interest in this work and for valuable criticism on the manuscript. We are also much indebted to many research students for stimulating discussions. We gratefully acknowledge financial support from the Swedish State Council of Technical Research and from the Air Force Office of Scientific Research of the Air Research and Development Command, United States Air Force under contract No. AF 61(052)–40.

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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:

$$a = 9.751 \pm 0.006 \text{ Å} \qquad \alpha = 115.7 \pm 0.1°$$
$$b = 10.681 \pm 0.006 \qquad \beta = 87.2 \pm 0.1$$
$$c = 9.531 \pm 0.006 \qquad \gamma = 116.4 \pm 0.1$$

The space group is $P\bar{1}$ 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 $R_2\text{Se}$ and $R_2\text{Te}$ 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 ± 0.1°		C$_1$–Te–C$_7$	101.1 ± 1.0°
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 $(p\text{-ClC}_6\text{H}_4)_2\text{TeI}_2$ is definitely not a molecular complex of the type found for $C_4H_8Se_2 \cdot 2 I_2$ (which involves $\text{Se} \cdots \text{I–I}$ 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 $\text{Se} \cdots \text{I–I}$ and $\text{S} \cdots \text{I–I}$ 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 $(p\text{-}ClC_6H_4)_2TeI_2$ 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:

$$a = 9.751 \pm 0.006 \text{ Å} \qquad \alpha^* = 62° 35' \pm 03'$$
$$b = 10.682 \pm 0.006 \qquad \beta^* = 79° 45' \pm 05'$$
$$c = 9.531 \pm 0.006 \qquad \gamma^* = 61° 59' \pm 03'$$
$$\alpha = 115.70 \pm 0.10° \qquad V = 788.8 \text{ (Å)}^3$$
$$\beta = 87.20 \pm 0.10$$
$$\gamma = 116.35 \pm 0.10$$

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 $P\bar{1}$ 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 0·15 mm. 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 $h0l$ and $0kl$ 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 inter-layer 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. Two-dimensional 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* $(\times 10^4)$

	x	y	z	$\sigma(x)$	$\sigma(y)$	$\sigma(z)$
Te	8042	9834	2412	0001	0001	0001
I_1	7757	9351	9130	0001	0001	C001
I_2	8022	0378	5692	0001	0001	0001
Cl_1	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}	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

	B_{11}	B_{22}	B_{33}	B_{12}	B_{13}	B_{23}
Te	2·60	3·24	2·96	2·80	3·50	3·03
	(0·04)	(0·04)	(0·05)	(0·06)	(0·16)	(0·07)
I_1	4·53	5·42	3·16	4·5	5·6	4·6
	(0·05)	(0·06)	(0·05)	(0·1)	(0·2)	(0·1)
I_2	4·32	4·74	3·25	3·8	3·3	4·0
	(0·05)	(0·06)	(0·06)	(0·1)	(0·2)	(0·1)
Cl_1	3·9	4·8	6·8	0·9	5·6	4·2
	(0·2)	(0·3)	(0·3)	(0·4)	(0·4)	(0·5)
Cl_2	9·6	4·3	6·7	9·6	0·3	3·4
	(0·4)	(0·2)	(0·4)	(0·6)	(0·6)	(0·5)

(b) Isotropic factors for carbon atoms

C_1	3·9	(0·3)	C_5	4·0	(0·3)	C_9	5·7	(0·5)
C_2	4·2	(0·3)	C_6	4·2	(0·4)	C_{10}	4·7	(0·4)
C_3	4·1	(0·4)	C_7	3·0	(0·3)	C_{11}	4·3	(0·3)
C_4	4·0	(0·4)	C_8	4·0	(0·3)	C_{12}	3·6	(0·3)

Table 3. *Amplitudes and orientations of atomic vibration ellipsoids in* $(ClC_6H_4)_2TeI_2$

	Root-mean-square displacement along axis of vibration ellipsoid (Å)	Direction Cosines of ellipsoid axes with respect to orthogonal axes		
		X	Y	Z
Te	0·208	0·436	−0·899	0·052
	0·195	0·185	0·146	0·972
	0·178	0·881	0·414	−0·230
I_1	0·272	0·448	−0·866	−0·225
	0·238	0·879	0·380	0·289
	0·191	0·165	0·327	−0·931
I_2	0·261	−0·724	0·669	0·166
	0·231	−0·687	−0·721	−0·092
	0·200	−0·058	0·180	−0·982
Cl_1	0·335	−0·542	0·672	−0·504
	0·284	−0·506	0·218	0·835
	0·206	−0·671	−0·708	−0·222
Cl_2	0·374	−0·717	−0·561	0·414
	0·306	−0·488	−0·021	−0·873
	0·173	−0·498	0·828	0·258

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

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: $hk0(0\cdot910)$, $hk1(0\cdot976)$, $hk4(0\cdot923)$, $hk6(0\cdot916)$ and $hk7(0\cdot943)$. The indicated changes on the remaining five levels (representing approximately half of the data) were less than 2% and no changes were made.

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 $0\cdot0004$ with an average shift of $0\cdot0002$. All other shifts in positional and vibrational parameters were less than the corresponding standard deviations of the final values listed in Tables 1 and 2(a).

Following one more cycle of refinement of the heavy atoms, these were used as the basis of a three-dimensional $(F_o - F_c)$ 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 $5 \cdot 0$ Å^2.

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 $5 \cdot 0$ Å^2) 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 $\pm 1 \cdot 5$ electrons per Å^3 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 $7 \cdot 2\%$ for all observed reflections.

Discussion of the structure

The observed molecular structure of $(ClC_6H_4)_2TeI_2$ 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 is along X and b is in the plane XY. The transformation equations are then:

$$X \text{ (Å)} = ax + (b \cos \gamma)y + (c \cos \beta)z$$
$$Y \text{ (Å)} = (b \sin \gamma)y - (c \sin \beta \cos \alpha^*)z$$
$$Z \text{ (Å)} = (c \sin \beta \sin \alpha^*)z$$

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

to that found in $(CH_3)_2TeCl_2$ (Christofferson, Sparks & McCullough, 1958) and other chlorides and bromides of R_2Se and R_2Te compounds, but is in sharp contrast to the molecular complex type of bonding observed in dibenzylsulfide.I_2 (Rømming, 1960) and in the iodine complexes of dithiane and diselenane (Chao & McCullough, 1960, 1961).

Table 5. *Bond distances in* $(ClC_6H_4)_2TeI_2$ *in* Å
Standard deviations in parentheses

Te–I$_1$	2·947	(0·002)	Te–I$_2$	2·922	(0·002)
Te–C$_1$	2·13	(0·02)	Te–C$_2$	2·10	(0·02)
Cl$_1$–C$_4$	1·75	(0·03)	Cl$_2$–C$_{10}$	1·74	(0·03)
C$_1$–C$_2$	1·39	(0·03)	C$_7$–C$_8$	1·40	(0·03)
C$_2$–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$_{10}$–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	(0·015)
Cl–C Average	1·745	(0·020)
C–C Average	1·39	(0·02)

Table 6. *Angles in* $(ClC_6H_4)_2TeI_2$ *in degrees*
Standard deviations in parentheses

(a) Bond angles

I$_1$–Te–I$_2$	173·5(0·1)		C$_1$–Te–C$_7$	101·1(1·0)
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$_7$	87·3(0·7)
Te–C$_1$–C$_6$	120·6(1·8)		Te–C$_7$–C$_{12}$	114·6(1·8)
Te–C$_1$–C$_2$	115·8(1·8)		Te–C$_7$–C$_8$	122·9(1·8)
C$_6$–C$_1$–C$_2$	123·0(2·5)		C$_{12}$–C$_7$–C$_8$	122·5(2·5)
C$_1$–C$_2$–C$_3$	119·2(2·5)		C$_7$–C$_8$–C$_9$	114·3(2·5)
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$_5$	122·4(2·5)		C$_9$–C$_{10}$–C$_{11}$	122·5(2·5)
Cl$_1$–C$_4$–C$_3$	118·5(2·0)		Cl$_2$–C$_{10}$–C$_9$	119·1(2·0)
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$_1$	117·2(2·5)		C$_{11}$–C$_{12}$–C$_7$	120·5(2·5)

(b) Angles showing distortion from 'ideal' molecular structure

Te–C$_1$ ··· C$_4$	171·6(1·2)	Te–C$_7$ ··· C$_{10}$	173·7(1·2)
Cl$_1$–C$_4$ ··· C$_1$	174·4(1·5)	Cl$_2$–C$_{10}$ ··· C$_7$	176·1(1·5)
Cl$_1$ ··· Te ··· Cl$_2$	111·1(0·2)		

Table 7. *Packing distances in* $(ClC_6H_4)_2TeI_2$

Atoms involved	Observed distance	Sum of van der Waals radii	Figure showing atoms involved
Te–I$_1$′	4·13 Å	4·35 Å	2(b)
Te–I$_2$″	4·46	4·35	2(b)
Te–Cl″′	3·91	4·00	2(c)
I$_1$–Cl$_1$′	4·09	3·95	2(c)
I$_1$–Cl$_2$″	3·92	3·95	2(c)
I$_2$–Cl$_1$′	4·06	3·95	2(c)
I$_2$–Cl$_2$″	3·79	3·95	2(c)
I$_1$–I$_1$′	4·14	4·30	2(b)
I$_1$′–I$_2$″	3·85	4·30	2(b)
I$_2$–I$_2$″	4·32	4·30	2(b)
C$_{12}$–Cl$_1$′	3·65	3·50	2(c)
*H$_{12}$–Cl$_1$′	(2·7)	3·0	2(c)
C$_2$–C$_3$′	3·40	3·40	2(c)
C$_3$–C$_3$′	3·45	3·40	2(c)
C$_{11}$–C$_{11}$′	3·40	3·40	2(c)
C$_{12}$–C$_{11}$′	3·48	3·40	2(c)

* On the assumption that H$_{12}$ is $1 \cdot 1$ Å from C$_{12}$ on the line from the center of the ring.

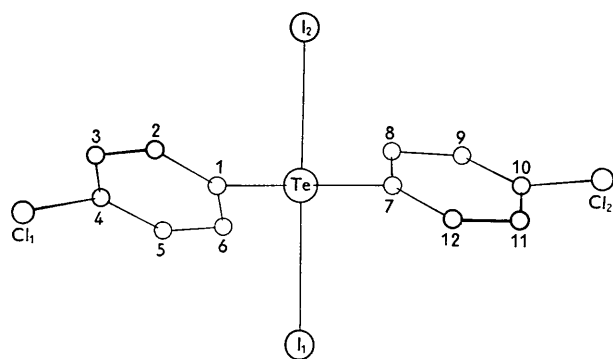Fig. 1. The molecular structure of $(p\text{-}ClC_6H_4)_2TeI_2$.

(a)

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 $(ClC_6H_4)_2TeI_2$, 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 $(CH_3)_2TeCl_2$ 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 $(VI) \cdots I\text{–}I$ 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 $(C_6H_5)_2TeBr_2$, $(C_6H_5)_2SeBr_2$ (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–I_1(2·947 Å) and Te–I_2(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 I_2, hence it is not surprising that the Te–I_1 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}, Cl_1 and Cl_2 to be in Plane 1,
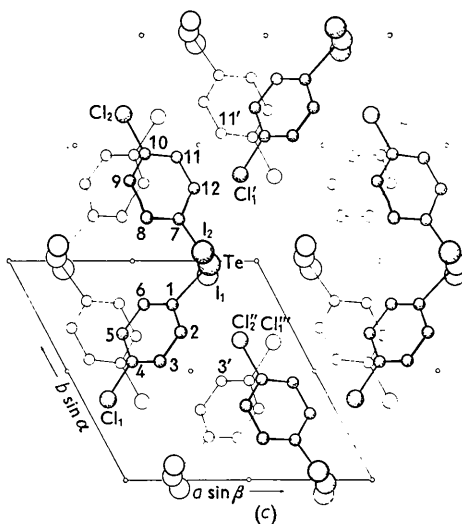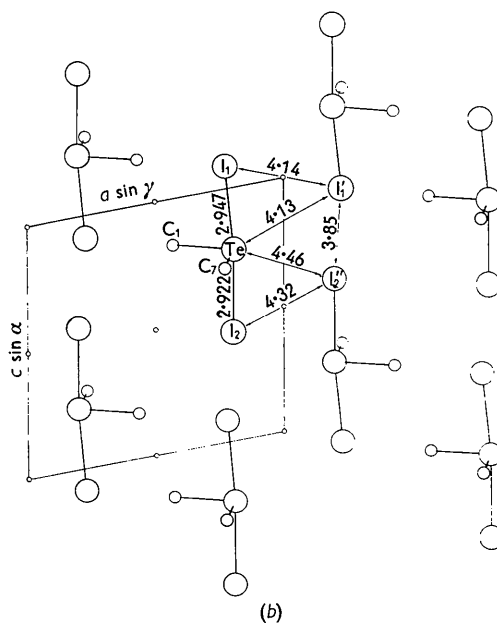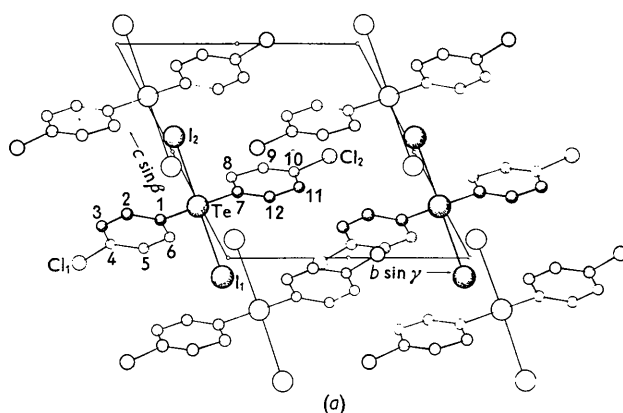

(b)

(c)

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 number	Atoms in L.S. fit	A	B	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 1 (Te, C_1, C_7)

Te	0.000	C_1	0.000	C_7	0.000
I_1	−2.941	C_2	0.660	C_8	0.608
I_2	2.918	C_3	0.559	C_9	0.552
Cl_1	−0.506	C_4	−0.228	C_{10}	0.000
Cl_2	0.118	C_5	−0.844	C_{11}	−0.632
		C_6	−0.776	C_{12}	−0.612

(b) Plane 2 (Phenyl group I)

C_1	0.002	C_4	0.020	Te	0.279
C_2	−0.005	C_5	−0.023	Cl_1	0.203
C_3	−0.006	C_6	0.012		

Mean distance of C atoms from Plane: 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}	−0.012	Cl_2	0.137
C_9	−0.013	C_{12}	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 $111 \cdot 1 \pm 0 \cdot 2°$ with the C_1–Te–C_7 bond angle of $101 \cdot 1 \pm 1 \cdot 0°$ 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 $(C_6H_5)_2TeBr_2$, 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 $97 \cdot 7°$ compared to the C_1–Te–C_1' angle of $93 \cdot 9°$. The difference in this case is more than three times the standard deviations of $0 \cdot 7°$ and $1 \cdot 2°$ respectively.

Further studies of appropriate R_2SeX_2 and R_2TeX_2 compounds are planned in order to learn more about the 'dihalide' versus the 'molecular complex' relationship.

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