with anisotropic temperature factors (fixed positional and thermal parameters for H atoms), final $R = 0{\cdot}028$ and $R_w = 0{\cdot}030$;* $F(000) = 500$.

Discussion. Table 1 shows the final atomic parameters. Fig. 1 shows a perspective drawing (Johnson, 1965) of the molecule. The coordination around the U atoms is the usual centrosymmetric distorted hexagonal bipyramid, O(5) and O(5ⁱ) being at 0·462 (6) Å from the plane defined by the other four O atoms around U. Table 2 contains a list of bond lengths and bond angles.

Most calculations were carried out with the XRAY70 system (Stewart, Kundell & Baldwin, 1970) on the Univac 1108 computer of the MEC (Madrid). Thanks are due to Professor S. García-Blanco for his sponsorship.

* Lists of structure factors, anisotropic thermal parameters and unrefined H-atom parameters have been deposited with the British Library Lending Division as Supplementary Publication No. SUP 38092 (18 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

Table 1. *Atomic parameters*

$$U_{eq} = \tfrac{1}{3}\sum_i\sum_j a_i^*a_j^*\mathbf{a}_i.\mathbf{a}_j\cos(\mathbf{a}_i,\mathbf{a}_j).$$

	x	y	z	U_{eq}(Å^2 × 10^4)
U	0	0	0	319 (1)
O(1)	0·0424 (4)	0·0804 (7)	0·2895 (10)	451 (20)
O(2)	0·1428 (5)	−0·0343 (7)	−0·1097 (15)	542 (31)
O(3)	0·0895 (5)	0·1975 (8)	−0·1688 (13)	527 (24)
O(4)	0·2095 (5)	0·1463 (13)	−0·2659 (18)	849 (39)
O(5)	0·0691 (4)	−0·2421 (7)	0·1460 (11)	473 (21)
N(1)	0·1480 (6)	0·1072 (11)	−0·1836 (17)	501 (31)
N(2)	0·1266 (5)	−0·4040 (9)	0·4510 (14)	452 (24)
C(1)	0·1099 (6)	−0·2653 (11)	0·3560 (16)	437 (27)
C(2)	0·1793 (9)	−0·4243 (15)	0·6941 (19)	728 (43)
C(3)	0·0997 (11)	−0·5446 (13)	0·3162 (26)	870 (59)

Table 2. *Bond lengths* (Å) *and bond angles* (°)

U–O(1)	1·766 (5)	O(1)–U–O(2)	93·9 (3)
U–O(2)	2·528 (9)	O(1)–U–O(3)	86·9 (3)
U–O(3)	2·521 (7)	O(1)–U–O(5)	87·1 (3)
U–O(5)	2·397 (6)	O(2)–U–O(3)	50·2 (2)
N(1)–O(2)	1·28 (1)	O(2)–U–O(5)	66·4 (2)
N(1)–O(3)	1·23 (1)	O(3)–U–O(5ⁱ)	64·4 (2)
N(1)–O(4)	1·23 (1)	O(5)–C(1)–N(2)	124·0 (8)
C(1)–O(5)	1·24 (1)	C(1)–N(2)–C(2)	121·6 (8)
C(1)–N(2)	1·30 (1)	C(1)–N(2)–C(3)	121·4 (8)
C(2)–N(2)	1·46 (1)	C(2)–N(2)–C(3)	116·9 (9)
C(3)–N(2)	1·43 (1)	O(2)–N(1)–O(3)	117·1 (9)
		O(2)–N(1)–O(4)	119·3 (9)
		O(3)–N(1)–O(4)	123·5 (9)

Symmetry operator: (i) $-x,-y,-z$.

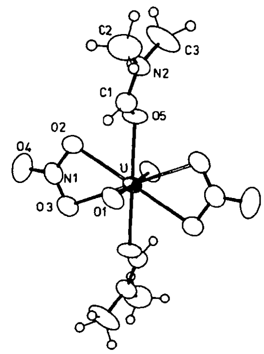

Fig. 1. Perspective drawing of the molecule. The U atom lies on a symmetry centre. Thermal ellipsoids are scaled at the 50% level.

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Acta Cryst. (1983). C**39**, 45–48

Structure of (*p*-Bromophenyl)dichloro(phenyl)tellurium(IV), $(C_6H_5)(C_6H_4Br)TeCl_2$

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(*Received* 26 *March* 1982; *accepted* 18 *August* 1982)

Abstract. $M_r = 431{\cdot}6$, triclinic, $P\bar{1}$, $a = 11{\cdot}257$ (7), $b = 10{\cdot}817$ (4), $c = 12{\cdot}358$ (5) Å, $\alpha = 82{\cdot}61$ (4), $\beta = 80{\cdot}72$ (5), $\gamma = 69{\cdot}38$ (4)°, $V = 1386$ (1) Å^3, $Z = 4$, $D_c = 2{\cdot}067$, $D_m = 2{\cdot}06$ Mg m^{-3}, Mo $K\alpha$, $\lambda = 0{\cdot}71069$ Å, $\mu = 5{\cdot}63$ mm^{-1}, 294 K. Final $R = 0{\cdot}048$, $R_{wF} = 0{\cdot}052$ for 3428 unique reflections. There are two independent molecules per unit cell and the crystal structure consists of discrete tetramers, in which

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individual molecules are linked through weak Te···Cl interactions.

Introduction. Crystallographic studies of organotellurium(IV) halides have shown intermolecular associations through interactions between Te and halogen atoms. Weak but significant Te···Br interactions were noted in $(C_6H_5)_2TeBr_2$ (Christofferson & McCullough, 1958), stronger Te···I interactions in several diiodides such as $(p\text{-}ClC_6H_4)_2TeI_2$ (Chao & McCullough, 1962) and significant Te···Cl interactions in some dichlorides including $(C_6H_5)_2TeCl_2$ (Alcock & Harrison, 1982), $(o\text{-}C_6H_{10}Cl)_2TeCl_2$ and $(o\text{-}C_6H_{10}Cl)(p\text{-}CH_3C_6H_4)TeCl_2$ (Cameron, Amero & Cordes, 1980). However, the arrangements of the individual molecules within these systems vary considerably, having been described variously as layers, infinite chains and tetramers.

Experimental. Preparation as described by Chadha & Miller (1982) followed by crystallization by slow evaporation of methylene chloride solution, density measured by flotation in CCl_4/CH_3I, 0·46 × 0·38 × 0·29 mm, Syntex $P2_1$ diffractometer, highly oriented graphite monochromator, data collected and processed as described earlier (Khan, Steevensz, Tuck, Noltes & Corfield, 1980); intensities of three monitor reflections did not change significantly during data collection; space group $P\bar{1}$ used, later assumed correct because of successful refinement; 5186 reflections ($2\theta_{max} = 50°$, $h \pm k \pm l$), 3428 [$I > 3\sigma(I)$] unique, Lorentz, polarization, absorption (minimum and maximum 3·73 and 7·11) corrections; positions of Te atoms obtained from a sharpened Patterson synthesis, positions of remaining non-H determined from a difference Fourier map; anisotropic blocked-matrix least-squares, minimizing $\sum w(|F_o| - |F_c|)^2$, 190 parameters in each cycle [these comprised parameters of the eight Te, Cl and Br of both molecules, those of the C atoms and the B (H) for one molecule, and a scale factor], $R = 0·05$; difference map at this stage showed peaks at some plausible H-atom positions, H atoms included in subsequent refinement in ideal positions (C—H = 0·95 Å, CCH = 120·0°) with individual isotropic temperature factors, $R = 0·048$ for 3428 reflections, $R_{wF} = 0·052$; in final two cycles of refinement largest shift/error 0·05, final difference map had no features of chemical significance, largest peak 0·8 e Å^{-3}, $F(000) = 808$, $w = 1/[\sigma^2(F) + pF^2]$, final $p = 0·02$; scattering factors for all non-H atoms, including anomalous-dispersion correction for Te, Br, Cl, obtained from Ibers & Hamilton (1974), for H from Stewart, Davidson & Simpson (1965); programs used included *SHELX* (Fourier and least-squares calculations, Sheldrick, 1977), *XANADU* (Roberts & Sheldrick, 1975), *ORTEP* (Johnson, 1965), *ABSORB* (Templeton & Templeton, 1973).

Discussion. The final atomic coordinates for non-H atoms are given in Table 1,* and important distances and angles are in Table 2.

In the solid state, (p-bromophenyl)dichloro(phenyl)tellurium(IV) exists as discrete tetramers as a result of significant secondary Te···Cl interactions (Fig. 1). There are two independently determined $(C_6H_5)(p\text{-}BrC_6H_4)TeCl_2$ molecules within the tetramer which display slight structural differences (Fig. 2). The tetrameric arrangement and secondary interactions are illustrated in Fig. 1(*a*). The structure is very similar to that of $C_{12}H_8OTeCl_2$ (Korp, Bernal, Turley & Martin, 1980) where a step-like structure with three different Te-Cl bond lengths was also noted. The structures of other species, such as $(CH_3)_2TeCl_2$ (Christofferson, Sparks & McCullough, 1958), $(p\text{-}ClC_6H_4)_2TeI_2$ (Chao & McCullough, 1962),

* Lists of structure factors, anisotropic thermal parameters, fractional coordinates for H atoms and equations for mean planes have been deposited with the British Library Lending Division as Supplementary Publication No. SUP 38109 (26 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

Table 1. *Final fractional coordinates and isotropic thermal parameters for non-*H *atoms with e.s.d.'s in parentheses*

	x	y	z	U_{eq}* (Å^2 × 10^3)
Te(1)	0·13522 (5)	0·02319 (5)	0·11762 (5)	42·5 (4)
Te(2)	0·22907 (6)	0·10688 (6)	−0·24266 (5)	44·1 (4)
Br(1)	0·4011 (2)	−0·3306 (2)	0·5616 (1)	148 (2)
Br(2)	0·3586 (1)	0·6258 (1)	−0·1037 (1)	76 (1)
Cl(1)	0·3447 (2)	−0·0734 (2)	−0·0029 (2)	55 (1)
Cl(2)	−0·0629 (2)	0·1215 (2)	0·2455 (2)	63 (2)
Cl(3)	0·4446 (3)	0·0147 (3)	−0·3378 (3)	80 (2)
Cl(4)	0·0049 (2)	0·2130 (2)	−0·1356 (2)	52 (1)
C(11)	0·2236 (9)	−0·0903 (9)	0·2537 (7)	46 (5)
C(12)	0·2119 (11)	−0·0333 (10)	0·3496 (8)	66 (4)
C(13)	0·2674 (13)	−0·1059 (13)	0·4404 (10)	80 (8)
C(14)	0·3301 (11)	−0·2382 (13)	0·4326 (9)	77 (7)
C(15)	0·3418 (12)	−0·2993 (12)	0·3389 (11)	87 (8)
C(16)	0·2853 (10)	−0·2244 (10)	0·2488 (8)	62 (5)
C(21)	0·1891 (9)	0·1891 (8)	0·1276 (7)	43 (4)
C(22)	0·1025 (10)	0·3168 (8)	0·1012 (7)	47 (5)
C(23)	0·1377 (13)	0·4240 (10)	0·1072 (8)	66 (5)
C(24)	0·2510 (13)	0·4102 (12)	0·1431 (8)	73 (7)
C(25)	0·3361 (12)	0·2866 (12)	0·1679 (8)	65 (7)
C(26)	0·3069 (9)	0·1729 (9)	0·1599 (7)	50 (5)
C(31)	0·2747 (8)	0·2670 (8)	−0·2022 (7)	41 (4)
C(32)	0·1994 (9)	0·3978 (10)	−0·2316 (8)	55 (5)
C(33)	0·2279 (9)	0·5028 (9)	−0·2039 (8)	55 (5)
C(34)	0·3262 (9)	0·4802 (9)	−0·1436 (7)	47 (5)
C(35)	0·4004 (9)	0·3520 (10)	−0·1135 (7)	54 (5)
C(36)	0·3755 (9)	0·2436 (9)	−0·1428 (7)	49 (5)
C(41)	0·1607 (9)	0·2052 (9)	−0·3921 (7)	45 (4)
C(42)	0·2352 (11)	0·2613 (11)	−0·4640 (7)	66 (6)
C(43)	0·1871 (14)	0·3333 (13)	−0·5606 (8)	74 (6)
C(44)	0·0691 (14)	0·3411 (13)	−0·5817 (9)	81 (7)
C(45)	−0·0019 (12)	0·2793 (13)	−0·5092 (9)	78 (7)
C(46)	0·0437 (10)	0·2113 (11)	−0·4138 (8)	61 (5)

* U_{eq} for non-H atoms is calculated from the refined anisotropic thermal parameters (deposited) ($U_{eq} = \frac{1}{3}\sum_i\sum_j U_{ij}a_i^*a_j^*\mathbf{a}_i.\mathbf{a}_j$).

Table 2. *Interatomic distances* (Å) *and angles* (°)

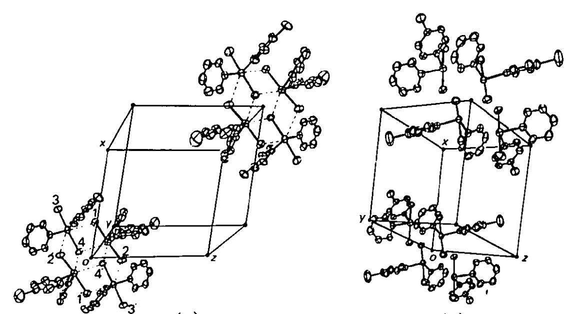
E.s.d.'s on average values are calculated with the use of the 'scatter formula': $\sigma = [\sum(d_i - \bar{d})^2/(N-1)]^{1/2}$ where d_i is the *i*th and $\bar{d}$ is the mean of *N* equal measurements.

Te(1)–Cl(1)	2·530 (2)	Te(2)–Cl(3)	2·437 (3)
Te(1)–Cl(2)	2·496 (2)	Te(2)–Cl(4)	2·590 (2)
Te(1)–C(11)	2·114 (9)	Te(2)–C(31)	2·109 (10)
Te(1)–C(21)	2·110 (11)	Te(2)–C(41)	2·124 (8)
Br(1)–C(14)	1·903 (11)	Br(2)–C(34)	1·876 (11)
C–C (mean)	1·381 (12)	C–C (mean)	1·380 (14)
Te(1)···Te(2)	4·459 (2)	Te(1)···Te(1′)	4·720 (2)
Te(1)···Cl(4)	3·723 (2)	Te(1)···Te(2′)	4·759 (3)
Te(2)···Cl(1)	3·500 (2)	Te(1)···Cl(4′)	3·413 (3)
		Te(2)···Cl(2′)	3·592 (2)

Cl(1)–Te(1)–Cl(2)	176·0 (1)	Cl(3)–Te(2)–Cl(4)	176·6 (1)
Cl(1)–Te(1)–C(11)	88·4 (2)	Cl(3)–Te(2)–C(31)	90·0 (2)
Cl(2)–Te(1)–C(11)	88·9 (2)	Cl(4)–Te(2)–C(31)	86·9 (2)
Cl(1)–Te(1)–C(21)	88·0 (2)	Cl(3)–Te(2)–C(41)	90·9 (2)
Cl(2)–Te(1)–C(21)	89·3 (2)	Cl(4)–Te(2)–C(41)	90·4 (2)
C(11)–Te(1)–C(21)	96·1 (4)	C(31)–Te(2)–C(41)	94·0 (4)
Te(1)–C(11)–C(12)	120·7 (6)	Te(2)–C(31)–C(32)	120·0 (8)
Te(1)–C(11)–C(16)	119·6 (7)	Te(2)–C(31)–C(36)	120·0 (6)
C–C–C (mean)	119·9 (20)	C–C–C (mean)	120·0 (9)
Te(1)–C(21)–C(22)	118·5 (8)	Te(2)–C(41)–C(42)	118·7 (8)
Te(1)–C(21)–C(26)	120·6 (6)	Te(2)–C(41)–C(46)	119·8 (7)
Cl(1)–Te(1)···Cl(4)	87·0 (2)	Cl(4)–Te(2)···Cl(1)	91·0 (1)
Cl(1)–Te(1)···Cl(4′)	103·4 (1)	Cl(4)–Te(2)···Cl(2′)	74·6 (2)
Cl(4)···Te(1)···Cl(4′)	97·3 (2)	Cl(1)···Te(2)···Cl(2′)	87·3 (2)

$(C_6H_5)_2TeBr_2$ (Christofferson & McCullough, 1958) and particularly $(C_6H_5)_2TeCl_2$ (Alcock & Harrison, 1982), which might have been assumed to be more closely related to $(C_6H_5)(p\text{-}BrC_6H_4)TeCl_2$, are slightly different with no more than two Te–*X* bond lengths reported in each case and identical monomeric units. As with $C_{12}H_8OTeCl_2$ (Korp *et al.*, 1980) the three Te–Cl bond lengths are associated with different degrees of secondary Te···Cl interactions. This can be clearly seen from the numbering of the Cl atoms in part of the tetramer in Fig. 1(*a*). Thus only Cl(3) has no contact with a neighboring Te atom within the sum of their van der Waals radii (4·0 Å) and Te(2)–Cl(3) is the shortest bond [2·437 (3) Å]. Both Te(1)–Cl(1) and Te(1)–Cl(2) are significantly longer [2·530 (2) and 2·496 (2) Å respectively] and each has one secondary close encounter Te(2)···Cl(1) [3·500 (2) Å] and Te(2)···Cl(2′) [3·592 (2) Å]. The slightly longer primary bond is associated with the shorter secondary bond so that the sum of the two bonds forming a bridge between molecules is ~ 6·0 Å. This is similar to the average sum of the two bridging Te–Cl distances in the tetrameric unit of solid $TeCl_4$ (5·9 Å) (Buss & Krebs, 1971), which has a cubane-type structure. The ratio of the unbridged Te–Cl bond length to the secondary bond in the unsymmetric bridge is very similar to that found for the Xe–F bond lengths in one form of XeF_6 in which individual XeF_6 molecules are also linked into tetrameric units by an unsymmetric bridge (Wells, 1975). The bridging system in (C_6H_5) $(p\text{-}BrC_6H_4)$ $TeCl_2$ also involves two secondary close encounters for Cl(4) [3·413 (3) and 3·723 (2) Å] leading to the longest terminal bond, Te(2)–Cl(4). Thus both environments about Te are essentially distorted octahedra. In molecules 1, which form the center of the bridging step system, there are essentially two equal-length Te–Cl terminal bonds while in molecules 2 the two terminal Te–Cl bond lengths differ considerably (Fig. 2). The atoms on the central step, which include C(11), C(21), Te(1), Cl(4′), Te(1′), C(11′), C(12′) and Cl(4) (Fig. 1*a*), are approximately in a plane. The Te(1)···Te(1′) distance of 4·720 (2) Å leaves ample room for the lone pair on each Te atom, even if they are stereochemically active and pointing towards each other.

The structural parameters of the two independently determined molecules are given in Table 2 and a view of the molecules showing the relationships of the planes of the phenyl and bromophenyl rings in Fig. 2. As in all R_2TeX_2 molecules, the monomeric unit may be based on a distorted trigonal bipyramid with the Cl atoms occupying the axial positions and the two phenyl rings and the supposed lone pair occupying the three equatorial positions. The Te–C bond lengths [average 2·11 (1) Å] are all essentially equal (see Table 2) and, as with the other R_2TeX_2 molecules, are close to that predicted from the sum of the single-bond covalent



(*a*) (*b*)

Fig. 1. Unit-cell packing of (C_6H_5) $(p\text{-}C_6H_4Br)TeCl_2$ indicating (*a*) the step-like structure of tetramers and (*b*) the relative orientation of the phenyl rings. H atoms are omitted for clarity.

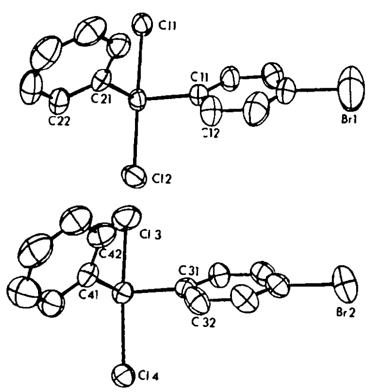


Fig. 2. *ORTEP* plot of the two independent molecules, 1 (top) and 2, of $(C_6H_5)(p\text{-}C_6H_4Br)TeCl_2$. The atoms are drawn with 50% probability ellipsoids.

radii. The C—Te—C angle is also within the range found for these species and given the differences in Te—Cl bond lengths and the secondary interactions in the two molecules, it is not surprising that it is slightly different in the two molecules [96·1 (4)° in 1 and 94·0 (4)° in 2]. This angle is less than the ideal of 120° and the distortion can be explained on the basis of lone-pair–bond-pair repulsions being greater than bond-pair–bond-pair repulsions. The dihedral angles involving the phenyl planes also differ slightly in the two molecules although the basic arrangements are similar, the phenyl and bromophenyl rings being in a 'propeller' rather than 'butterfly' arrangement. The dihedral angle between the TeCC plane and the phenyl ring is 41·9°* in molecule 1 and 32·1° in molecule 2 while that between the TeCC plane and the bromophenyl ring is 144·7° and 129·4° respectively. In the fused-ring system of $C_{12}H_8OTeCl_2$, the two independent molecules have similar angles at Te [90·7 (3°)] and the fused rings are folded so that they are 29·2° from coplanarity (*i.e.* have dihedral angle of *ca* 151°). The much smaller CTeC angle and slight fold are presumably associated with the relatively rigid system. There is no such internal rigidity in force in $(C_6H_5)(p\text{-}BrC_6H_4)TeCl_2$ so that the dihedral angle between the two rings (124·4° in 1 and 120·5° in 2) reflects a greater departure from planarity. The differences in all dihedral angles presumably reflect the overriding feature, which is clearly seen in Fig. 1(*b*), where the phenyl ring on molecule 1 lies parallel to the bromophenyl ring on molecule 2, while the phenyl ring on molecule 2 lies normal to the bromophenyl ring on molecule 1. Within the step-like structure, this arrangement probably minimizes non-bonding interactions between the ring systems on the same or adjacent molecules leading to an alternation of bromophenyl and phenyl rings around the tetrameric unit.

It has been almost universally suggested that the Te—X bond lengths in R_2TeX_2 compounds are unusually long even allowing for the fact that there is involvement in secondary interactions. However, the Te—Cl bond length of 2·437 (3) Å is close to or larger than the expected value for a Te—Cl bond (2·36 Å) if a pseudo-trigonal bipyramidal environment is assumed. (For equivalent bonds in, for example, gaseous PCl_5 the axial bonds are always longer than those in the equatorial plane. In PCl_5, there is a 10% increase in the covalent radius of P_{ax} compared to P_{eq}, and the same is true for the radii in other related species, such as SF_4, which have a lone pair. This difference can be rationalized as arising from the use of the less stable *d* orbitals of the central atom in hybridization involving the axial bonds or as arising from the formation of 2*e*—3 center bonds along the axis.) Whatever the rationale, the effective covalent radius of Te will be expected to be larger, by approximately 10%, along the axis than in the equatorial plane. Assuming the latter radius to be 1·34 Å from the Te—C bond length (1·34 + 0·78 = 2·12 Å), a value of 1·47 Å can be calculated for Te_{ax} leading to a predicted Te—Cl bond length of 2·47 Å, which is slightly larger than the experimental value [2·437 (3) Å] for the Te—Cl bond not involved in secondary interactions but still smaller than for those involved in such additional bonding.

* E.s.d.'s for the dihedral angles are ~ 1·0°.

This work was supported in part by Operating Grants from the Natural Sciences and Engineering Research Council of Canada.

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