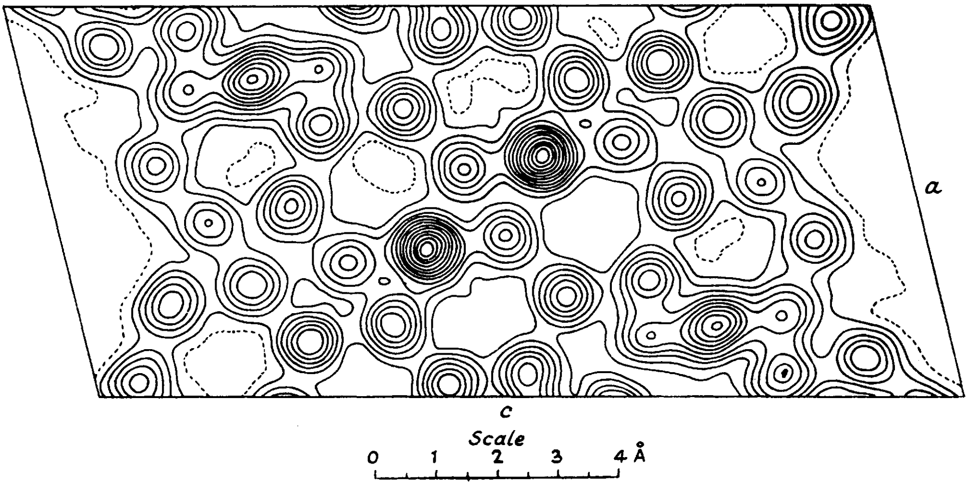
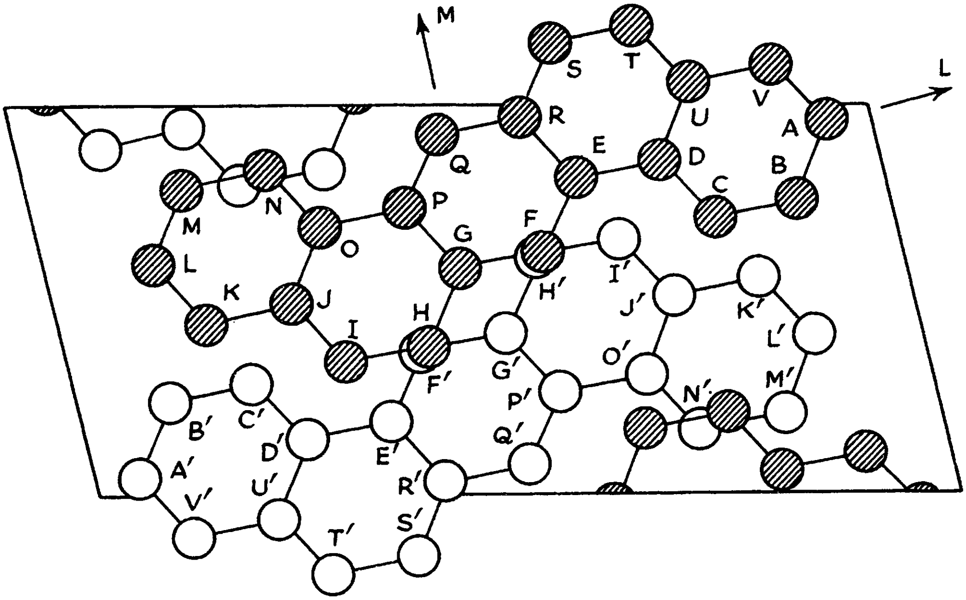
[1] Krishnan and S. Banerjee, *Z. Krist.*, 1935, **91**, 170.
[2] Iball, *Nature*, 1936, **137**, 361.
[3] J. M. Robertson and White, *J.*, 1947, 1001.
[4] Iball and J. M. Robertson, *Nature*, 1933, **132**, 750.

and all the bond lengths ascertained. The information finally obtained is thus more complete than that derived from the orthorhombic modification, and is discussed below. As the present work employs only two-dimensional Fourier methods the accuracy is not particularly high and the probable errors in bond length are about ±0·02 Å. The main features of the bond-length variations, however, are found to agree well with those obtained from the orthorhombic modification. It seems likely that more accurate results will only be possible by the use of three-dimensional methods, and the present analysis should provide the necessary first approximation for any such further refinement.

Fig. 1. *Projection along the* b *axis on* (010). *The molecules are inclined at about* 22° *to the projection plane. Each contour line represents a density increment of one electron per* Å^2, *the one-electron line being broken.*





Crystal Data.—1 : 2-5 : 6-Dibenzanthracene, $C_{22}H_{14}$; *M*, 278·3; m. p. 267·5°; *d*, calc. 1·288, found 1·282; monoclinic, *a* = 6·59, *b* = 7·84, *c* = 14·17 Å, β = 103·5°. Absent spectra, (0*k*0) when *k* is odd. Space group, $P2_1$ (C_2^2) or $P2_1/m$ (C_{2h}^2). $P2_1$ is indicated by this analysis. Two molecules per unit cell. No molecular symmetry required. Volume of the unit cell, 712 Å^3. Absorption coefficient for $\lambda = 1{\cdot}54$ Å, $\mu = 6{\cdot}74$ cm.$^{-1}$. Total number of electrons per unit cell = F(000) = 292.

The crystals were obtained from alcohol in the form of thin irregular plates, with only (001) prominently developed. The maximum thickness obtained (along *c*) was only about 0·1 mm., but it was possible to cut small needle-shaped specimens suitable for *X*-ray rotation photographs about the *a* and the *b* axis. Fairly complete intensity data were therefore collected for the (0*kl*) and (*h*0*l*) zones.

Structure Analysis.—Packing considerations show that the space group of higher symmetry, $P2_1/m$, is most improbable unless the molecules lie entirely in the (010) plane. However, evidence from magnetic-susceptibility measurements and that from *X*-ray intensities both show that the molecular planes are inclined at a small angle (about 20—25°) to the (010) plane. Space group $P2_1/m$ therefore appears to be excluded, and in what follows we assume the lower symmetry of $P2_1$.

The most outstanding reflection observed is (020) with F value of 159 (possible maximum about 200 at this angle). The situation is evidently similar to that observed in the orthorhombic modification, where the (200) reflection had a correspondingly high intensity. It can be safely assumed that the molecular plane is only inclined at a small angle to (010), and in particular that the long axis of the molecule (*L* in Fig. 1) must lie almost entirely in (010). A measure of the maximum degree of tilt of the other molecular axis (*M*) is obtained from the magnetic measurements due to Krishnan and Banerjee [5] who deduce an angle of about 25° between the molecular plane and (010).

A survey of the higher-order (*h*0*l*) reflections now shows that (00,13), $(10\bar{7})$, (209), (308), (302), $(30\bar{5})$, $(30\bar{1}\bar{1})$, and $(60\bar{3})$ are all strong. In this projection, along the two-fold axis, the structure has an effective centre of symmetry, and by studying the traces of these planes drawn in the projection, as has been described in detail in the analysis of the coronene structure,[6] positions of the molecules can be found which account for these enhancements. The weakness of the large-spacing reflections (100) and $(10\bar{1})$ also provides evidence concerning the overall positions of the two molecules and enable us to locate their centres at approximately $x = 1{\cdot}8$ Å, $z = 0{\cdot}5$ Å from the two-fold axis.

Trial calculations of the structure factors on this basis immediately yielded a considerable measure of agreement with the observed values. The parameters were then refined by a number of successive Fourier syntheses of the (*h*0*l*) structure factors. The final electron-density projection obtained is shown in Fig. 1, and the F values and phase constants of the terms included in this synthesis are given in Table 5.

By averaging certain distances as described more fully below (p. 929) the orientation of the molecule can be calculated on the assumption that the molecular axes *L* and *M* (Figs. 1 and 2) are at right angles and that the molecule is planar. The results are given in Table 1, where χ, ψ, and ω are respectively the angles which the molecular axes *L* and *M*, and their perpendicular *N* make with the *a*, *b*, and *c′* crystal axes (*c′* is taken perpendicular to *a* and *b*).

TABLE 1. *Orientation of the molecule in the crystal.*

$\chi_L = 91{\cdot}1°$, $\cos\chi_L = -0{\cdot}0331$; $\chi_M = 22{\cdot}4°$, $\cos\chi_M = 0{\cdot}9245$;
$\psi_L = 91{\cdot}5°$, $\cos\psi_L = -0{\cdot}0256$; $\psi_M = 67{\cdot}7°$, $\cos\psi_M = 0{\cdot}3795$;
$\omega_L = 2{\cdot}4°$, $\cos\omega_L = 0{\cdot}9991$; $\omega_M = 87{\cdot}7°$, $\cos\omega_M = 0{\cdot}0404$;

$\chi_N = 112{\cdot}3°$, $\cos{}_N\chi = -0{\cdot}3797$.
$\psi_N = 22{\cdot}3°$, $\cos\psi_N = 0{\cdot}9247$.
$\omega_N = 89{\cdot}2°$, $\cos\omega_N = 0{\cdot}0142$.

In the final electron-density map it will be noted that 18 out of the 22 independent atoms are resolved, although some are rather distorted by proximity to atoms of adjoining molecules. Co-ordinates were next assigned to the resolved atoms on the basis of this

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[5] Krishnan and S. Banerjee, *Z. Krist.*, 1935, **91**, 173.
[6] J. M. Robertson and White, *J.*, 1945, 607.

projection and of subsidiary difference syntheses, with allowance for overlap and series-termination effects. These co-ordinates are collected in Table 3 under $X(b)$ and $Z(b)$. Assuming that the molecule is strictly centrosymmetrical we can now obtain an accurate value for the co-ordinates of the molecular centre by taking the mean value of the x and z co-ordinates of the 7 pairs of atoms, A and L, B and M, etc. The co-ordinates of the 18 resolved atoms with respect to the molecular axes L and M can now be readily calculated by taking account of the orientation (Table 1) and the position of the molecular centre. These co-ordinates (in Å) are given in Table 3 under $L(b)$ and $M(b)$, and these figures provide the bond lengths directly.

We may now compare bond lengths between crystallographically independent atoms related by the assumed molecular centre of symmetry. The results are given in Table 2.

TABLE 2. *Bond lengths (in Å).*

AB = 1·44 LM = 1·39 Assumed mean value = 1·41
AV = 1·40 LK = 1·39 ,, ,, = 1·40
UV = 1·39 KJ = 1·40 ,, ,, = 1·40
DE = 1·40 OP = 1·40 ,, ,, = 1·40
UD = 1·45 OJ = 1·45 ,, ,, = 1·45
PG = 1·43 RE = 1·45 ,, ,, = 1·44

FIG. 2. *Dimensions of the molecule of* 1 : 2-5 : 6-*dibenzanthracene.*

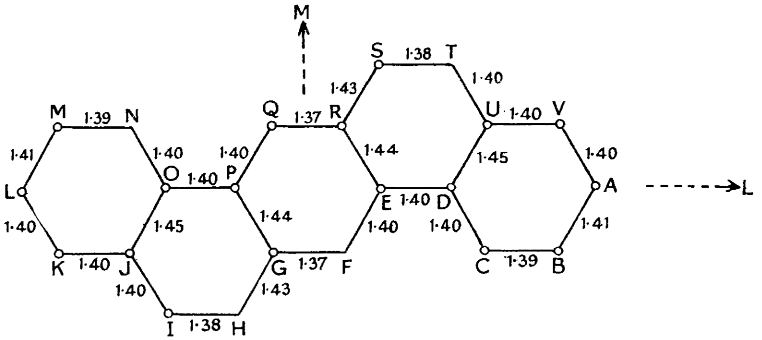

TABLE 3.

Co-ordinates. Origin on two-fold axis. x, y, z are expressed as fractions of the axial lengths, X, Y, Z, L, and M in Å. Space group, $P2_1$. General positions, x, y, z; $\bar{x}, \frac{1}{2} + y, \bar{z}$.

Atom	x	y	z	$X(a)$	$X(b)$	$Y(a)$	$Z(a)$	$Z(b)$	$L(a)$	$L(b)$	$M(a)$	$M(b)$
A	0·457	−0·017	0·447	3·017	3·030	−0·131	6·342	6·365	5·651	5·671	0·035	0·046
B	0·262	−0·073	0·392	1·729	1·712	−0·576	5·563	5·570	4·941	4·946	−1·186	−1·200
C	0·210	−0·072	0·292	1·385	1·385	−0·565	4·139	4·139	3·557	3·557	−1·249	−1·249
D	0·354	−0·012	0·242	2·332	2·340	−0·095	3·435	3·442	2·825	2·830	−0·062	−0·066
E	0·311	−0·007	0·141	2·054	2·040	−0·059	1·999	2·002	1·426	1·428	−0·061	−0·075
F	0·123	−0·061	0·081	0·813	—	−0·478	1·146	—	0·645	—	−1·216	—
G	0·083	−0·056	−0·018	0·548	0·554	−0·436	−0·259	−0·248	−0·725	−0·714	−1·197	−1·193
H	−0·114	−0·112	−0·074	−0·749	—	−0·883	−1·050	—	−1·444	—	−2·426	—
I	−0·152	−0·107	−0·174	−1·007	−1·007	−0·838	−2·465	−2·465	−2·823	−2·823	−2·397	−2·397
J	−0·006	−0·047	−0·223	−0·040	−0·038	−0·365	−3·158	−3·162	−3·544	−3·549	−1·203	−1·200
K	−0·055	−0·044	−0·324	−0·364	−0·360	−0·341	−4·593	−4·592	−4·939	−4·949	−1·237	−1·244
L	0·093	0·017	−0·372	0·615	0·630	0·131	−5·270	−5·254	−5·651	−5·632	−0·035	−0·024
M	0·289	0·073	−0·317	1·903	1·890	0·576	−4·493	−4·490	−4·941	−4·935	1·186	1·172
N	0·341	0·072	−0·217	2·247	—	0·565	−3·069	—	−3·557	—	1·249	—
O	0·197	0·012	−0·167	1·300	1·286	0·095	−2·365	−2·360	−2·825	−2·819	0·062	0·057
P	0·239	0·007	−0·066	1·578	1·570	0·059	−0·929	−0·932	−1·426	−1·423	0·061	0·048
Q	0·427	0·061	−0·005	2·819	2·819	0·478	−0·076	−0·076	−0·645	−0·645	1·216	1·216
R	0·468	0·056	0·094	3·084	3·070	0·436	1·329	1·342	0·725	0·735	1·197	1·201
S	0·664	0·112	0·149	4·381	4·381	0·883	2·120	2·120	1·444	1·444	2·426	2·426
T	0·704	0·107	0·249	4·639	—	0·838	3·535	—	2·823	—	2·397	—
U	0·557	0·047	0·298	3·672	3·674	0·365	4·228	4·222	3·544	3·538	1·203	1·205
V	0·606	0·044	0·399	3·996	3·984	0·341	5·663	5·652	4·939	4·929	1·237	1·230
Molecular centre,				1·816	—	0	0·535	—	—	—	—	—

These results appear to justify averaging the molecular co-ordinates $L(b)$ and $M(b)$ of Table 3 in pairs where possible (A and L, B and M, etc.), with the advantage that we can now derive all the bond distances in the molecule. The averaged molecular co-ordinates are given under $L(a)$ and $M(a)$ in Table 3, and the crystal co-ordinates obtained from them by combination with the orientation angles are given under $X(a)$, $Y(a)$, and $Z(a)$. The bond lengths finally derived from these co-ordinates are shown in Fig. 2, where the ringed atoms are those separately resolved in Fig. 1.

In Table 4 these bond-length measurements are summarized and compared with those derived from the orthorhombic modification. The results are seen to be in reasonably good agreement. The position of the atom K was very uncertain in the orthorhombic structure, and here the monoclinic results are more reliable, while for the bond lengths EF and FG the orthorhombic results are probably better. The Table gives also the best values derived from a consideration of the merits of both crystal structures.

TABLE 4. *Comparison of bond-length measurements (in Å) in monoclinic and orthorhombic dibenzanthracene.*

Bond	Mono-clinic	Ortho-rhombic	Best value	Calc. length [7]	Δ	Bond	Mono-clinic	Ortho-rhombic	Best value	Calc. length [7]	Δ
AB	1·41	1·41	1·41	1·40	0·01	*HI*	1·38	—	1·38	1·38	0·00
BC	1·40	—	1·40	1·39	0·01	*IJ*	1·40	—	1·40	1·42	0·02
CD	1·40	—	1·40	1·41	0·01	*JK*	1·40	1·44 ?	1·40	1·42	0·02
DE	1·40	1·41	1·41	1·44	0·03	*KL*	1·40	1·44 ?	1·40	1·39	0·01
EF	1·40 ?	1·38	1·39	1·41	0·02	*DU*	1·45	1·42	1·44	1·44	0·00
FG	1·37 ?	1·40	1·40	1·41	0·01	*RE*	1·44	1·44	1·44	1·44	0·00
GH	1·43	1·45	1·44	1·42	0·02						

The existence of exceptionally long bonds in the central ring at RE, and at GH and DU appears to be definitely confirmed. It is interesting to note that the distortion of the molecule can be detected quite readily on the electron density map by drawing a straight line through the atoms A, D, and E. This line is parallel to, but does not coincide with, the line through L, O, and P. The situation is exactly similar in the orthorhombic structure, when a line through A, D, and E did not pass through the origin.

In our previous paper [3] we discussed the expected values of the bond lengths from a simple consideration of the double-bond character of each link as assessed from the contributing Kekulé structures. Since that time more exact theoretical calculations of these bond lengths have been made by Vroelant and Daudel [7] and their results are given as " Calc. length " in Table 4. A very good overall agreement with our measurements is reached, the average discrepancy (Δ) being only slightly over 0·01 Å, with a maximum discrepancy of 0·03 Å for the bond DE.

From a consideration of our experimental data, and the agreements obtained between calculated and observed F values, we expect probable errors of about ±0·02 Å for our original directly measured bond lengths. The process of averaging the molecular co-ordinates, and in particular the fact that our final values are now based on two entirely independent crystal structures, will considerably increase the significance of these final results. The agreements obtained with the theoretical calculations are therefore encouraging.

Intermolecular distances have not been calculated in detail, but the closest contacts between atoms of adjacent molecules appear to be of the usual order of 3·5 and 3·6 Å, except between atom S on the standard molecule and O on the nearest rotated molecule, where the unusually small distance of 3·3 Å is observed.

EXPERIMENTAL

Small specimens were cut from the rather irregular plates obtained from alcohol and mounted for rotation, oscillation, and moving-film photographs about the principal crystallographic axes. For the *a* axis rotations the specimen weighed 0·108 mg. and had a cross section of

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[7] Vroelant and R. Daudel, *Bull. Soc. chim. France*, 1949, **16**, 36, 217; *Compt. rend.*, 1949, **228**, 399; Buu-Hoï, R. Daudel, and Vroelant, *Bull. Soc. chim. France.*, 1949, **16**, 211.

TABLE 5. *Measured and calculated values of the structure factor.*

hkl	$F_{meas.}$	$F_{calc.}$	$\alpha^{\circ}_{calc.}$
000	—	292	0
100	9	10	180
200	12	12	180
300	2	7	0
400	<2	3	180
500	4	6	180
600	<2	1	180
700	<2	1	0
800	<1	0	—
020	159	154	0
040	<4	16	0
060	12	8	180
001	41	41	0
002	34	34	180
003	15	18	0
004	10	8	180
005	8	8	0
006	11	7	180
007	2	3	0
008	4	4	180
009	<2	2	180
00,10	4	3	0
00,11	<2	1	180
00,12	6	6	0
00,13	13	14	0
00,14	2	1	0
00,15	<2	1	180
10,10	<2	2	0
109	3	0	—
108	4	4	180
107	7	11	180
106	20	20	0
105	<1	0	—
104	12	9	180
103	2	1	180
102	8	5	180
101	20	22	0
10$\bar{1}$	4	4	0
10$\bar{2}$	7	1	0
10$\bar{3}$	23	23	0
10$\bar{4}$	4	5	180
10$\bar{5}$	4	5	0
10$\bar{6}$	4	3	180
10$\bar{7}$	34	34	180
10$\bar{8}$	9	10	180
10$\bar{9}$	7	10	180
10,$\bar{1}\bar{0}$	6	6	180
10,$\bar{1}\bar{1}$	2	2	0
10,$\bar{1}\bar{2}$	2	3	0
10,$\bar{1}\bar{3}$	<2	0	—
20,16	1	1	180
20,15	<1	2	180
20,14	<2	1	180
20,13	<2	1	180
20,12	4	3	0
20,11	3	4	0
20,10	8	8	0
209	24	24	0
208	2	1	0
207	4	7	180
206	<2	1	0
205	<1	0	—
204	3	2	180
203	14	17	0
202	17	18	0
201	29	32	180
20$\bar{1}$	23	25	0
20$\bar{2}$	28	32	0
20$\bar{3}$	9	11	0
20$\bar{4}$	29	28	0
20$\bar{5}$	5	3	0
20$\bar{6}$	2	4	180
20$\bar{7}$	<1	1	180
20$\bar{8}$	<2	1	0
20$\bar{9}$	2	0	—
20,$\bar{1}\bar{0}$	2	4	0
20,$\bar{1}\bar{1}$	10	5	0
20,$\bar{1}\bar{2}$	5	6	180
20,$\bar{1}\bar{3}$	<2	0	—
30,11	<2	0	—
30,10	4	2	180
309	9	9	0
308	26	21	0
307	3	5	180
306	3	3	0
305	2	2	180
304	2	1	180
303	7	4	180
302	49	48	180
301	15	13	180
30$\bar{1}$	2	1	0
30$\bar{2}$	1	1	180
30$\bar{3}$	4	3	180
30$\bar{4}$	19	21	0
30$\bar{5}$	30	27	0
30$\bar{6}$	7	9	180
30$\bar{7}$	2	5	0
30$\bar{8}$	2	1	180
30$\bar{9}$	2	2	0
30,$\bar{1}\bar{0}$	9	9	180
30,$\bar{1}\bar{1}$	35	33	180
30,$\bar{1}\bar{2}$	5	3	180
30,$\bar{1}\bar{3}$	3	4	0
30,$\bar{1}\bar{4}$	<2	1	180
40,10	<2	0	—
409	2	2	0
408	5	4	180
407	<2	1	0
406	<2	0	—
405	2	1	180
404	<2	0	—
403	<2	2	180
402	3	4	180
401	7	4	180
40$\bar{1}$	8	9	180
40$\bar{2}$	4	1	180
40$\bar{3}$	6	5	180
40$\bar{4}$	2	5	0
40$\bar{5}$	15	14	180
40$\bar{6}$	3	2	180
40$\bar{7}$	<2	2	0
40$\bar{8}$	<2	0	—
40$\bar{9}$	<2	0	—
40,$\bar{1}\bar{0}$	2	1	0
40,$\bar{1}\bar{1}$	4	4	180
40,$\bar{1}\bar{2}$	7	7	180
40,$\bar{1}\bar{3}$	<2	0	—
40,$\bar{1}\bar{4}$	3	4	180
40,$\bar{1}\bar{5}$	<2	0	—
507	<2	2	0
506	2	2	0
505	5	5	0
504	6	8	0
503	2	2	180
502	<2	2	0
501	3	2	180
50$\bar{1}$	6	3	180
50$\bar{2}$	7	8	180
50$\bar{3}$	3	0	—
50$\bar{4}$	3	2	180
50$\bar{5}$	2	2	0
50$\bar{6}$	<2	1	0
50$\bar{7}$	2	2	0
50$\bar{8}$	4	4	180
50$\bar{9}$	2	2	180
50,$\bar{1}\bar{0}$	4	5	0
50,$\bar{1}\bar{1}$	<2	1	0
605	<2	0	—
604	2	2	180
603	<2	0	—
602	<2	0	—
601	<2	1	0
60$\bar{1}$	2	3	0
60$\bar{2}$	19	16	180
60$\bar{3}$	28	24	180
60$\bar{4}$	8	6	0
60$\bar{5}$	2	0	—
60$\bar{6}$	<2	1	0
60$\bar{7}$	<2	1	0
60$\bar{8}$	2	2	180
60$\bar{9}$	4	4	0
60,$\bar{1}\bar{0}$	<2	1	0
60,$\bar{1}\bar{1}$	<2	0	—
60,$\bar{1}\bar{2}$	<2	0	—
60,$\bar{1}\bar{3}$	<2	1	180
60,$\bar{1}\bar{4}$	<1	0	—
60,$\bar{1}\bar{5}$	2	3	180
703	<1	2	180
702	2	2	0
701	<2	1	180
70$\bar{1}$	<2	0	—
70$\bar{2}$	<2	1	180
70$\bar{3}$	3	2	0
70$\bar{4}$	<2	0	—
70$\bar{5}$	<2	0	—
70$\bar{6}$	<2	1	180
70$\bar{7}$	<2	1	0
70$\bar{8}$	3	1	180
70$\bar{9}$	3	3	0
70,$\bar{1}\bar{0}$	<1	2	0
801	<1	0	—
80$\bar{1}$	<1	0	—
80$\bar{2}$	<1	2	0
80$\bar{3}$	<1	0	—
80$\bar{4}$	2	2	180
80$\bar{5}$	2	2	180
80$\bar{6}$	2	2	180
80$\bar{7}$	<1	2	180
011	12	17	152
012	29	25	215
013	14	14	98
014	9	10	288
015	16	15	92
016	49	40	271
017	42	34	269
018	14	12	101
019	<4	3	134
021	22	16	347
022	23	22	231
023	12	15	353
024	5	7	143
025	7	6	9
026	13	6	137
027	4	8	72
028	7	10	103
029	5	6	84
02,10	<3	3	341
02,13	8	9	1
031	<5	9	177
032	19	19	182
033	7	8	93
034	<4	6	286
035	7	9	88
036	12	15	272

TABLE 5. (*Continued.*)

hkl	$F_{meas.}$	$F_{calc.}$	$\alpha^{\circ}_{calc.}$
037	5	8	265
038	<3	2	172
043	<4	4	23
044	7	4	211
051	<4	5	347
052	10	5	32
053	5	3	307
054	9	5	239
055	<4	3	86
05,10	8	6	133
061	<3	3	158
062	9	4	55
063	5	6	162
064	12	6	235
065	<3	1	19
069	7	3	249
071	<4	3	356
072	12	6	4
073	<4	6	287
074	10	5	233

0·15 × 0·56 mm. Other specimens employed were of similar size. Cu-$K\alpha$ radiation was used in all the photographic work, and approximate absorption corrections were calculated for a few of the stronger reflections only. The F values were derived by the usual formulæ, and the absolute scale was determined approximately by comparisons made on the two-crystal moving-film spectrometer[8] with previously measured standards. Intensity measurements were made on an integrating photometer, with visual estimations for the weaker spots. Although every care was taken with the measurements, the results are not expected to be particularly accurate owing to the rather thin and badly shaped specimens.

The Fourier calculations were carried out with three-figure strips, the *c* axis intervals being 60ths (0·236 Å), and the *a* axis interval 30ths (0·220 Å). For calculation of the orientation of the molecule, a mean hexagonal radius of 1·41 Å was chosen. The mean measured length of the lines *BV*, *CU*, *ES*, *GQ*, *IO*, and *KM* (see Fig. 1) is found to be 2·258 ± 0·03 Å. Hence

$$\psi_M = \sin^{-1}(2{\cdot}258/2{\cdot}44) = 67{\cdot}7^{\circ}$$

The mean value of the angles between the lines *VURQM*, *ADEPOL*, *BCGJK*, and the *a* axis gives

$$\eta_L = 91{\cdot}9^{\circ} \pm 0{\cdot}3^{\circ}$$

The mean value of the angles between *BV*, *CU*, *ES*, *GQ*, *IO*, *KM*, and the *a* axis gives

$$\eta_M = 2{\cdot}5^{\circ} \pm 1{\cdot}0^{\circ}$$

From these measurements, and the assumption of a planar molecule with the axes *L* and *M* at right angles, the orientation given in Table 1 was calculated, the nine relations given in the coronene analysis[6] being used.

From the final co-ordinates given in Table 3 the structure factors and phase constants were calculated for the two principal zones (*h*0*l*) and (0*kl*). These results are given in Table 5 under $F_{calc.}$ and $\alpha^{\circ}_{calc.}$ In these calculations an empirical scattering curve with the following *f* values was used :

$\sin\theta$ ($\lambda = 1{\cdot}54$)	0·1	0·2	0·3	0·4	0·5	0·6	0·7	0·8	0·9
f_c (max. = 100)	90·0	74·0	56·6	39·5	24·6	16·0	10·8	7·1	4·6

These values include an appropriate mean temperature factor, although there is some evidence that better agreements might be reached if different temperature factors were used for the two zones examined. The mean discrepancies between observed and calculated structure factors, expressed in the usual way, are 14·8% for the (*h*0*l*) zone and 21% for the (0*kl*) zone.

CHEMISTRY DEPARTMENT, UNIVERSITY OF GLASGOW.
FRICK LABORATORY, PRINCETON UNIVERSITY.

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[8] J. M. Robertson, *Phil. Mag.*, 1934, **18**, 729.