The Crystal Structure of α-Dimethyltellurium Dichloride*

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α-Dimethyltellurium dichloride crystallizes in the monoclinic system with the space-group symmetry $P2_1/c$. There are four molecules of $(CH_3)_2TeCl_2$ in the unit cell, the dimensions of which are:

$$a = 9\cdot552, \quad b = 6\cdot180, \quad c = 11\cdot314 \text{ Å (all } \pm0\cdot010 \text{ Å)}, \quad \beta = 97\cdot9\pm0\cdot1° .$$

The trial structure was determined by use of Fourier syntheses on (010) and (001) based on Weissenberg photographs prepared with Cu $K\alpha$ radiation. The structure was refined by use of a three-dimensional Fourier synthesis and five three-dimensional least-squares cycles based on Weissenberg photographs prepared with Mo $K\alpha$ radiation.

The molecular symmetry approximates $mm2$ and may be described as a trigonal-bipyramid with one equatorial position vacant. The observed bond distances and angles are:

Te–Cl$_1$	= 2·480±0·010 Å		Te–Cl$_2$	= 2·541±0·010 Å	
Te–C$_1$	= 2·08 ±0·03 Å		Te–C$_2$	= 2·10 ±0·03 Å	
Cl–Te–Cl	= 172·3±0·3°		C–Te–C	= 98·2 ±1·1°	
C$_1$–Te–Cl$_1$	= 87·6 ±0·7°		C$_2$–Te–Cl$_1$	= 86·4 ±0·8°	
C$_1$–Te–Cl$_2$	= 88·0 ±0·7°		C$_2$–Te–Cl$_2$	= 88·0 ±0·8°	

As in other molecules of the type R_3SbX_2, $R_2(Se,Te)X_2$, $RICl_2$, ClF_3, etc., the axial bonded distances to the halogen atoms are longer than the sums of the normal single covalent radii. An unusual feature of the dimethyltellurium dichloride structure is that the Cl–Te–Cl angle is bent toward the methyl groups. In the aromatic compounds such as diphenyltellurium dibromide the bending of these bonds is away from the organic groups. Fairly strong interaction between the tellurium atom of one molecule and one chlorine atom on each of two adjacent molecules is indicated. The positions of the additional chlorine atoms are approximately such as to complete the octahedron about the tellurium atom.

Introduction

The present investigation of the structure of α-dimethyltellurium dichloride was undertaken to increase our general knowledge of the stereochemistry of tetracovalent tellurium compounds. Preliminary work in this laboratory and that of Galloni & Pugliese (1950) showed that α-dimethyltellurium diiodide has a complex structure with 12 molecules of $(CH_3)_2TeI_2$ per unit cell in the space group $P2_1/c$. Further work on this compound was accordingly postponed in favor of the structurally simpler dichloride.

Crystallographic and intensity data

The α-dimethyltellurium dichloride used in the present study was prepared by the method of Vernon (1921). The substance is a white crystalline solid melting at 92 °C. Crystals are easily grown from ethyl alcohol and have a pronounced needle habit with elongation on the b axis of the monoclinic unit. The substance is

appreciably volatile and has a most disagreeable and persistent odor. For this reason, selected crystals were mounted in sealed X-ray capillaries for the diffraction study. The crystal used in the intensity measurements was a needle with cross-section 0·21 mm. by 0·26 mm. The preliminary two-dimensional study was carried out by use of Cu radiation due to lack of a shorter wavelength source at that time. Although absorption effects were quite pronounced, it is interesting to note that two thirds of the atomic positional parameters agreed within their standard deviations with the parameters resulting from the three-dimensional study based on Mo $K\alpha$ data. The linear absorption coefficient for $(CH_3)_2TeCl_2$ is 442 cm.$^{-1}$ for Cu $K\alpha$ radiation and 54 cm.$^{-1}$ for Mo $K\alpha$ radiation. The corresponding values for μr for the crystal used in the intensity measurements are 5·8 and 0·7 respectively. The latter was considered small enough to justify omission of absorption corrections to the molybdenum data. Rotation and Weissenberg photographs about the b and c axes were prepared with Cu $K\alpha$ radiation. Zero and upper level ($k = 0$ to $k = 5$) Weissenberg photographs as well as $hk0$ and $0kl$ precession photographs were prepared with Mo $K\alpha$ radiation. The intensity data were obtained by use of the multiple-film Weissenberg procedure, using 0·0025 cm. brass foil between

successive films. Intensities were estimated visually and corrected in the usual way to obtain $|F_o|$ values. In all, 1089 independent reflections were recorded with Mo $K\alpha$ radiation. The only systematic extinctions were those for $h0l$ with l odd and $0k0$ with k odd, thus indicating that the space group in $P2_1/c$. The lattice constants were determined by use of zero level Weissenberg and precession photographs prepared with Mo $K\alpha$ radiation. Powder photographs of CeO_2 ($a = 5\cdot411\pm0\cdot001$ Å) were superimposed on the films for calibration purposes. The resulting values are:

$$a = 9\cdot552\pm0\cdot010 \text{ Å}, \quad b = 6\cdot180\pm0\cdot010 \text{ Å},$$
$$c = 11\cdot314\pm0\cdot010 \text{ Å}, \quad \beta = 97\cdot9\pm0\cdot1°.$$

On the assumption of four molecules in the unit cell, the calculated value of the density is $2\cdot234$ g.cm.$^{-3}$.

Determination and refinement of the structure

Inspection of the $h0l$ data showed that the tellurium atom was near $x = 0\cdot18$, $z = 0\cdot16$. These values were used to fix the signs of the 123 (Cu $K\alpha$) $F(h0l)$ values in a Fourier synthesis on (010). This summation showed resolved maxima for all five atoms in the molecule. A second synthesis based on the first atomic positions gave a set of atomic positions which indicated no further sign changes. Further refinement was carried out by the least-squares routine of Sparks, Prosen, Kruse & Trueblood (1956) on SWAC. A Fourier synthesis on (001) using the 55 (Cu $K\alpha$) $F(hk0)$ values was less satisfactory. The tellurium atom and one chlorine atom, Cl_1, were clearly resolved but the second chlorine atom appeared as an unresolved doublet due to the nearness of its y parameter to $0\cdot75$. No maxima which could be attributed to the methyl groups appeared. A second Fourier synthesis resulted

in little change. On the assumption that the unresolved Cl_2 peak was due to the coalescence of two equal peaks of the size of that of the Cl_1 peak, a parameter value of $0\cdot780$ was derived for Cl_2. No attempt was made to refine the $hk0$ data by the least-squares routine. The positional parameters corresponding to this stage of the structure determination are given in Table 1.

When molybdenum radiation became available, a complete new set of photographs was prepared. The 1089 independent observed $|F(hkl)|$ values were used in the preparation of a three-dimensional Fourier synthesis. The tellurium and chlorine positions from the copper radiation study were used as the basis for the signs of the structure factors. In addition to the Te and Cl maxima, several smaller maxima appeared. Two of these coincided with the expected positions of the methyl group carbon atoms. The coordinates of the maxima were located by means of the 19 point SWAC routine.

Up to this point, only approximate inter-layer scaling had been applied. Since it was desirable to use more accurate scaling in the least-squares refinement, the Fourier parameters were used together with an isotropic temperature factor of $2\cdot16$ Å^2 (indicated by the copper data) to calculate a set of structure factors. For each of the six layers ($k = 0$ through $k = 5$) a plot of log (F_o/F_c) versus $\sin^2\theta/\lambda^2$ was constructed. The intercept in each case gave an improved scale factor to be applied to the F_o data for that layer. The improved isotropic temperature factors from the slopes of the graphs ranged from $2\cdot50$ Å^2 to $2\cdot77$ Å^2. The average of these, $2\cdot62$ Å^2, and the positional parameters from the three-dimensional Fourier synthesis were used as input in the first least-squares cycle, L.S.-1.

Table 1. *Atomic positional parameters in* $(CH_3)_2TeCl_2$

		Two-dimensional study (Cu radiation)		Three-dimensional study (Mo radiation)				
		Fourier and L.S.	Standard deviation	3-D Fourier	L.S.-1	L.S.-4	L.S.-5 (final)	Standard deviation
Te	x	0·1756	0·0006	0·1757	0·1758	0·1758	0·1758	0·0001
	y	0·1070	(0·0010)	0·1077	0·1080	0·1084	0·1084	0·0003
	z	0·1645	0·0005	0·1643	0·1643	0·1645	0·1645	0·0001
Cl_1	x	0·3622	0·0044	0·3575	0·3575	0·3570	0·3571	0·0008
	y	0·3990	(0·0050)	0·3928	0·3931	0·3937	0·3934	0·0016
	z	0·2136	0·0044	0·2152	0·2150	0·2144	0·2144	0·0007
Cl_2	x	0·0150	0·0035	0·0207	0·0204	0·0179	0·0176	0·0008
	y	0·7800	(0·0050)	0·7770	0·7772	0·7805	0·7806	0·0016
	z	0·1163	0·0029	0·1150	0·1151	0·1163	0·1163	0·0006
C_1	x	0·2430	0·0130	0·2605	0·2590	0·2586	0·2586	0·0028
	y	(0·9400)	—	0·9483	0·9501	0·9550	0·9545	0·0042
	z	0·3350	0·0100	0·3260	0·3244	0·3232	0·3227	0·0019
C_2	x	0·3261	0·0110	0·3149	0·3150	0·3137	0·3131	0·0027
	y	(0·9500)	—	0·9636	0·9665	0·9765	0·9767	0·0062
	z	0·0597	0·0090	0·0571	0·0566	0·0537	0·0533	0·0021
R		—	0·133	—	0·169	0·117	0·102	0·099	—

Values in parentheses were estimated.

As generally applied in this laboratory, the least-squares routine on SWAC makes provision for the simultaneous refinement of three positional and six vibrational parameters for each atom plus an over-all scaling factor for the F_o data. The anisotropic temperature factor applied to each atom is of the form:

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

The complete matrix of the coefficients of the normal equations for N atoms is then of the order $(9N+1)$. In the first three cycles the only elements of this matrix computed were the 3×3 matrix for the positional parameters of each atom and the 6×6 matrix for its vibrational parameters. There are, of course, five matrices of each kind, one for each of the five atoms. The shifts called for by these least-squares cycles were divided by two before input into the next cycle since experience had shown that the indicated shifts were too large. In the final two cycles of the least-squares refinement, the complete 46th order matrices were calculated. The sum of the squares of the residuals, $\Sigma W |\Delta F|^2$, which started at 20992 for the first cycle, was found to be nearly the same for the last two cycles (7320 and 7239), indicating that further refinement would probably do little to improve the parameters. In these cycles the full shifts indicated by the calculations were applied. The final parameters are listed with those from various stages of the structure determination in Table 1. The standard deviations given for the final parameters are from the inverse matrix element, D_{ii}^{-1}, rather than from the approximate form, $1/D_{ii}$. The differences between these two forms are negligible in the present case for the positional parameters. However, in the case of the vibrational parameters the more exact form gave standard deviations some 15% higher on the average than those given by the approximate form. The vibrational parameters are listed in Table 2 with their standard deviations in the more exact form.

The above form of the anisotropic temperature factors is based on the assumption that the vibrations of the individual atoms are ellipsoidal. The direction cosines of the axes of the vibration ellipsoid with respect to the crystallographic axes and the implied

root-mean-square displacement along each axis may be calculated for each atom from the B_{ii} and B_{ij} values for that atom. The resulting root-mean-square displacements and direction cosines are listed in Table 3 and are discussed later in relation to the molecular and crystal structure.

Table 3. *Amplitudes and orientations of atomic vibration ellipsoids in* $(CH_3)_2TeCl_2$

	Root-mean-square displacement along axis of vibration ellipsoid (Å)	Direction cosines of ellipsoid axis with respect to crystallographix axes		
		a	b	c
Te	0.181 ± 0.003	0.648	0.758	-0.158
	0.178	0.698	-0.628	-0.438
	0.144	0.305	-0.175	0.885
Cl_1	0.35 ± 0.01	-0.545	-0.128	0.896
	0.26	0.767	-0.476	0.321
	0.18	0.339	0.870	0.308
Cl_2	0.35 ± 0.01	-0.593	0.736	0.405
	0.22	0.341	-0.138	0.874
	0.21	0.730	0.662	-0.268
C_1	0.28 ± 0.04	0.953	0.266	-0.273
	0.17	0.192	-0.168	0.931
	0.13	-0.233	0.949	0.241
C_2	0.31 ± 0.04	-0.218	0.937	-0.240
	0.23	0.883	0.308	0.229
	0.16	-0.416	0.164	0.943

The observed structure factors used in the three-dimensional refinement are compared with those calculated on the basis of the final positional and vibrational parameters in Table 4. Within the limits covered by these observed reflections there were 693 additional reciprocal lattice points, reflections from which were not observed. For each of these a value of F_o(maximum) was estimated and values of F_c were calculated. The value of $\Sigma |F_o(\text{max.})|$ was 7042 and that of $\Sigma |F_c|$ was 5547 corresponding to average values of 10·0 and 8·0 per reflection, respectively. For 76% of the unobserved reflections, $|F_c|$ was less than $|F_o(\text{max.})|$. There were five cases where $|F_c|$ was greater than $2|F_o(\text{max.})|$ and the maximum deviation was for 6·3·$\overline{14}$ where $|F_c| = 2·5|F_o(\text{max.})|$. The average value of $||F_o(\text{max.})| - |F_c||$ was 4·3.

The following atomic scattering factors were used in the structure factor calculations: Te, Thomas–Fermi values (*Internationale Tabellen*, 1935) were corrected for dispersion for Mo $K\alpha$ radiation (Dauben & Templeton, 1955); Cl, the values for Cl⁻ (Berghuis *et al.*, 1955) were corrected to Cl° for $\sin \theta/\lambda$ values less than 0·25; C, the diamond carbon values of McWeeny (1954).

Discussion of the structure

The general features of the molecular structure of dimethyltellurium dichloride are similar to those of diphenylselenium dibromide (McCullough & Hamburger, 1941), diphenylselenium dichloride (McCul-

Table 2. *Final anisotropic temperature factors for* $(CH_3)_2TeCl_2$

(Standard deviations in parentheses)

	B_{11}	B_{22}	B_{33}	B_{12}	B_{13}	B_{23}
Te	2·38 (0·06)	2·53 (0·07)	1·74 (0·08)	0·21 (0·17)	-0.03 (0·05)	0·28 (0·15)
Cl_1	5·7 (0·3)	3·3 (0·4)	8·0 (0·4)	-1.4 (0·8)	-2.4 (0·6)	-2.7 (0·8)
Cl_2	5·3 (0·4)	6·8 (0·5)	4·4 (0·3)	-5.2 (0·7)	-0.9 (0·5)	2·9 (0·6)
C_1	5·5 (1·2)	1·7 (1·8)	2·4 (0·8)	2·3 (1·9)	-0.2 (1·6)	-0.7 (1·4)
C_2	4·3 (1·2)	7·0 (2·1)	2·6 (0·9)	-1.3 (2·6)	2·8 (1·6)	-2.4 (2·2)

Table 4. *Comparison of observed and calculated structure factors for α-dimethyltellurium dichloride*

h	k	l	F_o	F_c
00	00	04	120	106-
00	00	06	125	119
00	00	08	37	35-
00	00	10	39	42-
00	00	12	43	52
00	00	14	17	20-
01	00	16-	18	32-
01	00	14-	19	26
01	00	10-	57	64-
01	00	08-	75	76
01	00	06-	65	61
01	00	04-	170	211-
01	00	02-	132	160
01	00	02	155	171-
01	00	04	20	21
01	00	06	49	43
01	00	08	66	67-
01	00	10	32	30
01	00	12	34	37
01	00	14	37	47-
02	00	14-	32	44-
02	00	12-	40	45-
02	00	10-	17	15-
02	00	08-	122	128
02	00	06-	118	124-
02	00	04-	87	75-
02	00	02-	148	172
02	00	00	102	98-
02	00	02	46	40-
02	00	04	95	87
02	00	06	50	45-
02	00	08	34	32-
02	00	10	80	85
02	00	12	34	37-
02	00	14	20	27-
02	00	16-	28	33
03	00	16-	18	27
03	00	12-	52	59-
03	00	10-	58	60
03	00	08-	27	24
03	00	06-	129	127-
03	00	04-	70	63
03	00	02-	70	59
03	00	00	60	61-
03	00	02	51	46
03	00	04	67	60
03	00	06	127	125-
03	00	08	65	63
03	00	10	40	38
03	00	12	59	68-
04	00	16-	20	28
04	00	14-	33	42-
04	00	10-	69	72
04	00	08-	63	61-
04	00	06-	18	17-
04	00	04-	101	89
04	00	02-	56	51-
04	00	00	37	32-
04	00	02	128	134
04	00	04	125	119-
04	00	06	44	37-
04	00	08	98	98
04	00	10	39	42-
04	00	12	20	23-
04	00	14	25	37-
05	00	14-	29	35-
05	00	12-	36	42
05	00	10-	16	18
05	00	08-	58	59-
05	00	06-	53	48
05	00	04-	32	22
05	00	02-	125	127-
05	00	00	116	113
05	00	02	36	28
05	00	04	143	140-
05	00	06	82	80
05	00	08	37	34
05	00	10	49	56-
05	00	12	18	23
06	00	12-	31	38
06	00	16-	40	44-
06	00	06-	70	64
06	00	04-	102	95-
06	00	00	133	131
06	00	02	101	99-
06	00	04	20	15-
06	00	06	68	68
06	00	08	27	29-
06	00	10	18	19-
06	00	12	27	34-
07	00	16-	15	21-
07	00	14-	19	24
07	00	10-	43	44-
07	00	08-	61	58
07	00	04-	95	87-
07	00	02-	106	102
07	00	02	82	81-
07	00	04	44	40
07	00	06	18	19
07	00	08	43	49-
07	00	10	28	32
07	00	14	22	29-
08	00	12-	26	31-
08	00	08-	52	50
08	00	06-	68	64-
08	00	02-	65	62
08	00	00	54	49-
08	00	02	26	20-
08	00	04	49	49
08	00	06	34	34-
08	00	10	32	41
08	00	12	20	27-
09	00	12-	22	24-
09	00	10-	39	39
09	00	06-	53	51-
09	00	04-	51	47
09	00	00	57	48-
09	00	02	44	44
09	00	06	45	46-
09	00	12	21	29-
10	00	14-	17	21-
10	00	10-	23	24
10	00	08-	35	35-
10	00	04-	42	39
10	00	02-	38	35-
10	00	02	46	44
10	00	04	50	49-
10	00	08	32	34
10	00	10	18	26-
11	00	12-	20	22
11	00	08-	22	22-
11	00	06-	36	33
11	00	02-	36	34-
11	00	00	45	44
11	00	02	16	12-
11	00	04	31	34-
11	00	06	32	34
11	00	10	18	21-
12	00	12-	16	13
12	00	10-	18	20-
12	00	06-	22	20
12	00	04-	35	34-
12	00	02-	26	28
12	00	02	35	34-
12	00	06	20	24
12	00	08	16	20-
13	00	08-	20	21
13	00	02-	30	30
13	00	02	18	20-
13	00	04	18	21
14	00	06-	19	10-
14	00	00	22	21-
14	00	06	16	17-
15	00	04-	16	16
15	00	02	16	16
00	01	03	77	91-
00	01	04	109	112
00	01	05	11	14
00	01	06	37	33-
00	01	07	61	58-
00	01	08	59	58-
00	01	09	71	72-
00	01	10	44	47
00	01	11	15	13
00	01	13	24	26
00	01	14	28	31-
00	01	15	18	28-
01	01	14-	14	22
01	01	13-	32	40
01	01	12-	32	39-
01	01	11-	37	42-
01	01	09-	13	14-
01	01	08-	57	61
01	01	07-	84	93
01	01	06-	51	52-
01	01	05-	60	61-
01	01	03-	46	47-
01	01	03	110	112-
01	01	04	61	62-
01	01	05	110	120
01	01	06	80	79-
01	01	07	53	52-
01	01	09	31	31-
01	01	10	52	54-
01	01	11	49	56-
01	01	12	22	25-
01	01	13	17	18-
02	01	17-	16	19-
02	01	15-	15	24
02	01	12-	30	33-
02	01	11-	37	43-
02	01	10-	34	40
02	01	09-	46	47
02	01	07-	27	26-
02	01	06-	42	42-
02	01	05-	90	94-
02	01	04-	87	91
02	01	03-	12	19
02	01	02-	87	89-
02	01	00	50	46-
02	01	01	123	158-
02	01	02	100	115
02	01	03	71	70
02	01	05	51	49
02	01	06	82	87-
02	01	07	73	75-
02	01	08	47	46
02	01	09	36	37
02	01	11	24	26
02	01	12	23	30-
02	01	13	32	40
02	01	14	14	20
03	01	15-	24	30
03	01	14-	16	24-
03	01	13-	27	33-
03	01	11-	12	12-
03	01	10-	26	27
03	01	09-	56	58
03	01	08-	55	56-
03	01	07-	46	45
03	01	06-	54	48-
03	01	04-	32	29
03	01	03-	124	133
03	01	02-	107	106-
03	01	01-	82	94-
03	01	01	15	15
03	01	02	110	112
03	01	03	117	117
03	01	04	74	70-
03	01	05	83	73-
03	01	06	31	25-
03	01	07	18	16-
03	01	08	54	51
03	01	09	50	51
03	01	10	28	33-
03	01	11	23	26-
03	01	13	14	20-
03	01	15	18	27
04	01	13-	30	35-
04	01	12-	28	30
04	01	11-	27	30
04	01	10-	27	23-
04	01	09-	23	19
04	01	08-	21	20-
04	01	07-	69	69-
04	01	06-	72	71
04	01	05-	75	71
04	01	04-	40	34-
04	01	03-	38	31
04	01	02-	85	84-
04	01	01-	95	104-
04	01	00	89	91
04	01	01	85	84
04	01	02	31	24
04	01	04	76	74-
04	01	05	88	77-
04	01	06	51	47
04	01	07	33	31
04	01	08	15	13-
04	01	09	34	31
04	01	10	42	47-
04	01	11	26	30
04	01	12	26	30
05	01	15-	17	22-
05	01	11-	41	43
05	01	10-	39	41-
05	01	09-	42	42-
05	01	08-	17	22-
05	01	06-	54	48
05	01	05-	75	69
05	01	04-	82	77-
05	01	03-	90	89-
05	01	02-	11	8-
05	01	00	84	84
05	01	01	65	63
05	01	02	72	65-
05	01	03	53	48-
05	01	04	20	18
05	01	05	31	27-
05	01	06	28	21
05	01	07	62	64
05	01	08	42	42-
05	01	09	23	26-
05	01	10	16	16
05	01	12	20	23
05	01	13	21	30
05	01	14	15	23-
06	01	11-	18	22
06	01	10-	19	20-
06	01	09-	48	47-
06	01	08-	50	50
06	01	07-	51	48
06	01	06-	10	13-
06	01	04-	59	56-
06	01	03-	68	67-
06	01	01-	63	59
06	01	00	24	20-
06	01	01	40	36
06	01	02	24	17-
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Table 4 (cont.)

h	k	l	Fo	Fc		h	k	l	Fo	Fc		h	k	l	Fo	Fc		h	k	l	Fo	Fc		h	k	l	Fo	Fc
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03	03	08	76	66		09	03	05	18	19		04	04	06-	10	4		01	05	11-	27	27		08	05	02	13	12-
03	03	09	36	32-		09	03	08	17	19		04	04	05-	21	20		01	05	09-	17	15		08	05	03	38	40-
03	03	10	60	56-		09	03	10	28	29-		04	04	03-	25	27-		01	05	07-	59	45-		08	05	07-	24	28
03	03	14	27	30		10	03	06-	23	31		04	04	02-	42	47		01	05	06-	26	20		09	05	03-	27	32-
04	03	12-	40	45		10	03	02-	20	20-		04	04	00	43	46		01	05	05-	37	32		09	05	01-	33	37
04	03	10-	24	23-		10	03	00	32	35		04	04	01	18	18		01	05	03-	30	21		09	05	03	27	30-
04	03	08-	45	42-		10	03	01	16	16-		04	04	02	89	90-		01	05	02-	29	26-		10	05	05-	24	27-
04	03	07-	37	35		10	03	04	15	17-		04	04	03	30	34-		01	05	03	48	44						
04	03	06-	55	59		10	03	06	30	30		04	04	05	42	39		01	05	05	91	81-						
04	03	05-	20	23-		11	03	04-	35	39-		04	04	05	16	7		01	05	06	13	10						
04	03	02-	40	48-		11	03	00-	13	11		04	04	06	28	23		01	05	07	40	32						
04	03	01-	35	39		11	03	02	31	33-		04	04	07	26	23-		01	05	09	31	29-						
04	03	00	62	72		11	03	04	20	20		04	04	08	52	50-		01	05	11	37	39-						
04	03	01	49	49-		12	03	02-	20	26		04	04	10	33	28-		02	05	11-	37	35						
04	03	02	16	18-		12	03	00	17	20-		05	04	12-	20	26-		02	05	09-	32	26-						
04	03	04	79	71-		12	03	04	21	24																		
04	03	05	37	32																							

lough & Hamburger, 1942), the di-p-tolylselenium dihalides (Marsh & McCullough, 1950) and diphenyltellurium dibromide (Christofferson & McCullough, 1958). These structures may be considered to be slightly distorted trigonal bipyramids with one equatorial position vacant.

Table 5. Bond distances in (CH₃)₂TeCl₂

	Distance (Å)	Standard deviation (Å)
Te–Cl₁	2·480	0·010
Te–Cl₂	2·541	0·010
Te–C₁	2·08	0·03
Te–C₂	2·10	0·03
Te–C (average)	2·09	0·02

Table 6. Bond angles in (CH₃)₂TeCl₂

	Angle (°)	Standard deviation (°)
Cl–Te–Cl	172·3	0·3
C–Te–C	98·2	1·1
C₁–Te–Cl₁	87·6	0·7
C₁–Te–Cl₂	88·0	0·7
C₂–Te–Cl₁	86·4	0·8
C₂–Te–Cl₂	88·0	0·8

The molecular structure of $(CH_3)_2TeCl_2$ is shown in Fig. 1 while the bonded distances and bond angles are given in Tables 5 and 6 respectively. Two features, new to molecules of this type, appear here. One is the inequality of the Te–Cl distances of 2·480 Å and

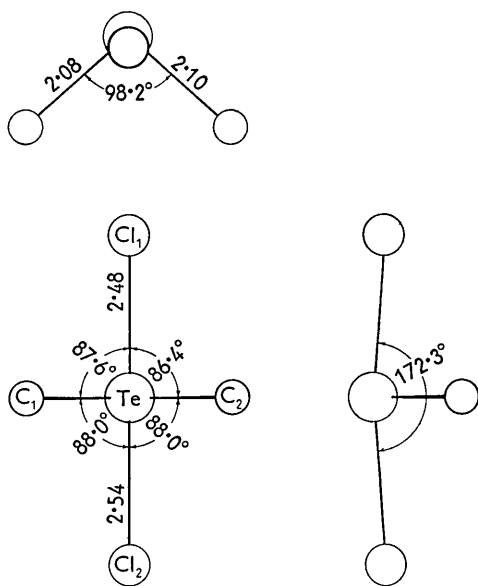Fig. 1. The molecular structure of α-dimethyltellurium dichloride. Distances are given in Å.

2·541 Å, each with a standard deviation of 0·010 Å. These are to be compared with a single, covalent bond radius sum of 2·36 Å. The difference between the two distances (0·061 Å) is six times the standard deviation and is therefore to be considered significant. A possible explanation for this difference is offered in terms of the intermolecular structure discussed later. The second feature is the deviation of the Cl–Te–Cl bond angle from 180° toward the methyl groups. In all other cases involving molecules of the type $R_2(Se,Te)X_2$ the observed deviations of the X–(Se,Te)–X bond angles from 180° have been in a direction away from the organic groups. It should be noted, however, that the organic groups in these cases have all been aromatic and bulkier than the methyl groups of the present example. Precedent for the type of apparent internal strain observed in $(CH_3)_2TeCl_2$ is found in ClF_3 (Burbank & Bensey, 1953; Smith, 1953). In this planar molecule, the axial F–Cl–F bond angle of 174° is bisected to give two F–Cl–F bond angles of 87°. Here, too, the axial bonded distances of 1·72 Å are longer than the equatorial bond distance of 1·62 Å. The sum of the single covalent bond radii is 1·63 Å in this case.

The observed Te–C bond distances of 2·08 Å and 2·10 Å in $(CH_3)_2TeCl_2$ have a standard deviation of 0·03 Å. The difference is therefore considered of no significance and the average value of 2·09 Å is accordingly taken as representative of the Te–C distance in this structure. This value is somewhat shorter than the sum of the single bond radii, 2·14 Å, and the distance 2·14±0·03 Å found in diphenyltellurium dibromide, but is longer than that found in di-p-tolyl telluride, 2·05±0·05 Å (Blackmore & Abrahams, 1955). The three experimental values are all consistent within

their respective standard deviations with the value 2·10 Å. However, consistency of Te–C bond distances in these three compounds is not necessary because of their different character (i.e. one aliphatic R_2TeX_2, one aromatic R_2TeX_2 and one aromatic R_2Te).

The C–Te–C bond angle of 98·2±1·1° is to be compared with the values 96·3±1·2° in diphenyltellurium dibromide, that of 101·0±2·7° in di-p-tolyl telluride, and those of 93·5±1·0° and 95·2±1·0° (average 94·4°) for C–Te–Te in p,p' dichlorodiphenyl ditelluride (Kruse, Marsh & McCullough, 1957). As expected, these tend to be some 5–10° smaller than the values in the corresponding selenium compounds. The C–Te–Cl bond angles are all slightly less than 90° and average 87·5°. The dihedral angle between the planes C–Te–C and Cl–Te–Cl is 88·3°. Although no molecular symmetry is required crystallographically, the molecule approximates closely to the symmetry m, and, somewhat less closely to the symmetry $mm2$.

The stereochemistry of molecules involving five pairs of electrons in the valency shell of the central atom has been discussed by Gillespie & Nyholm (1957), both in terms of the simple electrostatic theory of Sidgwick & Powell (1940) and on the basis of the calculations of Linnet & Mellish (1954) for $sp^3d_{z^2}$ hybridization. Both of these procedures lead to the conclusion that the molecular structure in these cases should be that of a trigonal-bipyramid. Distortion of the bond angles in dimethyltellurium dichloride from the ideal values: Cl–Te–Cl (180°), Cl–Te–C (90°) and C–Te–C (120°) can all be accounted for qualitatively on the basis of repulsive forces between the electron pairs about tellurium, which should be greater for lone-pair–bond-pair interaction than for bond-pair–bond-pair interaction. The lengthening of the axial Te–Cl bonds may be ascribed to equatorial-pair–axial-pair repulsion or to use of the 6s atomic orbital of Te (rather than the 5s) in the hybridization.

The packing arrangement is shown in Fig. 2 and
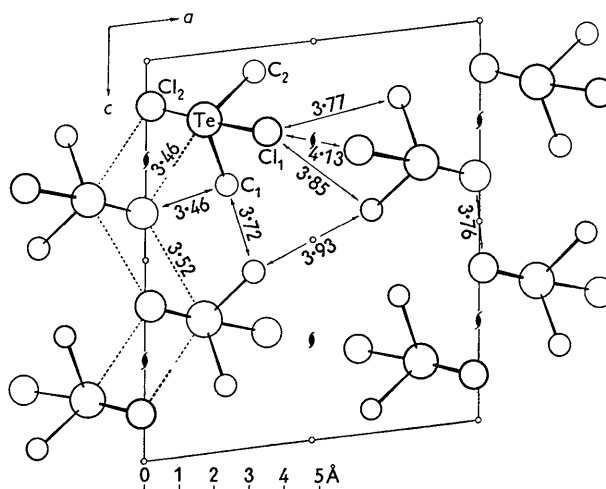
Fig. 2. Projection of the structure of α-dimethyltellurium dichloride on (010). Distances are given in Å.

Table 7. *Shortest non-bonded interatomic separations*
in $(CH_3)_2TeCl_2$ *in* Å

(a) Atoms within a given molecule

Cl_1–C_1	3·17	Cl_2–C_1	3·23
Cl_1–C_2	3·15	Cl_2–C_2	3·24

(b) Atoms in different molecules in same sheet

Te–Cl_2	3·46 (2_1)	Cl_2–C_1	3·46 (2_1)
Te–Cl_2	3·52 ($\bar{1}$)	Cl_2–C_2	3·77 ($\bar{1}$)
Cl_2–Cl_2	3·76 ($\bar{1}$)	Cl_1–C_2	4·00 ($2_1+\bar{1}$)
C_1–C_2	3·72 ($2_1+\bar{1}$)	Cl_1–C_1	3·84 (b)
		Cl_1–C_2	4·04 (b)

(c) Atoms in molecules in different sheets

Cl_1–C_1	3·77 (2_1)	Cl_1–C_2	3·85 (2_1)
		C_2–C_2	3·93 ($\bar{1}$)

(d) Sum of the van der Waals radii

Te–Cl	4·00	Cl–Cl	3·60
Te–CH_3	4·20	Cl–CH_3	3·80
		CH_3–CH_3	4·00

When the indicated atoms are in different molecules the symmetry operation relating the two molecules is given in parentheses.

the non-bonded separations are given in Table 7. An interesting feature of the packing is the close approach of the Te atom of one molecule to the chlorine atom, Cl_2, on each of two adjacent molecules. These additional chlorine atoms are approximately in the directions that would complete the octahedral coordination of Te. The Te–Cl separations involved here (3·46 Å and 3·52 Å) are somewhat shorter than the sum of the van der Waals radii (4·00 Å) for Te and Cl but are approximately 1·0 Å longer than the observed bonded separations. The result of these intermolecular attractive forces is to form loosely bonded sheets parallel to (100). In this respect also, the structure of $(CH_3)_2TeCl_2$ bears an interesting resemblance to that of ClF_3. The interaction thus indicated between molecules in a given sheet is quite weak, however, a fact which is in keeping with the relatively low melting point, 92 °C., of the solid. The packing contacts between molecules in adjacent sheets are all close to those corresponding to the sums of the van der Waals radii of the atoms or groups involved.

The chlorine atom, Cl_2, which is involved in the weak intermolecular bonding is the one at the longer bonded distance to tellurium in the same molecule. The lengthening of this bond relative to that of Te–Cl_1 may be the result of the weak bonds which this chlorine atom forms with two other tellurium atoms. The other chlorine atom, Cl_1, is 0·06 Å closer to the tellurium atom and is not involved in intermolecular contacts shorter than the sums of the corresponding van der Waals radii.

An analysis of the directions of the major axes of the vibration ellipsoids of the chlorine atoms (Table 3) shows that the principal vibrations of these atoms are nearly perpendicular to the directions of the respective Te–Cl bonds. In the case of Cl_1 the angle between the major axis of the ellipsoid and the direction of the Te–Cl, bond is 85°. The corresponding angle for Cl_2 is 71°. It is interesting to note further that the maximum vibrations of Cl_2 also make large angles (85° and 67°) with the directions of the looser bonds which this atom forms with the Te atoms in the molecules related by $\bar{1}$ and 2_1 respectively. It is thus believed that the vibrational parameters for the heavier atoms have some structural significance. A detailed analysis of the implied vibrations of the carbon atoms was not included. The observed vibrational parameters are less significant for these atoms because of the greater extent to which they are influenced by errors in the observed intensities and by the omission of the hydrogen atoms.

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