282. *The Crystal Structure of Hexamethylbenzene and the Length of the Methyl Group Bond to Aromatic Carbon Atoms.**

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The crystal structure of hexamethylbenzene has been re-investigated with the aid of the double Fourier series method of interpreting the intensity data. The projection along the *c* axis leads to an electron-density contour diagram in which two of the methyl carbon atoms are entirely resolved. The distances to the centre of the molecule are 2·92 A, which, with measurements on the ring, lead to a ring size of 1·39 A and methyl group bond lengths of 1·53 A. The lower values (1·47—1·49 A) previously reported for durene and dibenzyl may be less reliable because of the less favourable orientations of the molecules in the projections. The present result is in agreement with electron-diffraction data and shows that a methyl group bond attached to a fully substituted benzene ring has the same length as in saturated aliphatic hydrocarbons. The shorter single-bond lengths reported in stilbene, tolan, diphenyl, etc., are the result of conjugation of the side chain with the benzene nucleus.

The minimum intermolecular approach distances are 3·70 and 3·87 A between carbon atoms and 2·0—2·2 A between hydrogen atoms. Comparison with the closest intermolecular approach of hydrogen atoms in solid methane (1·97 A) shows that the hexamethylbenzene molecules are packed as closely as the hydrogen–hydrogen repulsions will allow. With the molecules lying very nearly in the (001) plane, the structure is triclinic instead of monoclinic because the former arrangement allows a closer packing amounting to a 9% greater density.

THE crystal structure of hexamethylbenzene was investigated by Lonsdale (*Proc. Roy. Soc.*, 1929, *A*, **123**, 494; *Trans. Faraday Soc.*, 1929, **25**, 352), who showed that the molecule is planar (except for the hydrogen atoms) and that it lies in the (001) crystallographic plane. In fixing the size of the molecule, Lonsdale calculated intensities for a number of trial structures, whose bond lengths are listed below :

Model	*b*	*c*	*d*	*e*	*f*	*g*	*h*
$C_{ar.}$–$C_{ar.}$, A	1·48	1·54	1·54	1·42	1·42	1·42	1·30
$C_{ar.}$–$C_{al.}$, A	1·48	1·54	1·48	1·48	1·42	1·36	1·30

Model *e* was chosen from this group on the basis of the comparison of calculated and observed intensities, with the conclusion that the carbon–carbon bonds in the benzene ring were 1·42 A long and those holding the methyl groups to the ring were 1·48 A long.

The length of the bonds by which the substituted groups are attached to the benzene ring in methylbenzenes is of special importance because it serves as the reference value for estimating the effect of conjugation on bond length in conjugated systems. The carbon–carbon bond length is always observed to be 1·54 A within about 0·02 or 0·03 A whenever the two atoms involved are each attached to four other atoms, as in diamond, ethane, propane, *iso*butane, *neo*pentane, and long-chain hydrocarbons (Brockway and Taylor,

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* A preliminary announcement of some of the results of this investigation was made at the meeting of the American Chemical Society, Baltimore, Maryland, April, 1939.

Ann. Reports, 1937, **34** 196); and this distance is regarded as characteristic of the carbon–carbon single bond. With the change of bond type to double or triple, the observed distances become 1·34 or 1·20 A. Intermediate values ranging from 1·48 to 1·39 A have been observed in a number of conjugated systems, including benzene and other molecules containing the benzene nucleus, cyanogen, diacetylene, and the oxalate group. For the bond holding a side chain to a benzene ring such intermediate values have been observed in durene, dibenzyl (Robertson, *Proc. Roy. Soc.*, 1933, *A*, **142**, 659; 1935, **150**, 348), stilbene, tolan (Robertson and Woodward, *ibid.*, 1937, *A*, **162**, 568; 1938, *A*, **164**, 436), and also in diphenyl (Dhar, *Indian J. Physics*, 1932, **7**, 43), *p*-diphenylbenzene (Pickett, *Proc. Roy. Soc.*, 1933, *A*, **142**, 333), and *pp'*-diphenyldiphenyl (*idem*, *J. Amer. Chem. Soc.*, 1936, **58**, 2299). The decrease from 1·54 A indicates that the bond type is different from that occurring in the saturated aliphatic hydrocarbons. In the last five of the seven molecules just named, the bond in question is part of a conjugated system, and it may be supposed that the accompanying resonance hybridisation is responsible for the intermediate character of the bond. On the other hand, the low values (1·47—1·48 A) reported for this bond in hexamethylbenzene, durene, and dibenzyl suggest that a single bond in this position is shorter than 1·54 A even in a non-conjugated system. The low values observed in these molecules have been quoted in support of the proposal (Glasstone, *Ann. Report*, 1936, **33**, 77) that "the conjugated resonating system of single and double linkages in the benzene nucleus can bring about a 'tightening up' of external bonds" in substituted benzenes.

From the foregoing considerations we might accept the value 1·48 A as the length characteristic of a carbon–carbon bond external to a benzene ring, and ascribe decreases below this value to the effect of conjugation. Accordingly, the external radius of a benzene carbon atom would be 0·71 A (0·77 A being taken for the radius of a methyl carbon). The consequences of this conclusion lead, however, to serious discrepancies. We should expect the separation of the rings in the diphenyl type of molecule to be 1·42 A with no allowance for the conjugation effects, and several hundredths of an Ångström unit less than this when the conjugation is taken into account; but the observed distance is 1·48 A. Predictions of the lengths of the side-chain-attaching bonds in stilbene and tolan (Penney and Kynch, *Proc. Roy. Soc.*, 1938, *A*, **164**, 409), based on calculations of the energy of the molecules and on the observed lengths of non-conjugated carbon–carbon bonds, gave excellent agreement with observation when the non-conjugated bond length was assumed to be 1·54 A. It would be difficult to understand this agreement if the non-conjugated length were in fact 1·48 A.

The accuracy of the value reported for hexamethylbenzene was questionable for two reasons. An electron-diffraction investigation (Pauling and Brockway, *J. Amer. Chem. Soc.*, 1937, **59**, 1223) on the vapour showed that the length, 1·54 A, for the methyl group bonds gave a better agreement between calculated and observed diffraction patterns than did the value 1·48 A. Also, Lonsdale's determination based on trial structures had not included a test of a side-chain bond length of 1·54 A (combined with a ring size of 1·42 A).* Because of this uncertainty in the observed value and of the importance of an accurate knowledge of the non-conjugated bond length, we have repeated the determination of the crystal structure of hexamethylbenzene.

The present investigation, based on a Fourier analysis of new and more extensive intensity data, leads to a ring size of 1·39 A and a methyl group bond length of 1·53 A. It is further found that the planar molecule is tilted out of the (001) crystal plane by about 1°, but apart from these modifications Lonsdale's previous structure is fully confirmed.

Our new figures for the bond lengths are probably accurate to within ±0·02 A, and are superior to the previous determinations in durene and dibenzyl because of the more favourable position of the hexamethylbenzene molecule in the crystal. Although the durene and

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* In 1929 an atom was thought of as having the same radius for all of its bonds irrespective of variations in bond type. For the combination of bond distances, 1·42 A and 1·54 A, in hexamethylbenzene it would have been necessary to postulate a methyl carbon atom with a diameter of 1·66 A. Because there was no evidence for a carbon atom of such a size, the foregoing combination of bond distances was not tested.

dibenzyl results were refined by a double Fourier analysis, yet the positions of the molecules in these crystals are such that no perfectly clear resolution of any of the methyl or methylene groups is possible in any two-dimensional analysis. Allowance had to be made for the overlapping effect of the neighbouring benzene carbon atoms in the projections, and it would now appear that this allowance may not have been sufficient. Furthermore, in these structures the radius of the benzene ring was assumed to be 1·41 A. If this is corrected to 1·39 A, the methyl group bond distances are automatically increased from the reported values of 1·47 A to 1·49 A. At present it seems most reasonable to assume that the remaining discrepancy between 1·49 A and our new value of 1·53 A in hexamethylbenzene is due to insufficient allowance for the overlapping effect of neighbouring atoms in the durene and dibenzyl structures.

We have attempted to check this point by recalculating the durene structure factors for a molecule with $C_{ar.}$–$C_{ar.}$ = 1·39 A and $C_{ar.}$–$C_{al.}$ = 1·54 A, and the orientation previously found. The results show that the sum of the discrepancies between the calculated and observed values becomes about 0·5% greater for the new figures. This change, however, is probably too small to be significant, and in general the figures are found to be extremely insensitive to the tested change in dimensions. We do not think that a more definite result can be obtained for durene until more accurate and more extensive intensity data are available. The same conclusion is probably true for dibenzyl. Both these crystals are volatile, and further more refined experimental work is consequently difficult.

The result of this investigation shows that the length of a methyl group bond external to benzene (fully substituted) is the same within the experimental error as the length of the single carbon–carbon bond in saturated aliphatic hydrocarbons. The resonance in the benzene ring itself accordingly has no important effect on the lengths of the external bonds. When the external bonds are observed to be less than about 1·53 A in length, the decrease is to be attributed to the influence of the attached group. Thus, in stilbene and the phenyl-substituted benzenes the carbon–carbon bond adjacent to the benzene ring is part of a conjugated system involving multiple bonds in the benzene nucleus and in the substituted group, and the observed decrease below 1·53 A is a measure of the conjugation effect. In the case of 1 : 2-diphenylbenzene and 1 : 3 : 5-triphenylbenzene, the molecules are not planar because of the repulsions between the phenyl groups (Lonsdale, *Z. Krist.*, 1937, **97**, 91); and although a complete structural analysis has not been made, it is very probable that the bonds between the benzene rings are longer than those in 1 : 4-diphenylbenzene because the departure from planarity inhibits the conjugation across this bond. In tolan, the " single " bond length is 1·40 A, a value 0·13 or 0·14 A less than the true single bond length. This decrease is probably due, not only to conjugation of the triple bond and the multiple bonds in the ring, but also to a change in the relative contribution of *s* and *p* atomic orbitals to the single bond on an atom also holding a triple bond. The short methyl group bond length, 1·46 A, observed in methylacetylene has been ascribed by Pauling, Springall, and Palmer (*J. Amer. Chem. Soc.*, 1939, **61**, 927) in part to the latter effect and in part to resonance with structures having two double carbon–carbon bonds and only two of the methyl hydrogens bonded. Here it may be simply noted that, whereas a single bond is shortened by an adjacent triple bond, there is no appreciable shortening of a single bond adjacent to a double bond or a benzene ring as shown by observations on methylethylenes (Pauling and Brockway, *ibid.*, 1937, **59**, 1223) and by the present result on hexamethylbenzene.

Analysis of the Structure.

Crystal Data.—Hexamethylbenzene, $C_{12}H_{18}$; *M*, 162·1; m. p. 164°; density, calc. 1·061, found 1·042. Triclinic. $a = 8{\cdot}92 \pm 0{\cdot}02$, $b = 8{\cdot}86 \pm 0{\cdot}02$, $c = 5{\cdot}30 \pm 0{\cdot}01$ A; $\alpha = 44° \ 27'$, $\beta = 116° \ 43'$, $\gamma = 119° \ 34'$; $d_{100} = 7{\cdot}66$, $d_{010} = 5{\cdot}96$, $d_{001} = 3{\cdot}66$ A; $\angle(010):(001) = 129° \ 18'$, $\angle(001):(100) = 80° \ 48'$, $\angle(100):(010) = 74° \ 0'$. Space group probably C_1' ($P\bar{1}$) rather than C_1' ($P1$). One molecule per unit cell. Molecular symmetry, centre. Volume of the unit cell = 252 A³. Absorption coefficient for *X*-rays, $\lambda = 1{\cdot}54$, $\mu = 5{\cdot}21$ per cm. Total number of electrons per unit cell = $F(000) = 90$.

The axial lengths and spacings differ slightly from Lonsdale's values, owing to a corrected value for the wave-length, but the angles are the same.

Experimental Measurements.—Small crystal specimens weighing about 0·1 mg. were mounted completely in the X-ray beam (filtered Cu-K_{α} radiation), and rotation photographs taken about the crystallographic axes. The intensities of the reflections were recorded on moving films, and measured on an integrating photometer. Considerable difficulty was experienced in cutting suitable crystal specimens owing to their great tendency to distort on the cleavage planes. The crystals were also found to perish rather rapidly in the X-ray beam, and a number of different specimens had to be employed in the work.

An attempt was made to obtain absolute values for the intensities by comparison with a diamond standard on the moving-film two-crystal spectrometer (Robertson, *Phil. Mag.*, 1934, **18**, 729), but the above difficulties tended to make the results inaccurate. The scale employed for the F values given below was finally obtained by correlation with the calculated values. One absolute measurement gave a value some 35% less than this scale, but the result is probably in error.

Structure Factors and Fourier Synthesis.—We know from Lonsdale's work (*loc. cit.*) that the hexamethylbenzene molecule lies practically in the (001) plane of the crystal. Consequently, the (*hk*0) set of structure factors and the corresponding projection of the structure along the c axis give far more complete information about the dimensions of the molecule than can be obtained from a study of any other zone. We have, therefore, confined our analysis principally to this zone, although a number of other reflections have been measured for confirmatory evidence.

The double Fourier series method was used. The coefficients, calculated from the measured intensities by the usual formulæ (mosaic crystal), are given in Table I. The phase constants, represented by the signs attached to these numbers, had to be derived by a preliminary trial analysis. For this purpose the molecular orientation given by Lonsdale (*loc. cit.*) was employed, and the structure factors were calculated for the following two models :

TABLE I.

Values and Signs of F (*hk*0).

		k.							
		0.	1.	2.	3.	4.	5.	6.	7.
	8	+1·0	−1·6	−1·1	—	—	—	—	—
	7	−3·0	−3·2	—	—	−1·4	—	—	—
	6	−1·6	−4·2	−2·8	+1·7	−0·8	—	—	—
	5	+1·2	+4·4	−3·4	—	—	−0·9	—	—
	4	−13·8	−2·0	−1·6	+2·3	+3·4	—	—	—
	3	−11·9	−17·7	−6·7	+3·0	+10·7	+4·3	—	—
	2	−10·4	−4·3	+2·2	−3·3	+5·6	+7·4	—	—
	1	+19·9	−5·4	+13·2	—	−3·8	—	—	—
h	0	+90·0	+17·1	−9·5	−9·2	−8·0	—	—	−1·1
	$\bar{1}$	—	+17·5	−4·4	−5·1	−9·7	—	+1·7	−2·3
	$\bar{2}$	—	−5·0	−7·6	+7·2	+1·7	−4·6	—	−0·9
	$\bar{3}$	—	+13·4	−6·0	−8·1	—	−1·6	+1·9	+1·2
	$\bar{4}$	—	+0·6	+1·4	−11·7	−7·4	−2·2	+4·3	+5·2
	$\bar{5}$	—	−4·8	−2·9	−5·6	−2·3	—	—	+4·2
	$\bar{6}$	—	−2·3	+6·2	+1·8	—	+1·4	—	—
	$\bar{7}$	—	—	+9·2	+9·3	+1·0	−1·0	−1·9	—
	$\bar{8}$	—	—	+1·8	+5·0	+2·1	—	−1·1	—
	$\bar{9}$	—	—	—	—	—	—	—	—
	$\overline{10}$	—	−1·5	−1·6	—	—	—	—	—

(1) $C_{ar.}$–$C_{ar.}$ = 1·39 A $C_{ar.}$–$C_{al.}$ = 1·48 A
(2) $C_{ar.}$–$C_{ar.}$ = 1·39 A $C_{ar.}$–$C_{al.}$ = 1·54 A

In both these cases precisely the same set of phase constants was obtained for all the measurable structure factors, and these are given in Table I. It will thus be quite clear that the value of the $C_{ar.}$–$C_{al.}$ distance which is obtained as a result of this Fourier synthesis is quite independent of the precise nature of the initial assumptions which have been made with regard to the molecular dimensions, and it does, in fact, amount to a direct determination.

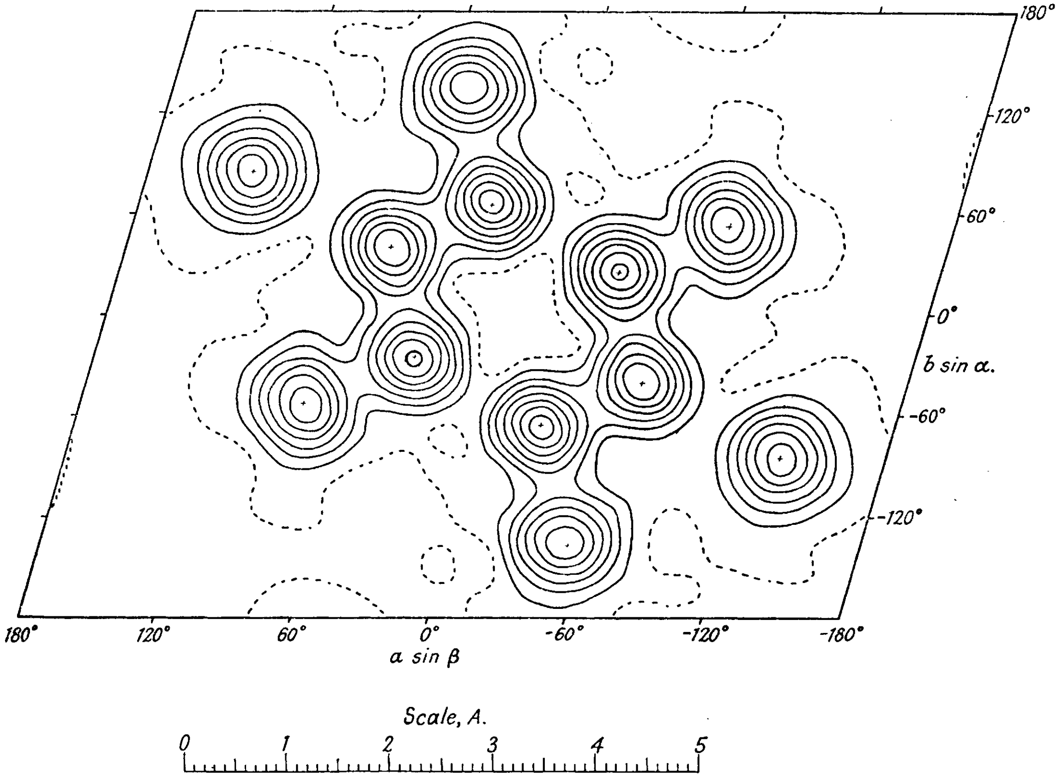
Orientation of the Molecule. Dimensions and Co-ordinates.—The results of the summation of the electron density series

$$\rho(xy) = \frac{1}{A}\sum_{-\infty}^{+\infty}\sum_{-\infty}^{+\infty} F(hk0)\cos 2\pi(hx/a + ky/b)$$

are represented by the contour map of Fig. 1, where the lines are drawn at unit electron intervals. It has been mentioned above that the scale of F values is not a true absolute one, but is derived by correlation with the calculated values. The density increments thus only approximate to one electron per A per line, and in fact, the peak values are somewhat higher than we should expect for a structure of this kind. These considerations, of course, have no effect on the atomic positions.

FIG. 1.

Hexamethylbenzene, c *axis projection.*



The projection has been drawn on a plane perpendicular to the c crystal axis. Owing to the triclinic axes, this projection plane does not coincide with any crystal plane, but is inclined at an angle of 46° 16′ to the (001) plane (and also approximately at this angle to the plane of the molecule). The sides of this projection plane are $a \sin \beta$ and $b \sin \alpha$, and the angle between them, γ^*, is 106° 0′. The area of the projection plane (A in the above equation) is equal to 47·5 A^2.

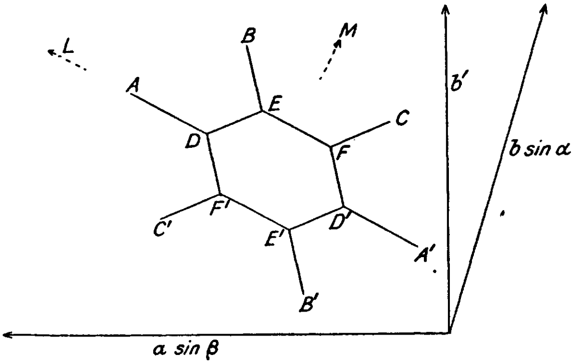
The inclination of the molecule to this plane causes considerable distortion in the projection, but fortunately the atoms A and D (compare Fig. 2) are very clearly resolved, and it is found that the line joining them lies very nearly in the projection plane. The measured distance between A and D is 1·53 A, and from D to the centre of the ring, 1·39 A.

The estimated centres of the other atoms are indicated by small crosses in Fig. 1, and these are found to lie on the *projection* of a regular plane hexagonal structure with $C_{ar.}$–$C_{ar.}$ = 1·39 A and $C_{ar.}$–$C_{al.}$ = 1·53 A.

The complete orientation of the molecule can be calculated from the projection. The line *L* (*AD*) makes an angle of 28° 30′ with the projected *a* axis, and *M* an angle of 116° 30′. The fact that these lines are not mutually perpendicular indicates a small rotation of the molecule about the *M* axis, and the observed foreshortening of the assumed hexagonal structure in the *M* direction [*r* (observed) /*R* (assumed) = sin ω_m = 0·6912] indicates a fairly large rotation about the *L* axis.

The orientation is most conveniently referred to an orthogonal system of axes. For these we choose the projected *a* axis (*a* sin β), another axis perpendicular to it and also lying in the plane of the projection (*b*′ in Fig. 2), and the crystallographic *c* axis along which the projection is made. The angles between the molecular axes, *L*, *M*, and their normal *N*, and these three orthogonal axes are then denoted by χ_L, ψ_L, ω_L, etc. The results are given below, together with the angles which the triclinic crystal axes make with these orthogonal axes. The co-ordinates of the atoms follow in Table II.

FIG. 2.



Orientation of molecular axes.

χ_L = 28° 34′ χ_M = 107° 58′ χ_N = 68° 35′
ψ_L = 61° 31′ ψ_M = 51° 47′ ψ_N = 128° 38′
ω_L = 91° 55′ ω_M = 43° 44′ ω_N = 46° 20′

Orientation of triclinic crystal axes.

χ_a = 26° 43′ χ_b = 101° 8′ χ_c = 90°
ψ_a = 90° 0′ ψ_b = 47° 41′ ψ_c = 90°
ω_a = 116° 43′ ω_b = 44° 27′ ω_c = 0°

Orientation of normal to (001) *plane* = c*, *etc.*

χ_{c^*} = 69° 39′ Angle between *c** and *L* = 91° 8′
ψ_{c^*} = 129° 18′ ,, ,, ,, *M* = 89° 59′
ω_{c^*} = 46° 16′ ,, ,, ,, *N* = 1° 7′

TABLE II.

Co-ordinates referred to triclinic crystal axes; centre of symmetry as origin.

Atom.	*x*, A.	$2\pi x/a$.	*y*, A.	$2\pi y/b$.	*z*, A.	$2\pi z/c$.
A CH	3·318	133·9°	2·069	84·1°	−0·082	−5·6°
B CH	1·287	51·9	3·359	136·5	−0·040	−2·7
C CH	−2·030	−81·9	1·289	52·4	0·043	2·9
D C	1·580	63·8	0·985	40·0	−0·039	−2·6
E C	0·613	24·7	1·598	64·9	−0·018	−1·2
F C	−0·967	−39·0	0·613	24·9	0·020	1·4

Intermolecular Distances and Arrangement of Molecules in the Crystal.

The grouping of the molecules in the crystal is illustrated by the extended contour map of Fig. 3, showing the relations of nine molecules in a normal projection along the *c* axis.

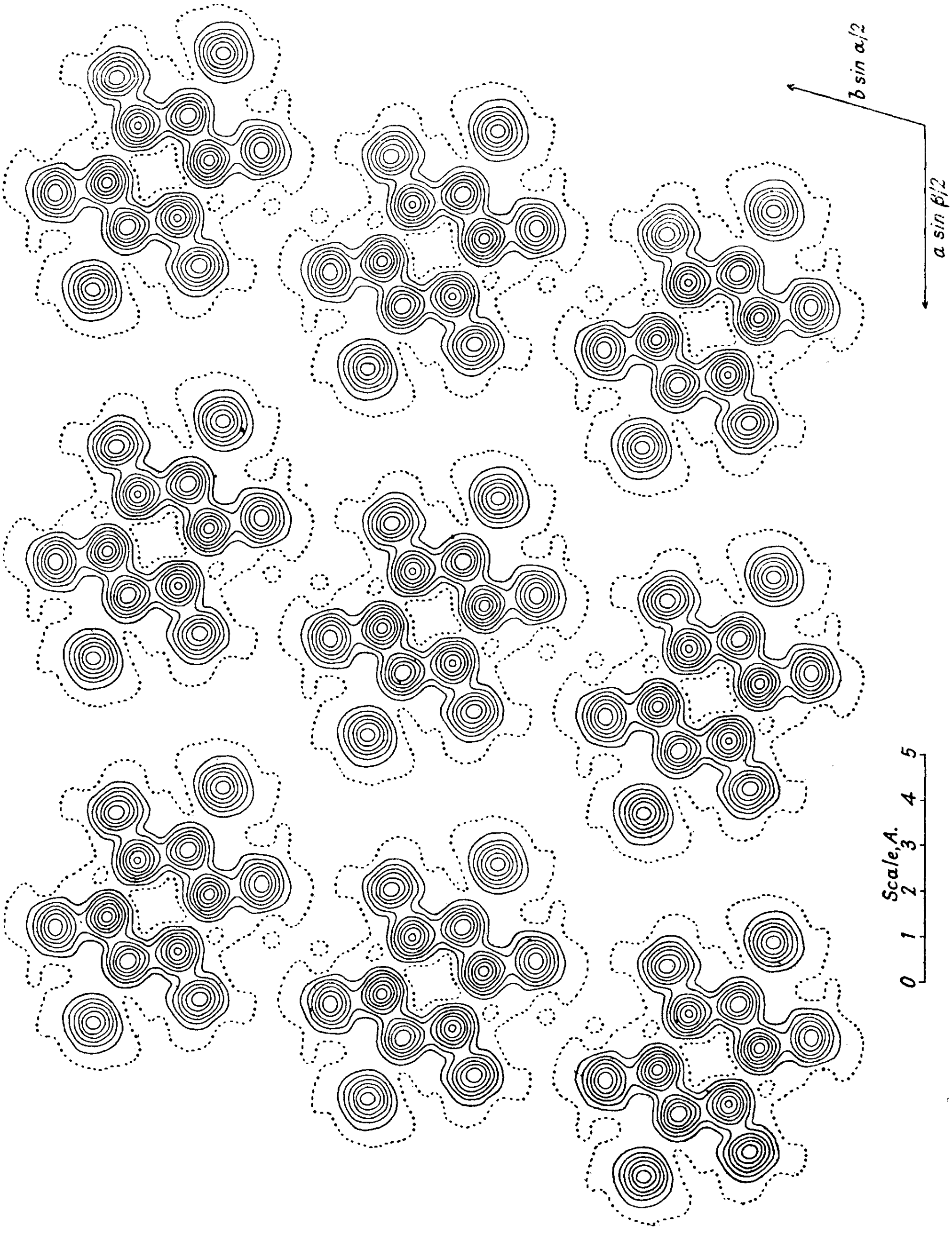


FIG. 3.
Group of molecules in c *axis projection.*

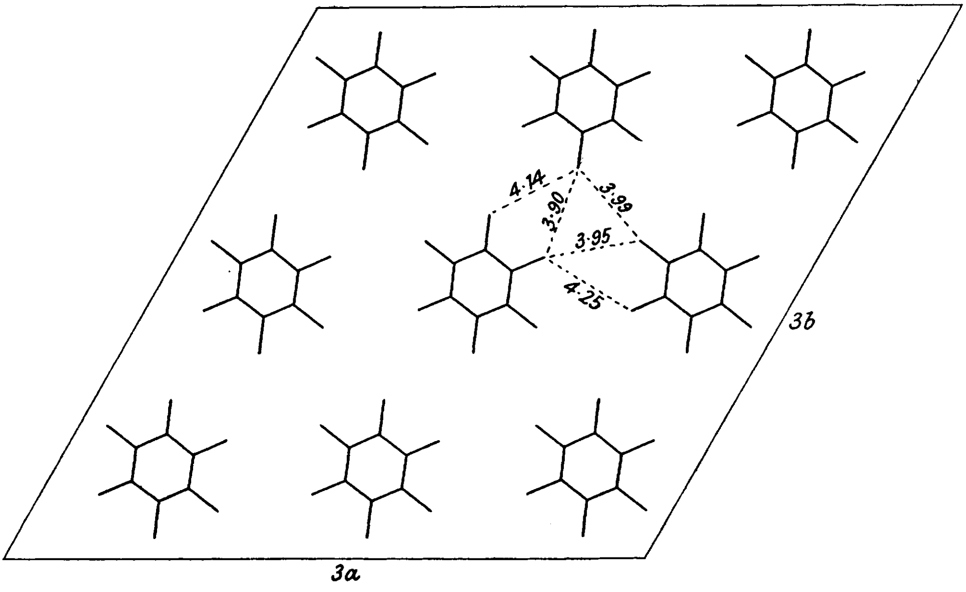
The arrangement of a single layer of molecules in the (001) plane is indicated in Fig. 4, with some of the distances of closest approach between adjoining methyl carbon atoms also shown. These distances, 3·90, 3·95, and 3·99 A, are to be compared with the corresponding value in durene of 3·93 A. The shortest distances between methyl atoms in adjoining

(001) layers are 3·87 and 3·98 A, the first being identical with the value observed for similarly disposed molecules in the durene structure. The shortest carbon–carbon intermolecular distances, 3·70 and 3·78 A, are observed in the (100) layer of molecules, where a methyl carbon in one molecule lies almost directly over an atom in the ring in the molecule below.

The packing of the molecules in the crystal is determined by the equilibrium distances between the hydrogen atoms in different molecules. Mack (*J. Amer. Chem. Soc.*, 1932, **54**, 2161) has discussed the packing arrangement in the hexamethylbenzene structure in some detail, and has given two figures to show how the space between the carbon atoms is occupied by hydrogen atoms. The hydrogen separations can be computed only if the positions of the atoms are determined, and this information is not afforded by the *X*-ray analysis. The carbon–hydrogen bond lengths in the methyl groups are very probably the same as those in methane, for which the band-spectroscopic value (Ginsburg and Barker, *J. Chem. Physics*, 1935, **3**, 668) is 1·093 A. The angle between the carbon–hydrogen bonds in methane is 109° 28′, but it is probably smaller in the methyl groups because of the repulsions between hydrogen atoms in adjacent groups in the same hexamethylbenzene molecule. It has been suggested by Pauling (*Physical Rev.*, 1930, **36**, 430) that a transition point observed in the heat-capacity curve at —122° marks the beginning of rotation of the methyl goups. If the methyl groups are rotating at about 20°, where the *X*-ray photographs were taken, the hydrogen atoms in adjacent methyl groups would approach each other within 1·50 A ($\widehat{\mathrm{HCH}}$ angles being assumed to be 109° 28), as compared with distances of 1·78 A between hydrogen atoms in the same methyl group. If the $\widehat{\mathrm{HCH}}$ angle is decreased to 102° 10′ and the $\widehat{\mathrm{CCH}}$ angle increased to 116° 5′, the hydrogen atom separations within a methyl group and between adjacent methyl groups on the same molecule become equal at 1·70 A. The separations between adjacent hydrogen atoms in *different* molecules in the (001) layer may now be calculated by using C–H = 1·09 A and CCH = 116° with the resulting values ranging from 2·00 A to 2·25 A. In solid methane, where the close approach of the molecules is also limited by repulsions between hydrogen atoms, the molecules lie in a face-centred cubic arrangement with the edge of the unit cell equal to

FIG. 4.

A single layer of molecules in the (001) *plane.*



5·88 A (Mooy, *Proc. K. Akad. Wetensch. Amsterdam*, 1931, **34**, 550). It is believed (Pauling, *loc. cit.*) that the molecules are rotating in the temperature region from —253° to the m. p. at —184°; and this would bring hydrogen atoms on different molecules within 1·97 A of each other. This value compared with 2·00 A, the smallest hydrogen–hydrogen intermolecular distance observed in hexamethylbenzene, shows that the hydrogen interactions are indeed the limiting factor in the molecular packing and explains the relatively large carbon–carbon intermolecular distances.

The symmetry of the (001) layer is nearly hexagonal (*i.e.*, with $a = b$ and $\gamma = 120°$). The deviations amounting to 0·7% difference between a and b and an angle deviation of 26′ may afford a more compact fitting-in of the methyl groups in the (001) layer, but are certainly influenced by the nature of the stacking of successive layers. If we attempt to build up a hexagonal or monoclinic structure by placing the centres of the molecules directly over those in the layer below and allow 2·00 A for the closest approach of hydrogen atoms, the interplanar spacing will be about 4·00 A. In the observed structure the upper layer is translated so that the molecular centres lie over intermediate positions in the lower layer and the methyl groups no longer lie directly over each other. This allows the layer spacing to decrease to the observed value of 3·66 A, which represents an increase of about 9% in the density. For this reason the structure as a whole deviates from hexagonal or monoclinic symmetry in spite of the nearly hexagonal arrangement of the (001) layer. The (001) spacing of 3·66 A is larger than the layer spacing in graphite, *viz.*, 3·40 A, by an amount which allows for the accommodation of the hydrogen atoms with inter-hydrogen separations ranging upwards from 2·0 A.

It may be noted that the deviations from hexagonal symmetry include a slight tilt of the molecules out of the (001) plane. The tilt corresponds to a rotation of 1° 8′ about an axis through the molecule parallel to the b axis.

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