group is well located and does not show any unusual structural features.

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Structure of Phenyltellurium Trichloride

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Abstract. [Te(C_6H_5)]Cl$_3$, M_r = 311·07, triclinic, $P\bar{1}$, a = 16·687 (3), b = 8·616 (2), c = 7·471 (1) Å, α = 90·79 (2), β = 114·18 (1), γ = 112·30 (2)°, V = 888·21 Å^3, Z = 4 (with two independent molecules in the asymmetric unit), D_c = 2·326, D_o = 2·33 Mg m^{-3}. 2661 observed [$I \geq 2\cdot3\ \sigma(I)$] reflections were used in the refinement and gave a final discrepancy index of R = 0·025. The structure is polymeric with bridging Cl atoms; each Te atom lies in an octahedral environment surrounded by four Cl atoms, a C atom and a lone pair of electrons.

Introduction. The literature contains a number of crystallographic studies of alkyl- and aryltellurium trihalides (Kobelt & Paulus, 1971; McCullough & Knobler, 1976; McCullough, 1977; Knobler & McCullough, 1977; Bergman & Engman, 1979). The tellurium halide skeletal structures of these compounds are all, to some extent, different, showing varying degrees of halogen bridging.

At present, it is unclear which are the factors which influence these crystal structures. Therefore, to improve present information on $RTeX_3$ compounds, we now report the structure of PhTeCl$_3$. This compound was of further interest in connection with previous vibrational spectroscopic studies (McWhinnie & Thavornyuti-karn, 1972) on phenyltellurium trihalides in which a

dimeric structure (PhTeX_3)$_2$ containing bridging halogen atoms was proposed for chloro and iodo derivatives and some kind of polymeric arrangement was inferred for the bromo compound.

Precession and Weissenberg photographs were used to determine approximate cell dimensions and the diffraction symbol for the crystals. A suitable crystal (0·18 × 0·16 × 0·25 mm) for data collection was mounted in a Lindemann capillary and accurate cell dimensions were determined by least-squares refinement of 20 accurately measured reflections (2θ = 28–35°, Mo $K\alpha$ radiation). Data were collected at 293 K using a Picker FACS-I four-circle diffractometer [λ(Mo $K\alpha$) = 0·70926 Å] with a graphite mono-chromator and a scintillation detector with pulse-height discrimination. The take-off angle was 3° and a symmetrical θ–2θ scan (2° min^{-1}) of (1·6 + 0·692 tan θ)° was used. Stationary-crystal stationary-counter background counts of 10% of the scan time were taken at each side of the scan. A peak profile analysis was performed on each reflection and the intensity and its associated error determined by the method of Grant & Gabe (1977). Intensity measurements of two standards every 70 reflections showed no evidence of crystal deterioration and no instability of the detection system.

Intensities were measured for 3129 independent reflections ($2\theta \leq 50°$), of which 2661 were classed observed [$I \geq 2\cdot3\sigma(I)$]. Lorentz, polarization and.

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Table 1. *Final positional parameters* ($\times 10^5$ *for* Te; $\times 10^4$ *for* Cl *and* C) *and temperature factors* ($\times 10^4$ *for* Te *and* Cl; $\times 10^3$ *for* C) *for phenyltellurium trichloride*

Estimated standard deviations in the least significant figure are given in parentheses. $U_{eq} = [\frac{1}{3}(U_{11}^2 + U_{22}^2 + U_{33}^2)]^{1/2}$.

	x	y	z	U/U_{eq} (Å^2)
Te(1)	17749 (3)	63891 (4)	3766 (5)	250 (2)
Te(2)	17574 (3)	37531 (4)	53281 (5)	278 (2)
Cl(1)	855 (1)	6801 (2)	−2830 (2)	393 (9)
Cl(2)	867 (1)	6900 (2)	1906 (3)	427 (9)
Cl(3)	820 (1)	2042 (2)	6835 (3)	449 (9)
Cl(4)	836 (1)	1823 (2)	2193 (2)	431 (9)
Cl(5)	2977 (1)	6041 (2)	−1037 (2)	393 (9)
Cl(6)	2991 (1)	5918 (2)	3949 (2)	385 (9)
C(1)	2770 (4)	9029 (7)	1331 (8)	28 (1)
C(2)	2374 (5)	10209 (8)	941 (10)	40 (1)
C(3)	3026 (5)	11946 (9)	1603 (10)	46 (2)
C(4)	3994 (6)	12427 (1C)	2603 (12)	54 (2)
C(5)	4364 (5)	11198 (9)	2945 (11)	45 (2)
C(6)	3743 (5)	9495 (8)	2307 (9)	36 (1)
C(7)	2748 (4)	2596 (7)	6324 (8)	27 (1)
C(8)	3741 (4)	3620 (7)	7244 (9)	34 (1)
C(9)	4367 (5)	2846 (9)	7913 (11)	45 (2)
C(10)	3991 (6)	1057 (9)	7612 (11)	51 (2)
C(11)	2995 (5)	69 (9)	6658 (11)	46 (2)
C(12)	2367 (5)	832 (8)	6011 (10)	39 (1)

absorption corrections ($\mu = 4 \cdot 282$ mm^{-1}) have been applied.

The structure was solved by Patterson and Fourier methods. H atoms were included as fixed contributions in their calculated positions. Full-matrix least-squares refinement with anisotropic temperature factors for Te and Cl atoms and isotropic temperature factors for all other atoms gave final agreement factors of $R = 0 \cdot 025$ ($R = \sum ||F_o| - |F_c||/\sum |F_o|$) and $R_w = 0 \cdot 045$ $\{R_w = [\sum w(|F_o| - |F_c|)^2/\sum w|F_o|^2]^{1/2}\}$. A weighting scheme was applied on the basis of the standard deviations $[w = 1/(\sigma F)^2]$. Atomic scattering factors including anomalous dispersion for Te and Cl were taken from *International Tables for X-ray Crystallography* (1974). Final positional and thermal parameters are given in Table 1.* The computer programs used here have been cited previously (Einstein & Jones, 1972).

Discussion. Bond parameters are contained in Table 2 and the molecular structure is shown in Fig. 1. There are two independent PhTeCl$_3$ molecules in the asymmetric unit which have very similar coordination geometry. Each Te atom lies in an irregular octahedral environment with a Te—C bond of $2 \cdot 13$ Å, two Te—Cl

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* Lists of structure factors, anisotropic thermal parameters and H-atom parameters have been deposited with the British Library Lending Division as Supplementary Publication No. SUP 36361 (21 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

terminal bonds of *ca* $2 \cdot 37$ Å, two Te—Cl bridge bonds of *ca* $2 \cdot 75$ Å, and a lone pair of electrons, constituting the vertices of the octahedron.

The angles between the Te—C and Te—Cl bonds range from $84 \cdot 9$ (2) to $92 \cdot 3$ (2)°, whereas angles between adjacent Te—Cl bonds range from $85 \cdot 40$ (5) to $95 \cdot 64$ (6)°.

Te(1) and Te(2) lie $0 \cdot 10$ and $0 \cdot 05$ Å, respectively, out of the mean planes described by the four Cl atoms surrounding them.

The two bridging interactions associated with Cl(5) and Cl(6) give rise to a continuous polymeric Cl-bridged chain. The angles about the bridging Cl atoms are Te(1)—Cl(6)—Te(2) = $104 \cdot 53$ (5) and Te(1')—

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

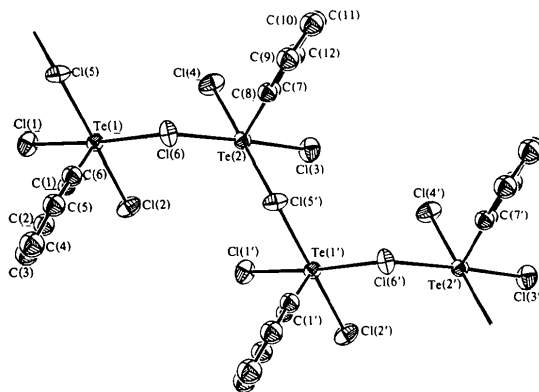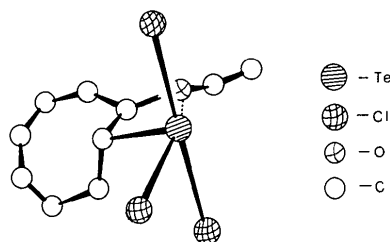|			
Te(1)—C(1)	2·135 (6)	C(1)—C(2)	1·384 (8)
Te(1)—Cl(1)	2·376 (2)	C(2)—C(3)	1·404 (9)
Te(1)—Cl(2)	2·388 (2)	C(3)—C(4)	1·354 (10)
Te(1)—Cl(5)	2·722 (2)	C(4)—C(5)	1·395 (10)
Te(1)—Cl(6)	2·761 (2)	C(5)—C(6)	1·370 (9)
Te(2)—C(7)	2·131 (5)	C(6)—C(1)	1·364 (8)
Te(2)—Cl(3)	2·372 (2)	C(7)—C(8)	1·392 (8)
Te(2)—Cl(4)	2·370 (2)	C(8)—C(9)	1·377 (9)
Te(2)—Cl(6)	2·767 (2)	C(9)—C(10)	1·400 (10)
Te(2)—Cl(5')	2·771 (2)	C(10)—C(11)	1·391 (10)
		C(11)—C(12)	1·371 (10)
		C(12)—C(7)	1·380 (8)
C(1)—Te(1)—Cl(1)	92·3 (2)	Te(1)—C(1)—C(2)	116·7 (4)
C(1)—Te(1)—Cl(2)	90·5 (2)	Te(1)—C(1)—C(6)	120·5 (4)
C(1)—Te(1)—Cl(5)	84·9 (2)	C(1)—C(2)—C(3)	116·8 (6)
C(1)—Te(1)—Cl(6)	86·4 (1)	C(2)—C(3)—C(4)	121·1 (7)
Cl(1)—Te(1)—Cl(2)	95·64 (6)	C(3)—C(4)—C(5)	120·3 (7)
Cl(1)—Te(1)—Cl(5)	88·20 (5)	C(4)—C(5)—C(6)	119·7 (7)
Cl(1)—Te(1)—Cl(6)	173·56 (5)	C(5)—C(6)—C(1)	119·3 (6)
Cl(2)—Te(1)—Cl(5)	174·09 (7)	C(6)—C(1)—C(2)	122·8 (5)
Cl(2)—Te(1)—Cl(6)	90·68 (6)	Te(2)—C(7)—C(8)	119·8 (4)
Cl(5)—Te(1)—Cl(6)	85·40 (5)	Te(2)—C(7)—C(12)	117·7 (4)
		C(7)—C(8)—C(9)	118·8 (6)
C(7)—Te(2)—Cl(3)	92·3 (2)	C(8)—C(9)—C(10)	119·4 (7)
C(7)—Te(2)—Cl(4)	91·4 (2)	C(9)—C(10)—C(11)	120·4 (7)
C(7)—Te(2)—Cl(6)	85·9 (2)	C(10)—C(11)—C(12)	120·5 (6)
C(7)—Te(2)—Cl(5')	85·04 (2)	C(11)—C(12)—C(7)	118·4 (6)
Cl(3)—Te(2)—Cl(4)	94·49 (6)	C(12)—C(7)—C(8)	122·5 (5)
Cl(3)—Te(2)—Cl(6)	174·33 (8)		
Cl(3)—Te(2)—Cl(5')	89·10 (6)	Te(1)—Cl(6)—Te(2)	104·53 (5)
Cl(4)—Te(2)—Cl(5')	175·08 (9)	Te(1') Cl(5')—Te(2)	105·05 (5)
Cl(4)—Te(2)—Cl(6)	90·92 (6)		
Cl(5')—Te(2)—Cl(6)	85·40 (5)		

Fig. 1. The polymeric structure of PhTeCl$_3$ [*ORTEP* diagram (Johnson, 1965), 50% probability contours for all atoms]. Te(1) is at x,y,z and Te(1') at $x, y, 1 + z$.

Table 3. *Comparison of some bond parameters of known RTeCl₃ structures*

	PhTeCl₃	(ClCH₂CH₂) TeCl₃[c]	(C₈H₁₂OC₂H₅) TeCl₃[d]
Te(1)–Cl(1)[a]	2·376 (2) Å	2·386 (3) Å	2·355 (1) Å
Te(1)–Cl(2)	2·388 (2)	2·386 (3)	2·481 (1)
Te(1)–Cl(5)	2·722 (2)	2·717 (3)	2·505 (1)
Te(1)–C(1)	2·135 (6)	2·16 (1)	2·172 (3)
Te(1)–Cl(6)	2·761 (2)	2·717 (3)	–
Cl(1)–Te(1)–C(1)	92·3 (2)°	92·7°	93·65 (9)°
Cl(2)–Te(1)–Cl(5)	174·09 (7)	(b)	176·24 (4)
Cl(2)–Te(1)–C(1)	90·5 (2)	82·5	88·10 (9)
Cl(2)–Te(1)–Cl(1)	95·64 (6)	(b)	92·00 (4)

(a) The numbering schemes of (ClCH₂CH₂)TeCl₃ and (C₈H₁₂OC₂H₅)TeCl₃ have been altered to be consistent with that of molecule (1) of the present compound. *(b)* These values were not reported. *(c)* Kobelt & Paulus (1971). *(d)* Bergman & Engman (1979).

Fig. 2. The monomeric structure of (C₈H₁₂OC₂H₅)TeCl₃ (Bergman & Engman, 1979).

Cl(5′)–Te(2) = 105·05 (5)°. The bond parameters of the phenyl rings are comparable to those of the Te-bonded phenyl rings found in the (2-biphenylyl)-TeX₃ series (McCullough & Knobler, 1976; McCullough, 1977; Knobler & McCullough, 1977).

A comparison of the structure of PhTeCl₃ with the previously reported RTeCl₃ systems (Kobelt & Paulus, 1971; Bergman & Engman, 1979) is shown in Table 3. It appears from the very limited information reported by Kobelt & Paulus (1971) that the polymeric structure of (ClCH₂CH₂)TeCl₃ is isostructural with that of PhTeCl₃. In contrast, (C₈H₁₂OC₂H₅)TeCl₃ (Bergman & Engman, 1979) is quite different, being essentially monomeric with Te lying in a trigonal-bipyramidal environment, in which two Cl atoms occupy axial positions, and a further Cl atom, a C atom and a lone pair of electrons occupy equatorial positions. It is interesting to note, however, that this geometry (Fig. 2; Table 3) is quite similar to the 'monomer' geometry within the PhTeCl₃ chain. It appears that the additional contacts between 'monomers' in PhTeCl₃ which result in chain formation also cause elongation of one of the Te–Cl bonds within the PhTeCl₃ unit, e.g. Te(1)–Cl(5) = 2·722 (2) Å, *cf.* the corresponding distance in (C₈H₁₂OC₂H₅)TeCl₃ of 2·505 (1) Å (Bergman & Engman, 1979). Chain formation of the type found in PhTeCl₃ and (ClCH₂CH₂)TeCl₃ (Kobelt & Paulus, 1971) is unlikely in (C₈H₁₂OC₂H₅)TeCl₃ due to a weak Te···O intramolecular interaction [2·419 (2) Å] which blocks the bridging site at Te. Weak intramolecular interactions of this kind are also found in the (2-biphenylyl)TeX₃ series (McCullough & Knobler,

1976; McCullough, 1977; Knobler & McCullough, 1977) where very similar 'monomer' geometries are also observed. In the Cl-bridged polymeric structures found for PhTeCl₃ and (ClCH₂CH₂)TeCl₃ it is obvious that the ligands are sterically incapable of such intramolecular interactions. It would seem, therefore, for the chloro RTeX₃ derivatives at least, that the steric nature of the ligand plays a major role in the type of structure adopted.

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