Table 1. *Selected geometric parameters (Å, °)*

P1—C1	1.796 (4)	P1—C19	1.795 (4)
P1—C7	1.794 (4)	O1—C21	1.239 (7)
P1—C13	1.789 (4)	O2—C21	1.210 (7)
C1—P1—C7	108.9 (2)	C7—P1—C19	109.4 (2)
C1—P1—C13	107.1 (2)	O1—C21—O2	126.1 (6)
C1—P1—C19	110.8 (2)	O1—C21—C20	116.1 (5)
C7—P1—C13	110.8 (2)	O2—C21—C20	117.8 (6)

H atoms bonded to C were treated using a riding model with $U(\mathrm{H}) = 1.5U_{\mathrm{eq}}(\mathrm{C})$. Water H atoms were placed at calculated positions with $U = 0.05$ Å^2. For the O3 water molecule, one of the H atoms is necessarily disordered over two positions.

Data collection: *CAD-4/PC* (Kretschmar, 1994). Cell refinement: *CELDIM* (Enraf–Nonius, 1988). Data reduction: *XCAD*4 (Harms, 1997). Program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997*a*). Program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997*b*). Molecular graphics: *ORTEP*II (Johnson, 1976). Software used to prepare material for publication: *SHELXL*97.

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Supplementary data for this paper are available from the IUCr electronic archives (Reference: DA1039). Services for accessing these data are described at the back of the journal.

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Butyldichloro(phenylethynyl)tellurium(IV)

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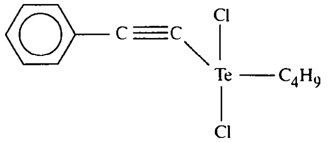
Abstract

In the title compound, $[\mathrm{TeCl_2(C_4H_9)(C_8H_5)}]$ ($\mathrm{C_{12}H_{14}Cl_2Te}$), the intramolecular geometry around the $\mathrm{Te^{IV}}$ is pseudo-trigonal bipyramidal, with the Cl atoms in the apical positions and the Te lone pair occupying the fifth position in the equatorial plane. Taking into account the intermolecular secondary Te···Cl1 contact of 3.266 (1) Å, *trans* to the Te—$\mathrm{C_{vinyl}}$, the structure may be regarded as pseudo-octahedral. Distances and angles are: Te—Cl 2.486 (1) and 2.551 (1), Te—C 2.020 (3) and 2.146 (3) Å; Cl—Te—Cl 173.81 (3), Cl—Te—C 89.94 (10), 86.59 (9), 87.84 (10) and 87.98 (9), and C—Te—C 97.66 (13)°. All of the C atoms lie in a plane, with the Te atom displaced 0.2220 (2) Å from the plane in the direction of Cl2.

Comment

Butyltelluroalkynes are important intermediates in organic synthesis, since they permit the stereospecific synthesis of vinylic tellurium species (Comasseto *et al.*, 1997), which in turn are precursors of other vinyl metal derivatives such as vinyl lithium, copper, zinc, magnesium, sodium and calcium. In previous papers, we reported the synthesis (Dabdoub *et al.*, 1988) and reactions (Dabdoub & Comasseto, 1988; Dabdoub & Cassol, 1995) of these acetylenic tellurium species. Reaction of acetylenic tellurides with Br or I produces organyltellurium trihalides and the corresponding 1,1,2-trihaloethylenes, instead of the expected diorganyl tellurium dihalides (Dabdoub *et al.*, 1990). However, reaction of telluroacetylenes with an excess of sulfurylchloride in petroleum ether at 273 K affords the corresponding dichlorotelluroacetylenes in high yield. In this way, the phenylethynyl(butyltelluro) dichloride was obtained in 97% yield. Due to our interest in the structure of organotellurium compounds in general (Zukerman-Schpector *et al.*, 1995; Zukerman-Schpector, Caracelli, Dabdoub & Dabdoub, 1996; Zukerman-Schpector, Caracelli, Dabdoub, Dabdoub & Pereira, 1996), and diorganyltelluro dichlorides in particular, the crystal structure of the title compound, (I), which was obtained as described by Dabdoub *et al.* (1990), was determined.



(I)

In (I), the Te^{IV} atom adopts a primary four-coordinate geometry based on a pseudo-trigonal bipyramidal polyhedron, formed by four bonds to two Cl and two C atoms of the ligands and one lone pair of electrons which, together with the C atoms, occupy equatorial sites, while the Cl atoms occupy axial positions. This configuration is in complete agreement with the valence-shell electron-pair repulsion (VSEPR) model (Gillespie, 1972). The average quadrupole angle, α_4^E, for the Te lone pair of electrons is 112.13°, a value typical for TeX_4E configurations (Zukerman-Schpector *et al.*, 1995, and references therein). The Te—Cl axial lengths are 0.19 and 0.13 Å longer than the sum of the normal covalent radii (2.36 Å; Ziolo & Troup, 1983), and may be compared with the values found in other $TeCl_2RR'$ type compounds (Dabdoub *et al.*, 1990; Zukerman-Schpector *et al.*, 1995; Singh *et al.*, 1990). The Te—C bond distances of 2.146 (3) and 2.020 (3) Å are close to the predicted values of 2.142 and 2.000 Å, using the Pauling (1960) radius for Te (1.37 Å), Csp^3 (0.772 Å) and Csp (0.630 Å). The C—Te—C angle of 97.66 (13)° is in the range found in other compounds (Zukerman-Schpector, Caracelli, Dabdoub, Dabdoub & Pereira, 1996).

There is a secondary intermolecular interaction between Te and $Cl1^i$ [symmetry code: (i) $-x$, $-y$, $1 - z$] of 3.266 (1) Å. This distance is less than the sum of the van der Waals radii (Pauling, 1960) of the Te and Cl of 4.00 Å, and is slightly longer than the Te—$Cl_{bridging}$ distances found in triphenyltellurium chloride [3.142 (1)–3.234 (1) Å; Ziolo & Extine, 1980]. With this interaction, which is approximately *trans* to C_{vinyl} [C1—Te···$Cl1^i$ 169.50 (11)°], the arrangement about the Te atom should be described as a distorted pseudo-octahedron, with the lone pair of electrons occupying the fourth equatorial site (Singh *et al.*, 1990), as seen in Fig. 1. This secondary bond links the molecules into chains parallel to **c**. The distortions of the coordination geometry from the ideal octahedral values (90 and 180°) can be explained in terms of the lone pair of electrons occupying an equatorial position between C1 and $Cl1^i$. The Cl—Te—C angles are slightly less than 90°, so that the Te—C bonds are bent slightly away from the lone pair, as might be expected from the VSEPR theory, resulting in a Cl—Te—Cl angle of 173.81 (3)°.

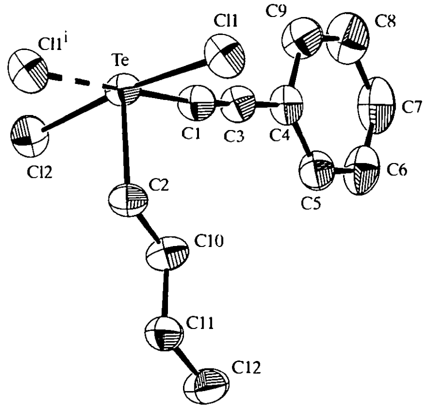


Fig. 1. The molecular structure of (I), showing 50% probability displacement ellipsoids [symmetry code: (i) $-x$, $-y$, $1 - z$]. H atoms have been omitted for clarity.

The carbon moiety is essentially planar, as can be seen by the σ_{av} $\{\sigma_{av} = [(\Sigma_i d_i^2)/(N-3)]^{1/2}\}$ value of 0.036 Å. The greatest deviation is that of the Te atom, which is displaced 0.2220 (2) Å from the plane, towards the Cl2 atom. The acetylenic C1—C3 bond length of 1.196 (4) Å is very close to the value of 1.203 (2) Å found for C≡C in acetylene (Nes & Bolhius, 1979) and may be compared with the value of 1.210 (11) Å found in bis(*p*-methoxyphenyltelluro)ethyne (de Matheus *et al.*, 1991).

Experimental

The title compound was synthesized as described by Dabdoub *et al.* (1990).

Crystal data

$C_{12}H_{14}Cl_2Te$
$M_r = 356.73$
Triclinic
$P\bar{1}$
$a = 8.7610\ (5)$ Å
$b = 8.8907\ (4)$ Å
$c = 10.4403\ (6)$ Å
$\alpha = 112.419\ (4)°$
$\beta = 106.101\ (5)°$
$\gamma = 96.407\ (4)°$
$V = 700.30\ (6)$ Å^3
$Z = 2$
$D_x = 1.692$ Mg m^{-3}
D_m not measured

Mo $K\alpha$ radiation
$\lambda = 0.71073$ Å
Cell parameters from 25 reflections
$\theta = 2.4$–$25.5°$
$\mu = 2.474$ mm^{-1}
$T = 293$ K
Irregular
0.35 × 0.25 × 0.10 mm
Colourless

Data collection

Enraf–Nonius CAD-4 diffractometer
$\omega/2\theta$ scans
Absorption correction: ψ scans (North *et al.*, 1968)
$T_{min} = 0.685$, $T_{max} = 0.781$

2481 reflections with $F^2 > 2\sigma F^2$
$R_{int} = 0.008$
$\theta_{max} = 25.46°$
$h = -10 \rightarrow 10$
$k = 0 \rightarrow 10$
$l = -12 \rightarrow 11$

2786 measured reflections
2605 independent reflections

3 standard reflections
  frequency: 30 min
  intensity decay: 0.4%

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.028$
$wR(F^2) = 0.075$
$S = 1.122$
2605 reflections
143 parameters
H-atom parameters
  constrained

$w = 1/[\sigma^2(F_o^2) + (0.0534P)^2 + 0.2809P]$
  where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} < 0.001$
$\Delta\rho_{\max} = 1.286$ e Å^{-3}
$\Delta\rho_{\min} = -1.252$ e Å^{-3}
Extinction correction: none
Scattering factors from
  International Tables for Crystallography (Vol. C)

Table 1. *Selected geometric parameters (Å, °)*

Te—C1	2.020 (3)	Te—Cl1	2.551 (1)
Te—C2	2.146 (3)	C1—C3	1.196 (4)
Te—Cl2	2.486 (1)		
C1—Te—C2	97.66 (13)	C1—Te—Cl1	87.84 (10)
C1—Te—Cl2	89.94 (10)	C2—Te—Cl1	87.98 (9)
C2—Te—Cl2	86.59 (9)	Cl2—Te—Cl1	173.81 (3)

H atoms were refined with fixed geometry, each riding on a carrier atom, with an isotropic displacement parameter equal to 1.5 (for methyl-H atoms) or 1.2 (for the other H atoms) times that of the carrier atom. The highest peak and the deepest hole in the final difference Fourier map were at 0.95 and 0.94 Å from Te, respectively.

Data collection: *CAD*-4 *Software* (Enraf–Nonius, 1989). Cell refinement: *CAD*-4 *Software*. Data reduction: *MolEN* (Fair, 1990). Program(s) used to solve structure: *SHELXS*86 (Sheldrick, 1990). Program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997). Molecular graphics: *ZORTEP* (Zsolnai, 1995). Software used to prepare material for publication: *SHELXL*97.

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Supplementary data for this paper are available from the IUCr electronic archives (Reference: GS1025). Services for accessing these data are described at the back of the journal.

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Methyl (2*S*)-2-[(5*R*)-3,5-diphenyl-4,5-dihydro-1,2,4-oxadiazol-4-yl]-3-phenylpropanoate

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Abstract

In the title compound, $C_{24}H_{22}N_2O_3$, the 4,5-dihydro-1,2,4-oxadiazole ring system is in an envelope conformation with the C1, N1, C8 and N2 sets of atoms in a common plane with O1 0.110 (3) Å out of this plane. The chiral C atom in the five-membered ring, C1, is in the *R* configuration, which was identified by referring to the known configuration of the atom C15 in the (*S*)-phenylalanine moiety.

Comment

4,5-Dihydro-1,2,4-oxadiazole derivatives are important pharmaceutical agents with antiviral (Franco *et al.*,