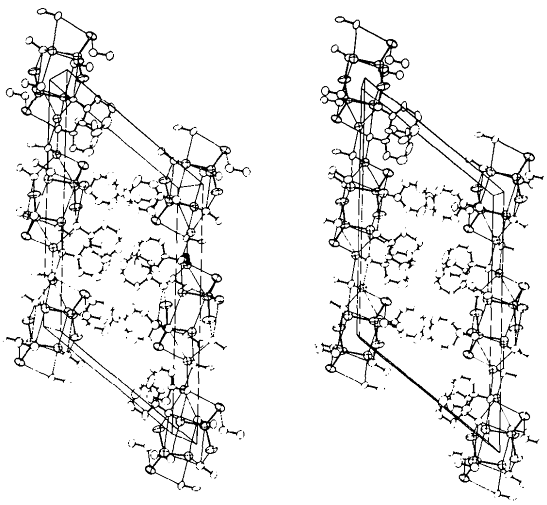

Fig. 3. Stereoview approximately along the b axis. The c axis is vertical. Hydrogen-bonded Cl–N contacts are indicated by single lines. Co and Cl are drawn with principal ellipses. Cyclohexyl rings outside the unit cell and hydrogens are omitted for clarity.

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Structure of Dichlorobis(*p*-methoxyphenyl)tellurium(IV), [$TeCl_2(C_7H_7O)_2$]

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Abstract. $M_r = 412\cdot6$, triclinic, $P\bar{1}$, $a = 10\cdot243$ (5), $b = 12\cdot480$ (4), $c = 13\cdot654$ (4) Å, $\alpha = 109\cdot22$ (2), $\beta = 80\cdot42$ (3), $\gamma = 77\cdot30$ (3)°, $V = 1553$ (1) Å^3, $Z = 4$, $D_x = 1\cdot76$, $D_m = 1\cdot74$ Mg m^{-3}, λ(Mo $K\alpha$) = 0·71069 Å, $\mu = 2\cdot09$ mm^{-1}, $F(000) = 800$, $T = 294$ K, final $R = 0\cdot028$ for 3406 unique observed reflections. The structure consists of isolated step-like tetramers in which two independent molecules and their centrosymmetric equivalents are linked through Te···Cl secondary interactions. The Te—C and Te—Cl bonds occupy

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the equatorial and axial positions respectively in the saw-horse structure. The phenyl rings are in a propeller arrangement.

Introduction. Crystal-structure analyses of various diorganotellurium dichlorides, R_2TeCl_2, have shown that a majority of compounds pack in loose sheets or infinite chains (Alcock & Harrison, 1982; Cameron, Amero & Cordes, 1980; Chadha, Drake & Hencher, 1983; Chadha & Drake, 1984; Kobelt & Paulus, 1971; Christofferson, Sparks & McCullough, 1958) through Te···Cl secondary interactions, and only two compounds, $(C_6H_5)(p\text{-}BrC_6H_4)TeCl_2$ (Chadha, Drake & Khan, 1983) and $C_{12}H_8OTeCl_2$ (Korp, Bernal, Turley & Martin, 1980), crystallize as discrete step-like tetramers. As part of our studies on secondary bonding in organotellurium compounds (Chadha, Drake & Hencher, 1983; Chadha, Drake & Khan, 1983; Chadha & Drake, 1984; Chadha, Drake & Khan, 1984; Chadha, Drake, Khan & Singh, 1984), we present herein the crystal structure of dichlorobis(*p*-methoxyphenyl)tellurium, $(p\text{-}CH_3OC_6H_4)_2TeCl_2$, which exists as a step-like tetramer.

Experimental. Preparation as described by Bergman (1972) followed by slow evaporation of CH_3CN solution, density measured by flotation in CCl_4/CH_3I, crystal 0·15 × 0·19 × 0·38 mm, Syntex $P2_1$ diffractometer, highly oriented graphite monochromator, cell parameters from 15 strong reflections ($15 < 2\theta < 30°$), data collected and processed as described earlier (Chadha, Drake & Khan, 1983); intensities of three monitor reflections changed only by 5% during data collection, corrected for by applying a scale factor; 4298 reflections ($4 < 2\theta < 45°$, h 0→11, k −12→13, l −14→14), 3406 [$I > 3\sigma(I)$] unique, Lorentz, polarization corrections, no absorption correction; positions of Te and Cl atoms obtained by direct methods (*SHELX*, 1977) and confirmed by three-dimensional Patterson synthesis, positions of remaining non-H determined from a difference Fourier map; anisotropic blocked-matrix least squares minimizing $\sum w(|F_o| - |F_c|)^2$, 199 parameters in each cycle (these comprised parameters of all Te and Cl atoms of both molecules, those of the O and C atoms for one molecule, and a scale factor), $R = 0.034$; 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, HCH = 109·5 and CCH = 120°), methyl H atoms refined as a group with isotropic U values assigned 0·01 Å^2 greater than the atoms to which they are attached, $R = 0.028$ for 3406 reflections, $R_w = 0.033$; in final cycle of refinement largest shift/error 0·1, final difference map had no features of chemical significance, largest peak 0·8 e Å^{-3} at (0·413, 0·634, 0·360); $w = 1/[\sigma^2(F) + pF^2]$, final $p = 0.0001$; scattering factors for all non-H atoms, including anomalous-dispersion correction for Te, Cl, obtained from Ibers & Hamilton (1974), for H from Stewart, Davidson & Simpson (1965); programs used include *SHELX* (Fourier and least-squares calculations, Sheldrick, 1977), *XANADU* (Roberts & Sheldrick, 1975) and *ORTEP* (Johnson, 1965).

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

The crystal-structure analysis shows the packing of $(p\text{-}CH_3OC_6H_4)_2TeCl_2$, *A* (Fig. 1) is similar to those of $(C_6H_5)(p\text{-}BrC_6H_4)TeCl_2$, *B* (Chadha, Drake & Khan, 1983) and $C_{12}H_8OTeCl_2$, *C* (Korp *et al.*, 1980). All of these compounds form discrete tetramers through Te···Cl secondary interactions with the Te_4Cl_6 unit adopting the step-like structure and a similar geometry around each Te atom. However, closer comparison reveals some interesting features. The Te—C bonds, forming the equatorial positions in the saw-horse (pseudo-trigonal bipyramidal) structure (Fig. 2) are essentially of equal length (average 2·11 Å) in all three compounds. The C—Te—C angles, which differ by 2° for the two independent molecules in *B* [96·1 (4) and 94·0 (4)°], differ by only 1° in *A* [97·0 (2) and 95·9 (2)°] (Table 2). However, all differ considerably from the angle of 90·7 (3)° found in the fused-ring system of *C*. The Te—Cl bonds which occupy the axial positions again differ in length in accord with the number of secondary Te···Cl interactions. The molecules (1 and 1′) forming the central step have Te—Cl bonds of intermediate length and the Cl atoms are each involved in one secondary interaction. In *A* the two Te—Cl bonds are virtually identical [2·514 (2) and 2·518 (1) Å; v.u. = 0·82 and 0·83†] (Table 2) but in *B*, where the *R* groups differ, they differ considerably [2·496 (2) and 2·530 (2) Å; v.u. = 0·85 and 0·80]. Additional distortion is also evident in the molecules (2′ and 2) which make up the 'upper' and 'lower' steps in both *A* and *B*. For these molecules, one Cl atom is involved in two secondary interactions leading to the weakest Te—Cl bond and the other is free of interactions and thus forms the strongest Te—Cl bond. However, the differences in bond lengths are less marked for the symmetrically substituted *A* [2·569 (1) and 2·474 (1) Å; v.u. 0·75 and 0·90] (Table 2) than for the unsymmetrically substituted *B* [2·590 (2) and 2·437 (3) Å; v.u. = 0·72 and 0·95].

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* 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 39419 (27 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

† Te—Cl bond lengths are converted to bond valences according to Brown & Wu (1976).

Table 1. *Final fractional coordinates with e.s.d.'s in parentheses and equivalent isotropic thermal parameters* ($\times 10^3$) *for non-*H *atoms*

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

	x	y	z	U_{eq}(Å^2)
Te(1)	0·38322 (3)	0·60352 (3)	0·41955 (2)	43·1
Te(2)	0·25471 (3)	0·75692 (3)	0·78753 (2)	42·3
Cl(1)	0·3837 (1)	0·7965 (1)	0·5564 (1)	60
Cl(2)	0·3797 (2)	0·4149 (1)	0·2787 (1)	67
Cl(3)	0·2454 (2)	0·9512 (1)	0·9202 (1)	65
Cl(4)	0·2590 (1)	0·5558 (1)	0·6517 (1)	47
O(1)	−0·2415 (4)	0·8113 (3)	0·4629 (4)	73
O(2)	0·6272 (5)	0·7777 (4)	0·0730 (3)	95
O(3)	−0·3188 (4)	0·9910 (4)	0·7347 (4)	79
O(4)	0·0088 (5)	0·6178 (4)	1·1607 (3)	77
C(11)	0·1716 (4)	0·6770 (4)	0·4350 (4)	39
C(12)	0·0794 (5)	0·6140 (4)	0·4487 (4)	56
C(13)	−0·0578 (5)	0·6626 (5)	0·4585 (5)	64
C(14)	−0·1050 (5)	0·7733 (4)	0·4541 (4)	47
C(15)	−0·0135 (5)	0·8366 (4)	0·4414 (4)	53
C(16)	0·1253 (5)	0·7879 (4)	0·4327 (4)	54
C(17)	−0·2981 (6)	0·9279 (5)	0·4646 (6)	85
C(21)	0·4617 (5)	0·6609 (4)	0·2988 (4)	41
C(22)	0·5782 (5)	0·6958 (4)	0·3016 (4)	49
C(23)	0·6309 (6)	0·7337 (5)	0·2246 (5)	61
C(24)	0·5658 (6)	0·7379 (5)	0·1437 (4)	56
C(25)	0·4490 (6)	0·7007 (5)	0·1400 (4)	63
C(26)	0·3960 (6)	0·6605 (5)	0·2165 (4)	56
C(27)	0·5535 (9)	0·8030 (8)	−0·0007 (6)	129
C(31)	0·0593 (5)	0·8338 (4)	0·7680 (4)	42
C(32)	0·0308 (5)	0·9424 (4)	0·7603 (4)	54
C(33)	−0·0954 (5)	0·9923 (5)	0·7490 (4)	60
C(34)	−0·1960 (5)	0·9328 (5)	0·7449 (4)	49
C(35)	−0·1651 (5)	0·8241 (5)	0·7530 (4)	58
C(36)	−0·0391 (5)	0·7738 (5)	0·7635 (5)	59
C(37)	−0·4258 (6)	0·9361 (6)	0·7333 (6)	93
C(41)	0·1756 (5)	0·7067 (4)	0·9130 (4)	43
C(42)	0·2428 (5)	0·6011 (4)	0·9184 (4)	50
C(43)	0·1912 (6)	0·5687 (5)	1·0012 (4)	63
C(44)	0·0721 (6)	0·6415 (5)	1·0777 (4)	57
C(45)	0·0056 (6)	0·7496 (5)	1·0737 (4)	55
C(46)	0·0565 (5)	0·7827 (5)	0·9925 (4)	53
C(47)	0·0616 (7)	0·5030 (5)	1·1633 (5)	87

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

Te(1)–Cl(1)	2·518 (1)	Te(2)–Cl(3)	2·474 (1)
Te(1)–Cl(2)	2·514 (2)	Te(2)–Cl(4)	2·569 (1)
Te(1)–C(11)	2·105 (4)	Te(2)–C(31)	2·121 (5)
Te(1)–C(21)	2·113 (5)	Te(2)–C(41)	2·110 (6)
C–C (mean)	1·379 (12)*	C–C (mean)	1·376 (12)
C(14)–O(1)	1·345 (6)	C(34)–O(3)	1·361 (7)
O(1)–C(17)	1·434 (8)	O(3)–C(37)	1·415 (9)
C(24)–O(2)	1·350 (9)	C(44)–O(4)	1·362 (8)
O(2)–C(27)	1·428 (11)	O(4)–C(47)	1·431 (8)
Te(1)···Te(1′)	4·472 (1)	Te(1)···Te(2)	4·583 (1)
Te(1)···Te(2′)	4·773 (1)		
Te(1)···Cl(4)	3·501 (1)	Te(2)···Cl(1)	3·446 (1)
Te(1)···Cl(4′)	3·559 (1)	Te(2)···Cl(2′)	3·675 (2)
Cl(2)–Te(1)–Cl(1)	177·9 (1)	Cl(4)–Te(2)–Cl(3)	178·8 (1)
Cl(2)–Te(1)–C(11)	89·3 (1)	Cl(4)–Te(2)–C(31)	89·0 (1)
Cl(1)–Te(1)–C(11)	89·6 (1)	Cl(3)–Te(2)–C(31)	90·1 (1)
Cl(2)–Te(1)–C(21)	90·4 (1)	Cl(4)–Te(2)–C(41)	89·0 (1)
Cl(1)–Te(1)–C(21)	88·0 (1)	Cl(3)–Te(2)–C(41)	90·3 (1)
C(11)–Te(1)–C(21)	97·0 (2)	C(31)–Te(2)–C(41)	95·9 (2)
Te(1)–C(11)–C(12)	119·9 (4)	Te(2)–C(31)–C(32)	120·1 (4)
Te(1)–C(11)–C(16)	119·9 (4)	Te(2)–C(31)–C(36)	119·8 (4)
C–C–C (mean)	119·9 (8)	C–C–C (mean)	120·0 (8)
Te(1)–C(21)–C(22)	118·7 (4)	Te(2)–C(41)–C(42)	120·6 (3)
Te(1)–C(21)–C(26)	120·4 (4)	Te(2)–C(41)–C(46)	119·5 (4)
C(14)–O(1)–C(17)	118·4 (5)	C(34)–O(3)–C(37)	117·9 (5)
C(24)–O(2)–C(27)	117·7 (6)	C(44)–O(4)–C(47)	118·2 (4)
Cl(1)–Te(1)···Cl(4)	81·7 (1)	Cl(4)–Te(2)···Cl(1)	82·2 (1)
Cl(2)–Te(1)···Cl(4′)	81·3 (2)	Cl(4)–Te(2)···Cl(2′)	78·3 (2)
Cl(4)···Te(1)···Cl(4′)	101·4 (1)	Cl(1)···Te(2)···Cl(2′)	79·6 (2)
Te(1)–Cl(1)···Te(2)	99·2 (1)	Te(2)–Cl(4)···Te(1)	96·8 (1)
Te(1)–Cl(2)···Te(2′)	99·2 (2)	Te(2)–Cl(4)···Te(1′)	101·1 (1)
		Te(1)···Cl(4)···Te(1′)	78·6 (1)

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

In *C*, where the phenyl rings are fused, they take up a slight butterfly arrangement. By contrast, the phenyl rings in both *A* and *B* are in a propeller rather than butterfly arrangement. In *A* the dihedral angles between the TeCC plane and the phenyl rings are 40·2 and 37·3°* in molecule 1 and 46·4 and 38·6° in molecule 2. The corresponding angles in *B* are 41·9 and 35·3° in molecule 1 and 50·6 and 35·3° in molecule 2. The dihedral angles between the planes of the rings are also very similar in both compounds (55·3 and 60·2° in molecules 1 and 2 respectively for *A* and 55·6 and 59·5° in *B*). Thus the packing of the phenyl rings is apparently an important factor. It is clear from the torsion angles C(13)–C(14)–O(1)–C(17), 176·8°, and C(43)–C(44)–O(4)–C(47), −6·7°, and Fig. 2 that the orientation of a methoxy group [O(1)C(17)] in molecule 1 differs from the counter methoxy group

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

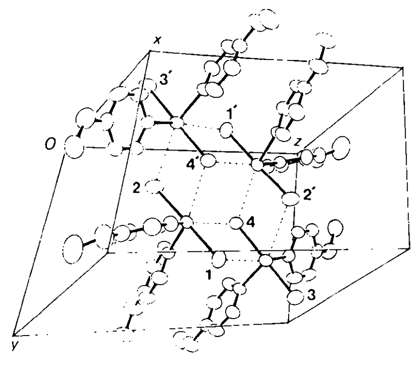

Fig. 1. Unit-cell packing of (p-$CH_3OC_6H_4)_2TeCl_2$ indicating the step-like structure of the tetramer about $\frac{1}{2},\frac{1}{2},\frac{1}{2}$. H atoms are omitted for clarity.

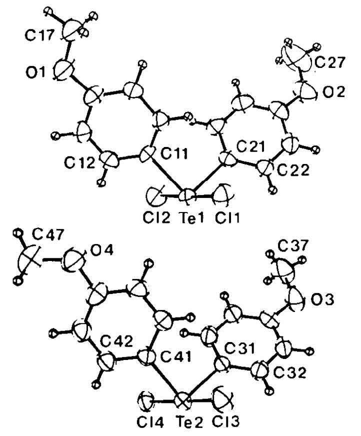

Fig. 2. *ORTEP* plot of the two independent molecules, 1 (top) and 2, of (p-$CH_3OC_6H_4)_2TeCl_2$. The atoms are drawn with 50% probability ellipsoids.

Table 3. *Comparison of some non-bonded distances* (Å) *and angles* (°) *in the tetramers of* (p-$CH_3OC_6H_4)_2TeCl_2$ (*A*), (p-$BrC_6H_4)(C_6H_5)TeCl_2$ (*B*) *and* $C_{12}H_8OTeCl_2$ (*C*)

	Step	*A*	*B*	*C*
Te$\cdots$Te'	Vertical*	4·678 (1)	4·609 (2)	4·594 (3)
	Central	4·472 (1)	4·720 (2)	4·793 (3)
TeClTe'	Vertical	99·1 (1)	83·0 (2)	98·9 (1)
	Central	78·6 (1)	82·7 (2)	88·0 (1)
ClTeCl'	Vertical	80·9 (1)	96·8 (2)	80·9 (1)
	Central	101·4 (1)	97·3 (2)	92·0 (1)

* Averaged for upper and lower step.

[O(4)C(47)] in molecule 2, thus minimizing the repulsions. Distortions in the central step formed by Te(1')$\cdots$Cl(4)$\cdots$Te(1)$\cdots$Cl(4') also appear to be designed to minimize repulsion. Thus in *C*, this central step approximates to a rectangle with the Cl$\cdots$Te$\cdots$Cl angle being 92·0 (1)° and the Te$\cdots$Te distance across the step being 4·793 (3) Å (Table 3). The shortest Te$\cdots$Te distance in this compound is in fact between molecules 1 and 2 and averages 4·594 (3) Å. In *B*, where the alternating packing of substituted and non-substituted rings presumably helps alleviate the repulsion between substituents, there is some distortion around the central rectangle so that the Cl$\cdots$Te$\cdots$Cl angle is now 97·3 (2)° with the Te$\cdots$Te distance slightly reduced to 4·720 (2) Å. However, in *A*, where methoxy groups on molecules 1 and 2 are in fairly close proximity, the distortion is larger so that the Cl$\cdots$Te$\cdots$Cl angle is now 101·4 (1)° and the Te$\cdots$Te distance reduced to 4·472 (1) Å. This has the effect of elongating the vertical steps so that the Te(1)$\cdots$Te(2) distances are now longer [on average 4·678 (1) Å] and the methoxy groups slightly further apart. In $TeCl_4$ (Buss & Krebs, 1971) in which the tetramer has all four Te atoms in the alternate vertices of an approximate cube, the Te$\cdots$Te distance is 4·309 (1) Å, considerably shorter than the shortest distance in *A*.

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[2,2-Di(2-pyridyl)-1,3-dioxolane-*N*,*N'*]dichloropalladium(II), $[PdCl_2(C_{13}H_{12}N_2O_2)]$

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Abstract. $M_r = 405·6$, monoclinic, $P2_1/c$, $a = 9·767$ (1), $b = 19·224$ (3), $c = 15·351$ (3) Å, $\beta = 90·34$ (1)°, $V = 2882$ (2) Å^3, $Z = 8$, $D_x = 1·869$ (1) g cm^{-3}, Mo $K\alpha$, $\lambda = 0·71073$ Å, $\mu = 16·45$ cm^{-1}, $F(000) = 1600$, $T = 296$ K, $R = 0·031$ for 4502 observations (of 5078 unique data). The title molecule consists of a central Pd^{II} atom bonded to two pyridine nitrogens and two chlorine atoms. The coordination geometry of Pd is square planar with slight tetrahedral distortion. The asymmetric unit

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