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The Crystal Structure of Di-p-Chlorodiphenyltellurium Diiodide

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Crystals of $(p-\text{ClC}_6\text{H}_4)_2\text{TeI}_2$ are triclinic with the following cell dimensions:

$a = 9.751 \pm 0.006 \text{ Å}$	$\alpha = 115 \cdot 7 \pm 0 \cdot 1^{\circ}$
$b = 10.681 \pm 0.006$	$\beta = 87 \cdot 2 \pm 0 \cdot 1$
$c = 9.531 \pm 0.006$	$\gamma = 116 \cdot 4 \pm 0 \cdot 1$

The space group is $P\overline{1}$ and Z=2.

The Te, I and Cl atoms were located by use of two-dimensional Patterson and Fourier syntheses but location of the carbon atoms required a three-dimensional $(F_o - F_c)$ synthesis based on approximately 2500 independent $|F_o|$ values. The structure was refined by use of full-matrix least-squares procedures and was checked by a final $(F_o - F_c)$ synthesis.

The molecular structure approximates the symmetry 2 and is similar to structures already reported for the dichlorides and dibromides of several R_2Se and R_2Te compounds. The observed bond distances and bond angles are:

$Te-I_1$	2.947 ± 0.002 Å	$Te-I_2$	2.922 ± 0.002 Å
$Te-C_1$	2.13 ± 0.02	$Te-C_7$	2.10 ± 0.02
$Cl_1 - C_4$	1.75 ± 0.03	$Cl_2 - C_{10}$	1.74 ± 0.03
$I_1 - Te - I_2$	$173.5 \pm 0.1^{\circ}$	C ₁ -Te-C ₇	$101 \cdot 1 \pm 1 \cdot 0^{\circ}$
C ₁ –Te–I ₁	87.3 ± 0.7	$C_7 - Te - I_1$	88.1 ± 0.7
$C_1 - Te - I_2$	89.1 ± 0.7	C ₇ -Te-I ₂	87.3 ± 0.7

Although $(p\text{-ClC}_6H_4)_2\text{TeI}_2$ is definitely not a molecular complex of the type found for $C_4H_8\text{Se}_2.2\text{I}_2$ (which involves $\text{Se}\cdots\text{I}-\text{I}$ bonding) the long Te–I distances and the short (3.85 Å) I_1-I_2 separation observed in the present study suggest some tendency toward molecular complex bonding.

Introduction

Previous studies on compounds of the type R_2SeCl_2 , R_2SeBr_2 , R_2TeCl_2 and R_2TeBr_2 have shown that

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molecules of these substances contain nearly linear X-Se-X and X-Te-X bonding (Christofferson & McCullough, 1958). By contrast, the iodine complexes of 1,4 diselenane and 1,4 dithiane have been found to contain nearly linear Se \cdots I-I and S \cdots I-I bonding (Chao & McCullough, 1960, 1961). No com-

plete structural study of a compound of the type R_2TeI_2 has, as yet, appeared in the literature. Of the several compounds of this type available for study, preliminary investigations indicated that di-p-chlorodiphenyltellurium diiodide would be the most promising.

Experimental

Di-p-chlorodiphenyltellurium was prepared by the method of Lederer (1916). The product was purified by recrystallization from methanol and the diiodide was prepared by mixing solutions of the components in carbon tetrachloride. Crystals suitable for the X-ray study were grown by slow evaporation of a solution in ethylene chloride. Crystals of $(p-ClC_6H_4)_2TeI_2$ are garnet-red in color and display triclinic holohedral symmetry. Weissenberg and precession camera photographs prepared by use of Mo radiation indicated the following cell dimensions, based on Mo $K\alpha = 0.7107$ Å:

 $a = 9.751 \pm 0.006 \text{ Å}$ $\alpha^* = 62^\circ 35' + 03'$ $= 10.682 \pm 0.006$ $\beta^* = 79^\circ 45' \pm 05'$ b $= 9.531 \pm 0.006$ С $\gamma^* = 61^\circ 59' \pm 03'$ $\alpha = 115.70 \pm 0.10^{\circ}$ $V = 788 \cdot 8 (\text{Å})^3$ $\beta = 87.20 \pm 0.10$ $\gamma = 116.35 \pm 0.10$

The density, as determined by flotation, is 2.5 g.cm.⁻³ while that calculated from the X-ray data for $2(ClC_6H_4)_2TeI_2$ in the unit cell is 2.544 g.cm.⁻³. The space group was therefore assumed to be $P\overline{1}$ with two non-centrosymmetric molecules in the unit cell.

Three-dimensional intensity data were obtained by use of a crystal elongated on c and 0.10 mm. to 0.15mm. in thickness. The calculated linear absorption coefficient for molybdenum radiation is 65 cm.⁻¹ and the corresponding value for μr is 0.5. No corrections were made for absorption in the specimen. Zero and upper level Weissenberg photographs about the c axis and sets of precession photographs including the h0land 0kl nets were prepared. The multiple-film technique with 0.025 mm. brass foil interleaves was employed in preparing the Weissenberg intensity films while graduated sets of timed exposures were used for the precession data. The latter were used for interlayer scaling of the Weissenberg data and in the preliminary two-dimensional trial structure determination and refinement.

Structure determination and refinement

With the aid of Patterson and electron density summations along the a, b and c axes, approximate tellurium, iodine and chlorine positions were obtained. Twodimensional difference syntheses based on the positions of the five heavy atoms failed to give clearly recognizable positions for the individual carbon atoms although the general positions of the phenyl groups were indicated. Use of three-dimensional procedures therefore became necessary.

Table 1. Final position parameters and their standard deviations $(\times 10^4)$

	\boldsymbol{x}	y	\boldsymbol{z}	$\sigma(x)$	$\sigma(y)$	$\sigma(z)$
Te	8042	9834	2412	0001	0001	0001
Ι,	7757	9351	9130	0001	0001	C001
I_2	8022	0378	5692	0001	0001	0001
СĪ,	1066	3705	9802	0006	0007	0008
Cl_2	7637	6410	4802	0009	0007	0009
C_1	5693	8027	1802	0021	0022	0023
C_2	5437	6762	2068	0022	0023	0025
C_3	3993	5458	1519	0023	0024	0025
C_4	2831	5442	0685	0023	0024	0025
C_5	3063	6715	0469	0022	0023	0025
C ₆	4543	8038	0989	0022	0023	0025
C ₇	7724	1826	3099	0017	0017	0019
C ₈	6468	1961	3796	0019	0020	0022
C ₉	6500	3423	4240	0029	0030	0032
C_{10}^{-}	7658	4619	4060	0024	0025	0027
C ₁₁	8876	4485	3338	0022	0023	0025
C_{12}^{11}	8913	3047	2865	0020	0020	0022

Table 2. Temperature factors in $(ClC_6H_5)_2TeI_2$ Standard deviations in parentheses

(a) Anisotropic factors for heavy atoms

Ге	B_{11} 2.60 (0.04)	$B_{22} \ 3.24 \ (0.04)$	$B_{33} \\ 2.96 \\ (0.05)$	B_{12} 2.80 (0.06)	$B_{13} \\ 3.50 \\ (0.16)$	$B_{23} \\ 3.03 \\ (0.07)$
[1	4 ·53 (0·05)	5·42 (0·06)	3·16 (0·05)	4.5 (0.1)	5·6 (0·2)	4·6 (0·1)
[₂	4.32 (0.05)	4·74 (0·06)	3·25 (0·06)	3·8 (0·1)	3·3 (0·2)	4·0 (0·1)
Cl1	3·9 (0·2)	4·8 (0·3)	6·8 (0·3)	0·9 (0·4)	5·6 (0·4)	$4 \cdot 2 \\ (0 \cdot 5)$
CI <u>2</u>	9·6 (0·4)	$4 \cdot 3$ (0·2)	6·7 (0·4)	9·6 (0·6)	0·3 (0·6)	${3\cdot 4} \ (0\cdot 5)$

(b) Isotropic factors for carbon atoms

Te

 I_1

 I_2

С,	3.9	(0.3)	C ₅	4 ·0	(0.3)	C ₉	5.7	(0.5)
C_2	$4 \cdot 2$	(0.3)	C ₆	$4 \cdot 2$	(0.4)	C ₁₀	4.7	(0.4)
C_3	4·1	(0.4)	C_7	$3 \cdot 0$	(0.3)	C11	$4 \cdot 3$	(0.3)
C ₄	4 ·0	(0.4)	C ₈	4 ·0	(0.3)	C ₁₂	$3 \cdot 6$	(0.3)

Table 3. Amplitudes and orientations of atomic vibration ellipsoids in (ClC₆H₄)₂TeI₂

	Root-mean-square displacement along	Directic axes with	on Cosines o respect to	f ellipsoid orthogonal
	ellipsoid (Å)	X	$\frac{axes}{Y}$	Z
Te	$0.208 \\ 0.195 \\ 0.178$	$0.436 \\ 0.185 \\ 0.881$	$-0.899 \\ 0.146 \\ 0.414$	$0.052 \\ 0.972 \\ - 0.230$
I	0.272 0.238 0.191	$0.448 \\ 0.879 \\ 0.165$	$-0.866 \\ 0.380 \\ 0.327$	$-0.225 \\ 0.289 \\ -0.931$
I_2	0·261 0·231 0·200	-0.724 - 0.687 - 0.058	$0.669 \\ -0.721 \\ 0.180$	0.166 - 0.092 - 0.982
Cl ₁	$0.335 \\ 0.284 \\ 0.206$	-0.542 - 0.506 - 0.671	$0.672 \\ 0.218 \\ -0.708$	$-0.504 \\ 0.835 \\ -0.222$
Cl_2	$0.374 \\ 0.306 \\ 0.173$	-0.717 -0.488 -0.498	-0.561 - 0.021 - 0.828	$0.414 \\ -0.873 \\ 0.258$

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Table 4. Observed and calculated structure factors

The data are separated into groups having common values of k and l. The three columns in each group list values of h, F_o and F_c , in that order

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11.2. 14.1. 11.2. 14.1. 11.2. 14.1. 11.2. 14.1. 11.2. 14.1. 12. 14.1. 14.
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3 12.1	-68.2	5 24.2 -23.7	5 28.1 -31.0	K=-12. L= 5	K. 3. L. 6	6 24.1 25.6	0 11.4 10.6	-3 20.4 -21.5	-2 20.4 -18.0	
	7.112		0 14.0 -19.7	-3 18.0 16.6	-10 29.6 -31.0	10 2008 -2104	1 1443 1344	-1 32.9 35.6	J 4.1 5.0	-1 53.8 -30.
7 07.1	6/.0			-1 19.4 -20.3	-0 47.9 51.2	2 12.5 -13.6		0 12.1 11.0	2 10.1 11.0	. 24 23.
7 62.9		-10 12.6 16.1	10 10 -22.0	0 20.8 -21.8	-/ 30.9 30.7			1 40.4 -41.4	4 13.3 -17.6	1 59.3
	- 50 - 8	-9 11-5 8.8	1	A 29.4 -10.0		8 24.2 21.2	-7 34-1 32-3	1 11 - 16-2		1 49.4
1. 30.7	32.4	-7 17.9 -15.9	-16 13.6 18.5	5 24.3 -25.4		9 10-9 6-5	-6 73-2 67-7		12.9 12.4	A 31+2 -27+
11 16.5	18+1	-4 37.1 36.7	-9 20.6 22.1	6 16 6 13-2	-3 66-8 75-6	10 20.5 -13.6	-4 112.2 -97.2	5 14-5 17-5		5 19.9
K=-:u+ L=	4	-2 43.1 -43.6	-8 15.5 -7.5	7 33.5 33.6	-2 27.6 28.8	K= -P. L= 6	-3 56.6 -53.1	6 42.6 -42.7	- 13.5 14.5	6 10.4 3.
-2 18.5	-15.5	-1 39.2 -38.9	-7 33.8 -36.4	513- 1- 5	-1 98.1 -49.2	-2 21.8 -18.6	-2 64.8 60.3	7 12.6 -11.7	-1 17.9 -12.4	8 17.4 -19.
-1 12.6	-6.0	J 40.8 37.8	-6 14.7 -19.4	v 13.6 -13.8	0 52.5 -54.0	U 18.7 19.4	0 20.3 -15.9	A 13.7 13.0	-2 27.9 -26.1	
v 21.6	20.4	1 64.1 65.2	-5 34.8 36.5	1 13.0 9.0	1 15.9 14.6	2 11.7 -11.5	1 88.4 -83.8	9 24.8 28.1	0 23-1 24-1	
1 28.8	30.4	3 51+2 -51+4	-4 39.6 43.8	2 20.3 19.8	2 49.4 49.0	4 25.0 28.1	2 17.9 -21.4	<10, L= 7	1 12.6 16.1	
	-22.3	4 29.4 -27.6	-2 43.4 -45.1	4 21.5 -19.4	3 18.1 15.2	6 17.1 -18.5	3 50.4 52.3	-3 16.2 -11.4	3 26.2 -29.7	-5 22.1 21.
		2 16-8 21-1		5 12+3 -15+1	4 26.6 -26.3			-1 24.2 24.9	4 9.6 -8.3	54.5
6 40.8	40.8		1 14.1 21.1	7 18.3 18.0	2.1 -22.2	9 11.2 9.0	7 18.9 -18.8	1 3 13.4 15.9	6 20.4 19.0	-2 46.38.
7 10.1	-8.7		2 13.4 -12.3					1 13.7 -13.3	K8. L. B.	-1 33.2 -28.
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11 15-1	19.2	-3 45.3 -45.8	-4 29.6 30.4	-5 96.3 -89.7	-4 10.1 -7.5	3 21.1 -22.8	0 12.5 8.8	7 30-0 -29-1	0 34-5 34-9	
U-1	4	-2 14.8 15.2	-3 25.5 25.4	-4 16.5 -14.9	-3 49.1 46.5	4 15.7 18.7	R 4. L. 7	8 14.1 13.5	1 19.3 26.8	
- 11.3	12.9	3 12.9 -10.3	-1 33.7 -29.8	-3 92.9 91.4	-2 38.2 40.5	5 22.6 27.6	-9 27.0 -24.9	9 23.0 26.4	2 15.9 -14.6	
1 17-1	23.2	3 85.3 63.0	0 17.8 -18.6	-2 89.0 87.3	-1 23.8 -22.7	6 11.7 -14.3	-8 31.9 -30.7	Ke-11. Le 7	3 21+1 -21+4	-1 -1 -1 -1
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8 26.5	-26+0	9 11.4 -7.6	7 19.9 18.9	4 68.0 -65.7	6 10.5 -10.9	3 9.9 -9.8	-2 72.2 64.5	6 13.7 -12.7	-2 38.9 -17.5	
9 14.0	-9.4	10 15.1 -14.9	8 28.4 28.4	5 62.5 -61.4	7 52.3 52.3	4 12.0 12.4	-1 91.5 114.5	7 22.4 -24.4	5 32.2 32.0	15.1 -10
14.3	15.4	5	10 23.1 -23.2	6 12.6 4.6	8 32.6 28.2	5 15.0 17.0	3 60.1 61.7	9 18.8 20.6	1 27.4 28.4	1 10.2 14-5
		-7 11.9 13.6	1	7 40.8 41.1	9 19.6 -19.2	1 12.8 -15.3	69.6 20.2		2 27.6 -27.6	0 36.4 34.4
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8 21.4	-20.0	-1 36.2 -37.5	0 20.6 20.2	-6 45.2 -46.2	-5 54.2 -55.9	6 14.7 -14.2	K5. L. 7	K- 1. L- 8	-2 28.1 -29.4	
		0 40.3 38.5	1 17.5 17.6	-5 92.4 -96.2	-4 12.3 14.3	7 17.6 -18.6	-9 17.8 -16.5	-5 19.0 -16.5	0 33.1 34.3	-2 47.6 -19-1
	2.0.0	1 45.7 46.5	3 18.6 -13.5	-3 110.4 124.2	-3 63.5 68.7	9 16-1 15-1	-8 23.6 -21.9	-2 13.1 12.8	1 30.4 30.6	-1 21-1 -20-3
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-4 39.3	- 34 . 5	6 23.0 22.6	-3 31.8 33.0	2 93.6 93.8	2 22 4 29.4	-6 33.1 29.6	-2 44.6 48.9	-1 24.7 26.3	3 23.5 23.6	K3. L. 9
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-2 14.0	11.1	-7 18.3 -18.2	0 26.8 -15.7	4 51.2 -47.5	4 17.9 -18.2		0 13.7 14.9	-1 23.1 -23.9	K11. L. 8	-2 25.1 -26.4
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6 19.4	22.2	2 27.1 -12.4	5 28.2 -31.1		-0 15.5 4.3	5 16-6 15-2	6 69.9 -64.3		1 2445 2641	2 20.0 21.4
8 17.3	-13.3	3 53.0 58.3	7.18.0 16.0	-10 22.9 -21.4	-5 11.9 -6.5	7 15.6 -14.2	7 24.5 -25.5	2 19-6 -20-9	2 200 - 200	3 42.8 -39.4
K# 1. L#	5	4 41.3 43.7	8 12.5 13.3	-8 29.6 29.6	-3 32.7 32.4	K. 1. L. 7	8 19.0 19.9	3 12.4 -7.6	A 19-7 19-4	4 43.8 -4.4
-10 21.8	22.7	5 38.2 -38.4	K. 9, L. 5	-7 34.8 30.2	-2 33.2 34.2	-9 15.4 -21.9	9 33.6 25.1	5 -2 1 1	8 18-6 -20-0	5 22.7 19.2
-8 27.8	-30+1	6 32.1 -32.9	-9 14.7 14.5	-6 14.1 -14.7	-1 20.4 -19.7	-7 25.2 26.3	K= -6+ L= 7	-5 24.3 -24.4	Se-12. 1. 8	
-4 14 1	-14.8	7 14.8 15.5	-7 16.8 -21.6	-5 68.3 -69.3	J 78.6 -78.6	-5 27.2 -26.6	-0 17.4 -15.4	-4 19.0 -19.4	-2 21.1 -20.1	9 20.7 14.1
-6 /2 1	22.4	8 30.8 33.0	-> 16.6 16.8	-4 11.5 -10.6	3 54.5 56.2	11.7 -7.6	-7 16-2 10-3	-3 26.6 28.4	0 22.6 18.9	
	-12.4	10 19.0 -23.0		-3 96.8 106.4	4 23.9 -22.6			-2 29.9 32.2	1 26.7 23.3	-9 17.9 15.3
-2 14.3	-10.9		0 14.7 15.1	-2 /4-7 84-6	2 2003 -0204	0 9.0 7.6	-4 41.2 -44.9	0 27.0 -32.3	3 36.0 -34.0	-7 23.6 -25.3
5 10.5	14.4	-7 12.5 -11.6	K9. L. 5	111.6 -166.6	A 31.6 27.9	1 9.8 5.6	-3 67.9 -66.0	A 24-8 -24-5	30.9 27.0	-6 15.9 -:5.8
1 50.0	18.9	-6 15.5 -16.1	-4 12.7 17.0	2 103-1 109-8	9 18.9 -18.1	2 10.4 -14.0	-2 29.9 29.7	K 3. L 8	7 14.9 -11.4	-5 19.5 20.4
2 11.7		-> 27.6 27.7	-3 33+1 33+0	3 73.3 67.1	10 27.0 -25.1	K1, L- 7	-1 02.9 97.1	-4 13+1 -12+8	8 19.3 -21.2	
5 15.1	- 10.0	-4 39.2 40.8	-1 43.4 -40.8	4 55-1 -54-2	K- 5-L- 6	-9 31.7 -32.5	0 16-2 10-6	-3 22.7 -25.1	K=-13+ L= 8	-2 2203 -2400
6 28.2	30.3	-2 26.6 -28.7	1 11.7 12.2	5 61.0 -65.9	-10 20.0 -21.7	-7 14 4 17	1 86.9 -99.9	-1 28.6 26.6	1 23.5 19.0	2 16-0 15-9
(* -1+ L*	5		2 39.6 42.9	7 50.0 49.1	-9 15.6 10.9	-6 49-8 46-6	1 61.2 66.9	0 19.9 20.7	3 29.8 -26.8	K
-1. 16.1	14.8	1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1	3 9.3 12.1	A 10-0 16-1	-7 14-3 12.0	-5 11.3 -13.4	4 85-6 85-2		5 22.1 19.2	-2 10.7 -11.9
-8 22.4	-25.7	3 33.2 -35.3	4 27.6 -31.8	9 18.3 -22.2	-6 35.2 -39.3	-4 56.4 -51.7	6 71.0 -63.6	-4 1448 -1441	6 19.5 19.9	-1 25.6 -19.4
-6 48.7	47.4	4 11.3 -14.0	5 28.9 -30.6	10 19.6 -20.5	-5 23.6 -25.6	-3 20.8 -19.2	7 38.0 -35.2	-2 13.9 13.9	K- 0. 1. 9	2 12-8 17-1
-7 20.7	26.8	5 17.0 17.9	6 20.4 20.1	K= 2. L= 6	-4 16.4 18.1	-2 49.4 50.0	8 21.6 23.3	0 31+7 -35+0	-9 16.6 20.6	3 22.6 -23.0
-1 -1 0		6 14.0 15.5	7 26.6 25.7	-10 35.0 -34.7	-3 26.7 30.0	-1 46.2 45.0	9 32.6 31.3	2 28.2 31.6	-7 29.0 -26.5	
-2 20.1	18.8	K -5, L 5		-8 53.1 55.7	-1 29.4 -29.7	14.4 -22.3		3 12.9 12.6	-6 33.1 -30.8	7 14-1 16-8
0 39.3	-26+1	-0 10.1 -10./	10 20.3 -22.4		0 13.0 -16.4	2 14.8 -18.9		2/10 - 10.3	-5 17.9 15.9	8 18.5 -17.8
1 42.7	-45.9	1 18.4 -20.8	5 10 1 5			3 12 4 9.2	-4 36-8 -19-1		-4 54.0 53.0	9 20.0 -14.9
2 16.6	14.2	2 5.6 -9.3	-7 14.4 -15.7	-3 99-5 111-6		4 27.5 25.0	-3 49.7 -46.1	-1 21.0 22.4	-3 17.6 11.7	K5, L. 9
3 34.8	36.2	3 25.8 27.0	-5 14.4 16.8	-2 -0.9 -1.1	1 15.8 -21.1	6 15.5 -6.6	-2 24.1 24.4	0 18-6 14-9	-2 34.2 -36.0	3 14.7 -11.8
7 16.7	18.2	4 19-1 20-5	-4 14.5 9.5	-1 85-1 -86-1	2 19.5 23.9	7 17.0 -10.1	-1 77.3 87.7	2 21-0 -21-9	-1 30.5 -6.2	* 23.9 -22.9
9 15-1	-16.8	5 34.0 -32.5	-2 14.8 -14.1	0 90.3 -88.0	3 34.5 43.7	K= 2. L= 7	0 27.9 23.8	K	1 62.7 41.1	6 22.6 21.4
	·	6 37.7 -37.6	K=-10, L= 5	1 33-1 27-6	4 8.7 -6.2	-7 13.7 18.2	2 70.7 -75.0	-4 13.5 -12.7	3 49.2 -48.2	2 14.7
	10.1	7 11.4 14.3	-5 14.4 -13.8	2 78.2 78.5	5 49.3 -55.8	-3 13.7 13.3	3 39.4 35.0	-2 25.2 26.7	4 23.4 -22.4	1 Aut 17.6
-7 14-4	-17.8	8 31.8 36.1	13.6 10.2	3 14-5 15-7	6 22.9 -27.3	-1 14.0 -12.5	• 101.9 99.9	0 24.7 -26.7	5 18.5 19.3	11.3 -11.4
-6 13.3	13.1	10 15.6 -19.9	-1 13.3 -12.1	34.2 -33.4	32.9 36.0	27.0	7 39.3 -70.4	2 29.5 30.1	6 25.6 23.8	6 16.7 13.5
-5 35.7	34.8	-10 11.1	0 28.8 -24.9	6 16-1 7.4	9 11.0 -4 4	-8 23.6 -24.4	A 32.1 32.7	- 33.9 -34.8	K 1. L 9	7 12.7 13.3
-4 14.2	11.7	-9 17.8 20.8	1 21.0 22.1	7 15.4 17.0	10 19.3 -23.4	-7 25.4 28.7	9 32.5 36.5	6 17.7 10.0	-7 26.3 22.5	K# -7, L# 9
-3 23.5	-22-1	-7 34.1 -35.9	2 39.3 40.3	K2. L. 6	K 6. L 6	-6 52.7 52.4	K+ -8+ L+ 7	7 21.8 18.1	-6 38-2 -14-0	-1 15.7 11.1
-2 29.1	-29+1	-6 21.3 -23.3	4 32.3 -32.9	-8 20.2 20.0	-8 19.0 23.0	-4 83.1 -75.6	-6 17.0 16.8	K+ 5.L+ 8	-5 16-1 10-3	1 19.7 -15.4
-1 20.5	-19.7	-5 32.6 33.0	5 22.4 -21.8	-7 26.2 22.8	-6 27.4 -27.8	-3 43.4 -40.0	-4 17.6 -25.4	-3 24.4 -25.5	-4 59.6 40.4	1 12-1 11-9
1 11.4	11.6	-4 40.4 41.9	7 27.0 27.5	-6 16.8 -16.9	-5 14.4 -12.4	-2 61.6 61.4	-3 33.1 -33.4	-1 22.4 22.5	-2 57.3 -58.9	2 16.7 -15.4
3 30-4	-29.8	-2 49.9 -51.7	1 13.6 11.6	-3 67.2 -66.2	14.4 14.5	1 60.2 -66.8	-2 12.6 10.7	2 17.6 -18.t	-1 36.8 -34.5	L
4 19.0	-21.2	-1 (***) -23.6	1 10 14.7 -18.4	20.8 -29.7	-3 20.4 19.4	3 24.8 27.4	-1 50.7 53.9	5	0 36.9 35.7	-1 11.5 12.1
\$ 20.2	19.8	1 33.0 34.4	Ke-11. L= 5	-2 42.2 02.1	5 -6. 1. 6	4 37.7 18.5	1 52.2 -44.4	4 47+2 18+0	1 51.7 49.3	1 12.0 -12.6
6 23.6	26.9	3 26-9 -30-4	-3 19.7 20.1	0 111.5 -115.0	-4 21.8 17.0	6 14.4 -18.9	2 54.9 -41.7	y 27.9 -28.0	3 36.6 -36.9	3 24.1 20.9
(* -2, L*	· .	K6. L. 5	-1 31.1 -27.9	2 129.8 124.7	-3 16.3 -12.1	7 16.0 -14.9	3 24.6 25.7	5 18.4 -20.0	5 19,0 17.2	Ke -9. Le 9
-8 18.3	-20.1	-6 14.0 -15.7	0 26-1 -25-5	3 77.8 78.2	-2 10.4 -10.5	K+ 3+ L+ 7	4 68.0 77.2	6 14.6 17.0	6 20.9 17.5	1 10.8 -13.4
	12.0	-4 26.4 22.6	1 21.3 22.9	4 77.3 -74.4	1 10.8 -10.9	-8 18.3 16.8	5 11.0 10.7	7 22.8 22.7	K= -1. L= 9	3 14-9 13-2
- 10.9	-13-0	-3 9.6 12.2	41.3 42.9	5 100.5 -94.2	2 6.3 -8.7	-7 14.0 9.9	6 60.8 -49.8	K* 6+ L* 8	-9 16.6 12.7	1 17.6
		-1 22.7 -17.8	1 1 10.1 -11.6	0 11.2 7.6	3 32.3 38.6	-0 21.4 -19.2	7 39.4 -40.0	-3 23.4 -25.0	-7 20.4 -18-9	1 1 1 1 1 1 1 1 1 1

-3 14.9 -2 12.3 14.0

9 39.6 K -9, L

Table 4 (cont.)

The three-dimensional data consisted of zeroth through ninth level Weissenberg photographs about c, supplemented by several intersecting precession nets. Some 2500 independent observed reflections were used. Before carrying out a three-dimensional difference synthesis to locate the carbon atoms, two cycles of three-dimensional least-squares refinement on the heavy atoms were computed by use of the full-matrix routines on the IBM 709. During this refinement, it became apparent that some adjustment of the interlayer scaling was indicated. The following factors, derived from $\Sigma |F_c|/\Sigma |F_o|$ for a given level, were accordingly applied for the remainder of the refinement: hk0(0.910), hk1(0.976), hk4(0.923), hk6(0.916) and hk7(0.943). The indicated changes on the remainder

15.3 18.8 31.6 28.3 26.6

-2 35.0 35.6

ing five levels (representing approximately half of the data) were less than 2% and no changes were made.

23.6

-6 32.0 -5 17.1 -4 52.9 + 22+2 15+8 6 22+3 -18+2

19.4 -1 20.8 38.2 K. -6. L. 7 -5 19.6

The rescaling could not have caused more than small shifts in the positional and vibrational parameters of the heavy atoms. In the cycle of least-squares refinement immediately following the rescaling, the maximum shift in the positional parameters of the iodine atoms was 0.0004 with an average shift of 0.0002. All other shifts in positional and vibrational parameters were less than the corresponding standard deviations of the final values listed in Tables I and 2(a).

Following one more cycle of refinement of the heavy atoms, these were used as the basis of a threedimensional $(F_o - F_c)$ synthesis. All twelve carbon atoms were clearly resolved with little false detail and another cycle of least-squares refinement was carried out on the heavy atoms including the carbon atoms with fixed positions and a fixed isotropic temperature factor of 5.0 Å².

In the next step, two three-dimensional least squares cycles were computed for refinement of the carbon atom positions. In these cycles, individual isotropic temperature parameters (initially 5.0 Å²) were applied to the carbon atoms while the heavy atom positional and anisotropic temperature parameters were held fixed. A final, full-matrix least-squares cycle was then computed which simultaneously refined all 94 parameters, 9 for each heavy atom, 4 for each carbon atom and the scale factor. The resulting atomic positional parameters and their standard deviations are shown in Table 1 and the temperature parameters are shown in Table 2. A final $(F_o - F_c)$ synthesis based on all 17 atoms showed numerous small maxima, some of which were high enough to correspond to hydrogen atoms. However, it was not surprising that there was little correlation between the positions of these maxima and those expected for hydrogen. The maximum fluctuations in the difference synthesis were within the range ± 1.5 electrons per Å³ and there were no significant maxima or minima in the vicinities of the atomic positions.

The observed structure factors are compared in Table 4 with those computed on the basis of the final positional and temperature parameters. The atomic scattering factors used for tellurium and iodine were those of Thomas & Umeda (1957), those for chlorine were the values of Dawson (1960) while for carbon, the graphite values of McWeeney (1954) were used. The atomic scattering factors were not corrected for dispersion as the corrections for Mo $K\alpha$ would have been less than the uncertainties in the individual values. The final value of $R = \Sigma ||F_o| - |F_c|| / \Sigma |F_o|$ was 7.2% for all observed reflections.

Discussion of the structure

The observed molecular structure of $(\text{ClC}_6\text{H}_4)_2\text{TeI}_2$ is shown in Fig. 1 and the packing arrangement is shown in Fig. 2. Tables 5, 6 and 7 list the bond distances, bond angles and the more significant non-bonded separations respectively. In order to simplify the computation of interatomic distances, bond angles, least-squares planes and related quantities, it was found convenient to transform the atomic coordinates to a set of isometric orthogonal axes, X, Y and Z. The origin is taken coincident with that of the crystallographic axes and the latter are so oriented that a_{\perp} is along X and b is in the plane XY. The transformation equations are then:

$$X (Å) = ax + (b \cos \gamma)y + (c \cos \beta)z$$

$$Y (Å) = (b \sin \gamma)y - (c \sin \beta \cos \alpha^*)z$$

$$Z (Å) = (c \sin \beta \sin \alpha^*)z$$

The molecular structure of $(ClC_6H_4)_2TeI_2$ is similar

to that found in $(CH_3)_2$ TeCl₂ (Christofferson, Sparks & McCullough, 1958) and other chlorides and bromides of R_2 Se and R_2 Te compounds, but is in sharp contrast to the molecular complex type of bonding observed in dibenzylsulfide. I₂ (Rømming, 1960) and in the iodine complexes of dithiane and diselenane (Chao & McCullough, 1960, 1961).

Table 5. Bond distances in (ClC₆H₄)₂TeI₂ in Å Standard deviations in parentheses

	otar	idara deviati	ions in parenth	eses	
Te-I	2.947	(0.002)	$Te-I_2$	2.922	(0.002)
Te-C,	$2 \cdot 13$	(0.02)	$Te-C_2$	$2 \cdot 10$	(0.02)
Cl₁–C₄	1.75	(0.03)	$Cl_2 - \overline{C_{10}}$	1.74	(0.03)
$C_1 - C_2$	1.39	(0.03)	$C_7 - C_8$	1.40	(0.03)
$C_{9}^{-}C_{3}^{-}$	1.38	(0.03)	$C_8 - C_9$	1.42	(0.03)
$C_3 - C_4$	1.41	(0.03)	$C_{9} - C_{10}$	1.35	(0.03)
$C_4 - C_5$	1.38	(0.03)	$C_{10} - \hat{C}_{11}$	1.38	(0.03)
$C_5 - C_6$	1.41	(0.03)	$C_{11} - C_{12}$	1.42	(0.03)
$C_6 - C_1$	1.40	(0.03)	$C_{12} - C_7$	1.41	(0.03)
	Te-	C Average	2.115 (0.0	015)	
	Cl-0	C Average	1.745 (0.0	(20)	
	CC	Average	1.39 (0.0)2)	

Table 6. Angles in (ClC₆H₄)₂TeI₂ in degrees Standard deviations in parentheses

(a) Bond angles

I ₁ -Te-I ₂	$173 \cdot 5(0 \cdot 1)$	C ₁ -Te-C ₇	$101 \cdot 1(1 \cdot 0)$
$I_1 - Te - C_1$	87.3(0.7)	I_2 -Te- C_1	89.1(0.7)
$I_1 - Te - C_7$	88.1(0.7)	$I_2 - Te - C_7$	$87 \cdot 3(0 \cdot 7)$
$Te-C_1-C_6$	120.6(1.8)	$\overline{Te}-C_7-C_{12}$	114.6(1.8)
$Te-C_1-C_2$	$115 \cdot 8(1 \cdot 8)$	$Te-C_7-C_8$	122.9(1.8)
$C_{6} - C_{1} - C_{2}$	123.0(2.5)	$C_{12} - C_7 - C_8$	$122 \cdot 5(2 \cdot 5)$
$C_1 - C_2 - C_3$	119.2(2.5)	$C_7 - C_8 - C_9$	$114 \cdot 3(2 \cdot 5)$
$C_2 - C_3 - C_4$	118.5(2.5)	$C_{8}-C_{9}-C_{10}$	123.7(2.5)
$C_{3}-C_{4}-C_{5}$	$122 \cdot 4(2 \cdot 5)$	$C_{9}-C_{10}-C_{11}$	$122 \cdot 5(2 \cdot 5)$
$Cl_1 - C_4 - C_3$	118.5(2.0)	$Cl_2 - C_{10} - C_9$	$1] 9 \cdot 1 (2 \cdot 0)$
$Cl_1 - C_4 - C_5$	119.1(2.0)	$Cl_2 - C_{10} - C_{11}$	118.5(2.0)
$C_4 - C_5 - C_6$	119.6(2.5)	$C_{10}-C_{11}-C_{12}$	116.6(2.5)
$C_{5}-C_{6}-C_{1}$	$117 \cdot 2(2 \cdot 5)$	$C_{11}-C_{12}-C_7$	120.5(2.5)

(b) Angles sł	nowing dist	ortion fron	n 'ideal' m	olecular	structure
$Te-C_1 \cdots C_4$	171.	6(1.2)	$Te-C_7 \cdot \cdot$	• C ₁₀ 1	173.7(1.2)
$Cl_1 - C_4 \cdot \cdot \cdot C_1$	174∙	4(1.5)	$Cl_2 - C_{10}$	$\cdot \cdot \tilde{C}_7$ 1	$176 \cdot 1(1 \cdot 5)$
$\operatorname{Cl}_1 \cdot \cdot \cdot \operatorname{Te} \cdot \cdot$	$\cdot \operatorname{Cl}_2$ 111 \cdot	1(0.2)			

Table 7. Packing distances in (ClC₆H₄)₂TeI₂

		Sum of	Figure
Atoms	Observed	van der Waals	showing
involved	distance	radii	atoms involved
$Te-I_1'$	4·13 Å	4·35 Å	2(b)
$Te-I_{a}^{\prime\prime}$	4.46	4.35	2(b)
TeCl ₁ ″″	3.91	4 ·00	2(c)
I ₁ -Cl ₁ ⁷	4.09	3.95	2(c)
I ₁ -Cl ₉ ″	3.92	3.95	2(c)
ICl_	4.06	3.95	2(c)
ICl_''	3.79	3.95	2(c)
I,-I,″	4.14	4.30	2(b)
I,'–ĺ,''	3.85	4·3 0	2(b)
II_″	4.32	4.30	2(b)
C1, -Cl, '	3.65	3.50	2(c)
*H1, -C1,'	(2.7)	$3 \cdot 0$	2(c)
CC_'	3.40	3.40	2(c)
$C_{a}^{\prime}-C_{a}^{\prime}$	3.45	3.40	2(c)
C,,-Ĉ,,′	3.40	$3 \cdot 40$	2(c)
$C_{12}^{11} - C_{11}^{11}$	3.48	$3 \cdot 40$	2(c)

* On the assumption that H_{12} is 1.1 Å from C_{12} on the line from the center of the ring.



Fig. 1. The molecular structure of $(p-\text{ClC}_6\text{H}_4)_2\text{TeI}_2$.

As in all molecules of the $R_2(VI)X_2$ (non complex) type, the axial bond distances are longer than the sum of the single-bond covalent radii. In $(CIC_6H_4)_2TeI_2$, the average Te–I distance of 2.93 Å is 0.23 Å longer than the radius sum, 2.70 Å. The difference in this case is considerably greater than the 0.15 Å and 0.17 Å lengthenings observed in $(CH_3)_2TeCI_2$ and in $(C_6H_5)_2TeBr_2$ (Christofferson & McCullough, 1958). This effect is probably due to the greater tendency for the iodide to be like the molecular complexes with $(VI) \cdots I-I$ bonding. Further evidence of this tendency is found in the short I_1-I_2 distance of 3.85 Å. No short Cl–Cl or Br–Br contacts were observed in the chloride and bromide.

In (C₆H₅)₂TeBr₂, (C₆H₅)₂SeBr₂ (McCullough & Hamburger, 1941) and the di-p-tolylselenium chloride and bromide (McCullough & Marsh, 1950), the molecules are required crystallographically to have a 2-fold axis. Although the molecular structure of $(ClC_6H_4)_2TeI_2$ approximates the symmetry 2, there are significant and interesting deviations. In the first place the distances Te-I₁(2.947 Å) and Te-I₂(2.922 Å) differ by more than 10σ . This difference may be due to the fact that an I_1 atom is only 4.13 Å from a second Te atom and the fact that pairs of I_1 atoms are only 4.14 Å apart. The sums of the corresponding van der Waals radii are 4.35 Å and 4.30 Å respectively. Although these 'non-bonded' interactions of I_1 are weak, there are no compensating interactions involving I₂, hence it is not surprising that the Te-I₁ distance is slightly longer than that for $Te-I_2$.

An analysis of the molecular structure in terms of the least-squares planes in Table 9 also reveals distortions from ideal symmetry. If the molecule had the symmetry 2, then Plane 1 through Te, C_1 and C_7 should divide the molecule into pairs of atoms equidistant from the plane. In fact, one might have expected the atoms C_4 , C_{10} , C_1 and C_2 to be in Plane 1,







Fig. 2. (a) Projection of the structure down the a axis. (b) Projection of the structure down the b axis. Only the central portion of the molecule is shown in order to emphasize certain features of the packing. (c) Projection of the structure down the c axis.

 Table 8. Equations of least-squares planes expressed in the form:

$$AX + BY + CZ + D = 0$$

(Orthogonal coordinates)

Plane num- ber	Atoms in L.S. fit	A	В	C	D
1	Te, C_1, C_7	0.00484	-0.33677	0.94158	8 ∙557
2	Phenyl group I (C ₁ –C ₆)	0.50043	-0.00519	-0.86576	- 7.501
3	Phenyl group II (C ₇ –C ₁₂)	0.43432	-0.05922	0.89881	10.715

Table 9. Distances of atoms from L.S. planes, in Å

(a)	Plane I (Te, C_1 , C	7)			
\mathbf{Te}	0.000	C_1	0.000	C ₇	0.000
I,	-2.941	C ₂	0.660	C_8	0.608
$\hat{\mathbf{I}_2}$	2.918	C_3	0.559	C ₉	0.552
ĊĪ,	-0.506	C_4	-0.228	C ₁₀	0.000
Cl_2	0.118	C_5	-0.844	C ₁₁	-0.635
_		C_6	-0.776	C ₁₂	-0.615

(b) Plane 2 (Phenyl group I)

C ₁	0.002	C4	0.020	${ m Te}$	0.279
C ₂	-0.002	C_5	-0.023	Cl ₁	0.203
C_3	-0.006	C_6	0.015	-	
-	Mean distance	e of Cat	oms from Pl	ane: 0.011 Å.	

(c) Plane 3 (Phenyl group II)

C_{7}	0.006	$C_{10} = 0.019$	Te	0.110
C'8	0.000	$C_{11}^{10} = -0.012$	Cl ₂	0.132
C ₀	-0.013	$C_{10}^{} = 0.000$	-	

Mean distance of C atoms from Plane: 0.008 Å.

even though not required by the symmetry 2. Not only are three of the latter atoms out of Plane 1, the atoms do not pair off as anticipated. Inspection of the data for the planes through the two phenyl groups shows that the rings themselves are planar within the standard deviations of the carbon atoms. However, the Te and Cl atoms are significantly out of the planes of their respective rings. Further evidence of molecular distortion is found in the comparison of the $Cl_1 \cdots Te \cdots Cl_2$ angle of $111 \cdot 1 \pm 0 \cdot 2^{\circ}$ with the C1–Te–C7 bond angle of $101 \cdot l \pm 1 \cdot 0^\circ$ and this emphasizes the danger of using the former as a measure of the bond angle at the central atom. All of the irregularities noted above are so much greater than the standard deviations involved that their reality can scarcely be doubted. It is interesting to note that although bonds to the phenyl groups may be bent out of plane by several degrees, the rings themselves retain their planarity.

A study of the distortion of the molecules in relationship to the intermolecular packing shows that the observed distortion permits a more efficient packing. If one keeps the Te, I_1 , I_2 , C_1 and C_7 atoms fixed in their observed positions and then arranges the remaining atoms according to an ideal (undistorted) model, the shortest I–Cl, Cl–C (and Cl–H) packing distances become some 0.25 to 0.35 Å shorter.

In reviewing the structure of $(C_6H_5)_2$ TeBr₂, a similar distortion of the molecular structure was noted. In that case, the Te atom was observed to be 0.134 Å out of the least-squares plane of the six carbon atoms, while the ring is again planar, within standard deviations. Also the angle $C_4 \cdots Te \cdots C'_4$ is 97.7° compared to the C_1 -Te- C'_1 angle of 93.9°. The difference in this case is more than three times the standard deviations of 0.7° and 1.2° respectively.

Further studies of appropriate $R_2 \text{Se} X_2$ and $R_2 \text{Te} X_2$ compounds are planned in order to learn more about the 'dihalide' versus the 'molecular complex' relationship.

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