Fig. 2. Projection along [100] of the packing of [H₂pic][PtCl₃(Me₂SO)].

displaced from the mean plane passing through them by -0.003 (2), 0.029 (4), -0.009 (2), 0.030 (4) and -0.008 (2) Å, respectively. The structural parameters of $[PtCl_3(Me_2SO)]^-$ are quite comparable to those of the same complex in the structure of the potassium salt (2) (Melanson, Hubert & Rochon, 1976) in which the values of the Pt—Cl bonds were

2.302 (6), 2.318 (5) and 2.296 (6) Å, and the Pt—S bond 2.193 (5) Å.

In contrast, some differences in the IR spectra of (1) and (2) have been found. (i) The stretching S—O falls at a lower frequency in (1) with respect to (2) [$\nu_{S=O}$: 1060 cm^{-1} (1), 1100 cm^{-1} (2)]; (ii) The stretching Pt—Cl (Cl trans to sulfoxide) decreases from 309 cm^{-1} (1) to 290 cm^{-1} (2), probably due to the weakness of the bond determined by the hydrogen bond with the 2-carboxypyridinium cation.

The packing of the structure, shown in Fig. 2, is determined by an intermolecular hydrogen bond involving the —OH group of the pyridine-2-carboxylic acid moiety and the O atom of the dimethyl sulfoxide moiety [$O(2)\cdots O(1)$ ($x + \frac{1}{2}, \frac{1}{2} - y, 1 - z$) $= 2.570$ (12) Å, $O(2)$—$H(2)$—$O(1)$ ($x + \frac{1}{2}, \frac{1}{2} - y, 1 - z$) $= 163°$].

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Structure of Dichlorobis(p-phenoxyphenyl)tellurium(IV)

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Abstract. [TeCl₂(C₁₂H₉O)₂], $M_r = 536.9$, monoclinic, $P2_1/c$, $a = 8.061$ (5), $b = 21.694$ (5), $c = 12.606$ (7) Å, $\beta = 101.5$ (2)°, $V = 2160$ (2) Å^3, $Z = 4$, $D_x = 1.652$ cm^{-3}, Mo $K\alpha$, $\lambda = 0.701069$ Å, $\mu = 16.45$ cm^{-1}, $F(000) = 1056$, room temperature, $R = 0.028$, $wR = 0.030$ for 2626 observed reflections [$I \geq 2.5\sigma(I)$]. The Te atom is in a pseudo trigonal-bipyramidal configuration with the lone pair in one of the equatorial positions. Distances Te—Cl $= 2.506$ (1), 2.510 (1) Å; Te—C $= 2.107$ (3), 2.129 (4) Å; Cl—Te—Cl $= 177.21$ (1)°; Cl—Te—C $= 90.7$ (1), 89.2 (1), 88.6 (1), 88.7 (1)°; C—Te—C $= 98.7$ (1)°.

Introduction. Diorganyl ditellurides and diorganyl tellurides constitute an important class of starting

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materials for the preparation of other organotellurium compounds (Petragnani & Comasseto, 1986). The well known synthetic route whereby diaryl ditellurides, arenetellurenyl halides (generated *in situ*) are treated with Grignard reagents to produce unsymmetrical aryl alkyl tellurides (Petragnani, Torres & Wynne, 1975) has been used as a general method for preparing other organotellurium compounds (Dabdoub, Dabdoub, Comasseto & Petragnani, 1986). Because of the increasing interest in the field of organic chemistry, a series of dihalobis(aryl)tellurium(IV) compounds were prepared following the procedure described by Drew (1926). A structural study of the title compound was undertaken in order to examine the bonding and molecular geometry.

Experimental. Prismatic red-brown crystals suitable for X-ray study ($0.16 \times 0.08 \times 0.03$ mm), Enraf–Nonius CAD-4 diffractometer, using the 'flat ψ mode' to minimize absorption. Unit-cell parameters by least squares from 25 reflections with θ between 6 and 13°; 3192 unique reflections collected, 2626 considered observed with $I \geq 2.5\sigma(I)$; ω–2θ scan mode, hkl range: $-8 \leq h \leq 8$, $-0 \leq k \leq 23$, $0 \leq l \leq 14$, θ limit 25°; scan range $\Delta\theta = (0.80 + 0.34\tan\theta)°$; no significant decay from monitoring of three standard reflections. Lorentz–polarization corrections, no absorption correction. Structure solved by heavy-atom methods (*SHELX*76; Sheldrick, 1976). Te atom located from Patterson functions, remaining atoms (except H9) by subsequent Fourier maps. Anisotropic full-matrix least-squares refinement on F of non-H atoms (*SHELX*76). H9 position was calculated for C—H = 0.96 Å; isotropic temperature-factor refinement for H atoms ($U = 0.0836$ Å²); 314 parameters refined, $R = 0.028$, $wR = 0.030$, $w = 0.7213/[\sigma^2(F) + 0.00109F^2]$; max. $(\Delta/\sigma) = 0.064$. Residual electron density within -0.94 and 0.47 e Å⁻³ near the Te atom. Scattering factors (except tellurium) from *International Tables for X-ray Crystallography* (1974, Vol. IV); scattering factors for tellurium from Forsyth & Wells (1959). Drawing by *PLUTO* (Motherwell & Clegg, 1978). All calculations were performed on a Digital MicroVAX II.

Discussion. The atomic parameters are given in Table 1.* A view of the molecule with the atomic numbering scheme is shown in Fig. 1, and the molecular packing in Fig. 2. Table 2 gives bond distances and angles.

Table 1. *Atomic coordinates* ($\times 10^4$, $\times 10^5$ *for* Te) *with e.s.d.'s in parentheses and equivalent isotropic temperature factors* (Å²) *for non-H atoms*

$$B_{eq} = (8\pi^2/3)\Sigma_i\Sigma_j U_{ij}a_i^*a_j^*\mathbf{a}_i.\mathbf{a}_j.$$

|	x	y	z	B_{eq}
Te	87768 (3)	6455 (1)	63321 (2)	3·64
Cl1	9647 (1)	1530 (1)	7599 (1)	5·43
C1	6759 (5)	475 (2)	7127 (3)	3·66
Cl2	7772 (1)	−243 (1)	5095 (1)	4·76
C2	6712 (6)	−85 (2)	7625 (3)	4·71
C3	5374 (7)	−203 (2)	8170 (4)	5·85
C4	4173 (5)	241 (2)	8192 (3)	4·91
C5	4254 (6)	794 (2)	7706 (4)	5·07
C6	5548 (5)	925 (2)	7168 (3)	4·63
O1	2910 (5)	154 (2)	8776 (3)	7·43
C7	1900 (6)	−374 (2)	8590 (4)	4·84
C8	1325 (7)	−609 (3)	9461 (4)	6·17
C9	269 (7)	−1111 (3)	9325 (4)	6·82
C10	−188 (6)	−1380 (3)	8336 (5)	6·61
C11	390 (6)	−1144 (3)	7471 (4)	5·85
C12	1444 (6)	−638 (2)	7595 (4)	4·99
C13	7540 (5)	1280 (2)	5144 (3)	3·70
C14	6053 (5)	1126 (2)	4460 (3)	4·14
C15	5315 (5)	1534 (2)	3666 (3)	4·63
C16	6111 (5)	2092 (2)	2556 (3)	4·65
C17	7573 (6)	2244 (2)	4239 (4)	5·35
C18	8290 (6)	1839 (2)	5047 (3)	5·11
O2	5404 (5)	2529 (1)	2795 (2)	6·10
C19	4692 (5)	2333 (2)	1751 (3)	4·40
C20	3274 (6)	2641 (2)	1224 (4)	5·59
C21	2617 (6)	2490 (3)	157 (4)	6·27
C22	3320 (6)	2036 (3)	−354 (4)	5·97
C23	4735 (7)	1741 (3)	176 (4)	6·13
C24	5439 (6)	1894 (2)	1233 (3)	5·52
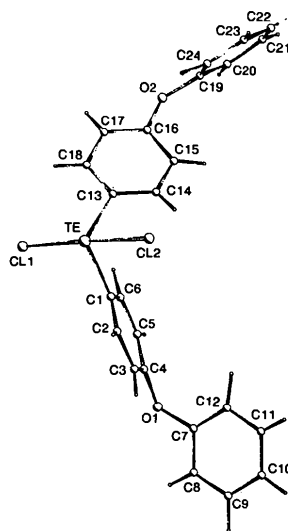
Fig. 1. A view of the molecule showing the atomic numbering.

The bonding in the molecule is consistent with the predictions of classical bonding models for AB_4E molecules (Gillespie, 1970). Cl atoms are axial with a Cl—Te—Cl angle of 172·2° whereas two C atoms are placed in equatorial positions. The Te^{IV} lone pair of electrons possibly occupies the vacant equatorial

Table 2. *Interatomic distances (Å) and angles (°) with e.s.d.'s in parentheses*

Cl1—Te	2·506 (1)	C11—C10	1·368 (7)
Cl—Te	2·107 (3)	C12—C11	1·376 (7)
Cl2—Te	2·510 (1)	C14—C13	1·370 (5)
Cl3—Te	2·129 (4)	C18—C13	1·372 (6)
C2—C1	1·370 (5)	C15—C14	1·379 (6)
C6—C1	1·390 (5)	C16—C15	1·391 (6)
C3—C2	1·414 (6)	C17—C16	1·354 (5)
C4—C3	1·370 (6)	O2—C16	1·386 (5)
C5—C4	1·353 (6)	C18—C17	1·382 (6)
O1—C4	1·383 (5)	C19—O2	1·393 (5)
C6—C5	1·383 (6)	C20—C19	1·375 (6)
C7—O1	1·398 (5)	C24—C19	1·361 (6)
C8—C7	1·373 (6)	C21—C20	1·383 (7)
C12—C7	1·362 (6)	C22—C21	1·360 (7)
C9—C8	1·373 (7)	C23—C22	1·361 (7)
C10—C9	1·358 (7)	C24—C23	1·380 (6)
Cl—Te—Cl1	88·6 (1)	C11—C10—C9	119·8 (5)
Cl2—Te—Cl1	177·2 (1)	C12—C11—C10	120·7 (5)
Cl2—Te—Cl	88·7 (1)	C11—C12—C7	119·1 (4)
Cl3—Te—Cl1	89·2 (1)	C14—C13—Te	120·9 (3)
Cl3—Te—Cl	98·7 (1)	C18—C13—Te	118·8 (3)
Cl3—Te—Cl2	90·7 (1)	C18—C13—C14	120·3 (4)
C2—C1—Te	117·9 (3)	C15—C14—C13	119·8 (4)
C6—C1—Te	120·5 (3)	C16—C15—C14	119·4 (4)
C6—C1—C2	121·5 (3)	C17—C16—C15	120·6 (4)
C3—C2—C1	118·5 (4)	O2—C16—C15	122·0 (4)
C4—C3—C2	119·5 (4)	O2—C16—C17	117·3 (4)
C5—C4—C3	121·0 (4)	C18—C17—C16	119·7 (4)
O1—C4—C3	120·8 (4)	C17—C18—C13	120·1 (4)
O1—C4—C5	118·0 (4)	C19—O2—C16	118·7 (3)
C6—C5—C4	120·9 (4)	C20—C19—O2	117·1 (4)
C5—C6—C1	118·5 (4)	C24—C19—O2	121·9 (4)
C7—O1—C4	119·2 (3)	C24—C19—C20	120·8 (4)
C8—C7—O1	116·7 (4)	C21—C20—C19	118·4 (5)
C12—C7—O1	122·7 (4)	C22—C21—C20	121·1 (5)
C12—C7—C8	120·6 (4)	C23—C22—C21	119·7 (4)
C9—C8—C7	119·6 (5)	C24—C23—C22	120·2 (5)
C10—C9—C8	120·2 (5)	C23—C24—C19	119·7 (4)
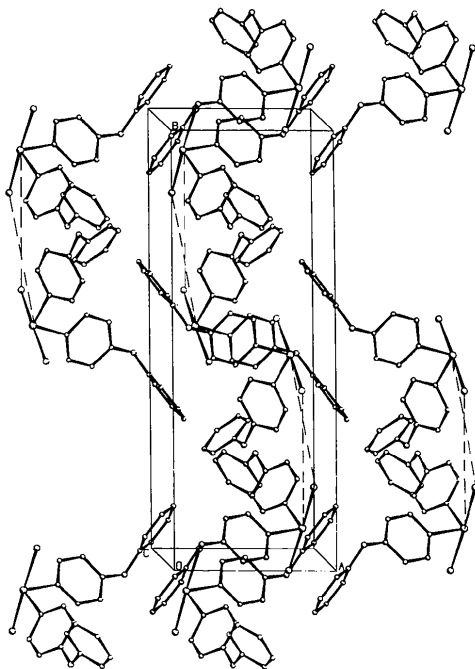
Fig. 2. Packing diagram, view down c. Intermolecular contacts are shown as dashed lines.

position in the trigonal bipyramid as Ziolo and co-workers reported in their study on electron density for dimethyltellurium dichloride (Ziolo & Troup, 1983). The Te—Cl bond lengths are similar to those found in other $TeCl_2R_2$ compounds, 2·47–2·55 Å (Alcock & Harrison, 1982; Ziolo & Troup, 1983; Husebye, Meyers, Zingaro, Comasseto & Petragnani, 1987). The Te—C bond distances are close to those predicted from the sum of the single-bond covalent radii, as in other R_2TeCl_2 molecules (Chadha, Drake & Kahn, 1983; Chada, Drake & Hencher, 1983; Castellano, Zukerman-Schpector, Ferreira & Comasseto, 1986). The C—Te—C and Cl—Te—Cl angles are also within the range reported for those compounds.

Intermolecular contacts are present: Te···Cl2' $(2 - x, -y, 1 - z)$ 3·71 Å, and Te···C12'' $(x - 1, y, z)$ 3·68 Å (shorter than the sum of respective van der Waals radii 3·81 and 3·83 Å), giving a distorted octahedral arrangement about the Te atom.

The phenyl rings are planar within experimental accuracy (r.m.s. deviation = 0·0044 Å; δ_{max} = 0·0073 Å for C1, r.m.s. deviation = 0·0024 Å, δ_{max} = 0·0037 Å for C9, r.m.s. deviation = 0·0077, δ_{max} = 0·0105 for C15, r.m.s. deviation = 0·0102, δ_{max} = 0·0146 for C21). The bond lengths and angles in the organic moiety are within the expected range of values.

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