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The Structure of Decachloropyrene, C₁₆Cl₁₀: an Overcrowded Molecule

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Decachloropyrene is monoclinic, space group $P2_1/n$, with $a=21.462$ (10), $b=7.494$ (5), $c=10.803$ (7) Å, $\beta=92.8$ (1)°, $Z=4$. Least-squares refinement with 2655 reflexions gave a final R of 0.038 for 236 parameters. The molecule is saddle-shaped, the maximum deviations from planarity being ca 1 Å for Cl and ca 0.5 Å for C atoms. The mean nearest-neighbour Cl...Cl distance in the molecule is 3.003 (1) and the mean C-Cl distance 1.719 (1) Å. The C-C distances are similar to those of pyrene itself. The molecules are stacked in such a way that half the molecule is sandwiched between two neighbouring molecules and the other half is essentially free. The packing forces result in a deviation from $mm2$ molecular symmetry: both the out-of-plane deformations and the Cl...Cl distances are smaller for the half of the molecule which is compressed.

Introduction

Decachloropyrene is an overcrowded molecule; if it were planar there would be Cl...Cl distances, *e.g.* Cl(2)...Cl(4), of only 2.4 Å whereas the sum of the van der Waals radii is 3.6 Å, and the shortest Cl...Cl distances found in similar compounds are about 3.0 Å, as in octachloronaphthalene (Gafner & Herbstein, 1963). The strain may be relieved by a splaying of angles and by out-of-plane displacements. The ultraviolet spectrum of C₁₆Cl₁₀ is quite different from that of other substituted pyrenes (Mosby, 1955) suggesting that the pyrene skeleton is non-planar. Possible ways in which pyrene can deviate from planarity are indicated in Fig. 1. We find the molecule to be saddle-shaped, *i.e.* model I; packing forces however cause it to deviate from the ideal $mm2$ symmetry.

Crystal data

C₁₆Cl₁₀, $M=546.7$. Monoclinic, $a=21.462$ (10), $b=7.494$ (5), $c=10.803$ (7) Å, $\beta=92.8$ (1)°, $U=1735$ Å³,

$Z=4$, $D_c=2.09$ g cm⁻³. Space group $P2_1/n$. Packing coefficient 0.77. $\mu(\text{Mo } K\alpha)$ 15.9 cm⁻¹. The compound crystallizes from dioxane as yellow needles elongated along [010].

Experimental

The crystals were provided by Arne Berg.

A crystal, 0.01 × 0.14 × 0.015 cm, was mounted along **b** and intensities measured out to $\sin \theta_{\max}=0.5$ with a computer-steered Supper diffractometer (Kryger, 1975). Monochromatic Mo $K\alpha$ radiation was used with a scintillation counter and a pulse-height analyser. 2655 independent reflexions, for which $F_o^2 < 3.0\sigma(F_o^2)$ according to counting statistics, were used in the subsequent calculations. No correction was applied for absorption.

Determination and refinement of the structure

The structure was determined by direct methods (*MULTAN*, Germain, Main & Woolfson, 1971). Least-squares refinement of atomic coordinates, anisotropic thermal parameters, a scale factor and an isotropic extinction coefficient, g , gave a final R of 0.038 ($R_w=0.040$) for 236 parameters.

The value obtained for g was 5.2 (6) × 10⁻⁷ with f

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assumed to be unity; the minimum value of $F_o/F_o(\text{corr})$ was 0.84. A final difference map showed a maximum electron density of $0.35 \text{ e } \text{Å}^{-3}$.

Atomic coordinates and thermal parameters are listed in Table 1.*

The thermal motion of the atoms was analysed, assuming that the molecule could be treated as a rigid body (Schomaker & Trueblood, 1968). **T**, **L**, and **S** are given in Table 2. The value of **L** was used to correct the bond lengths for thermal motion.

* A list of structure factors has been deposited with the British Library Lending Division as Supplementary Publication No. SUP 31311 (12 pp., 1 microfiche). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 13 White Friars, Chester CH1 1NZ, England.

Bond lengths and selected short intramolecular distances are given in Table 3, angles within the molecule in Table 4. The atomic numbering and bond labelling are in Fig. 2(a). Torsion angles and out-of-plane angles are shown in Fig. 2(b), short intermolecular distances in Table 5.

Computational details

Calculations were carried out on RC4000 and CDC6400 computers with the following programs: Data reduction (Kryger, 1975), averaging of symmetry-related reflexions, *DSORTH*, State University of New York at Buffalo; Fourier syntheses, *JIMDAP*, A. Zalkin, Lawrence Radiation Laboratory; full-matrix least-squares refinement, *LINUS* (Busing, Martin &

Table 1. Fractional atomic coordinates ($\times 10^5$) and thermal parameters ($\text{Å}^2 \times 10^{-4}$) and their standard deviations

	<i>x</i>	<i>y</i>	<i>z</i>	<i>U</i> ₁₁	<i>U</i> ₂₂	<i>U</i> ₃₃	<i>U</i> ₁₂	<i>U</i> ₁₃	<i>U</i> ₂₃
Cl(1)	95844 (5)	17228 (16)	-14471 (13)	291 (5)	784 (7)	860 (9)	-32 (5)	139 (5)	-17 (7)
Cl(2)	90173 (4)	8152 (15)	9768 (10)	344 (5)	767 (7)	543 (6)	8 (5)	-121 (5)	-35 (6)
Cl(4)	79814 (5)	-14328 (13)	19178 (9)	592 (6)	594 (6)	316 (5)	58 (5)	-61 (5)	76 (5)
Cl(5)	65938 (5)	-10958 (15)	19810 (9)	551 (6)	805 (7)	291 (5)	-188 (6)	106 (4)	36 (5)
Cl(7)	57294 (5)	20136 (17)	12657 (11)	480 (6)	944 (8)	554 (7)	39 (6)	197 (5)	-279 (6)
Cl(8)	49384 (5)	27237 (16)	-10686 (13)	304 (5)	819 (7)	891 (9)	126 (5)	83 (6)	-93 (7)
Cl(9)	53961 (5)	20113 (17)	-35995 (12)	532 (7)	818 (7)	639 (8)	217 (6)	-199 (6)	57 (6)
Cl(11)	63678 (6)	1882 (15)	-49715 (9)	704 (7)	701 (6)	311 (5)	-88 (5)	-66 (6)	-4 (5)
Cl(12)	77295 (5)	-1538 (14)	-50710 (9)	761 (8)	575 (6)	288 (5)	188 (5)	159 (5)	8 (4)
Cl(14)	88614 (5)	15740 (14)	-38793 (11)	537 (6)	640 (6)	589 (7)	105 (5)	317 (5)	176 (5)
C(1)	88175 (15)	10794 (45)	-14605 (38)	263 (17)	415 (19)	590 (24)	56 (15)	72 (17)	9 (18)
C(2)	85496 (15)	6716 (47)	-3506 (35)	266 (17)	415 (18)	441 (21)	26 (15)	-5 (16)	-26 (17)
C(3)	79155 (15)	3231 (41)	-3194 (31)	319 (18)	318 (16)	309 (17)	9 (14)	21 (15)	-41 (14)
C(4)	75948 (16)	-2562 (43)	7625 (30)	365 (20)	378 (17)	259 (17)	-10 (15)	-29 (15)	-29 (14)
C(5)	69721 (17)	-864 (46)	8007 (30)	423 (20)	440 (19)	228 (16)	-90 (16)	69 (15)	-57 (15)
C(6)	66107 (14)	7008 (42)	-2160 (30)	273 (16)	351 (16)	317 (17)	-74 (14)	48 (14)	-94 (14)
C(7)	60165 (16)	14059 (47)	-1272 (35)	308 (17)	454 (19)	436 (21)	-73 (16)	107 (16)	-124 (17)
C(8)	56636 (16)	18162 (46)	-11903 (38)	250 (17)	415 (19)	570 (25)	-1 (15)	22 (18)	-102 (18)
C(9)	58896 (16)	15100 (44)	-23623 (35)	348 (19)	348 (17)	455 (22)	-6 (15)	-65 (17)	7 (17)
C(10)	65086 (15)	9748 (39)	-24843 (31)	344 (18)	269 (15)	330 (18)	10 (14)	-16 (15)	9 (15)
C(11)	68049 (17)	6179 (42)	-36409 (30)	500 (22)	296 (16)	246 (17)	-4 (16)	-13 (16)	47 (14)
C(12)	74301 (18)	4915 (43)	-36849 (31)	531 (23)	341 (17)	249 (18)	83 (16)	111 (16)	38 (15)
C(13)	78339 (15)	6895 (41)	-25902 (31)	381 (19)	270 (15)	313 (19)	79 (14)	74 (15)	37 (14)
C(14)	84746 (16)	10213 (42)	-25691 (34)	379 (19)	342 (17)	433 (20)	81 (15)	182 (17)	52 (16)
C(15)	75462 (15)	5087 (38)	-14320 (30)	312 (17)	254 (15)	282 (17)	20 (13)	51 (14)	-22 (13)
C(16)	68817 (14)	6774 (40)	-13874 (30)	270 (15)	282 (14)	295 (17)	-10 (13)	25 (13)	-26 (14)

Table 2. **T**, **L**, and **S** and their estimated standard deviations relative to an orthogonal axial system with *A* parallel to **a** and *C* parallel to **c***

T is in $\text{Å}^2 \times 10^{-4}$, **L** in $(^\circ)^2$, and **S** in $(^\circ) \text{Å} \times 10^{-4}$. **A_L** and **A_M** are matrices for transforming the principal axes of **L** and the molecular axes respectively to the orthogonal axes.

$$\mathbf{T} = \begin{pmatrix} 298 & 7 & 22 \\ & 179 & -31 \\ & & 268 \end{pmatrix} \quad \mathbf{L} = \begin{pmatrix} 10.6 & -0.1 & 0.1 \\ & 6.9 & -0.1 \\ & & 8.4 \end{pmatrix} \quad \mathbf{S} = \begin{pmatrix} 563 & -641 & 1734 \\ -741 & -595 & -105 \\ 818 & -395 & 33 \end{pmatrix}$$

$$\sigma(\mathbf{T}) = \begin{pmatrix} 8 & 8 & 7 \\ & 13 & 9 \\ & & 9 \end{pmatrix} \quad \sigma(\mathbf{L}) = \begin{pmatrix} 0.5 & 0.3 & 0.2 \\ & 0.3 & 0.2 \\ & & 0.3 \end{pmatrix} \quad \sigma(\mathbf{S}) = \begin{pmatrix} 225 & 93 & 170 \\ 81 & 152 & 75 \\ 142 & 77 & 2047^* \end{pmatrix}$$

R.m.s. $\delta = 0.0033$ where $\delta = U_{ij} \text{ obs.} - U_{ij} \text{ calc.}$

$$\mathbf{A}_L = \begin{pmatrix} 0.9992 & -0.0228 & 0.0341 \\ 0.0354 & 0.0731 & -0.9967 \\ 0.0204 & 0.9971 & 0.0738 \end{pmatrix} \quad \mathbf{A}_M = \begin{pmatrix} 0.9957 & -0.0796 & -0.0475 \\ -0.0394 & 0.1003 & -0.9942 \\ 0.0839 & -0.9918 & -0.0967 \end{pmatrix}$$

* The trace of **S** has been set to zero, e.s.d. of deleted *S*(3,3) is given.

Table 3. Bond lengths and selected short intramolecular distances l (Å), and the corresponding distances corrected for thermal vibration

	l	l_{corr}		l	l_{corr}
<i>a</i> C(1)—C(2)	1.389 (5)	1.393	<i>g</i> C(1)—Cl(1)	1.714 (4)	1.718
<i>a</i> C(1)—C(14)	1.375 (5)	1.379	<i>g</i> C(8)—Cl(8)	1.710 (4)	1.714
<i>a</i> C(7)—C(8)	1.379 (5)	1.383	<i>h</i> C(2)—Cl(2)	1.713 (4)	1.718
<i>a</i> C(8)—C(9)	1.397 (5)	1.400	<i>h</i> C(7)—Cl(7)	1.715 (4)	1.720
<i>b</i> C(2)—C(3)	1.388 (5)	1.391	<i>h</i> C(9)—Cl(9)	1.706 (4)	1.710
<i>b</i> C(6)—C(7)	1.388 (5)	1.391	<i>h</i> C(14)—Cl(14)	1.726 (4)	1.730
<i>b</i> C(9)—C(10)	1.400 (5)	1.403	<i>i</i> C(4)—Cl(4)	1.710 (4)	1.714
<i>b</i> C(13)—C(14)	1.397 (5)	1.400	<i>i</i> C(5)—Cl(5)	1.720 (4)	1.724
<i>c</i> C(3)—C(15)	1.414 (5)	1.418	<i>i</i> C(11)—Cl(11)	1.708 (4)	1.713
<i>c</i> C(6)—C(16)	1.418 (5)	1.422	<i>i</i> C(12)—Cl(12)	1.727 (3)	1.732
<i>c</i> C(10)—C(16)	1.415 (5)	1.419	Cl(1)—Cl(2)	3.019 (3)	3.026
<i>c</i> C(13)—C(15)	1.429 (4)	1.432	Cl(1)—Cl(14)	2.988 (3)	2.995
<i>d</i> C(3)—C(4)	1.452 (5)	1.455	Cl(8)—Cl(7)	3.018 (3)	3.025
<i>d</i> C(5)—C(6)	1.440 (5)	1.443	Cl(8)—Cl(9)	2.998 (3)	3.006
<i>d</i> C(10)—C(11)	1.454 (5)	1.458	Cl(2)—Cl(4)	3.006 (2)	3.014
<i>d</i> C(12)—C(13)	1.439 (5)	1.443	Cl(5)—Cl(7)	3.054 (2)	3.062
<i>e</i> C(15)—C(16)	1.435 (4)	1.438	Cl(9)—Cl(11)	2.952 (3)	2.960
<i>f</i> C(4)—C(5)	1.345 (5)	1.348	Cl(12)—Cl(14)	2.988 (3)	2.996
<i>f</i> C(11)—C(12)	1.348 (5)	1.351	Cl(4)—Cl(5)	2.993 (2)	3.000
			Cl(11)—Cl(12)	2.940 (2)	2.948

Table 4. Bond angles (°)

The lower case letters refer to the notation in Fig. 2, e.g. *ab* means the angle between bonds *a* and *b*.

<i>aa</i> C(14)—C(1)—C(2)	121.2 (3)	<i>df</i> C(3)—C(4)—C(5)	120.5 (3)
<i>aa</i> C(7)—C(8)—C(9)	121.1 (3)	<i>df</i> C(6)—C(5)—C(4)	121.0 (3)
<i>ab</i> C(1)—C(2)—C(3)	120.7 (3)	<i>df</i> C(10)—C(11)—C(12)	121.4 (3)
<i>ab</i> C(6)—C(7)—C(8)	119.8 (3)	<i>df</i> C(13)—C(12)—C(11)	121.6 (3)
<i>ab</i> C(8)—C(9)—C(10)	120.4 (3)	<i>ag</i> C(2)—C(1)—Cl(1)	119.5 (3)
<i>ab</i> C(13)—C(14)—C(1)	120.3 (3)	<i>ag</i> C(14)—C(1)—Cl(1)	119.3 (3)
<i>bc</i> C(2)—C(3)—C(15)	118.1 (3)	<i>ag</i> C(7)—C(8)—Cl(8)	119.3 (3)
<i>bc</i> C(7)—C(6)—C(16)	119.0 (3)	<i>ag</i> C(9)—C(8)—Cl(8)	119.5 (3)
<i>bc</i> C(9)—C(10)—C(15)	117.8 (3)	<i>ah</i> C(1)—C(2)—Cl(2)	117.3 (3)
<i>bc</i> C(14)—C(13)—C(15)	118.0 (3)	<i>ah</i> C(8)—C(7)—Cl(7)	117.7 (3)
<i>bd</i> C(2)—C(3)—C(4)	125.5 (3)	<i>ah</i> C(8)—C(9)—Cl(9)	116.4 (3)
<i>bd</i> C(5)—C(6)—C(7)	124.5 (3)	<i>ah</i> C(1)—C(14)—Cl(14)	116.6 (3)
<i>bd</i> C(9)—C(10)—C(11)	126.2 (3)	<i>bh</i> C(3)—C(2)—Cl(2)	121.8 (3)
<i>bd</i> C(12)—C(13)—C(14)	125.8 (3)	<i>bh</i> C(6)—C(7)—Cl(7)	122.2 (3)
<i>cd</i> C(4)—C(3)—C(15)	116.5 (3)	<i>bh</i> C(10)—C(9)—Cl(9)	123.0 (3)
<i>cd</i> C(5)—C(6)—C(16)	116.5 (3)	<i>bh</i> C(13)—C(14)—Cl(14)	122.8 (3)
<i>cd</i> C(9)—C(10)—C(16)	117.8 (3)	<i>di</i> C(3)—C(4)—Cl(4)	120.6 (3)
<i>cd</i> C(12)—C(13)—C(15)	116.2 (3)	<i>di</i> C(6)—C(5)—Cl(5)	119.3 (3)
<i>ce</i> C(3)—C(15)—C(16)	119.8 (3)	<i>di</i> C(10)—C(11)—Cl(11)	120.8 (3)
<i>ce</i> C(6)—C(16)—C(15)	118.9 (3)	<i>di</i> C(13)—C(12)—Cl(12)	120.4 (3)
<i>ce</i> C(10)—C(16)—C(15)	120.6 (3)	<i>fi</i> C(5)—C(4)—Cl(4)	118.3 (3)
<i>ce</i> C(13)—C(15)—C(16)	119.6 (3)	<i>fi</i> C(4)—C(5)—Cl(5)	119.1 (3)
<i>cc</i> C(3)—C(15)—C(13)	120.4 (3)	<i>fi</i> C(12)—C(11)—Cl(11)	117.6 (3)
<i>cc</i> C(6)—C(16)—C(10)	120.3 (3)	<i>fi</i> C(11)—C(12)—Cl(12)	117.6 (3)

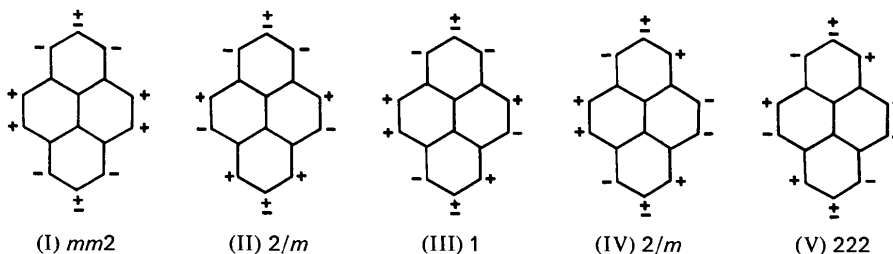


Fig. 1. Possible modes of out-of-plane distortion and their maximum symmetries; + and - denote displacements from the plane defined by the six central atoms, \pm is the displacement from the plane defined by the neighbouring atoms and may be in either direction.

Table 5. Intermolecular contacts less than 3.65 Å

Symmetry code

(i)	$1\frac{1}{2}-x, -\frac{1}{2}+y, -\frac{1}{2}-z$	(v)	$1-x, -y, -z$
(ii)	$x, y, 1+z$	(vi)	$\frac{1}{2}+x, \frac{1}{2}-y, -\frac{1}{2}+z$
(iii)	$1\frac{1}{2}-x, -\frac{1}{2}+y, \frac{1}{2}-z$	(vii)	$2-x, -y, -z$
(iv)	$\frac{1}{2}+x, \frac{1}{2}-y, \frac{1}{2}+z$		

Molecules within a stack are related by symmetry operation (i).

Cl(1)—Cl(9 ⁱ)	3.531 (3)	Cl(16)—Cl(14 ⁱ)	3.483 (4)
Cl(4)—Cl(11 ⁱ)	3.615 (3)	Cl(4)—Cl(12 ⁱⁱ)	3.459 (3)
Cl(11)—Cl(2 ⁱ)	3.538 (3)	Cl(5)—Cl(11 ⁱⁱⁱ)	3.487 (3)
Cl(11)—Cl(1 ⁱ)	3.477 (4)	Cl(4)—Cl(7 ⁱⁱⁱ)	3.512 (3)
Cl(11)—Cl(2 ⁱ)	3.406 (4)	Cl(5)—Cl(2 ⁱⁱⁱ)	3.497 (3)
Cl(12)—Cl(6 ⁱ)	3.422 (3)	Cl(1)—Cl(9 ^{iv})	3.588 (4)
Cl(12)—Cl(16 ⁱ)	3.579 (4)	Cl(2)—Cl(9 ^{iv})	3.389 (2)
C(1)—Cl(9 ⁱ)	3.484 (4)	Cl(8)—Cl(5 ^v)	3.600 (3)
C(6)—Cl(14 ⁱ)	3.384 (4)	Cl(14)—Cl(8 ^{vi})	3.427 (3)
Cl(14)—C(9 ⁱ)	3.648 (5)	Cl(1)—Cl(2 ^{vii})	3.568 (2)

Levy, 1962; Coppens & Hamilton, 1970); distances and angles, *ORFFE* (Busing, Martin & Levy, 1964); drawings, *ORTEP* (Johnson, 1965).

The quantity minimized was $r = \sum w(|F_o| - |F_c|)^2 / \sum w|F_o|^2$ where $w = [(\sigma(F_o^2) + 1.02F_o^2)^{1/2} - |F_o|]^{-2}$. The scattering factors were those of Cromer & Mann (1968). R and R_w are defined as $R = \sum ||F_o| - |F_c|| / \sum |F_o|$ and $R_w = [\sum w(|F_o| - |F_c|)^2 / \sum w|F_o|^2]^{1/2}$.

Discussion

The decachloropyrene molecule is not planar but is saddle-shaped as in model I (Fig. 1); the deviations from planarity are given in Table 6 which gives atomic coordinates in a molecular axial system. The central part of the pyrene molecule is almost planar, *i.e.* C(3),

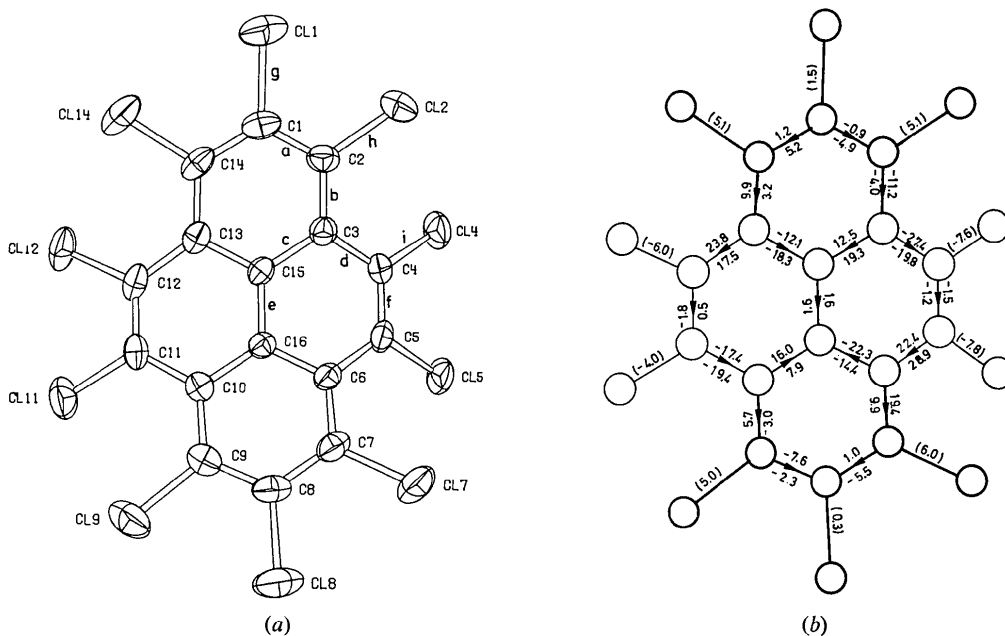


Fig. 2. (a) The molecule showing the numbering of the atoms and the labelling of the bonds. (b) Torsion angles and, in parentheses, the angles between C—C bonds and the plane defined by the neighbouring three atoms. Standard deviations are in the range 0.4 to 0.5°. A positive torsion angle $i-j-k-l$ is defined such that when looking along $j-k$ a clockwise rotation makes $i-j$ superimpose $k-l$. In the diagram the arrows point from j towards k .

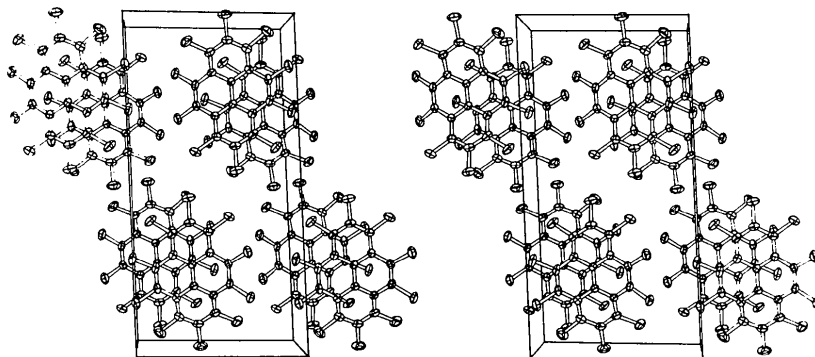


Fig. 3. A stereo view of the unit cell contents as seen down $[0\bar{1}0]$; a is up the page, c across.

C(6), C(10), C(13), C(15), and C(16). Torsion about bonds of type *c* together with a splaying of angles *bd*, *bh*, and *di* (Table 7) and out-of-plane displacements of the substituent groups suffice to increase the short Cl...Cl distance from 2.4 to 3.003 (1) Å, which is similar to that found in other halogenated aromatic compounds: octachloronaphthalene 3.032 (2) Å, 1,3,6,8-tetrafluoro-2,4,5,7,9,10-hexachloropyrene, 2.968 (2) Å (Hazell & Weigelt, 1976) and 1,10-dichloro-3,8-dimethyl-4,7-phenanthroline, 3.082 (2) Å (Herbstein & Kapon, 1972).

Table 6. Coordinates, in Å, relative to an axial system calculated for the atoms marked with asterisks

X is along the molecule, Z perpendicular to the molecule, the standard deviations are approximately 0.004 Å for C atoms and 0.001 Å for Cl atoms.

	X	Y	Z
C(1)	-3.406	-0.007	0.631
C(2)	-2.756	-1.213	0.382
C(3)*	-1.418	-1.233	0.002
C(4)	-0.669	-2.419	-0.387
C(5)	0.679	-2.409	-0.379
C(6)*	1.410	-1.237	0.038
C(7)	2.738	-1.244	0.456
C(8)	3.422	-0.050	0.590
C(9)	2.809	1.174	0.292
C(10)*	1.437	1.228	0.002
C(11)	0.671	2.427	-0.319
C(12)	-0.680	2.426	-0.295
C(13)*	-1.430	1.239	0.038
C(14)	-2.778	1.201	0.413
C(15)*	-0.719	-0.001	-0.040
C(16)*	0.720	0.004	-0.040
Cl(1)	-5.005	-0.022	1.261
Cl(2)	-3.625	-2.658	0.710
Cl(4)	-1.467	-3.770	-1.076
Cl(5)	1.532	-3.728	-1.091
Cl(7)	3.522	-2.679	0.988
Cl(8)	5.046	-0.070	1.136
Cl(9)	3.784	2.570	0.449
Cl(11)	1.455	3.852	-0.853
Cl(12)	-1.493	3.850	-0.852
Cl(14)	-3.692	2.626	0.773

Table 7. Mean values of selected angles, showing the splaying of angles on going from C₁₆H₁₀ to C₁₆F₄Cl₆ to C₁₆Cl₁₀

	C ₁₆ H ₁₀	C ₁₆ F ₄ Cl ₆	Δ	C ₁₆ Cl ₁₀	Δ
<i>bd</i>	122.1 (1)	123.6 (2)	1.5	125.5 (2)	3.4
<i>bh</i>	118.9 (2)	121.6 (2)	2.7	122.5 (2)	3.6
<i>di</i>	118.7 (2)	120.8 (2)	2.1	120.3 (2)	1.6

The C-C distances are very similar to those in pyrene and substituted pyrenes (Table 8); comparison has been made with structures determined by X-ray diffraction as there are systematic differences between the bond distances determined by X-ray and neutron diffraction (Hazell, Larsen & Lehmann, 1972). Although deviations from planarity should lead to an increase in bond distances, the changes observed do not correlate with the torsion angles.

Table 8. Comparison of mean bond lengths (Å) with those of pyrene

The values for pyrene are the mean of the observed values for pyrene (Allmann, 1970), 2,7-di-*t*-butylpyrene (Hazell & Lomborg, 1972) and pyrene/TCNE (Larsen, Little & Coppens, 1975). τ is the mean torsion angle for the bond, Δ the difference between the values for C₁₆Cl₁₀ and C₁₆H₁₀.

	C ₁₆ H ₁₀	C ₁₆ Cl ₁₀	Δ	τ (°)
<i>a</i>	1.388 (1)	1.389 (3)	0.001 (3)	3.3 (2)
<i>b</i>	1.399 (1)	1.395 (3)	-0.004 (3)	7.5 (2)
<i>c</i>	1.421 (1)	1.423 (3)	0.002 (3)	15.3 (2)
<i>d</i>	1.437 (1)	1.450 (3)	0.013 (3)	22.1 (2)
<i>e</i>	1.423 (1)	1.438 (4)	0.015 (4)	1.6 (3)
<i>f</i>	1.345 (1)	1.350 (4)	0.005 (4)	1.0 (3)

The packing is shown in Fig. 3. The crystal is composed of stacks of molecules with the stack axes parallel to **b**. The molecules within a stack are related by a screw axis and do not overlap completely, which results in part of the molecule being essentially free. The packing forces result in one half of the molecule being compressed resulting in smaller out-of-plane deformations, $\langle|\Delta|\rangle = 0.812$ for Cl(8) to Cl(14) and $\langle|\Delta|\rangle = 1.025$ Å for Cl(1) to Cl(7). The Cl...Cl distances in the compressed half of the molecule are also shorter, 2.981 (1) compared with 3.025 (1) Å. A similar effect has been observed by Gafner & Herbstein (1963) for octachloronaphthalene.

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