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Structural Studies of Polychlorinated Hydrocarbons.
III. The *cis* and *trans* Isomers of Tetrachlorostilbene

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The *cis* and *trans* isomers of 1,2-bis(4-chlorophenyl)-1,2-dichloroethylene, $C_{14}H_8Cl_4$, are monoclinic, space group $P2_1/c$. The 107 parameters describing the *trans* isomer [$a = 6\cdot002\,(5)$, $b = 14\cdot500\,(12)$, $c = 7\cdot630\,(5)$ Å, $\beta = 94\cdot55\,(2)°$, $Z = 2$, $D_x = 1\cdot596$ g cm^{-3}] were refined *versus* the 854 most significant single-crystal X-ray reflexions to an R of 0·043. The 195 parameters of the *cis* isomer [$a = 8\cdot062\,(8)$, $b = 28\cdot560\,(12)$, $c = 6\cdot118\,(6)$ Å, $\beta = 97\cdot60\,(2)°$, $Z = 4$, $D_x = 1\cdot513$ g cm^{-3}] were refined *versus* the 1017 most significant reflexions to an R of 0·048. The molecules of both isomers were found to be nonplanar. The C—C=C bond angles at the ethylene bridge were significantly greater than 120 (125) for the *cis* isomer and less than 120° (118°) for the *trans* isomer. The apparently general C—C—C bond-angle distribution of *p*-chlorophenyl rings is discussed.

Introduction

The present determination of the crystal structures of the *cis* and *trans* isomers of 1,2-bis(4-chlorophenyl)-1,2-dichloroethylene continues a series of investigations at this Institute on the structures of polychlorinated hydrocarbons (Söderholm, Sonnerstam, Norrestam & Palm, 1976). The present compounds, both tetrachlorinated stilbenes (*cf.* Fig. 1), will accordingly be referred to as the *cis*-tetrachlorostilbene and *trans*-tetrachlorostilbene isomers. They can also be regarded as isomers of the DDT metabolite 2,2-bis(4-chlorophenyl)-1,1-dichloroethylene (DDE), and are formed from the former under certain conditions (Göthe, Jensen & Wachtmeister, 1977).

Three-dimensional single-crystal X-ray diffraction data were collected on a single-crystal diffractometer by the θ–2θ scan technique (scan interval in θ: $1\cdot6 + 0\cdot6\tan\theta$), with graphite-monochromatized Cu K radiation. The intensity data were corrected for polarization, Lorentz and crystal-absorption effects. The structures were solved by conventional applications of direct methods followed by difference electron density calculations and full-matrix least-squares refinements (Hughes's weighting scheme). Further details of the calculations are given in Table 1. The scattering factors used were those in *International Tables for X-ray Crystallography* (1974). During the structure determination of the *trans* isomers a doubled maximum appeared at the C atom positions of the ethylene bridge. This was taken as an indication of disorder of the *trans*-tetrachlorostilbene structure and both positions were included in the subsequent calculations. Full-matrix least-squares refinements of the resulting struc-

Table 1. *Some relevant details of the data collection and of the structure determinations*

	cis-Tetrachlorostilbene	*trans*-Tetrachlorostilbene
Crystal size	0·06 × 0·08 × 0·46 mm	0·10 × 0·16 × 0·28 mm
Linear absorption coefficient (μ)	75·2 cm^{-1}	79·3 cm^{-1}
Total number of measured independent reflexions	1602	1003
Acceptance limit $\delta(I_{\rm net})/I_{\rm net}$	0·33	0·20
Accepted reflexions	1017	854
Normalized structure factors ($\geq$1·5) used	191	141
Best triple relations	974	411
Number of solutions of triple relations	4	4
Parameters to describe the final structural model	195	107
Final linear R value based on accepted reflexions	0·048	0·043

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ture models, with anisotropic temperature factors for the nonhydrogen and isotropic for the H atoms, were carried out until the parameter shifts were well below their e.s.d.'s.*

Table 2. *cis-Tetrachlorostilbene: fractional atomic coordinates and hydrogen isotropic temperature factors with e.s.d.'s*

	x	y	z	B (Å^2)
Cl(α)	−0·0710 (3)	0·2953 (1)	0·2219 (4)	
Cl(4)	0·6105 (3)	0·2969 (1)	−0·3381 (4)	
Cl(α')	−0·1215 (3)	0·3889 (1)	0·4507 (4)	
Cl(4′)	0·3820 (4)	0·5626 (1)	0·1494 (5)	
C(α)	0·0589 (8)	0·3422 (3)	0·1849 (11)	
C(1)	0·1945 (8)	0·3319 (2)	0·0551 (11)	
C(2)	0·1622 (11)	0·3120 (3)	−0·1538 (13)	
C(3)	0·2903 (10)	0·3005 (3)	−0·2723 (13)	
C(4)	0·4508 (9)	0·3107 (3)	−0·1852 (12)	
C(5)	0·4850 (11)	0·3307 (3)	0·0144 (13)	
C(6)	0·3582 (9)	0·3413 (3)	0·1367 (12)	
C(α')	0·0323 (9)	0·3831 (3)	0·2774 (11)	
C(1′)	0·1239 (10)	0·4262 (3)	0·2442 (13)	
C(2′)	0·1320 (12)	0·4432 (3)	0·0419 (16)	
C(3′)	0·2141 (12)	0·4850 (4)	0·0106 (17)	
C(4′)	0·2824 (11)	0·5095 (3)	0·1854 (17)	
C(5′)	0·2727 (16)	0·4940 (4)	0·3935 (17)	
C(6′)	0·1942 (15)	0·4521 (4)	0·4195 (18)	
H(2)	0·072 (7)	0·304 (2)	−0·174 (9)	2·6 (13)
H(3)	0·255 (8)	0·288 (3)	−0·422 (11)	5·2 (15)
H(5)	0·586 (7)	0·339 (2)	0·077 (9)	2·9 (12)
H(6)	0·404 (9)	0·359 (3)	0·282 (12)	6·9 (18)
H(2′)	0·094 (8)	0·430 (3)	−0·091 (12)	5·4 (17)
H(3′)	0·210 (10)	0·495 (3)	−0·151 (14)	8·0 (20)
H(5′)	0·340 (9)	0·505 (3)	0·533 (14)	7·0 (19)
H(6′)	0·229 (12)	0·436 (4)	0·562 (16)	10·7 (29)

Discussion

The final atomic coordinates and thermal parameters are listed in Tables 2–5. Fig. 1 displays the structural formula for the planar form of the *cis* isomer, together with the atomic labelling used. The H and Cl atoms have been assigned the same atomic labels as the C atoms to which they are bonded. As discussed above, the crystal structure of the *trans* isomer, in which the molecules themselves possess a centre of symmetry at the midpoint of the ethylene bridge, is somewhat disordered. Disordered structures appear to be a very common feature of *trans*-stilbenes (*cf.* Finder, Newton & Allinger, 1974) and related compounds such as the azobenzenes (*e.g.* Brown, 1966*a*, *b*). In the present study this disorder was approximated by including atom C(α) with equal occupancy in two positions denoted by C(α) and C(α') respectively. Given this approximation, the observed bond angles and bond lengths for the *trans* isomer, especially in the neighbourhood of the ethylene bond, may be affected by systematic errors. The low R value (0·043) obtained in the least-squares refinement of the derived structural

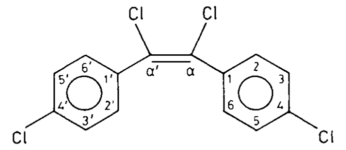

Fig. 1. Schematic structural formula for a hypothetical planar form of the *cis* isomer of 1,2-bis(*p*-chlorophenyl)-1,2-dichloroethylene (*cis*-tetrachlorostilbene).

Table 3. *cis-Tetrachlorostilbene: anisotropic thermal parameters* (× 10^4) *with e.s.d.'s*

The temperature factor expression used is $\exp[-(h^2b_{11} + k^2b_{22} + l^2b_{33} + hkb_{12} + hlb_{13} + klb_{23})]$.

	b_{11}	b_{22}	b_{33}	b_{12}	b_{13}	b_{23}
Cl(α)	184 (4)	16 (1)	597 (9)	−13 (2)	169 (9)	11 (3)
Cl(4)	242 (5)	23 (1)	474 (8)	15 (2)	280 (9)	0 (3)
Cl(α')	258 (5)	21 (1)	512 (8)	6 (2)	358 (10)	−2 (3)
Cl(4′)	421 (7)	17 (1)	860 (13)	−33 (3)	528 (15)	19 (4)
C(α)	160 (12)	13 (2)	364 (22)	6 (6)	71 (28)	8 (8)
C(1)	177 (14)	10 (1)	336 (23)	−2 (6)	84 (29)	−5 (8)
C(2)	162 (16)	17 (2)	427 (31)	−15 (7)	84 (38)	5 (10)
C(3)	251 (18)	15 (2)	292 (24)	−11 (8)	73 (35)	−3 (9)
C(4)	176 (14)	13 (1)	354 (24)	−2 (6)	110 (29)	4 (8)
C(5)	164 (15)	19 (2)	396 (29)	−8 (7)	49 (36)	−14 (10)
C(6)	178 (14)	14 (1)	341 (23)	7 (7)	−15 (33)	1 (8)
C(α')	214 (14)	15 (2)	353 (22)	9 (7)	178 (30)	6 (9)
C(1′)	288 (17)	13 (2)	327 (26)	22 (8)	179 (34)	−22 (10)
C(2′)	371 (22)	14 (2)	411 (34)	8 (9)	232 (44)	−11 (11)
C(3′)	406 (24)	17 (2)	451 (35)	22 (10)	262 (47)	29 (12)
C(4′)	314 (19)	15 (2)	560 (36)	−7 (8)	400 (44)	−5 (12)
C(5′)	571 (34)	26 (2)	405 (37)	−83 (13)	315 (59)	−47 (13)
C(6′)	511 (29)	22 (2)	463 (38)	−82 (12)	294 (53)	12 (14)

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* A list of structure factors has been deposited with the British Library Lending Division as Supplementary Publication No. SUP 32040 (3 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 13 White Friars, Chester CH1 1NZ, England.

Table 4. *trans-Tetrachlorostilbene: fractional atomic coordinates and hydrogen isotropic temperature factors with e.s.d.'s*

	x	y	z	B (Å^2)
Cl(α)	0·0599 (2)	−0·0024 (1)	−0·2706 (1)	
Cl(4)	0·5902 (2)	0·3647 (1)	0·1112 (2)	
C(α)	0·0573 (11)	0·0265 (6)	−0·0527 (14)	
C(α')	−0·0310 (13)	−0·0260 (7)	−0·0638 (14)	
C(1)	0·1778 (5)	0·1107 (3)	0·0302 (6)	
C(2)	0·3893 (6)	0·1055 (3)	0·1129 (6)	
C(3)	0·5165 (5)	0·1834 (3)	0·1373 (5)	
C(4)	0·4293 (5)	0·2665 (2)	0·0798 (4)	
C(5)	0·2198 (6)	0·2730 (3)	−0·0012 (4)	
C(6)	0·0948 (6)	0·1943 (3)	−0·0261 (5)	
H(2)	0·447 (7)	0·041 (3)	0·153 (5)	6·2 (8)
H(3)	0·669 (7)	0·178 (3)	0·203 (5)	6·4 (10)
H(5)	0·157 (6)	0·335 (3)	−0·040 (5)	4·9 (8)
H(6)	−0·050 (8)	0·199 (3)	−0·091 (6)	6·9 (10)

model does however support the correctness of the overall conformation of the *trans* isomer.

The molecular conformations obtained for the two different *trans* isomers and for the *cis* isomer are shown in Fig. 2. The molecules of unsubstituted *trans*-stilbenes (Finder, Newton & Allinger, 1974) and of the conformationally related unsubstituted *trans*-azobenzenes (Brown, 1966*a*, *b*; Hope & Victor, 1969) are almost planar. On the other hand, *o*-substituted *trans*-azobenzenes (Graeber & Morosin, 1974) and α-substituted *trans*-stilbenes (Plieth & Repmann, 1967) deviate significantly from planarity, probably because of steric hindrance by the bulky substituents. Steric hindrance also appears to be the reason for the nonplanarity of such related *cis* isomers as *cis*-azobenzene (Mostad & Rømming, 1971). Accordingly, on steric grounds we would expect both the *cis* and *trans* isomers of tetrachlorostilbene to deviate from planarity. In Tables 6 and 7 least-squares planes through the phenyl rings and the ethylene system are listed for each molecule. The deviations from the least-squares planes through the ethylene systems by the Cl atoms at the *para* positions of the phenyl rings are significant. The conformations of the molecules can be approximately described by the two torsion angles, along the C(α)–C(1) and C(α')–C(1′) bonds respectively, for rotation of the phenyl groups out of the strictly planar molecular conformation. For the *cis* isomer these torsion angles are 54·2 and 54·5°, while the *trans* isomer torsion angles for the two different disordered positions of the ethylene bridge are significantly larger, 75·2 and 74·9°. The four different torsion angles along the ethylene bond deviate from 0 and 180° by less than 2° for the *trans* isomers and by 5–7° for the *cis* isomer. This distortion of the planarity of the ethylene part of the *cis* isomer is also evident from the calculations of least-squares planes. Thus, the

Table 6. *trans-Tetrachlorostilbene: deviations of the nonhydrogen atoms from least-squares planes*

The atoms indicated by an asterisk were omitted from the calculations of the planes. Atomic positions generated by inversion are indicated by (i).

	Deviation from plane I		Deviation from plane II
Cl(α)	0·000 Å	Cl(α)	−0·002 Å
Cl(α)(i)	0·000	Cl(α)(i)	0·002
C(α)	−0·002	C(α')	−0·012
C(α)(i)	0·002	C(α')(i)	0·012
C(1)	0·000	C(1)	0·003
C(1)(i)	0·000	C(1)(i)	−0·003
*Cl(4)	−0·032	*Cl(4)	−0·025
*Cl(4)(i)	0·032	*Cl(4)(i)	0·025

	Deviation from plane III	Plane	R.m.s. deviations of the atoms from the planes
C(1)	0·002 Å	I	0·002 Å
C(2)	−0·004	II	0·011
C(3)	0·003	III	0·004
C(4)	0·001		
C(5)	−0·003		
C(6)	0·002		
*C(α)	0·436		
*C(α')	−0·448		
*Cl(4)	0·005		

Table 5. *trans-Tetrachlorostilbene: anisotropic thermal parameters* ($\times 10^4$) *with e.s.d.'s*

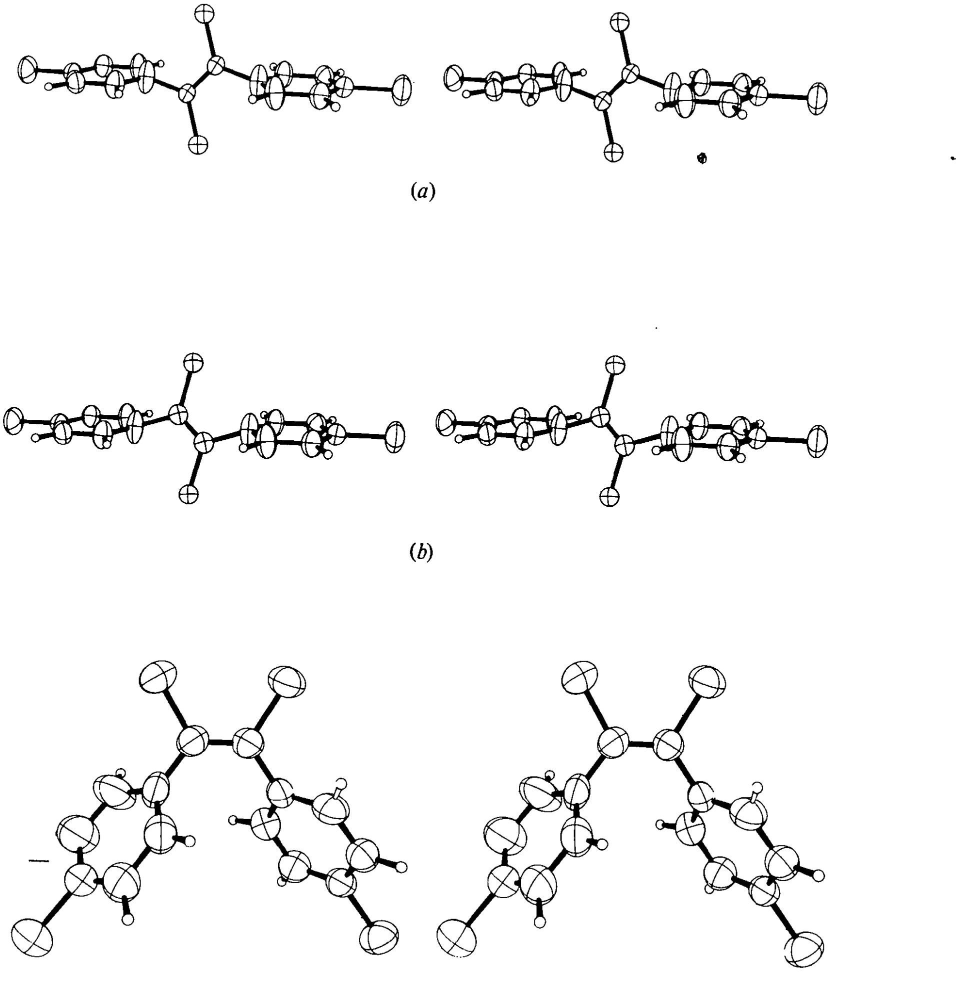
The temperature factor expression used is $\exp[-(h^2b_{11} + k^2b_{22} + l^2b_{33} + hkb_{12} + hlb_{13} + klb_{23})]$.

	b_{11}	b_{22}	b_{33}	b_{12}	b_{13}	b_{23}
Cl(α)	327 (3)	43 (1)	131 (2)	−35 (2)	46 (3)	−3 (2)
Cl(4)	417 (4)	47 (1)	304 (3)	−126 (2)	−25 (4)	−21 (2)
C(α)	206 (18)	33 (4)	136 (18)	−5 (16)	16 (25)	−18 (11)
C(α')	175 (17)	38 (5)	166 (20)	15 (16)	38 (25)	5 (12)
C(1)	212 (9)	33 (2)	419 (11)	−10 (6)	−61 (14)	−20 (6)
C(2)	238 (9)	38 (2)	353 (9)	5 (6)	−37 (14)	18 (7)
C(3)	225 (9)	46 (2)	216 (7)	−25 (6)	−1 (12)	−8 (6)
C(4)	273 (9)	40 (2)	152 (6)	−45 (6)	51 (10)	−17 (5)
C(5)	325 (10)	36 (2)	193 (6)	−4 (6)	1 (12)	18 (5)
C(6)	253 (9)	38 (2)	270 (8)	5 (6)	51 (13)	−4 (6)

ethylene part (plane I in Table 7) of *cis*-tetrachlorostilbene gives the highest r.m.s. deviation, 0·085 Å, of the atoms from any of the calculated planes. The conformations of the molecules are apparently to a large extent determined by short non-bonded intramolecular interactions. Thus, in the *cis* isomer the Cl(α)···Cl(α') intramolecular distance is 3·07, the Cl(α)···C(1) and Cl(α')···C(1′) distances are both 2·70 and the Cl(α)···C(2) and Cl(α')···C(2′) distances are 3·19 and 3·15 Å respectively. In the *trans* isomer, the Cl(α)···C(1) and Cl(α)···C(1′) intramolecular distances are 2·86 and 2·88, while Cl(α)···C(6) and Cl(α)···C(2′) are 3·41 and 3·39 Å respectively. The stilbene conformations obtained agree to some extent with those recently found in gas electron diffraction studies of *cis* and *trans*-stilbene (Trætteberg, Frantsen, Mijlhoff & Hoekstra, 1975; Trætteberg & Frantsen, 1975). However, their torsional angles describing the orientations of the phenyl groups are considerably smaller (43 and 32° respectively) than those found in the present study (54 and 75° respectively). A possible explanation might be the steric effects of the dichloro substitution of the ethylene group, which gives rise to a number of short non-bonded intramolecular interactions as discussed above.

In Fig. 3 the packing in the two crystal structures is illustrated. As seen from this figure and from Tables 8 and 9, there are no remarkably short contact distances between the molecules in the crystal structures, the shortest C···C contact distance being 3·44, the shortest C···Cl 3·42 and the shortest Cl···Cl 3·52 Å.

The intramolecular bond distances and bond angles for the two stilbene isomers are listed in Tables 10–13. The Cl—C bond lengths, ranging from 1·72 to 1·74 Å,



(*a*)

(*b*)

(*c*)

Fig. 2. Stereoscopic views of (*a*), (*b*) the molecular geometries of the two conformers of *trans*-tetrachlorostilbene, and of (*c*) *cis*-tetrachlorostilbene. The nonhydrogen atoms are represented by their thermal ellipsoids, while the hydrogens are drawn with constant radii.

Table 7. *cis-Tetrachlorostilbene: deviations of the nonhydrogen atoms from least-squares planes*

The atoms indicated by an asterisk were omitted from the calculations of the planes.

	Deviation from plane I		Deviation from plane II
Cl(*a*)	0·064 Å	C(1)	–0·006 Å
Cl(*a*′)	–0·068	C(2)	0·014
C(*a*)	0·007	C(3)	–0·010
C(*a*′)	0·002	C(4)	0·000
C(1)	–0·070	C(5)	0·007
C(1′)	0·066	C(6)	–0·004
*Cl(4)	–0·357	*C(*a*)	–0·040
*Cl(4′)	0·357	*Cl(4)	–0·003

	Deviation from plane III	Plane	R.m.s. deviation of the atoms from the planes
C(1′)	–0·008 Å	I	0·085 Å
C(2′)	0·012	II	0·013
C(3′)	–0·005	III	0·012
C(4′)	–0·005		
C(5′)	0·009		
C(6′)	–0·002		
*C(*a*′)	0·060		
*Cl(4′)	0·008		

agree well with those found in some DDT derivatives by DeLacy & Kennard (1972): average 1·74 (2) Å. The average C—C bond lengths in the three independently determined phenyl groups are 1·369 (6) for the *trans* isomer, and 1·372 (16) and 1·360 (21) Å for the *cis* isomer. These values are lower than the 'standard' value of 1·394 (5) Å (Sutton, 1965), possibly because of the electronegativity of the Cl substituents (Bent, 1961) and/or because the bond lengths have not been corrected for thermal effects in the present two structures. The larger the thermal vibrations are for the atoms forming the phenyl rings, the larger are the deviations from ideal $6/m$ symmetry; the average r.m.s. thermal displacements of the atoms of the phenyl rings are 0·235 Å for the *trans* isomer and 0·249 and 0·305 Å for the rings of the *cis* isomer. The corresponding r.m.s. deviations of the atoms from least-squares planes are 0·004, 0·012 and 0·013 Å respectively, while the e.s.d.'s from 120° of the C—C—C bond angles within the phenyl rings are 1·0, 1·3 and 1·7° respectively. Apart from thermal effects, the distortions of the ring bond angles may well be systematic, since similar distortions are observed in several other *p*-chloro substituted phenyl rings. In the present structures the C—C—C bond angles within the phenyl rings at the

Table 8. *cis-Tetrachlorostilbene: intermolecular distances less than* 3·8 Å *between nonhydrogen atoms, with e.s.d.'s*

Symmetry code

None	x,	y,	z	(iv)	$1-x$,	$1-y$,	$-z$
(i)	$x-1$,	$\frac{1}{2}-y$,	$\frac{1}{2}+z$	(v)	$-x$,	$1-y$,	$-z$
(ii)	x,	$\frac{1}{2}-y$,	$\frac{1}{2}+z$	(vi)	$1-x$,	$1-y$,	$1-z$
(iii)	$-x$,	$1-y$,	$1-z$				

Cl(*a*)···Cl(4)(i)	3·662 (4) Å	Cl(4′)···C(3′)(iv)	3·776 (11) Å
Cl(*a*)···C(2)(ii)	3·623 (9)	C(2′)···C(3′)(v)	3·443 (14)
Cl(*a*′)···Cl(4′)(iii)	3·698 (5)	C(2′)···C(4′)(v)	3·700 (13)
Cl(*a*′)···C(5′)(iii)	3·727 (12)	C(3′)···C(3′)(v)	3·542 (20)
Cl(4′)···C(5)(iv)	3·423 (9)	C(5′)···C(5′)(v)	3·740 (25)

Table 9. *trans-Tetrachlorostilbene: intermolecular distances less than* 3·8 Å *between nonhydrogen atoms, with e.s.d.'s*

Symmetry code

None	x,	y,	z	(iii)	$1-x$,	$-y$,	$-z$
(i)	$-x$,	$-y$,	$-1-z$	(iv)	x,	$\frac{1}{2}-y$,	$z-\frac{1}{2}$
(ii)	$x-1$,	$\frac{1}{2}-y$,	$z-\frac{1}{2}$	(v)	x,	$\frac{1}{2}+y$,	$\frac{1}{2}-z$

Cl(*a*)···Cl(*a*)(i)	3·517 (3) Å	C(3)···C(4)(v)	3·533 (5) Å
Cl(*a*)···Cl(4)(ii)	3·513 (3)	C(3)···C(5)(v)	3·457 (5)
Cl(*a*)···C(2)(iii)	3·739 (5)	C(4)···C(5)(v)	3·573 (5)
Cl(*a*)···C(3)(iii)	3·738 (4)	C(4)···C(6)(v)	3·788 (5)
Cl(4)···C(3)(iv)	3·675 (5)	C(5)···C(6)(v)	3·790 (5)
C(2)···C(5)(v)	3·644 (6)		

C(1) positions are less than 120° and the ring angles at the chlorine-substituted *para* C atom C(4) are all greater than 120°. Furthermore, the ring angles at the *ortho* positions are all greater than 120° while five of the six ring angles at the *meta* positions are less than 120°. This distribution of bond angles appears to be a characteristic feature of *p*-chlorophenyl groups, though it is scarcely statistically significant here. The same distribution of C—C—C bond angles can be found in, for example, the DDT derivatives studied by X-ray diffraction (DeLacy & Kennard, 1972). A calculation of average phenyl ring angles from the latter and from the present study (altogether eleven observations of the thermally uncorrected *p*-chlorophenyl ring geometry) gives the following values: 118·4 at C(1), 121·1 at the *ortho* position, 119·0 at the *meta* position and 121·2° at the *para* position (e.s.d.'s *ca* 1°). The significance of these observations is strengthened by the experimentally supported (see, for example, Carter, McPhail & Sim, 1966; Hope & Victor, 1969) hypothesis that such electronegative substituents on C as Cl affect the orbital hybridization in such a way that the *p* content of the C sp^2 hybrid orbital directed towards the Cl substituent tends to increase (Bent, 1961). Thus, the *s* content of the C sp^2 orbitals directed towards the adjoining, more electropositive C atoms is increased and so accordingly is the C—C—C bond angle. Distortions of phenyl rings due to substitution effects in general have very recently been discussed by Domenicano, Vaciago & Coulson (1975*a*, *b*). Their suggestions are fully supported by the present study.

In the dichloroethylene group, the Cl—C=C angles (average 119·6°) are closer to the ideal sp^2 value of 120° than the C—C=C and Cl—C—C bond angles. Thus in the *cis* isomer the C—C=C angles average 125·2°, while the corresponding angles average 118·1° in the *trans* isomer. This difference in the C—C=C angles between the *cis* and *trans* isomers is probably a significant feature; a similar difference is observed for the

Table 10. *cis-Tetrachlorostilbene: intramolecular bond distances with e.s.d.'s*

C(1)–C(2)	1·391 (10) Å	Cl(α)–C(α)	1·734 (8) Å
C(2)–C(3)	1·378 (12)	Cl(α)–C(α)	1·742 (7)
C(3)–C(4)	1·364 (11)	Cl(4)–C(4)	1·734 (8)
C(4)–C(5)	1·344 (11)	Cl(4′)–C(4′)	1·743 (9)
C(5)–C(6)	1·378 (11)	H(2)–C(2)	0·77 (6)
C(6)–C(1)	1·374 (10)	H(3)–C(3)	0·99 (7)
C(1′)–C(2′)	1·339 (13)	H(5)–C(5)	0·88 (6)
C(2′)–C(3′)	1·390 (14)	H(6)–C(6)	1·04 (8)
C(3′)–C(4′)	1·334 (14)	H(2′)–C(2′)	0·91 (8)
C(4′)–C(5′)	1·360 (15)	H(3′)–C(3′)	1·03 (9)
C(5′)–C(6′)	1·372 (16)	H(5′)–C(5′)	1·00 (9)
C(6′)–C(1′)	1·363 (14)	H(6′)–C(6′)	1·00 (10)
C(1)–C(α)	1·464 (9)		
C(1′)–C(α′)	1·462 (12)		
C(α)–C(α′)	1·328 (12)		

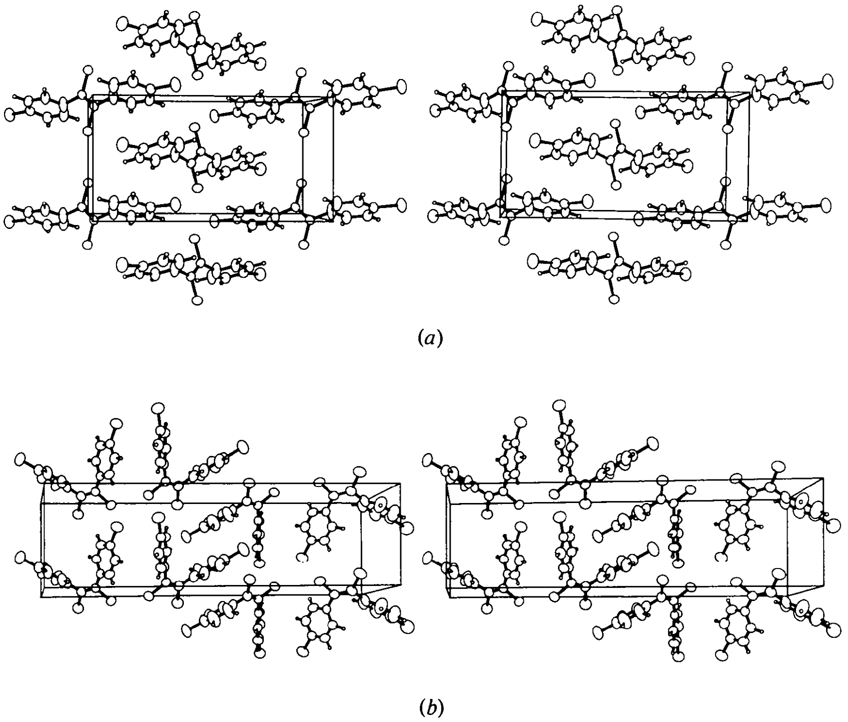


Fig. 3. Stereoscopic packing diagrams of (*a*) the *trans*-tetrachlorostilbene structure viewed perpendicular to the *bc* plane and of (*b*) the *cis*-tetrachlorostilbene structure viewed perpendicular to the *ab* plane.

C—N=N angles of the conformationally related azobenzenes (Mostad & Rømming, 1971). The large C—C=C angle (126°) found in *trans*-stilbene (Finder *et al.*, 1974; Bernstein, 1975) probably arises from disorder in the crystal structure, since the angle found in the non-disordered structure (Plieth & Repmann, 1967) of *trans-p,p′*-dichloro-1,2-diethylstilbene is 118°.

Table 11. *cis-Tetrachlorostilbene: intramolecular bond angles* (°) *with e.s.d.'s*

C(1)—C(2)—C(3)	121·2 (8)	Cl(α)—C(α)—C(1)	115·0 (6)
C(2)—C(3)—C(4)	118·8 (8)	Cl(α)—C(α)—C(α′)	119·4 (6)
C(3)—C(4)—C(5)	121·1 (8)	Cl(4)—C(4)—C(3)	118·3 (6)
C(4)—C(5)—C(6)	120·6 (8)	Cl(4)—C(4)—C(5)	120·6 (7)
C(5)—C(6)—C(1)	120·4 (7)	Cl(α′)—C(α′)—C(1′)	114·7 (6)
C(6)—C(1)—C(2)	117·9 (7)	Cl(α′)—C(α′)—C(α)	120·7 (7)
C(1′)—C(2′)—C(3′)	121·4 (9)	Cl(4′)—C(4′)—C(3′)	120·2 (9)
C(2′)—C(3′)—C(4′)	119·5 (10)	Cl(4′)—C(4′)—C(5′)	119·2 (8)
C(3′)—C(4′)—C(5′)	120·6 (10)	H(2)—C(2)—C(1)	110 (5)
C(4′)—C(5′)—C(6′)	118·6 (10)	H(2)—C(2)—C(3)	127 (5)
C(5′)—C(6′)—C(1′)	122·1 (10)	H(3)—C(3)—C(2)	115 (4)
C(6′)—C(1′)—C(2′)	117·6 (9)	H(3)—C(3)—C(4)	126 (4)
C(2)—C(1)—C(α)	121·2 (7)	H(5)—C(5)—C(4)	125 (4)
C(6)—C(1)—C(α)	120·9 (7)	H(5)—C(5)—C(6)	114 (4)
C(1)—C(α)—C(α′)	125·7 (7)	H(6)—C(6)—C(5)	111 (5)
C(1′)—C(α′)—C(α)	124·6 (7)	H(6)—C(6)—C(1)	128 (5)
C(2′)—C(1′)—C(α′)	121·4 (8)	H(2′)—C(2′)—C(1′)	128 (6)
C(6′)—C(1′)—C(α′)	120·8 (8)	H(2′)—C(2′)—C(3′)	110 (6)
		H(3′)—C(3′)—C(2′)	114 (5)
		H(3′)—C(3′)—C(4′)	126 (5)
		H(5′)—C(5′)—C(4′)	127 (5)
		H(5′)—C(5′)—C(6′)	112 (5)
		H(6′)—C(6′)—C(5′)	115 (6)
		H(6′)—C(6′)—C(1′)	119 (7)

Table 12. *trans-Tetrachlorostilbene: intramolecular bond distances with e.s.d.'s*

C(1)—C(2)	1·374 (5) Å	Cl(α)—C(α)	1·716 (11) Å
C(2)—C(3)	1·367 (6)	Cl(α)—C(α′)	1·744 (10)
C(3)—C(4)	1·373 (5)	Cl(4)—C(4)	1·726 (3)
C(4)—C(5)	1·359 (5)	H(2)—C(2)	1·03 (5)
C(5)—C(6)	1·371 (6)	H(3)—C(3)	1·01 (5)
C(6)—C(1)	1·367 (6)	H(3)—C(5)	1·01 (5)
C(1)—C(α)	1·529 (10)	H(6)—C(6)	0·97 (5)
C(α)—C(α)(i)	1·342 (18)		
C(1)—C(α′)	1·545 (10)		
C(α′)—C(α′)(i)	1·263 (21)		

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Table 13. *trans-Tetrachlorostilbene: intramolecular bond angles* (°) *with e.s.d.'s*

C(1)—C(2)—C(3)	120·2 (4)	C(2)—C(1)—C(α′)	113·5 (5)	H(2)—C(2)—C(1)	118 (3)
C(2)—C(3)—C(4)	119·2 (4)	C(6)—C(1)—C(α′)	124·0 (5)	H(2)—C(2)—C(3)	122 (3)
C(3)—C(4)—C(5)	121·4 (4)	C(1)—C(α′)—C(α′)(i)	118·9 (12)	H(3)—C(3)—C(2)	119 (3)
C(4)—C(5)—C(6)	118·8 (4)	Cl(α)—C(α)—C(1)	123·7 (6)	H(3)—C(3)—C(4)	122 (3)
C(5)—C(6)—C(1)	120·9 (4)	Cl(α)—C(α)—C(α)(i)	119·0 (10)	H(5)—C(5)—C(4)	120 (3)
C(6)—C(1)—C(2)	119·5 (4)	Cl(α)—C(α′)—C(1)	122·0 (7)	H(5)—C(5)—C(6)	121 (3)
C(2)—C(1)—C(α)	122·4 (5)	Cl(α)—C(α′)—C(α′)(i)	119·1 (11)	H(6)—C(6)—C(5)	121 (3)
C(6)—C(1)—C(α)	115·4 (5)	Cl(4)—C(4)—C(3)	119·0 (3)	H(6)—C(6)—C(1)	118 (3)
C(1)—C(α)—C(α)(i)	117·2 (11)	Cl(4)—C(4)—C(5)	119·5 (3)		