

spots from mixed regions are quite sharp, that the widths of most of the domains are not much less than about 1μ . Some smearing out along the columns in the X-ray photographs is observed which indicates some one-dimensional disorder.

The authors wish to express their sincere thanks to Professors E. Alexander and I. T. Steinberger for many helpful discussions and suggestions.

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The Crystal Structure of 1,8-Dichloro-9-methylanthracene

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(Received 3 September 1968)

1,8-Dichloro-9-methylanthracene, $C_{15}H_{10}Cl_2$, crystallizes in the orthorhombic space group *Pnma* with $a=7.13$, $b=19.46$, $c=8.76$ Å, $Z=4$, $D_{obs}=1.42$ and $D_{calc}=1.43$ g.cm⁻³. Thus a crystallographic mirror plane is imposed on the separate molecular units. The intensities of 772 reflexions were estimated visually from integrated Weissenberg photographs. Atomic parameters have been refined by full-matrix least-squares procedures to a conventional *R* index of 0.092. The chlorine and methyl carbon atoms were assigned anisotropic thermal parameters; the other atoms isotropic parameters. All hydrogen atoms have been located. There is a pronounced distortion of the anthracene skeleton, C(9) being displaced by 0.19 Å from the mean molecular plane. The methyl carbon displacement is 0.80 Å on the same side of the plane as C(9), while the chlorine displacement is 0.33 Å on the opposite side.

Introduction

There are now a number of structural data available relating to the molecular distortions which arise when naphthalene is *peri*-substituted. (For a review see Balasubramanian, 1966.) Hitherto, however, there appears to have been no structure analysis which could cast light on the related problem in the *peri*-substitution of anthracene.

The electronic absorption spectrum of 1-chloro-9-methylanthracene relative to that of 1-chloro-10-methylanthracene has been interpreted by Bouas-Laurent & Lapouyade (1965) as being consistent with distortions of the ground state molecular configuration of the 1,9(*peri*) substituted compound. In particular, the shift to longer wave-lengths of the band in the 3900 Å region, which accompanies *peri*-substitution, is believed to reflect the reduction in energy difference between the ground and excited electronic states to be expected as the result of molecular distortion. With a view to establishing the extent of such distortions, we began X-ray studies on crystals of 1-chloro-9-methylanthracene and 1,8-dichloro-9-methylanthracene. The relatively poor quality of the diffraction data obtainable from the monochloro compound at room temperature (22°C) caused us to abandon further work on it in favour of the dichloro compound in which the distortions would be expected to be even greater.

Experimental

A sample of 1,8-dichloro-9-methylanthracene was kindly supplied by Professor Henri Bouas-Laurent of the University of Bordeaux, France. Suitable crystals were mounted on glass fibres and appeared to be stable in air and to X-rays.

Crystal data

1,8-Dichloro-9-methylanthracene, $C_{15}H_{10}Cl_2$, $M=261.2$. Orthorhombic with $a=7.13(1)$, $b=19.46(3)$, $c=8.76(1)$ Å. ($\lambda=1.5418$ Å for Cu $K\alpha$ radiation. The numbers in parentheses here and elsewhere are estimated standard deviations in the least significant figures quoted). $U=1215$ Å³, $D_{obs}=1.42(2)$ g.cm⁻³ (by flotation). $Z=4$, $D_{calc}=1.43$ g.cm⁻³, $F(000)=536$, $\mu(Cu K\alpha)=45.4$ cm⁻¹, $\mu(Mo K\alpha)=5.1$ cm⁻¹. Systematic absences: $0kl$ for $(k+l)$ odd, $hk0$ for h odd.

Unit-cell dimensions were obtained from zero-level precession photographs with Polaroid film (Swink & Carpenter, 1967). Systematic absences of X-ray reflexions were consistent with space groups *Pnma* (which requires molecular symmetry *m*) and *Pn2₁a* (which requires no molecular symmetry). Intensity statistics (Wilson, 1949; Howells, Phillips & Rogers, 1950) favoured centrosymmetric *Pnma* and the structure has been solved and refined in this space group.

X-ray intensity data were obtained by visual estimation of integrated equi-inclination Weissenberg film packs obtained with Cu $K\alpha$ radiation. Within the levels (0---5*kl*), 1103 independent reflexions (75% of the Cu $K\alpha$ limiting sphere) were accessible. Of these, 331 were below the threshold of observation, leaving 772 which were used for structure solution and refinement. One crystal, approximately a cube, with edge 0.1 mm, was used for all levels. No absorption corrections were made. The Weissenberg data were placed on a common scale with the aid of (*h0l*) and (*hhl*) data obtained with Mo $K\alpha$ radiation on a precession camera. The crystal used for this purpose was a disc of thickness about 0.2 mm and diameter 1.0 mm with the crystallographic *b* axis coinciding with the axis of the disc. The spots produced on the precession films were, therefore, large and of uniform shape.

Initial computations were performed on an IBM 1620 by use of various local computer programs and local modifications of Mair's *SFLS* (block diagonal least-squares) and Van der Helm's *ICR1* (Fourier calculations). Solution and refinement of the structure were completed on an IBM 360/44 computer with 16K words of core storage and twin 2315 disc storage drives. Programs, which have been modified extensively and adapted to this hardware include Zalkin's *FORDAP* for Fourier calculations, the Busing-Martin-Levy *ORFLS* full-matrix least-squares and *ORFFE-II* error function programs and Pippy & Ahmed's *MEAN PLANE* program.

Solution and refinement of the structure

Initial values for the coordinates of all non-hydrogen atoms were obtained from the three-dimensional Patterson function. The distribution of peaks indicated a centrosymmetric arrangement for the molecules and refinement was commenced in space group *Pnma*. The atomic scattering factors for chlorine and carbon were taken from *International Tables for X-ray Crystallography* (1962), real dispersion corrections being applied for chlorine only; the scattering factor of hydrogen was that tabulated by Stewart, Davidson & Simpson (1965). The usual agreement index $R = \sum ||F_o| - |F_c|| / \sum |F_o|$ was reduced from 0.39 to 0.20 in four cycles of block-diagonal least squares, all atoms being refined isotropically. All atoms appeared to be correctly located except the methyl carbon atom which was relocated from an electron density difference map. Four further cycles reduced *R* to 0.18.

At this stage full-matrix least-squares refinement was commenced, the quantity $\sum w(F_o - S_q F_c)^2$ being minimized. Unobserved reflexions were given zero weight. Discrepancy indices are $R_1 = \sum ||F_o| - |S_q F_c|| / \sum |F_o|$ and the weighted *R* value $R_2 = (\sum w \Delta F^2 / \sum w F_o^2)^{1/2}$. Two cycles of refinement produced no significant changes in any parameters. A subsequent difference map showed several large peaks, the largest, of height 2.5 e.Å⁻³ being close to the chlorine atom. Accordingly,

in the next round of calculations the chlorine and methyl carbon atoms were allowed to vibrate anisotropically, temperature parameters for all other non-hydrogen atoms being fixed at the values given by the previous isotropic refinement. In addition, the contributions of the four independent ring hydrogen atoms were included with an isotropic thermal parameter of 6.0 Å², no parameters being refined for these atoms. Two cycles of refinement reduced *R*₁ and *R*₂ to 0.104 and 0.144, the weighting scheme being one based on scatter in the film factor ratios. Two further cycles varying all relevant parameters (including those for the four H atoms) reduced *R*₁ and *R*₂ to 0.095 and 0.131.

The largest peak given by the next difference map was of height 1.0 e.Å⁻³ and situated close to the chlorine atom. The next largest were several of height about 0.5 e.Å⁻³. Two of these were in positions expected to be occupied by methyl hydrogen atoms so as to maximize chlorine-hydrogen separation if the methyl group is not rotating freely and the hydrogen atoms are fixed. As the parameters for the ring hydrogen atoms appeared to have refined successfully, we were encouraged to attempt to refine parameters for the methyl hydrogen atoms as well. After several cycles the shifts for all hydrogen atom parameters were less than 0.1 of the estimated standard deviation, *R*₁ and *R*₂ being reduced to 0.092 and 0.126. This improvement in *R*₂ over the refinement without the methyl hydrogen atoms is highly significant (Hamilton, 1965). We take the successful least-squares refinement and the physical reasonableness of the resulting parameters as evidence that the methyl hydrogen atoms are fixed in the crystal.

Analysis of the weighting scheme showed that excessive weights were being given to medium and strong reflexions. A more appropriate set of weights was obtained by using Cruickshank's (1965) formula,

$$w = (a + |F_o| + bF_o^2)^{-1},$$

with $a = 4.0$, $b = 0.0167$. Several additional cycles

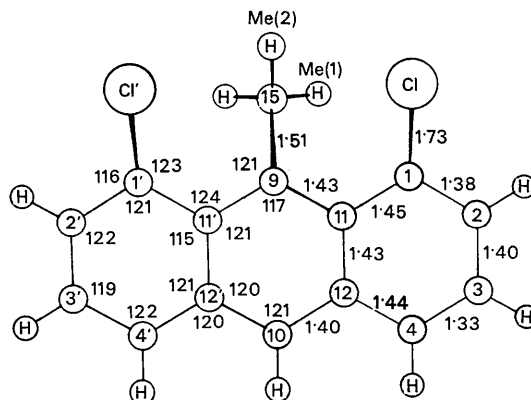


Fig. 1. Bond angles (degrees) and lengths (Å) and crystallographic numbering scheme for 1,8-dichloro-9-methylanthracene.

Table 1. Positional and thermal parameters

	x	y	z	β_{11}^*	β_{22}	β_{33}	β_{12}	β_{13}	β_{23}
Cl	0.0378 (3)	0.1078 (1)	0.1848 (3)	0.0262 (7)	0.00300 (5)	0.0238 (4)	0.0005 (1)	-0.0110 (4)	0.0016 (1)
C(15)	0.1067 (18)	0.25†	0.0666 (16)	0.0160 (31)	0.0034 (3)	0.0220 (20)	0.0†	-0.0031 (19)	0.0†
	x	y	z	B^\ddagger					
C(1)	-0.1298 (10)	0.1196 (3)	0.0450 (7)	3.45 (10)					
C(2)	-0.2181 (11)	0.0608 (4)	-0.0061 (7)	3.99 (12)					
C(3)	-0.3737 (11)	0.0630 (4)	-0.1034 (8)	4.23 (13)					
C(4)	-0.4464 (12)	0.1237 (4)	-0.1417 (9)	4.04 (13)					
C(11)	-0.1957 (9)	0.1871 (3)	-0.0019 (6)	2.89 (9)					
C(12)	-0.3635 (10)	0.1874 (3)	-0.0905 (7)	3.56 (11)					
C(9)	-0.1003 (14)	0.25†	0.0325 (9)	3.17 (15)					
C(10)	-0.4418 (15)	0.25†	-0.1367 (11)	3.73 (16)					
H(2)	-0.135 (12)	0.025 (5)	0.032 (9)	7.0 (21)					
H(3)	-0.427 (11)	0.011 (5)	-0.134 (11)	7.0 (21)					
H(4)	-0.538 (12)	0.143 (4)	-0.158 (9)	4.7 (18)					
H(10)	-0.589 (25)	0.25†	-0.175 (20)	11.5 (51)					
HMe(1)	0.198 (12)	0.205 (4)	0.021 (8)	5.3 (18)					
HMe(2)	0.194 (23)	0.25†	0.193 (17)	9.4 (40)					

* The form of the anisotropic thermal ellipsoid is $\exp[-(\beta_{11}h^2 + \beta_{22}k^2 + \beta_{33}l^2 + 2\beta_{12}hk + 2\beta_{13}hl + 2\beta_{23}kl)]$.

† Isotropic thermal parameter (\AA^2).

‡ Parameter fixed by symmetry.

using these weights produced no significant shifts in any parameter, the final values of R_1 and R_2 being 0.092 and 0.131. The final difference map using all 772 observed reflexions still showed the peak of height 1.0 e. \AA^{-3} close to the chlorine atom; the next peak of height 0.5 e. \AA^{-3} was approximately the height of a hydrogen atom in the structure. Analysis of the anisotropic thermal motion of the chlorine atom shows that the principal axis of vibration is perpendicular to the mean plane of the anthracene skeleton. The large residual peak lies, approximately, along the direction of this axis, 0.9 \AA from the chlorine atom and on the opposite side of the molecule. Assuming that the peak is genuine and does not arise from systematic errors in the data or series termination errors, it seems possible that the six-parameter model of anisotropic vibration for the chlorine thermal motion is inadequate. A check on inter-layer scaling (a single scale factor had been used throughout refinement) proved satisfactory in that refining separate scale factors for data from each film pack produced no significant improvement in the agreement factors.

Positional and thermal parameters and their standard deviations as estimated from the inverse matrix are listed in Table 1. In Table 2 are given the root mean-square thermal amplitudes of vibration which may be derived from the data of Table 1. Table 3 contains values, in electrons, of $10F_o$ and $10F_c$ for all 772 observed reflexions, the values of F_c being based on the parameters in Table 1. The principal axis of vibration of the methyl carbon atom is in the mirror plane at $y = \frac{1}{4}$ and perpendicular to the C(9)-C(15) bond. For both anisotropic atoms, the smallest axis of vibration is, approximately, directed along the bond joining the atom to the ring skeleton.

Table 2. Root mean square amplitudes of vibration (\AA)

	Minimum	Intermediate	Maximum
Cl	0.193 (3)	0.249 (3)	0.344 (3)
C(15)	0.197 (20)	0.254 (12)	0.296 (14)

Results and discussion

Molecular dimensions and the crystallographic numbering scheme are shown in Fig. 1. Selected interatomic distances and angles are given in Table 4. Deviations from various weighted least-squares planes are listed in Table 5. A convenient point of reference for describing the molecular shape is the exact plane in the central ring defined by atoms C(11), C(11'), C(12) and C(12') (plane IV). Deviations of carbon and chlorine atoms from this plane are shown in Fig. 2.

Overcrowding of the *peri*-substituents has been relieved by a combination of in-plane and out-of-plane deformations giving a chlorine-methyl carbon separation of 2.99 \AA ; values of 2.9-3.1 \AA are well established from previous crystallographic results (Avoyan, Struchkov & Dashevskii, 1966). The most striking deforma-

tions are out of plane. The chlorine atoms are 0.33 Å from the mean molecular plane (plane I) while atoms C(9) and the methyl carbon, C(15), are on the opposite side of this plane and 0.19 and 0.80 Å respectively from it. In-plane distortion has arisen from adjustments to bond lengths and bond angles. Bonds C(9)-C(11) (longer by 0.03 Å) and C(3)-C(4) (shorter by 0.04 Å) differ significantly from those reported for anthracene (Mason, 1964); differences in bond lengths for C(1)-C(11) (longer by 0.01 Å) and C(2)-C(3) (shorter by 0.02 Å), while not statistically significant, are logical extensions of the changes to C(9)-C(11) and C(3)-C(4). These adjustments, coupled with decreases in angles Cl-C(1)-C(2), C(1)-C(11)-C(12) and C(11)-C(9)-C(11') to 115.8, 115.4 and 117.4° respectively and with increases in angles Cl-C(1)-C(11) and C(1)-C(11)-C(9) to 123.0° and 124.0°, result in a non-bonded separation of 2.55 Å for C(1)-C(9) compared with 2.46 Å for C(4)-C(10). Bond lengths for C(9)-C(15) and C(1)-Cl are similar to values found for compounds with the methyl carbon and chlorine atoms in similar environments (Avoyan *et al.*, 1966).

A χ^2 test shows that the outer rings are significantly non-planar (plane VI). This is best explained as a folding of each ring about a line joining C(3) and C(11). The atoms C(1), C(2), C(3) and C(11) are essentially coplanar (plane II) as are C(4), C(12), C(3) and C(11) (plane III), the angles between these planes being 5.0°. Plane III makes an angle of 1.3°

with the central ring plane. Out-of-plane deformation in the central ring plane is mainly confined to C(9) (0.12 Å away).

The chlorine atom is 0.24 Å from plane II compared with 0.33 Å from the mean molecular plane (plane I). C(15) is 0.80 Å away from plane I, 0.69 Å off the central ring plane and only 0.33 Å from plane V, formed by C(9)-C(11) and C(11'). Thus, out-of-plane distortions of the anthracene skeletons can be explained in terms of the ring atoms which are bonded to substi-

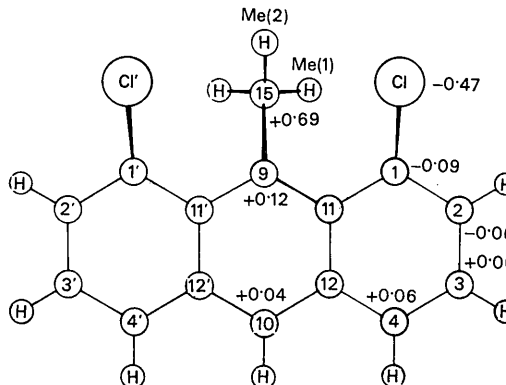


Fig. 2. Deviations (Å) of carbon and chlorine atoms of 1,8-dichloro-9-methylanthracene from the exact plane (IV) through carbon atoms 11, 11', 12, 12'.

Table 3. Structure factor amplitudes for 1,8-dichloro-9-methylanthracene (electrons $\times 10$)

The largest value of F_{calc} for the unobserved reflexions is 5.5 electrons.

K	L	OBS	CALC	K	L	OBS	CALC	K	L	OBS	CALC	K	L	OBS	CALC	K	L	OBS	CALC				
0	0	330	340	10	0	110	110	20	0	330	330	30	0	110	110	40	0	330	330	50	0	110	110
0	1	110	110	10	1	110	110	20	1	110	110	30	1	110	110	40	1	110	110	50	1	110	110
0	2	110	110	10	2	110	110	20	2	110	110	30	2	110	110	40	2	110	110	50	2	110	110
0	3	110	110	10	3	110	110	20	3	110	110	30	3	110	110	40	3	110	110	50	3	110	110
0	4	110	110	10	4	110	110	20	4	110	110	30	4	110	110	40	4	110	110	50	4	110	110
0	5	110	110	10	5	110	110	20	5	110	110	30	5	110	110	40	5	110	110	50	5	110	110
0	6	110	110	10	6	110	110	20	6	110	110	30	6	110	110	40	6	110	110	50	6	110	110
0	7	110	110	10	7	110	110	20	7	110	110	30	7	110	110	40	7	110	110	50	7	110	110
0	8	110	110	10	8	110	110	20	8	110	110	30	8	110	110	40	8	110	110	50	8	110	110
0	9	110	110	10	9	110	110	20	9	110	110	30	9	110	110	40	9	110	110	50	9	110	110
0	10	110	110	10	10	110	110	20	10	110	110	30	10	110	110	40	10	110	110	50	10	110	110
0	11	110	110	10	11	110	110	20	11	110	110	30	11	110	110	40	11	110	110	50	11	110	110
0	12	110	110	10	12	110	110	20	12	110	110	30	12	110	110	40	12	110	110	50	12	110	110
0	13	110	110	10	13	110	110	20	13	110	110	30	13	110	110	40	13	110	110	50	13	110	110
0	14	110	110	10	14	110	110	20	14	110	110	30	14	110	110	40	14	110	110	50	14	110	110
0	15	110	110	10	15	110	110	20	15	110	110	30	15	110	110	40	15	110	110	50	15	110	110
0	16	110	110	10	16	110	110	20	16	110	110	30	16	110	110	40	16	110	110	50	16	110	110
0	17	110	110	10	17	110	110	20	17	110	110	30	17	110	110	40	17	110	110	50	17	110	110
0	18	110	110	10	18	110	110	20	18	110	110	30	18	110	110	40	18	110	110	50	18	110	110
0	19	110	110	10	19	110	110	20	19	110	110	30	19	110	110	40	19	110	110	50	19	110	110
0	20	110	110	10	20	110	110	20	20	110	110	30	20	110	110	40	20	110	110	50	20	110	110

tuent [C(1) and C(9)] being forced out of plane in the direction of the substituent to which they are bonded.

Comparison with other overcrowded molecules

We know of no other reported crystal structure determination of an anthracene derivative with sub-

stituents in the 1,8,9 *peri* positions. However, the mechanism for the relief of overcrowding in the present case, a combination of out-of-plane deformations, and in-plane distortions involving changes to bond lengths and angles, is very similar to that generally observed for other overcrowded systems (Avoyan *et al.*, 1966).

Table 4. Selected distances (Å) and angles (°)

Intramolecular bonded distances		Bond angles	
C(1)—Cl	1.726 (7)	Cl—C(1)—C(2)	115.8 (5)
C(1)—C(2)	1.381 (9)	Cl—C(1)—C(11)	123.0 (5)
C(2)—C(3)	1.400 (10)	C(2)—C(1)—C(11)	120.6 (6)
C(3)—C(4)	1.333 (10)	C(1)—C(2)—C(3)	122.2 (7)
C(4)—C(12)	1.444 (9)	C(2)—C(3)—C(4)	119.3 (7)
C(11)—C(12)	1.426 (9)	C(3)—C(4)—C(12)	121.5 (8)
C(1)—C(11)	1.453 (8)	C(4)—C(12)—C(11)	120.6 (6)
C(11)—C(9)	1.433 (7)	C(4)—C(12)—C(10)	119.6 (7)
C(10)—C(12)	1.400 (8)	C(10)—C(12)—C(11)	119.7 (6)
C(9)—C(15)	1.506 (16)	C(12)—C(10)—C(12')	121.0 (9)
C(2)—H(2)	0.98 (9)	C(1)—C(11)—C(9)	124.0 (6)
C(3)—H(3)	1.11 (9)	C(1)—C(11)—C(12)	115.4 (5)
C(4)—H(4)	0.76 (8)	C(9)—C(11)—C(12)	120.6 (6)
C(10)—H(10)	1.11 (18)	C(11)—C(9)—C(11')	117.4 (8)
C(15)—HMe(1)	1.16 (8)	C(11)—C(9)—C(15)	120.5 (5)
C(15)—HMe(2)	1.27 (16)		
Intramolecular non-bonded distances		Dihedral angle*	
C(15)···Cl	2.994 (7)	Cl—C(1)—C(11) } C(15)—C(9)—C(11) }	34.8 (7)
C(1)···C(9)	2.548 (7)		
C(4)···C(10)	2.457 (8)		
Cl···HMe(1)	2.64		
Cl···HMe(2)	2.98		
Cl···H(2)	2.44		
Intermolecular distances†			
Cl···Cl	3.74		
Cl···C	3.36		
Cl···H	2.92		
C···C	3.53		
C···H	2.82		
H···H	2.2		

* Angles are between two plane each defined by three atoms.

† The shortest intermolecular distance of the type specified.

Table 5. Least-squares planes showing atomic deviations (Å)

Figures followed by an asterisk denote atoms not used to define the plane in question; additional atoms related by mirror plane were used in defining planes I, IV, V.

	I	II	III	IV	V	VI
C(1)	-0.023 (7)	-0.001 (7)	—	-0.089 (7)*	—	-0.020 (7)
C(2)	-0.024 (7)	0.002 (7)	—	-0.056 (7)*	—	-0.016 (7)
C(3)	0.027 (7)	-0.001 (7)	-0.006 (7)	0.056 (7)*	—	0.032 (7)
C(4)	0.001 (8)	—	0.014 (8)	0.056 (8)*	—	-0.002 (8)
C(11)	0.039 (6)	0.001 (6)	0.003 (6)	0	0	0.033 (6)
C(12)	-0.023 (7)	—	-0.009 (7)	0	—	-0.032 (7)
C(9)	0.188*	—	—	0.117*	0	—
C(10)	-0.017 (10)	—	—	0.036* (10)	—	—
Cl	-0.327*	-0.236*	—	-0.467*	—	-0.320*
C(15)	0.801*	—	—	0.690*	0.326*	—

Equations of planes referred to orthorhombic crystallographic axes. X, Y, Z are atomic coordinates in Å.

$$\begin{aligned}
 \text{I} & 0.5801X - 0.8145Z + 0.8349 = 0 \\
 \text{II} & 0.6906X - 0.0283Y - 0.7922Z + 0.9407 = 0 \\
 \text{III} & 0.5512X + 0.0215Y - 0.8341Z + 0.6802 = 0 \\
 \text{IV} & 0.5438X - 0.8392Z + 0.7445 = 0 \\
 \text{V} & 0.4056X - 0.9140Z + 0.5505 = 0 \\
 \text{VI} & 0.5816X - 0.0057Y - 0.8135Z + 0.8517 = 0
 \end{aligned}$$

In particular, the degree of out-of-plane deformation as given by the α parameter of Silverman & Yannoni (1967) agrees well with values obtained for systems as intrinsically overcrowded as 1,8-dichloro-9-methylanthracene. The angle α between planes formed by Cl-C(1)-C(11) and C(15)-C(9)-C(11) is 34.8° in this compound, compared with values of $25-40^\circ$ found for systems where the interacting atoms are at the ends of an hexagonal fragment of five atoms. The non-bonded separation for these atoms would be 2.4 \AA for exact trigonal bonding.

Molecular packing

Fig. 3 is a drawing of the contents of one unit cell projected on to the (010) plane. The packing is characterized by molecular pairs such as I and II which are related by glide planes perpendicular to the c axis. The anthracene skeletons of these pairs are practically perpendicular, the closest approach being 3.36 \AA between C(1) and Cl. Table 4 contains a list of the shortest intermolecular contacts between any two types of atom. With adjacent molecules perpendicular to each other, the crystal packing is thus of type 'A' (Robertson, 1951). Knowledge of the relative orientation of the monomer molecules may be useful in a study of the solid-state photodimerization of this compound (e.g. Schmidt, 1965; Craig & Sarti-Fantoni, 1966; Bouas-Laurent & Lapouyade, 1967).

The authors wish to thank Professor Henri Bouas-Laurent of the University of Bordeaux for suggesting this problem to us and for providing a sample. They are grateful to the originators of computer programs used in the work and also to Drs J.A. Ibers and R.J. Doedens for modifications incorporated in our local versions. Finally, they acknowledge grants for equipment made by the Research Committee of the New Zealand Universities Grants Committee.

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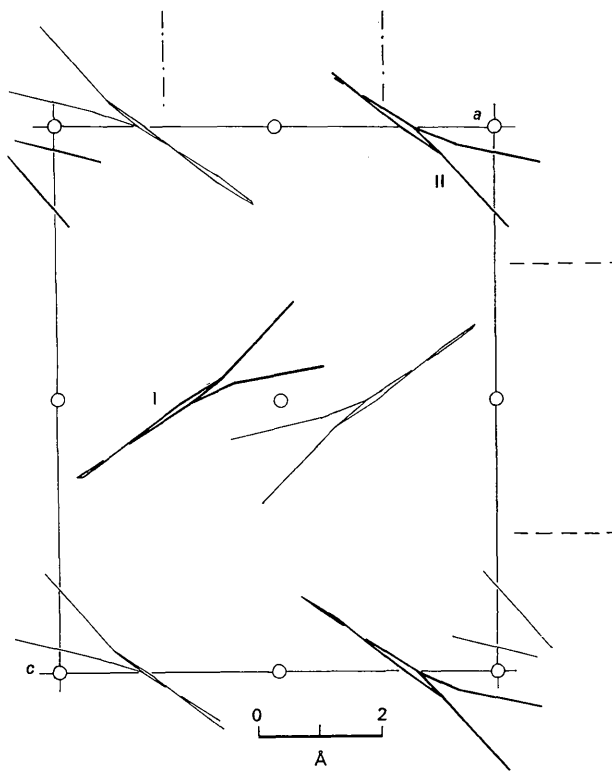


Fig. 3. Contents of the unit cell of 1,8-dichloro-9-methylanthracene projected onto the (010) face.