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The Structure of the Molecular Compound Decachloropyrene: Benzene, $C_{16}Cl_{10}:C_6H_6$

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The molecular compound between decachloropyrene and benzene is monoclinic, space group $P2_1/c$, with $a = 18.043$ (9), $b = 7.180$ (4), $c = 17.579$ (8) Å, $\beta = 98.75$ (0.2)°, $Z = 4$. Least-squares refinement with 3601 reflexions [$I > 3\sigma(I)$] gave $R = 0.046$ and $R_w = 0.053$ for 314 parameters. The molecule is saddle-shaped, the maximum deviations from planarity being ca 1 Å for Cl and ca 0.5 Å for C. The mean nearest-neighbour Cl...Cl distance in the molecule is 3.025 (1) Å, the mean C—Cl distance is 1.721 (1) Å. The geometry is similar to that found in decachloropyrene itself. The molecules pack in columns of alternating decachloropyrene and benzene molecules parallel to **b**.

Introduction

Decachloropyrene is an overcrowded molecule. The strain is relieved by a splaying of angles and by large out-of-plane displacements (Hazell & Jagner, 1976) to give a saddle-shaped molecule. Packing forces cause the decachloropyrene molecule to deviate from the ideal $mm2$ symmetry. The structure of decachloropyrene:benzene has been determined to compare the geometries of the decachloropyrene molecule in different environments. The decachloropyrene molecules

will be referred to as DCP and DCPB in the two compounds.

Crystal data

$C_{16}Cl_{10}:C_6H_6$, $M_r = 624.8$, monoclinic, $a = 18.043$ (9), $b = 7.180$ (4), $c = 17.579$ (8) Å, $\beta = 98.75$ (0.2)°, $U = 2251$ Å³, $Z = 4$, $D_c = 1.84$ g cm⁻³, space group $P2_1/c$. Packing coefficient 0.75, $\mu(\text{Mo K}\alpha)$ 12.6 cm⁻¹.

Table 1. Fractional atomic coordinates (for Cl and C $\times 10^4$; for H $\times 10^3$)

	<i>x</i>	<i>y</i>	<i>z</i>
Cl(1)	5484 (1)	2955 (2)	4709 (1)
Cl(2)	4678 (1)	2253 (2)	6058 (1)
Cl(4)	3421 (1)	-131 (2)	6465 (1)
Cl(5)	1747 (1)	-158 (2)	6133 (1)
Cl(7)	572 (1)	2400 (2)	5279 (1)
Cl(8)	-183 (1)	2883 (2)	3638 (1)
Cl(9)	668 (1)	2538 (2)	2301 (1)
Cl(11)	1898 (1)	95 (2)	1850 (1)
Cl(12)	3583 (1)	-36 (2)	2220 (1)
Cl(14)	4690 (1)	2759 (2)	3064 (1)
C(1)	4571 (2)	2229 (5)	4542 (2)
C(2)	4196 (2)	1866 (5)	5153 (2)
C(3)	3429 (2)	1333 (5)	5026 (2)
C(4)	2990 (2)	800 (5)	5611 (2)
C(5)	2229 (2)	784 (5)	5460 (2)
C(6)	1836 (2)	1302 (5)	4716 (2)
C(7)	1075 (2)	1825 (5)	4558 (2)
C(8)	729 (2)	2109 (5)	3810 (3)
C(9)	1122 (2)	1904 (5)	3194 (2)
C(10)	1881 (2)	1392 (5)	3320 (2)
C(11)	2322 (2)	936 (5)	2726 (2)
C(12)	3079 (2)	931 (5)	2879 (2)
C(13)	3469 (2)	1432 (5)	3630 (2)
C(14)	4216 (2)	2034 (5)	3783 (2)
C(15)	3057 (2)	1276 (5)	4252 (2)
C(16)	2250 (2)	1258 (5)	4096 (2)
C(17)	2838 (4)	6127 (8)	4015 (5)
C(18)	2380 (4)	6344 (8)	3326 (4)
C(19)	1627 (4)	6592 (8)	3313 (4)
C(20)	1341 (4)	6579 (8)	3966 (5)
C(21)	1803 (6)	6353 (9)	4659 (5)
C(22)	2550 (5)	6137 (9)	4679 (4)
H(17)	331 (4)	584 (9)	398 (4)
H(18)	253 (4)	641 (8)	281 (4)
H(19)	134 (4)	666 (8)	282 (4)
H(20)	90 (5)	677 (10)	404 (5)
H(21)	158 (4)	651 (9)	505 (4)
H(22)	286 (4)	589 (9)	520 (4)

Table 2. **T**, **L** and **S** for the decachloropyrene molecule

T is in $\text{\AA}^2 \times 10^{-4}$, **L** in deg^2 , **S** in $\text{\AA} \text{deg} \times 10^{-3}$. The trace of **S** has been set to zero, the e.s.d. of deleted S_{33} is given. R.m.s. $\delta u = 0.0054 \text{\AA}^2$. **T**, **L** and **S** are referred to orthogonal axes, **A**||**a**, **C**||**c*** and **B**⊥**A** and **C**.

<i>ij</i>	11	22	33	12	13	23
T_{ij}	260 (13)	174 (21)	251 (14)	0 (13)	25 (11)	-10 (14)
L_{ij}	13.8 (0.7)	4.6 (0.4)	8.1 (0.5)	0.1 (0.5)	2.1 (0.4)	0.4 (0.4)
S_{ij}	-47 (36)	44 (25)	22 (329)	4 (15)	-150 (27)	28 (12)
S_{ii}				26 (13)	13 (23)	-36 (12)

Experimental

The crystals, which were provided by Arne Berg, were obtained by crystallization from a benzene solution. As the crystals lose benzene on standing, the crystal, $0.3 \times 0.3 \times 0.4$ mm, was sealed in a Lindemann-glass capillary together with a piece of filter paper soaked in

Table 3. Bond lengths and selected short intramolecular distances *l* (\AA) and for decachloropyrene the corresponding distances corrected for thermal vibration

		<i>l</i>	<i>l</i> _{corr}
See Fig. 1(a) for the labelling of the bonds.			
<i>a</i>	C(1)–C(2)	1.378 (6)	1.382
<i>a</i>	C(1)–C(14)	1.396 (6)	1.399
<i>a</i>	C(7)–C(8)	1.383 (6)	1.386
<i>a</i>	C(8)–C(9)	1.388 (6)	1.392
<i>b</i>	C(2)–C(3)	1.419 (6)	1.422
<i>b</i>	C(13)–C(14)	1.401 (5)	1.403
<i>b</i>	C(6)–C(7)	1.410 (6)	1.413
<i>b</i>	C(9)–C(10)	1.402 (6)	1.405
<i>c</i>	C(3)–C(15)	1.425 (6)	1.428
<i>c</i>	C(13)–C(15)	1.416 (5)	1.420
<i>c</i>	C(6)–C(16)	1.412 (6)	1.416
<i>c</i>	C(10)–C(16)	1.427 (6)	1.431
<i>d</i>	C(3)–C(4)	1.442 (6)	1.446
<i>d</i>	C(12)–C(13)	1.445 (6)	1.448
<i>d</i>	C(5)–C(6)	1.439 (6)	1.443
<i>d</i>	C(10)–C(11)	1.444 (6)	1.448
<i>e</i>	C(15)–C(16)	1.440 (5)	1.443
<i>f</i>	C(4)–C(5)	1.359 (6)	1.362
<i>f</i>	C(11)–C(12)	1.351 (6)	1.353
<i>g</i>	C(1)–Cl(1)	1.711 (4)	1.714
<i>g</i>	C(8)–Cl(8)	1.720 (4)	1.723
<i>h</i>	C(2)–Cl(2)	1.715 (5)	1.719
<i>h</i>	C(14)–Cl(14)	1.712 (5)	1.717
<i>h</i>	C(7)–Cl(7)	1.716 (5)	1.721
<i>h</i>	C(9)–Cl(9)	1.718 (5)	1.722
<i>i</i>	C(4)–Cl(4)	1.717 (5)	1.722
<i>i</i>	C(12)–Cl(12)	1.725 (4)	1.729
<i>i</i>	C(5)–Cl(5)	1.710 (4)	1.715
<i>i</i>	C(11)–Cl(11)	1.721 (5)	1.726
	Cl(1)–Cl(2)	3.007 (4)	3.015
	Cl(2)–Cl(4)	3.012 (3)	3.020
	Cl(4)–Cl(5)	2.989 (3)	2.995
	Cl(5)–Cl(7)	3.025 (4)	3.033
	Cl(7)–Cl(8)	3.016 (5)	3.023
	Cl(8)–Cl(9)	3.006 (5)	3.015
	Cl(9)–Cl(11)	3.029 (3)	3.036
	Cl(11)–Cl(12)	3.012 (3)	3.018
	Cl(12)–Cl(14)	3.052 (4)	3.060
	Cl(14)–Cl(1)	3.029 (5)	3.036
	C(17)–C(18)	1.367 (9)	
	C(18)–C(19)	1.367 (9)	
	C(19)–C(20)	1.329 (10)	1.399 (3)*
	C(20)–C(21)	1.377 (11)	
	C(21)–C(22)	1.352 (11)	
	C(22)–C(17)	1.348 (10)	
	C(17)–H(17)	0.90 (7)	
	C(18)–H(18)	0.99 (6)	
	C(19)–H(19)	0.94 (6)	0.96 (3)*
	C(20)–H(20)	0.83 (8)	
	C(21)–H(21)	0.85 (7)	
	C(22)–H(22)	1.01 (7)	

* Values from constrained refinement.

the mother liquor. The crystal 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. 6536

Table 4. Bond angles ($^{\circ}$) compared with those of DCP

Lower-case letters refer to bonds, TL, TR, BL, BR refer to the top left and right and bottom left and right sides of the molecules (Fig. 1).

	TL	TR	BL	BR	Mean	DCP*
aa	121.1 (4)		121.1 (4)		121.1 (3)	121.2 (2)
ab	120.7 (4)	120.2 (4)	120.7 (4)	120.4 (4)	120.6 (2)	120.3 (2)
bc	117.6 (4)	118.6 (4)	117.9 (4)	118.1 (4)	118.1 (2)	118.2 (2)
bd	126.0 (4)	125.0 (4)	125.3 (4)	125.3 (4)	125.4 (2)	125.5 (2)
cc	120.6 (4)		120.7 (4)		120.7 (3)	120.4 (2)
cd	116.3 (4)	116.4 (3)	116.8 (4)	116.5 (3)	116.5 (2)	116.8 (2)
de	120.8 (4)	121.3 (4)	121.2 (4)	120.6 (4)	121.0 (2)	121.1 (2)
cf	119.9 (4)	119.2 (4)	119.4 (4)	119.5 (4)	119.5 (2)	119.7 (2)
ag	119.9 (3)	119.0 (3)	119.7 (4)	119.1 (4)	119.4 (2)	119.4 (2)
ah	116.9 (3)	117.8 (3)	117.0 (3)	117.1 (3)	117.2 (2)	117.0 (2)
bh	122.2 (4)	121.7 (3)	121.8 (3)	122.1 (4)	122.0 (2)	122.5 (2)
di	120.1 (3)	118.7 (3)	119.9 (3)	120.5 (3)	119.8 (2)	120.3 (2)
ei	118.5 (4)	119.2 (3)	118.3 (3)	118.4 (4)	118.6 (2)	118.2 (2)

* There are errors in Table 4 of DCP: *cf* and *de* are given as *ce* and *df*.

independent reflexions were measured of which 3602 had $F_o^2 > 3.0\sigma(F_o^2)$. No correction was made for absorption.

Determination and refinement of the structure

Direct methods (*MULTAN*, Germain, Main & Woolfson, 1971) gave the position of the decachloropyrene molecule. A Fourier synthesis following a few cycles of least-squares refinement showed the benzene molecule. Least-squares refinement of atomic coordinates, thermal parameters (anisotropic for Cl and C, isotropic for H) and an isotropic extinction factor, *g*, gave a final *R* of 0.046 ($R_w = 0.053$) for 314 parameters and 3601 reflexions. Reflexion 220 was omitted from the final cycles of refinement as it measured too small, possibly due to shadowing from the beam-stop; layers $k = 0$ and 1 had been measured without a beam-stop. Extinction correction could not correct fully for the discrepancy between the observed and calculated values for 220 although it made $F_o > F_c$ for all the other strong reflexions.

The value obtained for *g* was $1.7(2) \times 10^{-6}$ with \bar{i} assumed to be unity; the minimum value of $F_o/F_c(\text{corr.})$ was 0.81.

Atomic coordinates are listed in Table 1.* The thermal motion of the decachloropyrene molecule was analysed on the assumption that the molecule could be treated as a rigid body (Schomaker & Trueblood, 1968). The components of **T**, **L**, and **S** are given in Table 2. The value of **L** was used to correct the bond

* Lists of structure factors and thermal parameters have been deposited with the British Library Lending Division as Supplementary Publication No. SUP 32962 (17 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 13 White Friars, Chester CH1 1NZ, England.

Table 5. Close intermolecular contacts (\AA), Cl—Cl ≤ 3.65 ; Cl—C, C—C ≤ 3.5 ; Cl—H, C—H ≤ 3.0 , H—H $\leq 2.4 \text{\AA}$

Symmetry code

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

Molecules within a stack are related by symmetry operations (i) or (ii).

Cl(1)—Cl(1 ⁱⁱⁱ)	3.642	Cl(12)—Cl(14 ^{vii})	3.597
Cl(2)—Cl(12 ^{iv})	3.647	C(17)—Cl(1 ⁱⁱⁱ)	3.545
Cl(2)—Cl(14 ^{iv})	3.524	C(18)—C(11 ⁱⁱ)	3.459
Cl(5)—Cl(8 ^v)	3.507	C(19)—C(9 ⁱ)	3.485
Cl(5)—Cl(10 ^{iv})	3.573	C(19)—C(10 ⁱⁱ)	3.477
Cl(7)—Cl(10 ^{iv})	3.534	C(20)—C(8 ⁱ)	3.392
Cl(8)—Cl(11 ^{vi})	3.469	C(21)—C(7 ⁱ)	3.501

lengths for thermal motion. The thermal motion of the benzene molecule cannot be analysed in the same way since Schomaker & Trueblood's method does not work for circular planar molecules. The mean square amplitudes of vibration radial, tangential and perpendicular to the molecule were $U_{\text{rad}} = 0.0572$, $U_{\text{tan}} = 0.1206$, and $U_{\perp} = 0.0571 \text{\AA}^2$; cf. $U_{\text{rad}} = 0.0572$, $U_{\text{tan}} = 0.0934$, and $U_{\perp} = 0.0605 \text{ rad}^2$ for benzene itself (Cox, Cruickshank & Smith, 1958), suggesting that the correction to be applied to the C—C bonds is in the range 0.025 to 0.030 \AA . To obtain better parameters for the benzene molecule, refinements were carried out in which the benzene molecule was constrained to have *6/mmm* symmetry. The thermal motion was described by **TLX** in the early and by **TLS** in the later cycles, in both cases in the third cumulant expansion (Pawley & Willis, 1970; Prince & Finger, 1973). The *R* values

Table 6. *Coordinates (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 for C atoms and 0.001 Å for Cl atoms.

	X	Y	Z
C(1)	-3.422	0.075	0.609
C(2)	-2.814	-1.137	0.389
C(3)*	-1.447	-1.207	0.022
C(4)	-0.722	-2.400	-0.319
C(5)	0.635	-2.415	-0.319
C(6)*	1.393	-1.248	0.025
C(7)	2.747	-1.241	0.410
C(8)	3.423	-0.054	0.585
C(9)	2.790	1.162	0.399
C(10)*	1.442	1.209	0.022
C(11)	0.721	2.400	-0.343
C(12)	-0.627	2.409	-0.359
C(13)*	-1.389	1.250	0.025
C(14)	-2.724	1.267	0.442
C(15)*	-0.719	0.010	-0.046
C(16)*	0.720	-0.014	-0.046
Cl(1)	-5.053	0.131	1.112
Cl(2)	-3.750	-2.534	0.696
Cl(4)	-1.556	-3.753	-0.953
Cl(5)	1.429	-3.785	-0.946
Cl(7)	3.563	-2.672	0.867
Cl(8)	5.043	-0.073	1.152
Cl(9)	3.668	2.569	0.820
Cl(11)	1.556	3.759	-0.975
Cl(12)	-1.450	3.727	-1.093
Cl(14)	-3.450	2.711	0.913

Table 7. *Comparison of bond lengths with those in pyrene and in decachloropyrene*

j is the mean C—Cl distance. The values for pyrene are the means of the values observed for pyrene (Allmann, 1970), 2,7-di-*tert*-butylpyrene (Hazell & Lomborg, 1972) and pyrene: TCNE.

	$C_{16}H_{10}$	DCP	DCPB
a	1.388 (1)	1.389 (3)	1.390 (3)
b	1.399 (1)	1.395 (3)	1.411 (3)
c	1.421 (1)	1.423 (3)	1.423 (3)
d	1.437 (1)	1.450 (3)	1.446 (3)
e	1.425 (1)	1.438 (4)	1.443 (5)
f	1.345 (1)	1.350 (4)	1.357 (4)
j	—	1.719 (1)	1.721 (1)

Table 8. *Comparison of DCPB with DCP*

DCP₁ refers to atoms 1–7, DCP₂ to atoms 8–14. Δ is the deviation from planarity; for Δ_c only the C atoms attached to Cl are included in the mean.

Mean values (Å)	DCPB	DCP	DCP ₁	DCP ₂
Cl...Cl	3.025 (1)	3.003 (1)	3.025 (1)	2.981 (1)
$ \Delta _{Cl}$	0.953	0.919	1.025	0.812
$ \Delta _C$	0.417	0.414	0.447	0.414

obtained were $R = 0.047$ and $R_w = 0.054$ for 263 parameters and 3601 reflexions, the decachloropyrene parameters were kept fixed at the values from the conventional refinement and T_{22} was fixed at 0.0507 Å². The bond lengths obtained were C—C = 1.399 (3) and C—H = 0.96 (3) Å.

Bond lengths and short intramolecular distances are given in Table 3, angles within the molecule in Table 4. The atomic numbering and bond labelling are shown in Fig. 1(a), torsion angles and out-of-plane angles in Fig. 1(b). Short intermolecular distances are given in Table 5.

Computational details

Calculations were carried out with the following programs: data reduction (Kryger, 1975) and *DSORTH*, State University of New York at Buffalo; full-matrix least-squares refinement, *LINUS* (Coppens & Hamilton, 1970); constrained refinement, *KONSLs* (Pawley, 1972); 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 $w = \{[\sigma(F_o^2) + 1.03F_o^2]^{1/2} - |F_o|\}^{-2}$. The scattering factors were those of Cromer & Mann (1968) for Cl and C, and of Stewart, Davidson & Simpson (1965) for H. $R = \sum ||F_o| - |F_c|| / \sum |F_o|$ 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 saddle-shaped. The deviations from planarity are given in Table 6 which gives atomic coordinates in a molecular axial system. The mean Cl—Cl distance is 3.025 (1) Å, *cf.* octachloronaphthalene, 3.032 (2) Å (Gafner & Herbstein, 1963); decachloropyrene, 3.003 (1) Å, 1,3,6,8-tetrafluoro-2,4,5,7,9,10-hexachloropyrene, 2.968 (2) Å (Hazell & Weigelt, 1976) and decachlorophenanthrene, 3.033 (3) Å (Herbstein, Kapon & Merksamer, 1976). The mean C—C and C—Cl distances are compared with those for decachloropyrene and for pyrene in Table 7. The C—C distance in the benzene molecule, 1.399 (3) Å, is similar to that, 1.395 (4) Å, found by Cruickshank (1970) for benzene. The molecule is much more symmetric in DCPB than in DCP where packing forces result in one half of the molecule being compressed. The geometries of the two molecules are compared in Table 8 where it is seen that the deviations from planarity of DCPB are similar to those of the uncompressed half of DCP.

The packing is shown in Fig. 2. The crystal is composed of stacks of alternating decachloropyrene and benzene molecules. The benzene molecules are towards one end of the pyrene and somewhat skew, *cf.*

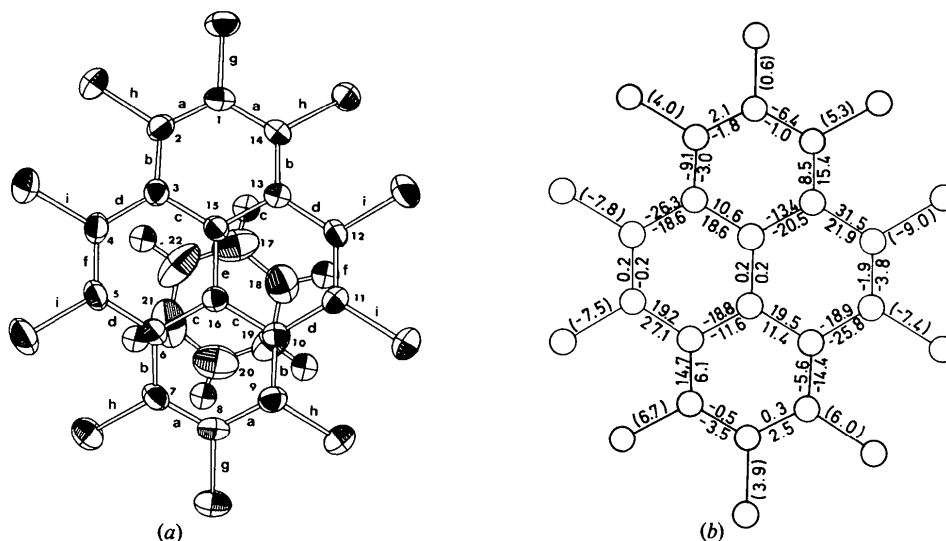


Fig. 1. (a) The molecules projected on the plane through C(3), C(6), C(10), C(13), C(15) and C(16) showing the numbering of the carbon atoms and the labelling of the bonds. Cl atoms and H atoms have the same numbering as the C atoms to which they are attached. (b) Torsion angles ($^{\circ}$) and, in parentheses, the angles between C-Cl bonds and the plane defined by the neighbouring three atoms. Standard deviations are *ca* 0.5 $^{\circ}$. A positive torsion angle $i-j-k-l$ is defined such that when looking along $j-k$ a clockwise rotation makes $i-j$ superimpose $k-l$.

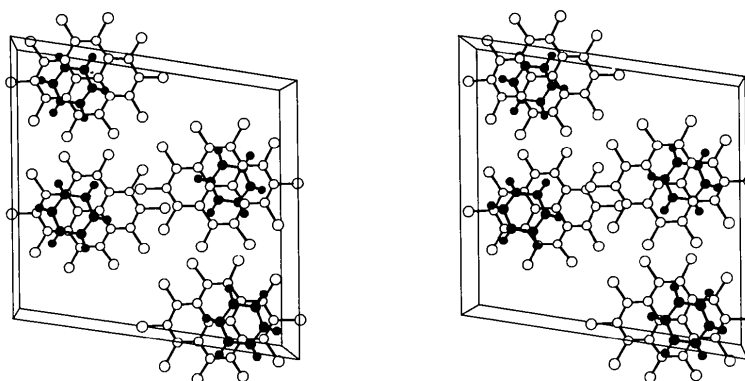


Fig. 2. A stereoview of the unit-cell contents as seen down **b**; **a** is across, **c** up the page.

the TCNE molecule in pyrene:TCNE (Larsen, Little & Coppens, 1975). The compound readily loses benzene. This, together with the fact that the crystals are not highly coloured, red-brown as compared to the dark yellow-brown of DCP, suggests that benzene is present as benzene of crystallization and that little charge transfer occurs.

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The Crystal Structure of the α Phase of *N*-(*p*-Tolyl)tetrachlorophthalimide

BY M. KAFTORY

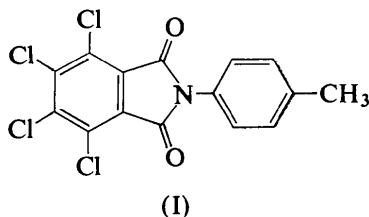
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Crystals of the title compound are orthorhombic, space group *Cmca*, $a = 6.906$ (4), $b = 25.191$ (13), $c = 17.020$ (9) Å, $Z = 8$. The crystal structure was solved by direct methods and refined to $R = 0.030$ (goodness of fit 0.99). The molecule occupies the space-group mirror (*m*) special position. The tetrachlorophthalimide part lies in the mirror plane and is necessarily planar; the *p*-tolyl part is bisected by this plane and is somewhat bow-shaped, presumably because of packing forces. The short Cl...O intermolecular contact of 2.984 Å suggests a charge transfer between the O atom as the donor and the Cl atom as the acceptor.

Introduction

N-(*p*-Tolyl)tetrachlorophthalimide (I) forms inclusion compounds (Pratt & Perkins, 1918) which are of special interest because it appears that only aromatic molecules of particular shapes can act as guests. Three different polymorphic forms of the host compound have been found during a study of the crystal chemistry and thermal stability of the system (Herbstein & Kaftory, 1977). The crystal structure of the stable polymorph (α phase) is reported here.



Experimental

Colourless needles, elongated along [100], may be obtained by the slow cooling of decalin, cyclo-

hexanone, cyclohexanone or *N,N*-dimethylformamide solutions. Intensities from a crystal, $0.40 \times 0.25 \times 0.30$ mm, were collected on an automated Hilger & Watts Y290 diffractometer with graphite-monochromatized Mo $K\alpha$ radiation ($\lambda = 0.71069$ Å, $\mu = 4.80$ cm⁻¹); 1433 independent reflexions were measured, of which 1230 were above background [$F_o > 1.2\sigma(F_o)$]. Crystal data are summarized in Table 1. The systematic absences indicate space groups *Cmca* or *C2ca*; intensity and *E* statistics suggest the presence of a centre of symmetry.

The structure was solved by *MULTAN* (Germain, Main & Woolfson, 1971). The *E* map of the best set of 205 phases (ABS FOM = 1.283) revealed the correct structure. The structure was refined by full-matrix

Table 1. *Crystal data for the α phase of N-(p-tolyl)-tetrachlorophthalimide*

$C_{15}H_7NO_2Cl_4$	$M_r = 375.03$
Orthorhombic	$\mu(\text{Mo } K\alpha) = 4.80 \text{ cm}^{-1}$
$a = 6.906$ (4) Å	Space group conditions:
$b = 25.191$ (13)	$hkl: h + k = 2n$
$c = 17.020$ (9)	$h0l: l = 2n; (h = 2n)$
$V = 2960.9$ Å ³	$hk0: h = 2n; (k = 2n)$
$Z = 8$	Space group <i>Cmca</i> (No. 64) or <i>C2ca</i>
$D_m = 1.630$ g cm ⁻³	
$D_x = 1.683$	

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