tautomer (I*b*). The four atoms of the triazene *N*-oxide group are closely planar ($\chi^2 = 4$). The average plane of the group forms a dihedral angle of 11 (1)° with the phenyl ring. This is probably due to repulsion between H(C2) and H(N1) atoms [H(C2)···H(N1) = 2·39 Å, C(2)—C(1)—N(1)—N(2) = 172·3 (4)°, C(2)—C(1)—N(1)—H(N1) = −13·6 (4)°]. N(1) and N(2) atoms do not deviate significantly from the phenyl ring [−0·056 (2) and −0·020 (2) Å, respectively], hence the delocalization is extended to these atoms, resulting in the short C(1)—N(1) distance of 1·403 (3) Å. The N(1) and O(1) atoms are *cis* to each other.

The four atoms of the amide group are highly planar ($\chi^2 = 0$), and the group is inclined at an angle of 27 (1)° to the average plane of the phenyl group. This probably results from steric hindrance between N(4) and C(5) and between the O(2) and C(3) atoms. The H(N42)···H(C5) distance is 2·21 (4) Å, which would be 2·02 Å if the two groups were coplanar.

Both of the amide hydrogen atoms participate in hydrogen bonding. H(N41) forms a bond to the O(2) atom of the neighbouring molecule related by an inversion centre, while H(N42) links an *a*-glide-plane-related molecule *via* O(2) [H(N41)···O(2) = 1·83 (4) Å, O(2)···H(N41)—N(4) = 170 (4)°; H(N42)···O(2) = 2·11 (5) Å, O(2)···H(N42)—N(4) = 166 (4)°].

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Trichloro(2-phenylthiophenyl)tellurium

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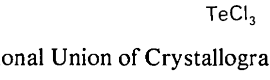
Abstract. [Te($C_{12}H_9S$)Cl_3], $M_r = 419{\cdot}2$, monoclinic, $P2_1/c$, $a = 9{\cdot}428$ (2), $b = 11{\cdot}878$ (1), $c = 13{\cdot}095$ (2) Å, $\beta = 96{\cdot}57$ (1)°, $V = 1456{\cdot}8$ Å^3, $D_x = 1{\cdot}91$ Mg m^{-3}, $Z = 4$, Mo $K\alpha$, $\lambda = 0{\cdot}71073$ Å, $\mu = 2{\cdot}77$ mm^{-1}, $F(000) = 800$, $T = 296$ K, $R = 0{\cdot}033$ for 2283 reflections with $I > 0{\cdot}5\sigma(I)$. In C_6H_5—S—C_6H_4—$TeCl_3$ the phenyl rings and C—Te and C—S bonds are normal, as is the T-shaped $TeCl_3$ group. There is a close contact between the *ortho* substituents Te and S.

Introduction. It was of interest to determine the structure of the title compound in order to (1) establish the coordination around Te and (2) find out how the Group VI *ortho* substituents, S and Te, affect each other and the remainder of the structure.



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Experimental. X-ray data were collected by The Molecular Structure Corporation, College Station, Texas, from a yellow needle-like crystal (0·15 × 0·15 × 0·25 mm) mounted on a glass fiber. D_m not determined. All data obtained with graphite-monochromatized Mo $K\alpha$ radiation from an Enraf–Nonius CAD-4 diffractometer. Monoclinic cell parameters calculated by least-squares refinement of 2θ values for 25 reflections. Intensities of 2698 reflections measured by scanning in 2θ ($2\theta_{\max} = 50°$). When all systematically absent reflections, as well as others for which $I < 0{\cdot}5\sigma(I)$, were eliminated, 2283 reflections remained. Intensities of three check reflections measured periodically showed no significant crystal decay. Corrections for Lorentz and polarization effects, but not for absorption since the crystal was small and $\mu = 2{\cdot}77$ mm^{-1}. A Patterson function yielded coordinates for Te, and electron-density maps and weighted least-squares refinements yielded parameters for Te, Cl, S and C atoms. After refinement with anisotropic temperature factors for Te, Cl and S, and with isotropic values for C, the positions of the nine H atoms were calculated (C–H = 1·08 Å). Each H atom was assigned the temperature factor of the C atom to which it was attached. All of the H-atom parameters were fixed, while the scale factor and all other atomic coordinates and anisotropic temperature factors were varied in weighted block-diagonal least-squares refinements until $(\Delta/\sigma)_{\max} < 0{\cdot}04$. $\sum w(|F_o| - |F_c|)^2$ minimized; $R = 0{\cdot}033$, $wR = 0{\cdot}042$; $w = 1/\sigma^2(F)$; $\sigma(I) = [\sigma_c^2 + (0{\cdot}05I)^2]^{1/2}$, with σ_c calculated from counting statistics; $S = 1{\cdot}15$ for 154 refined parameters. No correction for secondary extinction. The program *SHELX76* (Sheldrick, 1976), modified for a DEC 1144 computer, was used. Scattering factors, including anomalous-dispersion corrections, were taken from those supplied with the program and from Cromer & Liberman (1970), Cromer & Mann (1968) and Stewart, Davidson & Simpson (1965). The largest residues on a final difference density map were +0·42 and −0·58 e Å^{-3}.

Discussion. Final atomic parameters are given in Table 1.* An *ORTEP* drawing of the molecule is shown in Fig. 1 (Johnson, 1971) and some interatomic distances and angles are listed in Table 2. The weighted average of the C–C distances in phenyl ring *A* [C(1),...,C(6)] is 1·382 (3) [2] Å, and in phenyl ring *B* [C(7),...,C(12)] is 1·377 (7) [3] Å; the corresponding average C–C–C angles are 120·1 (6) [2] and 120·0 (5) [2]°. (When two values are given, the e.s.d.'s in parentheses have been calculated from the deviations of the individual values from the weighted mean, and those in square brackets from the e.s.d.'s of the individual

Table 1. *Fractional coordinates and equivalent isotropic temperature factors* (Å^2)

$U_{eq} = \frac{1}{3}\sum_i\sum_j U_{ij}a_i^*a_j^*(\mathbf{a}_i.\mathbf{a}_j)$. The e.s.d.'s of the last digit(s) are given in parentheses. H-atom parameters were not refined.

	x	*y*	*z*	U_{eq}
Te	0·14496 (3)	0·13267 (2)	0·08329 (2)	0·0444
Cl(1)	0·3160 (2)	0·2560 (1)	0·0062 (1)	0·0726
Cl(2)	0·1001 (1)	0·2766 (1)	0·1955 (1)	0·0695
Cl(3)	−0·0092 (1)	0·0018 (1)	0·1711 (1)	0·0677
S	0·3174 (1)	−0·0537 (1)	0·0096 (1)	0·0538
C(1)	0·3210 (4)	0·0691 (3)	0·1798 (3)	0·0408
C(2)	0·3840 (4)	−0·0217 (3)	0·1378 (3)	0·0440
C(3)	0·5016 (5)	−0·0729 (4)	0·1923 (4)	0·0594
C(4)	0·5504 (5)	−0·0329 (4)	0·2883 (4)	0·0648
C(5)	0·4881 (5)	0·0600 (4)	0·3296 (3)	0·0614
C(6)	0·3708 (5)	0·1117 (4)	0·2754 (3)	0·0515
C(7)	0·2568 (4)	−0·1953 (4)	0·0138 (4)	0·0528
C(8)	0·2774 (6)	−0·2602 (4)	−0·0704 (4)	0·0656
C(9)	0·2303 (7)	−0·3704 (5)	−0·0737 (6)	0·0881
C(10)	0·1693 (6)	−0·4156 (5)	0·0035 (7)	0·0926
C(11)	0·1454 (6)	−0·3502 (5)	0·0876 (5)	0·0895
C(12)	0·1911 (6)	−0·2383 (4)	0·0934 (4)	0·0707

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

Te–Cl(1)	2·477 (2)	C(4)–C(5)	1·388 (7)
Te–Cl(2)	2·324 (1)	C(5)–C(6)	1·387 (6)
Te–Cl(3)	2·497 (1)	C(6)–C(1)	1·382 (5)
Te···S	2·972 (1)	C(7)–C(8)	1·377 (7)
Te–C(1)	2·108 (4)	C(8)–C(9)	1·381 (8)
S–C(2)	1·765 (4)	C(9)–C(10)	1·332 (11)
S–C(7)	1·779 (5)	C(10)–C(11)	1·387 (10)
C(1)–C(2)	1·376 (5)	C(11)–C(12)	1·397 (8)
C(2)–C(3)	1·388 (6)	C(12)–C(7)	1·371 (7)
C(3)–C(4)	1·373 (7)		
Cl(1)–Te–Cl(2)	89·81 (4)	C(2)–S–C(7)	104·8 (2)
Cl(2)–Te–Cl(3)	90·53 (4)	S–C(7)–C(8)	115·4 (4)
Cl(3)–Te···S	93·13 (4)	S–C(7)–C(12)	123·4 (4)
S···Te–Cl(1)	84·40 (4)	C(6)–C(1)–C(2)	122·1 (4)
C(1)–Te–Cl(1)	87·2 (1)	C(1)–C(2)–C(3)	119·6 (4)
C(1)–Te–Cl(2)	94·1 (1)	C(2)–C(3)–C(4)	118·9 (4)
C(1)–Te–Cl(3)	87·8 (1)	C(3)–C(4)–C(5)	121·3 (4)
C(1)–Te···S	60·4 (1)	C(4)–C(5)–C(6)	120·0 (4)
Cl(1)–Te–Cl(3)	174·97 (4)	C(5)–C(6)–C(1)	118·0 (4)
Cl(2)–Te···S	154·01 (3)	C(12)–C(7)–C(8)	121·2 (4)
Te···S–C(2)	71·3 (1)	C(7)–C(8)–C(9)	118·8 (6)
Te–C(1)–C(2)	112·8 (3)	C(8)–C(9)–C(10)	121·6 (7)
Te–C(1)–C(6)	125·1 (3)	C(9)–C(10)–C(11)	120·0 (6)
S–C(2)–C(1)	115·2 (3)	C(10)–C(11)–C(12)	119·9 (6)
S–C(2)–C(3)	124·8 (3)	C(11)–C(12)–C(7)	118·5 (5)

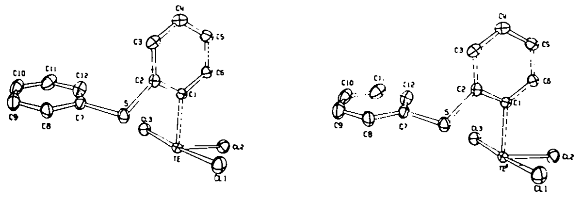

Fig. 1. Stereoscopic projection of [Te($C_{12}H_9S$)Cl_3].

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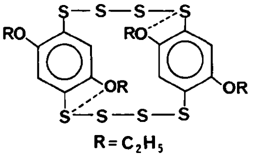
* Lists of structure factors, anisotropic thermal parameters, H-atom parameters, mean-planes and dihedral angles, and shortest intermolecular distances have been deposited with the British Library Lending Division as Supplementary Publication No. SUP 42359 (21 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

values.) The average C—C distances are 0·01 to 0·02 Å shorter than expected, with the greater deviation associated with ring *B*, where the thermal parameters are large. Also, there are large deviations in bond angles from 120° which do not seem to follow a simple pattern. The average C—S distance is 1·771 (7) [3] Å, which is slightly shorter than that proposed by Domenicano, Vaciago & Coulson (1975), 1·781 (3) Å. The distance Te—C = 2·108 (4) Å is normal (Mangion, Zingaro & Meyers, 1975). The unit [$TeCl_3$] is T-shaped with long distances Te—Cl = 2·490 (9) [1] Å in the linear part, with angle Cl(1)—Te—Cl(3) = 174·97 (4)°, and with Te—Cl(2) = 2·324 (1) Å as the short distance. These values are in agreement with those formed in other structures that involve Te—Cl bonds (Mangion, Zingaro & Meyers, 1975). An examination of the remaining bond angles around Te, all of which are close to 90°, makes it seem reasonable to describe qualitatively the Te bonding by use of the Te 5*p* orbitals, with Cl(1)—Te—Cl(3) a three-center bond.

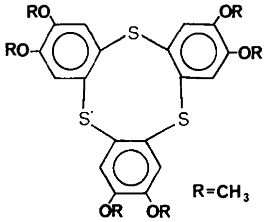
In addition to the atoms that are unequivocally bonded to Te, there is a short Te···S distance, 2·972 (1) Å, with 'adjacent' angles C(2)—C(1)—Te = 112·8 (3) and C(1)—C(2)—S = 115·2 (3)°. This geometry suggests a significant Te···S intramolecular interaction. The maximum deviation from the best plane through phenyl ring *A* is 0·013 Å for C(4). The deviations of other atoms from this plane are: Te −0·020, Cl(1), 2·455, Cl(2) 0·025, Cl(3) −2·514, S 0·177 Å. For comparison, the maximum deviation in phenyl ring *B* is for C(10) (0·016 Å) and S is only −0·017 Å from the plane. The angle between the rings is 78·8°.

Ricci & Bernal (1971) commented on close contacts between S and O in $C_{20}H_{24}O_4S_8$ (I).



(I)

The ethoxy groups, EtO, are nearly coplanar with their phenyl ring, and the phenyl rings are nearly parallel to one another. The average C—C—O angle next to 'adjacent' S is 115·3 (4)°, and C—C—S next to 'adjacent' O is 116·2 (4)°, with intramolecular S···O = 2·775 Å. Systematic correlations in S···S and S—C distances and for interior C—C—S angles were obtained by Cowie & Bennett (1976) for a series of metal derivatives of 1,2-dithiobenzene. In $Mo(S_2C_6H_4)_3$, the values are S···S = 3·110 (8), S—C = 1·727 (6) Å, C—C—S = 119·4°; and in $[N(CH_3)_4]_2[Zr(S_2C_6H_4)_3]$, S—S = 3·265 (14), S—C = 1·765 (7) Å, C—C—S = 122·0°. These variations are complicated by the presence of the metal species, but they serve to show that the Te···S distance in the present compound is extraordinarily short. In catechol, $C_6H_4(OH)_2$ (Brown, 1966), there is conflicting evidence for short contacts between adjacent O atoms; the C—C—O angles are 121·0 and 117·1°. Recent work by Von Deuten & Klar (1979, 1981) has shown for 1,2,4,5-tetramethoxybenzene, $C_{10}H_{14}O_4$, and for bis-(3,4-dimethoxyphenyl) sulfide, $C_{16}H_{18}O_4S$, that the 'adjacent' C—C—O angles vary from 114·9 (4) to 116·7 (2)°. In other work (Von Deuten, Kopf & Klar, 1979), for molecule (II), $C_{24}H_{24}O_6S_3$, and its CuBr adduct, it was found that 'adjacent' C—C—O angles varied from 114·4 (4) to 118·1 (16)°, while 'adjacent' C—C—S angles varied from 118·9 (14) to 130·1 (4)°. In (II), the C—S—C angle ranged from 100·9 (2) to 111·0°, compared to 104·8 (2)° in the present structure. There appears to be sufficient variety in the geometry of these benzene derivatives that have chalcogen atoms *ortho* to each other to warrant further studies.



(II)

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