To find what happens when (iii) holds, we define

$$X(\delta, \zeta) = \sum_{1}^{\infty} q(\delta, \zeta)^n \exp\,[2\pi i n \bar{b} \zeta]\,.$$

Under condition (ii), therefore,

$$|G|^2 = 4K^2F_0^2N_3(1+X+X^*)\,,$$

whereas under condition (iii)

$$|G|^2 = 4K^2F_0^2N_3(1+Y+Y^*)\,,$$

where

$$Y(\delta, \zeta) = \sum_{1}^{\infty} (-1)^n q(\delta, \zeta)^n \exp\,[2\pi i \bar{b} \zeta]\,.$$

Put $\zeta' = \zeta + 1/2\bar{b}$ and define δ' so that $\delta\zeta = \delta'\zeta'$. We note that q is a function of the product $\delta\zeta$ (see (A2)).

Then

$$Y(\delta, \zeta) = \sum_{1}^{\infty} q(\delta', \zeta')^n \exp\,[2\pi i n \bar{b} \zeta'] = X(\delta', \zeta')\,.$$

The net result is that for $|G|^2$ under (iii), we have the same function as under (ii), but displaced by an amount $1/2\bar{b} \simeq 2/a$ in ζ, so that spikes occur only at $l = 2, 6, 10, \ldots$. Under (iii), those are the points for which Bragg reflexions occur. The spike magnitude is found to be as before.

A similar treatment applies to case (iv). It is found that the spike intensity $|G|^2$ is a factor 2 less than above; the spike magnitude is, however, the same since these are the reflexions for which F is a factor $\sqrt{2}$ less.

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The Crystal Structure of Diphenyltellurium Dibromide*

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(*Received* 12 *September* 1957)

Diphenyltellurium dibromide crystallizes with the space-group symmetry $I4_1$. There are four molecules of $(C_6H_5)_2TeBr_2$ in the unit cell for which $a = 11{\cdot}421 \pm 0{\cdot}010$ Å and $c = 9{\cdot}817 \pm 0{\cdot}010$ Å. The trial structure was determined by means of two-dimensional Patterson and Fourier syntheses and refined by means of three-dimensional Fourier syntheses and the least-squares routine on SWAC. The observed bond distances are $2{\cdot}682 \pm 0{\cdot}003$ Å for Te–Br and $2{\cdot}14 \pm 0{\cdot}03$ Å for Te–C, while the observed bond angles are $178{\cdot}0 \pm 0{\cdot}2°$ for Br–Te–Br and $96{\cdot}3 \pm 1{\cdot}2°$ for C–Te–C. Packing distances are all consistent with accepted van der Waals radii.

Introduction

X-ray diffraction studies of a number of diarylselenium dihalides have shown that the molecules of these substances involve nearly linear X–Se–X bonds with the Se–C bonds in a plane perpendicular to the axis of the halogen atoms (McCullough & Hamburger, 1941, 1942; McCullough & Marsh, 1950). An interesting feature of the structure is the observed selenium–halogen bonded distance, which is approximately 0·2 Å longer than the sum of the single covalent bond radii of the atoms involved (McCullough, 1953). By contrast, the observed selenium–carbon distance appears to be normal.

The investigation of structures of the type R_2TeX_2 is of interest, both as a natural extension of the above studies of selenium compounds and because of the general lack of detailed structural studies of compounds of tetracovalent tellurium. Preliminary X-ray diffraction studies of several compounds of the above type indicated that diphenyltellurium dibromide with only one-half molecule in the asymmetric unit was most promising.

Crystallographic data

Diphenyltellurium dibromide was prepared by Mr N. J. Krilanovich by the method of Krafft & Lyons (1894). The material was purified by recrystallization

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* This research was sponsored, in its early part, by the Office of Ordnance Research of the U.S. Army under Contract Number DA-04-495-Ord-305 and, in its conclusion, by the National Science Foundation under Research Grant NSF-G 2354.

from ethylene chloride and the crystals used in the X-ray diffraction study were grown by slow evaporation of solutions in that solvent. The sulfur-yellow crystals melt at 203° C. and are described by Billows (1905) as being ditetragonal-bipyramidal with an axial ratio $c/a = 0{\cdot}8516$; however, only the forms $\{100\}$, $\{101\}$ and occasionally $\{001\}$ were noted. It is difficult to reconcile this symmetry class with the X-ray observations of the present authors. Rotation, Weissenberg and powder photographs confirm that the substance is tetragonal. A least-squares treatment of the measurements of powder photographs and spectrometer records prepared with filtered copper radiation (Cu $K\alpha = 1{\cdot}5418$ Å), both with and without an internal standard (Y_2O_3, $a = 10{\cdot}608 \pm 0{\cdot}002$ Å), gave the lattice constants

$$a = 11{\cdot}421 \pm 0{\cdot}010, \quad c = 9{\cdot}817 \pm 0{\cdot}010 \text{ Å} .$$

The value of c/a from the X-ray data is 0·8595, which is about 1% higher than the reported goniometric value. The fact that the latter was based on the measurement of only two angles (not in good agreement) probably accounts for the discrepancy.

The crystals are elongated on c and have approximately square cross-sections. Complete Weissenberg data were obtained about the c axis by use of a crystal 0·06 mm. × 0·06 mm. × 0·52 mm. Complete Weissenberg data were also obtained about the a axis by use of a crystal worn down to 0·09 mm. × 0·105 mm. × 0·12 mm. by selective dissolution. The longest dimension in this case was along the rotation axis. All intensity photographs were prepared by use of the multiple-film technique, and intensities were estimated visually by comparison with standard intensity strips prepared with the particular crystal specimen involved. Unfortunately it was necessary to use copper radiation, so that appreciable absorption effects were involved. The linear absorption coefficient in this case is 272 cm.$^{-1}$, which gives a value of 0·82 for μr for the c-axis data and of 1·4 for the a-axis data. Absorption corrections were applied to all data on the assumption of cylindrical specimens (Bradley, 1935). Additional small corrections were made for the upper-level photographs. The maximum corrections applied were 1·4 on the c-axis intensity data and 2·0 on the a-axis intensity data. Where a choice was permitted, intensities were taken from the c-axis photographs; thus about 70% of the data used were from this source. In all, some 760 independent reflections were possible under the conditions of radiation, space-group, and camera geometry. Of these, 720 were actually observed. The only systematic absences noted were those for $h+k+l \neq 2n$ and for $00l \neq 4n$. The space groups consistent with these observations are $I4_1$ and $I4_122$. An approximate density of 2·25 g.cm.$^{-3}$, observed by flotation in a mixture of ethylene bromide and bromoform, indicates four molecules in the unit cell. The density calculated from the X-ray data on this basis is 2·290 g.cm.$^{-3}$. The presence of only four molecules in the unit cell would require additional extinctions if the space group were $I4_122$, as indicated in the *International Tables for X-ray Crystallography* (1952). This space group can also be eliminated in the present case on the grounds that it requires the diffraction symmetry $4/mmm$, whereas $I4_1$ requires only $4/m$. Selection on this basis requires careful consideration of intensities, however, because of the special position of the tellurium atom and the nearly special position of bromine. These heavy atoms actually come close to satisfying the requirements of $I4_122$, but deviations from the diffraction symmetry $4/mmm$, due almost entirely to diffraction by the carbon atoms, are apparent on careful inspection. One final reason for discarding $I4_122$ in the present case is that the molecule would be required to have the symmetry 222, which in turn would require planar square bonds about tellurium. On the other hand, $I4_1$ requires only that the molecule have the expected symmetry, 2, found in the diarylselenium dihalides.

Placing four molecules of $(C_6H_5)_2TeBr_2$ in $I4_1$ requires that the Te atom be at $0, 0, z$, etc., in which z may be taken arbitrarily as zero. The asymmetric unit thus becomes one-half of the chemical molecule. In many cases the location of a heavy atom such as Te permits one to go directly to Fourier syntheses. However, in the present case, the Te atom does not contribute to reflections of the type $hk0$ with odd indices. For this reason, Patterson syntheses on (001) and on (100) were prepared in order to locate the bromine atom so that it could be used as a supplementary heavy atom. These syntheses indicated clearly that the bromine parameters were close to $x = 0{\cdot}235$, $y = 0$, $z = 0$. This near coincidence of the y and z parameters to zero was another source of difficulty, as these values complicate the problem of phase determination. It was noted that the Patterson peaks due to Te–Br and to Br–Br interaction were definitely elliptic in shape, indicating deviation from exact zero values for the bromine y and z parameters. Analysis of the eccentricities and slopes of the major axes of the ellipses gave approximate values for the bromine parameters, namely $y = -0{\cdot}008$ and $z = 0{\cdot}002$. A two-dimensional Fourier synthesis on (001) was then prepared. Although this did not result in resolved carbon maxima, the bromine position was confirmed and the parameter values $x = 0{\cdot}2347$ and $y = 0{\cdot}9906$ were obtained. On the basis of the bromine parameters $x = 0{\cdot}2347$, $y = 0{\cdot}9906$ and $z = 0{\cdot}002$, and the Te atom at $0, 0, 0$, a three-dimensional Fourier synthesis was prepared. A tentative isotropic temperature factor $B = 4{\cdot}5$ Å^2 was applied in calculating the structure factors and phases needed. In addition to the Te and Br maxima in their expected locations, a number of smaller maxima were observed, and six of these were selected as being due to carbon. A second three-dimensional Fourier synthesis based on tentative parameter values for all atoms was then prepared, the above isotropic temperature factor being again applied. The carbon maxima now doubled in size and

Table 1. *Positional parameters and R values for diphenyltellurium dibromide at various stages of refinement*

		Initial Fourier refinement	Least-squares refinement		Final Fourier refinement			Final least-squares parameters *	Final Fourier parameters *
			Atomic parameters	Standard deviation	F_o	F_c	Backshift corrections		
Te	x	0·0000	0·0000	—	0·0000	0·0000	—	0·0000	0·0000
	y	0·0000	0·0000	—	0·0000	0·0000	—	0·0000	0·0000
	z	0·0000	0·9987	0·0004	0·0012	0·0014	−0·0027	0·0000	0·0000
Br	x	0·2350	0·2346	0·0002	0·2348	0·2348	−0·0002	0·2346	0·2346
	y	0·9906	0·9907	0·0002	0·9906	0·9907	0·0000	0·9907	0·9906
	z	0·0015	0·0036	0·0004	0·0033	0·0036	0·0000	0·0049	0·0048
C_1	x	0·0017	0·0057	0·0017	0·0052	0·0059	−0·0002	0·0057	0·0050
	y	0·1367	0·1392	0·0017	0·1375	0·1370	0·0022	0·1392	0·1397
	z	0·8578	0·8473	0·0031	0·8541	0·8539	−0·0066	0·8486	0·8490
C_2	x	0·0881	0·0916	0·0024	0·0900	0·0896	0·0020	0·0916	0·0920
	y	0·2210	0·2262	0·0026	0·2231	0·2243	0·0019	0·2262	0·2250
	z	0·8612	0·8580	0·0031	0·8600	0·8588	−0·0008	0·8593	0·8607
C_3	x	0·0883	0·0915	0·0022	0·0893	0·0895	0·0020	0·0915	0·0913
	y	0·3138	0·3171	0·0023	0·3155	0·3164	0·0007	0·3171	0·3162
	z	0·7613	0·7630	0·0027	0·7612	0·7593	0·0037	0·7643	0·7664
C_4	x	0·0040	0·0018	0·0025	0·0025	0·0022	−0·0004	0·0018	0·0021
	y	0·3173	0·3221	0·0019	0·3202	0·3227	−0·0006	0·3221	0·3196
	z	0·6684	0·6715	0·0029	0·6693	0·6683	0·0032	0·6728	0·6740
C_5	x	0·9165	0·9119	0·0019	0·9139	0·9119	0·0000	0·9119	0·9139
	y	0·2317	0·2315	0·0017	0·2346	0·2321	−0·0006	0·2315	0·2340
	z	0·6583	0·6597	0·0021	0·6579	0·6594	0·0003	0·6610	0·6597
C_6	x	0·9192	0·9183	0·0018	0·9197	0·9196	−0·0013	0·9183	0·9184
	y	0·1434	0·1455	0·0017	0·1457	0·1461	−0·0006	0·1455	0·1451
	z	0·7533	0·7521	0·0029	0·7512	0·7514	0·0007	0·7534	0·7534
R		0·145	0·097	—	—	—	—	0·097	—

* The origin for the final parameters is taken at the tellurium atom.

the spurious maxima disappeared. The atomic positions and value of R corresponding to this stage are given in the first column of Table 1.

Refinement of the structure

The tentative positional parameters from the three-dimensional Fourier were used as input data in the least-squares refinement routine on SWAC (Sparks, Prosen, Kruse & Trueblood, 1956). Provision is made in this routine for individual anisotropic temperature factors and for their symmetry transformation, as required by the space group (Trueblood, 1956). The factor applied to each atom has the form

$$\exp\left[-(B_{11}h^2+B_{22}k^2+B_{33}l^2+B_{12}hk+B_{13}hl+B_{23}kl)\right].$$

An improved isotropic temperature factor $B = 4{\cdot}05$ Å^2 was taken as a starting point for the anisotropic factors in the refinement. Five cycles of refinement were carried out and the resulting positional parameters and R value are given in Table 1. The standard deviations listed are based on the determinant coefficients in the least-squares refinement.

The vibrational parameters, B_{ii} and B_{ij}, are listed with their indicated standard deviations in Table 2. No structural significance has been attached to these values. Except for the fact that the values for bromine average a little higher than those for carbon (4·73 versus 3·90), the values are about as expected.

As a check on the least-squares refinement, final three-dimensional F_o and F_c Fourier syntheses were computed. The atomic positional parameters used as input in both syntheses were those from the final least-squares cycle, but the average vibrational parameters from Table 2 were taken as individual isotropic temperature factors on each atom. A composite contour map of the F_o synthesis is shown in Fig. 1. The positions of the maxima in both syntheses were located by the 19-point routine (Sparks *et al.*, 1956) on SWAC and are listed in Table 1. Also listed in the table are the indicated backshift corrections and the final Fourier refinement parameters. The agreement of these parameters, which are based on isotropic temperature factors, with those from the least-squares refinement using anisotropic temperature factors shows that the latter have had little influence in the structure determination.

The greatest discrepancy between the least-squares parameters and the Fourier parameters is at C_5, which accounts for the larger differences in the distances and angles involving this atom in Tables 4 and 5. The Fourier parameters give a more consistent set of C–C bond distances, but the C–C–C bond angles are more consistent when the least-squares parameters are used. The value of R for the final least-squares positional parameters is 0·097 when the anisotropic factors are used, and 0·103 when one uses the isotropic (average) values. The values of F_c and $\cos\alpha$

Table 2. *Anisotropic atomic temperature factors*

(Standard deviations in parentheses)

	B_{11}	B_{22}	B_{33}	B_{12}	B_{13}	B_{23}	Average B_{ii}
Te	3·91	3·72	3·52	−0·2	*	*	3·72
	(0·07)	(0·07)	(0·08)	(0·1)	—	—	—
Br	4·20	5·25	4·73	0·7	−0·5	0·7	4·73
	(0·09)	(0·11)	(0·10)	(0·2)	(0·2)	(0·2)	—
C_1	3·1	2·2	5·4	1·9	−2·2	−2·0	3·53
	(0·6)	(0·4)	(1·0)	(0·8)	(1·2)	(1·2)	—
C_2	3·8	5·5	3·9	−0·7	−0·6	−2·6	4·41
	(0·8)	(1·0)	(0·8)	(1·4)	(1·5)	(1·6)	—
C_3	4·5	5·4	2·7	−0·6	2·6	0·5	4·17
	(0·7)	(0·8)	(0·5)	(1·3)	(1·7)	(1·9)	—
C_4	5·8	2·7	4·7	−2·4	−3·1	−1·7	4·39
	(1·0)	(0·6)	(1·0)	(1·2)	(1·6)	(1·2)	—
C_5	4·5	2·6	2·3	−0·6	3·1	−0·1	3·15
	(0·7)	(0·5)	(0·5)	(1·1)	(1·1)	(1·0)	—
C_6	3·7	3·6	3·8	1·8	−3·0	2·0	3·72
	(0·6)	(0·6)	(0·7)	(1·1)	(1·2)	(1·2)	—

* Values identically zero because of the special position of tellurium on the twofold axis.

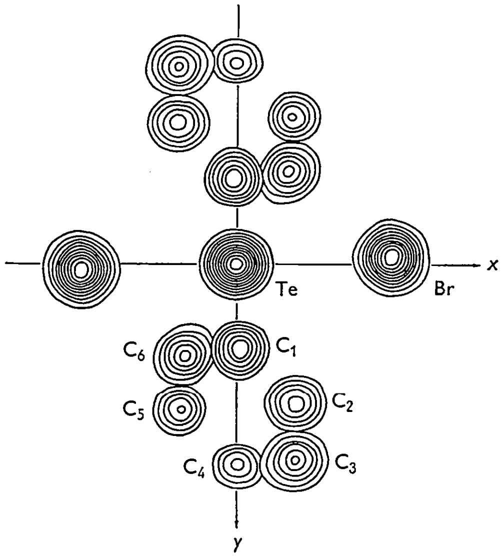

Fig. 1. Composite diagram of sections through atomic positions in the final three-dimensional F_o synthesis. Contour intervals are: 1 e.Å^{-3} for carbon, 5 e.Å^{-3} for bromine, and 10 e.Å^{-3} for tellurium. The zero contour is omitted throughout, also the 1 and 2 e.Å^{-3} contours on carbon, in order to minimize overlapping.

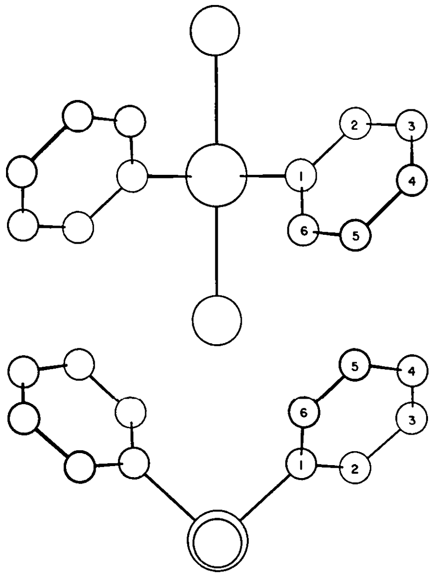

Fig. 2. Molecular structure of diphenyltellurium dibromide.

based on the final least-squares positional parameters and isotropic temperature factors are compared with the values of F_o in Table 3. The atomic scattering factors employed for tellurium and bromine were those of Thomas & Fermi, corrected for dispersion by use of the tables of Dauben & Templeton (1955). The carbon scattering factors were those of McWeeny (1954).

Discussion of the structure

The molecular structure of diphenyltellurium dibromide is shown in Fig. 2 and is similar to the structures found for chemically related molecules (McCullough, 1953). The observed bond distances and bond angles with their standard deviations from the least-squares refinement are listed in Tables 4 and 5. A view of the structure as a whole down the *c* axis is shown in Fig. 3 and the intermolecular packing distances are listed in Table 6.

The observed Te–Br bonded distance of 2·682 Å is, as expected, longer than the sum of the single covalent radii for these atoms: Te(1·37)+Br(1·14) = 2·51 Å. A discussion of this effect has been given by McCullough & Marsh (1950) in connection with the structures of the di-*p*-tolylselenium dihalides. The observed

Table 3. *Observed and calculated structure factors and values of* cos α(*hkl*)

(At the time these calculations were made, SWAC was programmed to print out values of cos α(*hkl*) rather than the more significant quantities *A*(*hkl*) and *B*(*hkl*). Although the cos α(*hkl*) values are ambiguous, they do give more information than $F_c(hkl)$ alone. For this reason the values are included.)

h	k	l	F_o	F_c	cos α
03	01	00	23	12	-1000
05	01	00	66	63	1000
07	01	00	34	28	-1000
09	01	00	37	34	1000
11	01	00	<11	3	1000
13	01	00	9	12	1000
00	02	00	186	190	1000
02	02	00	128	112	-1000
04	02	00	165	162	1000
06	02	00	37	24	1000
08	02	00	62	53	1000
10	02	00	15	0	1000
12	02	00	25	20	1000
14	02	00	15	15	1000
01	03	00	49	41	1000
03	03	00	16	16	-1000
05	03	00	57	55	1000
07	03	00	59	52	-1000
09	03	00	26	24	1000
11	03	00	28	26	-1000
13	03	00	< 8	2	1000
00	04	00	306	318	1000
02	04	00	129	119	1000
04	04	00	211	217	1000
06	04	00	109	110	1000
08	04	00	104	120	1000
10	04	00	55	66	1000
12	04	00	39	47	1000
14	04	00	16	23	1000
01	05	00	19	10	-1000
03	05	00	75	74	-1000
05	05	00	27	27	1000
07	05	00	44	47	-1000
09	05	00	31	30	1000
11	05	00	16	17	-1000
13	05	00	12	16	1000
00	06	00	111	119	1000
02	06	00	32	27	1000
04	06	00	73	80	1000
06	06	00	30	24	1000
08	06	00	45	45	1000
10	06	00	26	22	1000
12	06	00	19	20	1000
01	07	00	60	60	1000
03	07	00	12	14	-1000
05	07	00	51	56	1000
07	07	00	16	12	-1000
09	07	00	19	23	1000
11	07	00	8	12	-1000
00	08	00	154	160	1000
02	08	00	104	92	1000
04	08	00	117	115	1000
06	08	00	69	68	1000
08	08	00	60	67	1000
10	08	00	36	41	1000
12	08	00	23	29	1000
01	09	00	<11	6	1000
03	09	00	33	37	-1000
05	09	00	11	11	1000
07	09	00	25	31	-1000
09	09	00	< 9	0	-1000
11	09	00	< 6	3	-1000
00	10	00	59	74	1000
02	10	00	16	8	1000
04	10	00	28	39	1000
06	10	00	22	21	1000
08	10	00	24	25	1000
10	10	00	12	11	1000
01	11	00	12	12	1000
03	11	00	<11	6	-1000
05	11	00	27	32	1000
07	11	00	10	2	-1000
09	11	00	8	6	1000
00	12	00	60	70	1000
02	12	00	36	27	1000
04	12	00	40	45	1000
06	12	00	31	32	1000
08	12	00	23	31	1000
01	13	00	9	1	1000
03	13	00	13	19	-1000
05	13	00	< 7	1	-1000
00	14	00	24	32	1000
02	14	00	13	14	1000
04	14	00	12	20	1000
00	01	01	158	180	722
02	01	01	105	106	344
04	01	01	167	156	944
06	01	01	42	44	- 43
08	01	01	90	80	959
10	01	01	28	25	822
12	01	01	26	22	972
14	01	01	14	12	666
01	02	01	130	134	941
03	02	01	73	71	445
05	02	01	97	102	976
07	02	01	19	23	984
09	02	01	61	61	972
11	02	01	22	13	- 182
13	02	01	30	31	980
00	03	01	151	152	956
02	03	01	79	76	204
04	03	01	146	138	912
06	03	01	53	64	- 123
08	03	01	71	69	780
10	03	01	30	36	302
12	03	01	25	26	726
14	03	01	16	20	548
01	04	01	209	218	452
03	04	01	156	150	171
05	04	01	159	158	541
07	04	01	90	84	139
09	04	01	68	69	634
11	04	01	33	36	115
13	04	01	28	34	651
00	05	01	187	182	867
02	05	01	81	86	- 194
04	05	01	115	117	881
06	05	01	43	45	225
08	05	01	66	62	853
10	05	01	22	26	663
12	05	01	20	19	817
01	06	01	70	79	995
03	06	01	22	24	803
05	06	01	63	70	996
07	06	01	11	9	978
09	06	01	41	46	998
11	06	01	<10	7	941
13	06	01	13	15	1000
00	07	01	102	107	984
02	07	01	16	21	- 116
04	07	01	85	87	968
06	07	01	26	27	490
08	07	01	43	44	739
10	07	01	20	21	688
12	07	01	18	19	736
01	08	01	95	95	719
03	08	01	71	68	335
05	08	01	76	79	706
07	08	01	56	52	30
09	08	01	49	53	732
11	08	01	22	23	8
00	09	01	89	88	600
02	09	01	69	68	53
04	09	01	70	70	713
06	09	01	31	31	353
08	09	01	30	33	634
10	09	01	18	19	644
01	10	01	43	49	942
03	10	01	17	11	249
05	10	01	27	33	993
07	10	01	5	5	520
09	10	01	23	32	992
00	11	01	31	27	938
02	11	01	23	14	970
04	11	01	30	30	992
06	11	01	15	14	662
08	11	01	14	15	803
01	12	01	39	44	765
03	12	01	25	24	189
05	12	01	33	34	695
07	12	01	21	19	153
00	13	01	34	37	458
02	13	01	30	31	391
04	13	01	22	24	728
06	13	01	14	18	485
01	14	01	18	23	891
03	14	01	7	4	510
01	01	02	178	190	982
03	01	02	127	122	932
05	01	02	162	154	997
07	01	02	37	40	884
09	01	02	82	79	993
11	01	02	25	23	991
13	01	02	31	28	997
00	02	02	248	275	1000
02	02	02	52	41	- 959
04	02	02	132	135	998
06	02	02	16	15	922
08	02	02	58	65	1000
10	02	02	14	20	982
12	02	02	18	23	974
14	02	02	5	7	638
01	03	02	141	157	977
03	03	02	104	94	946
05	03	02	146	147	1000
07	03	02	51	48	963
09	03	02	99	97	992
11	03	02	31	30	989
13	03	02	37	41	1000
00	04	02	11	11	631
02	04	02	126	135	-1000
04	04	02	17	13	560
06	04	02	79	82	-1000
08	04	02	21	24	- 975
10	04	02	26	30	- 995
12	04	02	6	8	- 866
01	05	02	188	192	999
03	05	02	110	101	979
05	05	02	132	135	1000
07	05	02	41	44	967
09	05	02	71	76	998
11	05	02	16	14	994
13	05	02	29	31	1000
00	06	02	78	85	999
02	06	02	16	12	269
04	06	02	75	80	995
06	06	02	20	15	927
08	06	02	31	36	987
10	06	02	7	12	864
12	06	02	< 7	8	1000
01	07	02	84	87	996
03	07	02	37	34	926
05	07	02	87	87	1000
07	07	02	31	27	958
09	07	02	50	50	1000
11	07	02	17	14	987
00	08	02	5	9	943
02	08	02	56	59	- 971
04	08	02	24	19	- 808
06	08	02	35	37	- 950
08	08	02	10	12	- 674
10	08	02	8	13	- 911
12	08	02	4	9	- 996
01	09	02	103	98	997
03	09	02	56	46	998
05	09	02	81	87	996
07	09	02	38	37	993
09	09	02	41	44	999
11	09	02	18	17	998
00	10	02	43	48	996
02	10	02	14	9	126
04	10	02	27	26	959
06	10	02	12	7	999
08	10	02	14	14	970
10	10	02	7	9	961
01	11	02	40	46	998
03	11	02	19	14	999
05	11	02	32	40	1000
07	11	02	9	6	937
09	11	02	18	23	999
00	12	02	13	12	967
02	12	02	17	21	-1000
04	12	02	11	5	- 253
06	12	02	9	9	- 971
08	12	02	5	7	- 856
01	13	02	40	44	995
03	13	02	34	29	993
05	13	02	36	43	999
00	14	02	9	10	971
02	14	02	6	5	- 933
00	01	03	166	173	854
02	01	03	79	60	251
04	01	03	151	154	896
06	01	03	44	28	- 381
08	01	03	59	58	940
10	01	03	23	12	682
12	01	03	22	25	862
14	01	03	10	12	993
01	02	03	120	101	791
03	02	03	35	28	970
05	02	03	93	85	950
07	02	03	19	12	960
09	02	03	59	45	986
11	02	03	14	8	205
13	02	03	28	25	995
00	03	03	200	186	952
02	03	03	62	46	314
04	03	03	116	124	829
06	03	03	58	48	522
08	03	03	77	82	668
10	03	03	43	34	624
12	03	03	29	33	575
01	04	03	153	154	586
03	04	03	172	160	148
05	04	03	116	122	740
07	04	03	62	65	138
09	04	03	65	67	732
11	04	03	31	38	222
13	04	03	29	32	705
00	05	03	137	151	845
02	05	03	68	61	159
04	05	03	96	103	753
06	05	03	57	48	297
08	05	03	41	43	825
10	05	03	26	21	503
12	05	03	16	20	779
01	06	03	79	68	983
03	06	03	35	23	866
05	06	03	76	75	996
07	06	03	12	9	- 744
09	06	03	37	36	1000
11	06	03	< 8	2	950
00	07	03	95	91	970
02	07	03	17	14	- 617
04	07	03	54	56	972
06	07	03	29	25	645
08	07	03	32	32	963
10	07	03	29	24	480
12	07	03	13	14	604
01	08	03	83	82	558
03	08	03	65	59	39
05	08	03	65	68	636
07	08	03	37	40	- 51
09	08	03	43	50	718
11	08	03	22	24	111
00	09	03	70	78	746
02	09	03	62	51	124
04	09	03	66	68	723
06	09	03	42	38	359
08	09	03	22	25	845
10	09	03	20	21	595
01	10	03	53	45	968
03	10	03	32	20	850
05	10	03	42	36	984
07	10	03	13	2	993
09	10	03	21	21	990
00	11	03	35	35	998
02	11	03	16	9	996
04	11	03	27	31	949
06	11	03	17	13	769
08	11	03	16	17	928
01	12	03	31	33	842
03	12	03	26	28	98
05	12	03	25	30	716
07	12	03	16	19	435
00	13	03	31	33	614
02	13	03	23	20	445
04	13	03	22	25	574
01	14	03	14	16	968
03	14	03	4	12	145
00	00	04	268	290	1000
01	01	04	24	19	587
03	01	04	23	24	- 940
05	01	04	46	45	998
07	01	04	30	23	- 988
09	01	04	37	39	954
11	01	04	14	10	- 999
13	01	04	13	15	999
00	02	04	131	134	1000
02	02	04	15	10	- 657
04	02	04	124	119	997
06	02	04	18	9	560
08	02	04	56	42	997
10	02	04	24	18	998
12	02	04	32	27	982
01	03	04	54	52	918
03	03	04	22	20	637
05	03	04	25	26	878
07	03	04	32	33	902
09	03	04	23	22	972
11	03	04	24	22	- 981
13	03	04	6	4	999
00	04	04	211	215	1000
02	04	04	93	88	1000
04	04	04	199	209	1000
06	04	04	95	92	1000
08	04	04	104	106	1000
10	04	04	49	53	999
12	04	04	32	37	993
01	05	04	23	13	- 465
03	05	04	36	38	- 987
05	05	04	15	15	1000
07	05	04	14	11	- 966
09	05	04	21	20	962
11	05	04	14	15	-1000
13	05	04	< 3	8	1000
00	06	04	92	95	1000
02	06	04	19	13	449
04	06	04	67	68	992
06	06	04	9	17	557
08	06	04	29	31	991
10	06	04	21	19	981
12	06	04	19	17	996
01	07	04	51	51	980
03	07	04	19	16	890
05	07	04	21	17	958
07	07	04	9	11	- 971
09	07	04	13	15	980
11	07	04	10	10	- 993
00	08	04	106	107	999
02	08	04	77	69	995
04	08	04	102	103	995
06	08	04	57	54	1000
08	08	04	50	54	993
10	08	04	30	32	992
01	09	04	14	4	- 855
03	09	04	32	34	- 983
05	09	04	11	12	998
07	09	04	18	20	- 966
09	09	04	5	4	982
00	10	04	46	50	999
02	10	04	28	23	956
04	10	04	34	35	969
06	10	04	14	20	966
08	10	04	20	21	995
01	11	04	30	28	998
03	11	04	10	3	- 674
05	11	04	24	25	994
07	11	04	< 6	5	- 830
00	12	04	40	45	999
02	12	04	34	29	998
04	12	04	33	37	999
06	12	04	26	27	999
01	13	04	7	6	- 684
03	13	04	16	18	- 997
05	13	04	< 4	0	-1004
00	01	05	138	149	936
02	01	05	61	65	- 203
04	01	05	109	103	938
06	01	05	24	34	1
08	01	05	64	57	953
10	01	05	12	16	485
12	01	05	25	17	934
01	02	05	82	85	968
03	02	05	49	48	797
05	02	05	75	78	999
07	02	05	16	16	993
09	02	05	42	39	999
11	02	05	8	11	998
13	02	05	20	22	999
00	03	05	119	122	961
02	03	05	53	56	24
04	03	05	81	76	824
06	03	05	32	38	193
08	03	05	61	52	798
10	03	05	22	28	290
12	03	05	26	23	653
01	04	05	130	127	440
03	04	05	83	80	112
05	04	05	105	99	750
07	04	05	34	39	- 19
09	04	05	49	51	707
11	04	05	24	28	156
00	05	05	120	111	873
02	05	05	63	61	149
04	05	05	82	73	701
06	05	05	48	48	517
08	05	05	54	45	733
10	05	05	17	18	532
12	05	05	18	13	835
01	06	05	55	58	1000
03	06	05	17	15	998
05	06	05	61	67	946
07	06	05	16	9	- 663
09	06	05	33	36	995
11	06	05	4	7	981
00	07	05	64	73	977
02	07	05	16	20	7
04	07	05	33	37	985
06	07	05	16	18	928
08	07	05	29	26	839
10	07	05	13	17	651
01	08	05	75	65	597
03	08	05	56	42	338
05	08	05	67	59	754
07	08	05	31	30	- 25
09	08	05	33	38	662
00	09	05	62	59	831
02	09	05	45	44	1
04	09	05	54	49	702
06	09	05	32	31	368
08	09	05	27	24	848
10	09	05	10	12	658
01	10	05	25	33	967
03	10	05	10	12	906
05	10	05	22	27	987
07	10	05	4	6	999
09	10	05	11	18	1000
00	11	05	29	32	981
02	11	05	11	11	205
04	11	05	21	24	962
06	11	05	11	11	558
01	12	05	31	29	746
03	12	05	24	17	270
05	12	05	24	24	709
00	13	05	24	25	754
02	13	05	16	18	327
01	01	06	96	108	1000
03	01	06	81	74	970
05	01	06	91	85	1000
07	01	06	34	25	964
09	01	06	57	55	999
11	01	06	12	10	898
00	02	06	71	84	996
02	02	06	16	15	882
04	02	06	66	75	985
06	02	06	8	9	944
08	02	06	32	34	983
10	02	06	6	8	999
12	02	06	8	8	969
01	03	06	88	84	1000
03	03	06	71	60	989
05	03	06	75	79	999
07	03	06	44	43	983
09	03	06	59	64	1000
11	03	06	18	18	956
00	04	06	9	3	- 150
02	04	06	67	78	- 992
04	04	06	6	6	238
06	04	06	58	67	- 974
08	04	06	18	18	- 979
10	04	06	15	16	- 969
12	04	06	< 5	4	- 999
01	05	06	114	108	1000
03	05	06	65	64	990
05	05	06	65	64	995
07	05	06	34	32	998
09	05	06	43	44	998
11	05	06	10	12	962
00	06	06	49	46	996
02	06	06	13	4	890
04	06	06	61	69	991
06	06	06	14	11	953
08	06	06	26	29	979
10	06	06	8	7	927
01	07	06	55	55	999
03	07	06	36	27	1000
05	07	06	55	57	1000
07	07	06	32	30	1000
09	07	06	35	36	999
00	08	06	12	1	948
02	08	06	33	34	-1000
04	08	06	8	7	- 999
06	08	06	28	10	- 996
08	08	06	5	5	- 617
10	08	06	4	6	-1000
01	09	06	67	74	1000
03	09	06	40	32	994
05	09	06	48	53	1000
07	09	06	27	23	1000
09	09	06	28	33	1000
00	10	06	20	17	999
02	10	06	12	5	970
04	10	06	20	15	1000
06	10	06	4	3	912
08	10	06	4	6	999
01	11	06	22	25	998
03	11	06	11	8	718
05	11	06	20	26	998
00	12	06	6	1	744
02	12	06	8	10	- 987
04	12	06	6	3	- 798
00	01	07	106	102	493
02	01	07	40	31	20
04	01	07	68	70	936
06	01	07	31	21	365
08	01	07	45	47	924
10	01	07	22	15	835
12	01	07	8	15	980
01	02	07	42	41	997
03	02	07	15	15	106
05	02	07	47	42	1000
07	02	07	20	7	713
09	02	07	25	24	978
11	02	07	9	5	600
00	03	07	85	81	372
02	03	07	39	30	260
04	03	07	66	59	911
06	03	07	39	27	247
08	03	07	32	33	814
10	03	07	22	15	201
01	04	07	83	92	539
03	04	07	64	61	228
05	04	07	61	70	750
07	04	07	40	37	- 3
09	04	07	35	35	637
11	04	07	20	21	244
00	05	07	78	86	587
02	05	07	36	32	- 11
04	05	07	37	46	743
06	05	07	33	32	483
08	05	07	27	36	778
10	05	07	19	16	733
01	06	07	36	29	986
03	06	07	23	13	152
05	06	07	39	39	984
07	06	07	17	14	- 18
09	06	07	22	23	998
00	07	07	62	60	316
02	07	07	28	13	867
04	07	07	45	41	965
06	07	07	29	19	976
08	07	07	21	20	767
10	07	07	4	12	818
01	08	07	38	47	723
03	08	07	33	36	454
05	08	07	30	38	835
07	08	07	27	31	60
00	09	07	38	44	676
02	09	07	25	24	- 60
04	09	07	26	34	646
06	09	07	15	18	590
01	10	07	24	20	897
03	10	07	10	9	126
05	10	07	16	15	986
07	10	07	< 4	5	325

Table 3 (*cont.*)

h	k	l	F_o	F_c	cos α
00	11	07	24	24	210
02	11	07	14	7	790
04	11	07	18	18	961
01	12	07	16	23	731
00	00	08	136	143	996
01	01	08	<24	6	103
03	01	08	11	9	-192
05	01	08	<24	17	927
07	01	08	11	9	-845
09	01	08	<18	18	994
11	01	08	<10	2	-751
00	02	08	71	62	993
02	02	08	26	19	91
04	02	08	58	58	992
06	02	08	24	18	802
08	02	08	37	26	985
10	02	08	17	11	819
01	03	08	19	17	522
03	03	08	9	11	-17
05	03	08	16	12	685
07	03	08	15	18	-995
09	03	08	16	11	652
11	03	08	<6	12	-999
00	04	08	98	98	998
02	04	08	58	51	991
04	04	08	81	89	996
06	04	08	45	46	999
08	04	08	52	51	996
10	04	08	29	29	998
01	05	08	<18	6	-461
03	05	08	16	18	-981
05	05	08	<17	7	882
07	05	08	9	10	-891
09	05	08	10	14	1000
00	06	08	41	43	988
02	06	08	19	12	941
04	06	08	32	33	1000
06	06	08	13	8	622
08	06	08	26	23	931
01	07	08	19	23	999
03	07	08	<10	8	-472
05	07	08	16	15	980
07	07	08	<7	6	-920
09	07	08	3	8	984
00	08	08	58	59	999
02	08	08	44	43	991
04	08	08	49	53	997
06	08	08	27	28	1000
01	09	08	<15	3	-145
03	09	08	9	16	-1000
05	09	08	<10	4	957
07	09	08	3	12	-1000
00	10	08	25	28	1000
02	10	08	11	10	978
04	10	08	13	18	994
01	11	08	<8	9	962
03	11	08	<5	1	276
00	01	09	55	48	678
02	01	09	32	27	245
04	01	09	50	44	858
06	01	09	18	18	-22
08	01	09	27	19	884
10	01	09	<10	10	449
01	02	09	36	36	1000
03	02	09	24	17	999
05	02	09	35	40	987
07	02	09	13	13	999
09	02	09	22	20	937
00	03	09	39	47	206
02	03	09	27	21	265
04	03	09	42	42	846
06	03	09	20	20	334
08	03	09	28	27	894
01	04	09	47	48	587
03	04	09	38	44	92
05	04	09	40	42	607
07	04	09	22	25	285
09	04	09	24	24	701
00	05	09	45	48	480
02	05	09	28	30	79
04	05	09	41	37	852
06	05	09	16	20	222
08	05	09	23	17	747
01	06	09	26	30	997
03	06	09	17	16	976
05	06	09	22	28	987
07	06	09	9	7	990
00	07	09	23	27	207
02	07	09	16	16	-403
04	07	09	20	21	920
06	07	09	12	16	401
01	08	09	28	26	660
03	08	09	22	17	168
05	08	09	22	25	581
00	09	09	30	31	692
02	09	09	22	24	309
04	09	09	23	24	778
01	10	09	14	21	933
01	01	10	38	38	1000
03	01	10	38	32	986
05	01	10	34	35	1000
07	01	10	19	15	968
00	02	10	36	49	-946
02	02	10	11	5	-871
04	02	10	15	23	966
06	02	10	<13	1	816
08	02	10	12	16	985
01	03	10	42	40	993
03	03	10	40	30	960
05	03	10	37	37	1000
07	03	10	20	16	928
00	04	10	<17	3	87
02	04	10	18	23	-974
04	04	10	<16	2	517
06	04	10	8	13	-987
08	04	10	<7	5	-861
01	05	10	40	44	1000
03	05	10	31	28	986
05	05	10	33	38	999
07	05	10	14	14	960
00	06	10	15	16	-994
02	06	10	7	3	995
04	06	10	12	13	998
06	06	10	4	3	939
01	07	10	22	24	1000
03	07	10	18	13	947
05	07	10	21	24	1000
00	08	10	<10	2	-168
02	08	10	8	13	-994
04	08	10	<6	5	-996
00	01	11	29	26	587
02	01	11	23	21	594
04	01	11	27	30	866
06	01	11	16	6	691
01	02	11	19	16	963
03	02	11	17	6	731
05	02	11	14	11	1000
07	02	11	9	6	738
00	03	11	30	26	329
02	03	11	18	10	670
04	03	11	26	24	847
06	03	11	12	9	513
01	04	11	28	30	579
03	04	11	31	32	353
05	04	11	24	28	618
00	05	11	25	31	589
02	05	11	14	11	349
04	05	11	19	24	827
01	06	11	13	11	974
03	06	11	10	4	689
00	07	11	19	22	339
02	07	11	9	4	751
00	00	12	42	53	985
01	01	12	<13	4	775
03	01	12	6	1	173
00	02	12	25	23	999
02	02	12	14	9	276
04	02	12	19	22	989
01	03	12	6	5	960
03	03	12	<7	5	-815
00	04	12	30	34	999
02	04	12	16	16	979

Table 4. *Bonded distances in diphenyltellurium dibromide with their standard deviations*

Bond	Distance (Å), final least-squares parameters	Standard deviation (Å)	Distance (Å), final Fourier parameters
Te–Br	2·682	0·003	2·682
Te–C$_1$	2·18	0·03	2·18
Te–C*	2·14	—	2·14
C$_1$–C$_2$	1·40	0·03	1·40
C$_2$–C$_3$	1·40	0·04	1·39
C$_3$–C$_4$	1·36	0·04	1·36
C$_4$–C$_5$	1·46	0·03	1·41
C$_5$–C$_6$	1·34	0·03	1·37
C$_6$–C$_1$	1·37	0·04	1·37

* Based on position of center of phenyl group.

Table 5. *Bond angles in diphenyltellurium dibromide with their standard deviations*

Bonds	Angle (°), final least-squares parameters	Standard deviation (°)	Angle (°), final Fourier parameters
Br–Te–Br′	177·9	0·2	178·0
C$_1$–Te–C$_1'$	93·9	1·2	94·2
C–Te–C*	96·3	—	96·3
C$_1$–Te–Br	90·7	0·6	90·8
C$_1$–Te–Br′	90·8	0·6	90·5
C$_6$–C$_1$–C$_2$	121·7	2·3	122·7
C$_1$–C$_2$–C$_3$	118·5	2·5	117·5
C$_2$–C$_3$–C$_4$	118·2	2·4	118·0
C$_3$–C$_4$–C$_5$	123·4	2·4	125·4
C$_4$–C$_5$–C$_6$	115·3	2·0	114·8
C$_5$–C$_6$–C$_1$	122·7	2·1	121·5

* Based on position of center of phenyl group.

Table 6. *Shortest non-bonded interatomic distances in diphenyltellurium dibromide*

(All distances in Ångström units)

(*a*) Within a given molecule

Br–C$_1$	3·47	Br–C$_1'$	3·48
Br–C$_2$	3·46	Br–C$_6'$	3·40

(*b*) Between atoms in different molecules (Br atom in molecule at 0, ¼, ¼ taken as reference for all distances involving bromine)

Carbon atoms in molecule at 0, 0, 0:			
Br–C$_1$	4·25	Br–C$_2$	4·08
Carbon atoms in molecule at 0, 0, 1:			
Br–C$_4$	4·16	Br–C$_5$	4·11
Carbon atoms in molecule at ½, 0, ¾:			
Br–C$_3$	3·91	Br–C$_4$	4·04
Carbon atoms in molecule at −½, 0, ¾:			
Br–C$_4$	3·97	Br–C$_5$	3·90
Atoms in molecule at 0, 0, 0:			
Br–Te	3·93	Br–Br	4·60
Miscellaneous:			
C$_2$–C$_2'$	3·57	C$_2$–C$_3'$	3·65
C$_3$–C$_3'$	3·71	C$_3$–C$_4'$	3·69
C$_4$–C$_5'$	3·69	C$_5$–C$_5'$	3·60
Te–C(shortest)	4·62		

(*c*) Sum of van der Waals radii

Br–C(aromatic)	3·80	Te–C(aromatic)	4·05
Br–Br	3·90	Te–Br	4·15
C–C(aromatic)	3·70		

distance from the Te atom to C$_1$ is 2·18 Å with a standard deviation of 0·03 Å. In order to check on this important bond distance, the Te–C distance was evaluated in another (and almost independent) way. The positions of all six carbon atoms were averaged in order to locate the effective center of the phenyl group, the resulting position being at $x = 0{\cdot}0035$, $y = 0{\cdot}2303$, $z = 0{\cdot}7599$. It makes little difference, in this case, whether one uses the final least-squares or the final Fourier parameters. This point is 3·53 Å from the Te atom. If we subtract from this a C–C distance of 1·39 Å, the value 2·14 Å results. It is believed that this value is more reliable than that based on the position of C$_1$ alone, and it might be permissible to apply a smaller standard deviation to it. The sum of the single covalent bond radii for tellurium and carbon is 2·14 Å (1·37+0·77), in exact agreement with the more reliable of the two observed values above. Previously reported values for the Te–C distance are

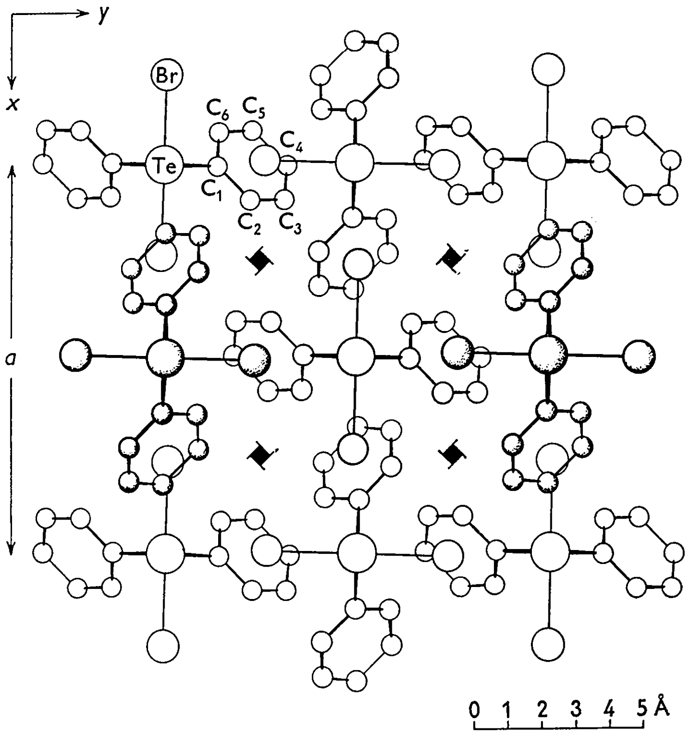

Fig. 3. The crystal structure of diphenyltellurium dibromide viewed down the *c* axis.

2·13±0·14 Å by Kruse, Marsh & McCullough (1957) in *p,p'*-dichlorodiphenyl ditelluride and 2·05±0·05 Å by Blackmore & Abrahams (1955) in di-*p*-tolyl telluride. The observed least-squares C–C distances in diphenyltellurium dibromide range from 1·36 Å to 1·41 Å, with an average of 1·38 Å. The deviations of the individual values from the average value are all less than the standard deviation.

The observed bond angle Br–Te–Br of 178·0±0·2° agrees well with the values of 177·5±1·0° and 177·0 ±1·0° found for Cl–Se–Cl and Br–Se–Br respectively in the di-*p*-tolylselenium dihalides by McCullough & Marsh (1950). In all three molecules the direction of the deviation is such that the halogen atoms are moved slightly away from the phenyl groups. When based on the positions of the atoms C_1 and C_1', the C–Te–C bond angle is 94·4±1·2°; however, if the centers of the phenyl rings are used, the angle is 96·3°. Again it is believed that this value is more reliable than the one based on C_1 alone. These angles may be compared with the value of 101·0±2·7° for C–Te–C in di-*p*-tolyl telluride reported by Blackmore & Abrahams (1955) and with the values 93·5±1·0° and 95·2±1·0° (average 94·4°) for Te–Te–C reported by Kruse *et al.* in *p,p'*-dichlorodiphenyl ditelluride. The C_1–Te–Br and C_1–Te–Br' bond angles in diphenyltellurium dibromide are 90·8±0·6° and 90·5±0·6° respectively, and the dihedral angle between the planes C_1–Te–C_1' and Br–Te–Br' is 90·0°. (If the centers of the phenyl rings are used as reference points, these angles are about 1° different.) The plane of the Te–C bonds is thus nearly perpendicular to the plane of the Te–Br bonds, a structurally interesting observation not required by the crystallographic point-group symmetry, 2, of the molecule. The C–C–C bond angles range from 114·8° to 125·4° with an average of 120·0°, which value must result if the ring is planar. The least-squares plane based on the tellurium atom and six carbon atoms (all seven weighted equally) has the equation

$$-0{\cdot}19422X+0{\cdot}18865Y+0{\cdot}21317Z = 1\ ,$$

where X, Y and Z are expressed in Ångström units. In order to simplify the computation, the least-squares plane was based on atoms in the molecule at the body-center, rather than on the molecule at the origin. Deviations of the individual atoms from this plane (in Å) are:

Te, 0·034; C_1, −0·051; C_2, 0·004; C_3, −0·004; C_4, 0·050; C_5, −0·010, and C_6, −0·028 .

With the exception of the Te atom, the individual deviations are less than $2\sigma(r)$ for the atoms involved. A least-squares plane based on the carbon atoms alone shows considerably lower deviations for the individual carbon atoms, but the Te atom is then 0·134 Å from the plane. These uncertainties in the positions of the carbon atoms are not unexpected in view of the heavy atoms involved in the molecule and the use of copper radiation; however, the more interesting features of the molecular structure are quite accurately determined. For steric reasons, the plane of the phenyl ring must avoid positions nearly parallel to the Br–Br axis and to the plane of the C–Te–C bonds. The former would cause intramolecular overlap of the *ortho* hydrogen atoms with bromine, while the latter would cause overlap between *ortho* hydrogen atoms in different rings of the same molecule and serious overlap of the ring with the bromine atoms of neighboring molecules along the 4_1 axis. In diphenyltellurium dibromide, the plane of the phenyl ring is rotated 56° from the plane of the C–Te–C bonds. The corresponding angle in diphenylselenium dibromide is approximately 60°, while that in the di-*p*-tolylselenium dihalides is approximately 40°. This angle is probably largely determined by the particular intermolecular packing arrangement, which is quite different in the three structures compared.

Within a given molecule, there are four Br–C contacts for each bromine atom of the order of 3·40–3·48 Å. Two of these for each bromine atom are the contacts with carbon atoms C_1 and C_1'. These distances cannot be lengthened by rotation of the plane of the phenyl group or by change in the C–Te–C angle. The shortest intermolecular Br–C contacts are at least 0·5 Å longer than the above and the eight shortest of these are listed in Table 6. In all cases, the hydrogen atoms are well removed from the lines of contact so that the half-thickness of a benzene ring, 1·85 Å, should be used as the effective van der Waals radius for carbon. On this basis the Br–C van der Waals radius sum is 3·80 Å and it is seen that intermolecular contacts start in this region. The shortest Br–Br contacts are 4·60 Å and 4·86 Å, well above the van der Waals radius sum of 3·90 Å, but the Te–Br contact of 3·93 Å is slightly less than the van der Waals radius sum of 4·15 Å. It is thus seen that the packing distances are all consistent with accepted van der Waals radii.

The authors gratefully acknowledge the assistance of the following:

1. The Office of Ordnance Research of the U.S. Army and the National Science Foundation for their financial assistance of this research.
2. The Numerical Analysis Research Project of the UCLA Department of Mathematics for use of SWAC, and the Office of Naval Research for their financial support of N.A.R.P.
3. Mr R. A. Sparks, Dr R. J. Prosen, Dr F. H. Kruse and Prof. K. N. Trueblood for many hours of assistance and instruction in the use of their SWAC routines.

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