Tetraorganotellurium(IV) Derivatives. Crystal and Molecular Structure of Tetraphenyltellurium–Benzene (1/8), $(C_6H_5)_4Te\cdot{}^1/_8C_6H_6$

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The crystal and molecular structure of tetraphenyltellurium–benzene (1/8) has been determined by a single-crystal X-ray diffraction study. The results represent the first structural characterization of a tetraorgano derivative of a group 6 element. The compound crystallizes in the space group $P\bar{1}$ with eight molecules per unit cell. Lattice parameters (23 ± 1 °C) are as follows: a = 14.547 (5) Å, b = 21.687 (7) Å, c = 13.140 (6) Å, α = 101.93 (3)°, β = 93.39 (3)°, γ = 89.46 (3)°, and V = 4052 (2) Å^3. The structure was determined by Patterson and Fourier methods from automatic diffractometer data using filtered Mo Kα radiation. Refinement by the least-squares technique led to a conventional R factor (on F) of 0.074 for 7893 reflections having $F_o^2 < 3\sigma(F_o^2)$. Tetraphenyltellurium has a distorted, ψ-trigonal-bipyramidal geometry with the axial phenyl groups bending toward the equatorial groups. Mean angles are as follows: C_{eq}–Te–C_{eq} = 108.6°, C_{ax}–Te–C_{ax} = 168.7 (7)°, and C_{eq}–Te–C_{ax} = 86.7 (3)°. The equatorial Te–C distances are normal with a mean of 2.13 (0) Å. The axial Te–C distances are elongated and range from 2.27 (1) to 2.31 (1) Å. These distances are the longest primary Te–C bond distances known. It is suggested that the relative thermal stability of the R_nTeX_{4-n} (n = 2, 4) compounds relates, in part, to the stability of the long, axial $M^{\delta+}\cdots L^{\delta-}$ bond. The stereochemistry about Te in the four independent molecules is identical. Each molecule, however, is conformationally unique due to phenyl group orientations. Short intermolecular contacts are absent, giving tellurium a genuine fourfold configuration. The closest Te–Te approach is 4.803 (1) Å.

Introduction

Tetraphenyltellurium is a relatively stable solid that decomposes on heating to diphenyl telluride and biphenyl.[2,3] It is one of the few stable tetraorganochalcogen molecules known. The molecule shows the reactivity of an organometallic compound as seen in its reactions with CH_2Cl_2 and $CHCl_3$ to form $(C_6H_5)_3TeCl$.[4] Although no structural work on the tetraorganochalcogens has been reported, tetraphenyltellurium, as an AB_4E molecule, is expected to have a ψ-trigonal-bipyramidal geometry similar to that, for example, of $(CH_3)_2TeCl_2$[5] or of gas-phase $TeCl_4$.[6] In the solid state, however, the presence of intermolecular interactions gives tellurium(IV) a coordination number higher than that expected from the compound's stoichiometry.[7–9] For example, solid tellurium tetrachloride possesses six-coordinate tellurium and is a tetramer.[10] Similarly, $(CH_3)_2TeCl_2$ is more accurately described as having a distorted octahedral geometry with intermolecular bonding.[11] In general, intermolecular bonding leads to five- and six-coordinate distorted octahedral geometries in the R_nTeX_{4-n} (n = 0–3) compounds.[7,8,12] When n = 4 and R is C_6H_5, the situation is not as predictable. Although the indium and gallium phenyls exhibit short intermolecular contacts,[13] none is observed in trimethyltelluronium tetraphenylborate due to steric or electronic constraints.[14] To date, structural examples of a genuine four-coordinate solid-state tellurium(IV) species appear to be unknown.[15]

As part of a larger effort to study the stereochemistry and bonding in hypervalent tellurium compounds, we have determined the structure of tetraphenyltellurium by X-ray diffraction techniques.[17] This example serves as the first structural characterization of a tetraorgano derivative of a group 6 element. Structural examples of groups 3, 4, and 5 heavier element phenyls are known.[18]

Experimental Section

Tetraphenyltellurium was prepared from diphenyltellurium dichloride and phenyllithium by the method of Wittig and Fritz.[2] The product was crystallized at 10 °C from a 3:1 mixture of anhydrous diethyl ether and benzene. The crystal density was not measured.

A crystal coated with dry Nujol was mounted randomly in a glass capillary. Unit cell parameters were obtained from a least-squares analysis of 25 reflections. Tetraphenyltellurium–benzene (1/8) crystallizes in the triclinic system: a = 14.547 (5) Å, b = 21.687 (7) Å, c = 13.140 (6) Å, α = 101.93 (3)°, β = 92.39 (3)°, γ = 89.46 (3)°, V = 4052 (2) Å^3, d_{calcd} = 1.46 g/cm^3 for Z = 8. A Delaunay reduction of the cell revealed no hidden symmetry.

Intensity data were collected at Molecular Structure Corp.[19] on an Enraf-Nonius CAD4 automatic diffractometer using gra-

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(15) The possibility that $(C_6H_5)_2TeBr_2$[16] is an exception to this statement has not been ruled out. The Te–Br contact is at or near the van der Waals distance and the bromine is in a stereochemically significant position. A situation similar to that in $(CH_3)_2TeCl_2$[11] is expected.
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phite-monochromatized Mo Kα radiation. The prism used measured 0.3 × 0.3 × 0.35 mm. The width of half-height from ω scans was 0.2°.

A total of 11 940 independent reflections were collected by the θ–2θ scan technique in the range $0 < 2\theta$ (Mo Kα) < 47°. A takeoff angle of 5.6° was used with a counter aperture width of 2.0 mm. The incident-beam collimeter diameter was 2.0 mm and the crystal to detector distance 21 cm. A variable scan rate of 8–20°/min (in 2θ) was used with stationary-crystal stationary-counter background counts where scan time per background time equaled 2.0. The scan range was from 2θ (Mo Kα_1) – 0.7° to 2θ (Mo Kα_2) + 0.7°.

Intensities and standard deviations of intensities were calculated as described previously.[20] The factor, p, introduced to downweight intense reflections was set to 0.05. Lorentz and polarization corrections were applied to the data. Extinction and absorption corrections were unnecessary. Psi scans of the relatively uniform prism showed less than 5% variation in transmission . The calculated linear absorption coefficient (Mo Kα), μ, is 15.2 cm^{-1}. Three representative reflections which were measured periodically showed a linear decrease in intensity with X-ray exposure. A total average decrease of 39% in the standard reflections was corrected for by a linear factor.

A data set consisting of the 4519 reflections with $2\theta < 40°$ (Mo Kα) was employed for solution and initial refinement of the structure. A sharpened Patterson map failed to yield unambiguous positions for the four independent tellurium atoms in the asymmetric unit. A structure factor calculation was carried out by assuming noncentrosymmetric $P1$ symmetry with a single tellurium atom placed at the origin. A Fourier map phased on this basis was used in conjunction with the Patterson map to fix the relative positions of the Te atoms. Once these were established, the coordinates were transformed to the centrosymmetric space group $P\bar{1}$; all subsequent calculations employed this symmetry. A structure factor calculation based on the four tellurium atoms gave an R ($=\sum||F_o| - |F_c||/\sum|F_o|$) value 0.459. Two cycles of least squares refinement and Fourier syntheses located all of the carbon atoms; with isotropic thermal parameters for all atoms, the R value stood at 0.061. At this point the data set was expanded to 7893 reflections, including all independent reflections having $F_o > 3\sigma(F_o)$. Because of the large number of parameters to be refined (413), each complete cycle of least squares was broken down into several smaller blocks. In view of the crystal decomposition during data collection, it seemed likely that the original values of $\sigma(F_o)$ were underestimated. A careful study of the goodness of fit, $[\sum w(F_o - F_c)^2/(\text{no. of reflections} - \text{no. of variables})]^{1/2}$, as the refinement progressed indicated that the standard deviations were too small by a factor of about 9.5. In subsequent calculations all values of $\sigma(F_o)$ were increased by this factor. Because of the prohibitive amount of computing time that would be required and because of the substantial decomposition of the crystal during data collection, anisotropic refinement of the model was not attempted. The hydrogen atoms were included as fixed contributions to the structure factors, assuming the normal ring geometry with C–H distances set at 0.95 Å. Refinement of the model was terminated with R at 0.074 and R_w ($=\sum w(|F_o| - |F_c|)^2/\sum w|F_o|^2$) at 0.065. A few of the parameters shifted by more than their standard deviations in the last cycles. Most of the large shifts were associated with carbon atoms meta or para to the tellurium position, reflecting the weakness of the isotropic model for these atoms. An additional complete cycle of refinement was carried out in order to determine if better convergence could be achieved. Some shifts greater than σ (parameter) were again noted, while the values for R and R_w remained unchanged; there was no improvement in the derived bond distances and angles. A final difference Fourier map showed several large peaks (ca. 1.1 e/Å^3) within 0.4 Å of the tellurium atoms. No other peaks exhibited electron densities higher than 15% of the observed carbon atom densities.

Scattering factors were taken from the compilation of Hanson et al.;[21] those for Te were corrected for the real and imaginary components of anomalous dispersion by using the values of Cromer.[22] The programs used are listed in an earlier publication.[20] In the least-squares refinement the function minimized was $\sum w(|F_o| - |F_c|)^2$ where $w = \sigma^{-2}(F)$.

The final positional and thermal parameters for the atoms are given in Table I. The hydrogen atom parameters and the observed and calculated structure factors are available as supplementary material.

Results and Discussion

Tetraphenyltellurium–benzene (1/8) crystallizes in the triclinic system with eight molecules in the unit cell. The unique conformation of each of the four independent molecules is illustrated in Figure 1, and distances and angles about Te are given in Table II. With the possible exception of two C–Te2–C angles, the stereochemistry about tellurium in the four molecules is identical within experimental error.

In the solid state, tetraphenyltellurium has a distorted, pseudo-trigonal-bipyramidal (ψ-tbp) geometry, similar to that observed in $(CH_3)_2TeCl_2$.[5] The third equatorial site is presumably occupied by the Te(IV) lone pair as has been found in the X–X electron deformation density study of dimethyltellurium dichloride.[11] The mean value[23] of the equatorial C–Te–C angles in $(C_6H_5)_4Te$ is 108.6 (1.3)° and is the largest known for the R_2TeX_2 molecules.[24] In $(C_6H_5)_2TeBr_2$[16] and $(p\text{-}ClC_6H_4)_2TeI_2$,[25] for example, the C–Te–C angles are 96.3 (1.2) and 101.1 (1.0)°, respectively. Although no correlation is implied, we note that the large angle is in keeping with the trend of increasing size of the axial ligands, bromine, iodine, and phenyl. The axial phenyls bend toward the equatorial groups with the C–Te–C angles ranging from 167.9 (4) to 170.8 (4)°. Thus, the C_{eq}–Te–C_{ax} angles are all acute with an observed range of 84.2 (4) to 88.5 (4)°. The direction of bend of the axial angles is consistent with the predictions of the VSEPR model[26] and is like that observed in $(CH_3)_2TeCl_2$[5] but opposite to that observed in Br_2.[16] The deviation of the axial angles from the idealized value of 180° is matched only by that in $[CH_3CH(Cl)CH_2]_2TeCl_2$.[27] Unfortunately, it is not yet possible to distinguish between the steric and electronic factors that affect the equilibrium structure of the Te(IV) AB_4E molecules. Moreover, it is possible that the lone pair participates in the bonding as has been suggested in other instances.[10,26]

The Te–C distances in the molecule fall into two groups. The equatorial Te–C distances have a mean value of 2.13 (0) Å[23] and are identical with the sum of the covalent radii[28a] and to the Te–C distances found in the $(C_6H_5)_3Te^+$ ion.[14,20,29,30] In keeping with the salient feature of axial elongation in the trigonal-bipyramidal AB_4E molecules, the Te–C axial distances range from 2.27 (1) to 2.31 (1) Å and represent the longest primary Te–C bond distances known.[31] Their bond order[28b] of approximately 0.5 is

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(23) The estimated variance of the mean is given in parentheses and is calculated as $[\sum(x-\bar{x})^2/(n(n-1))]^{1/2}$. "International Tables for X-Ray Crystallography", The Kynoch Press: Birmingham, England, 1972; Vol. II, p 89.
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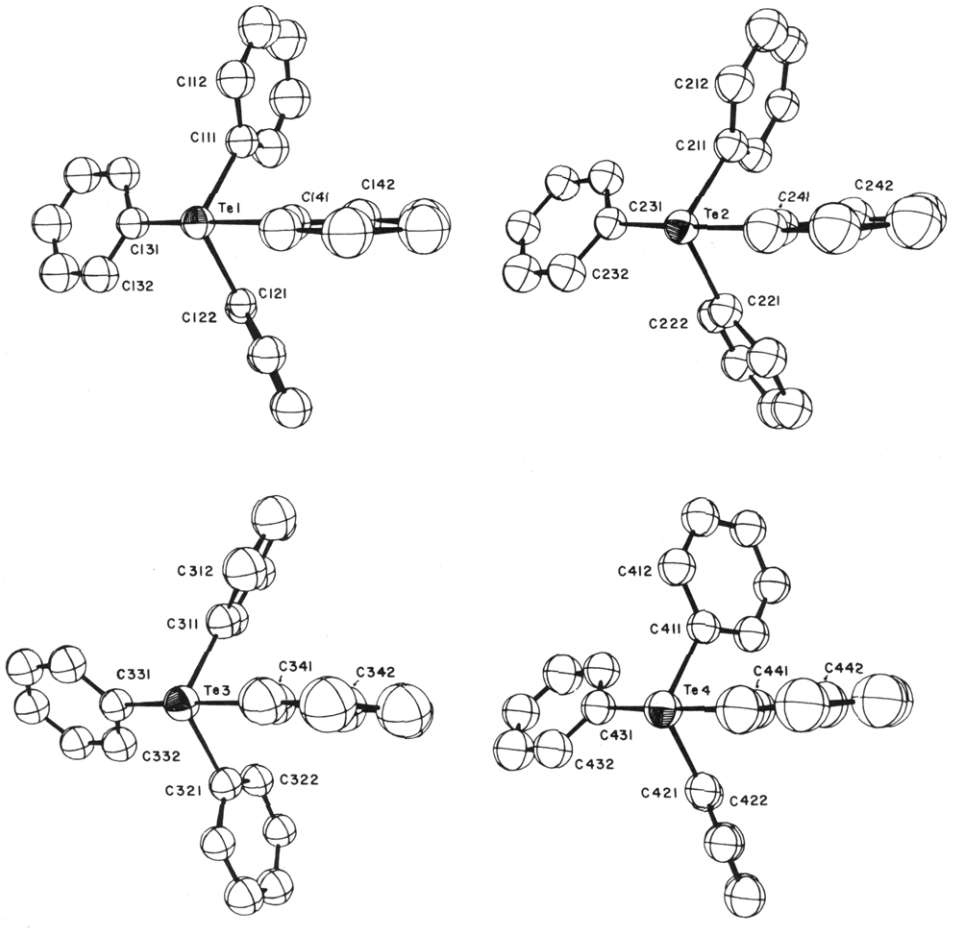

Figure 1. Atom labeling scheme of the four independent molecules of $(C_6H_5)_4Te$.

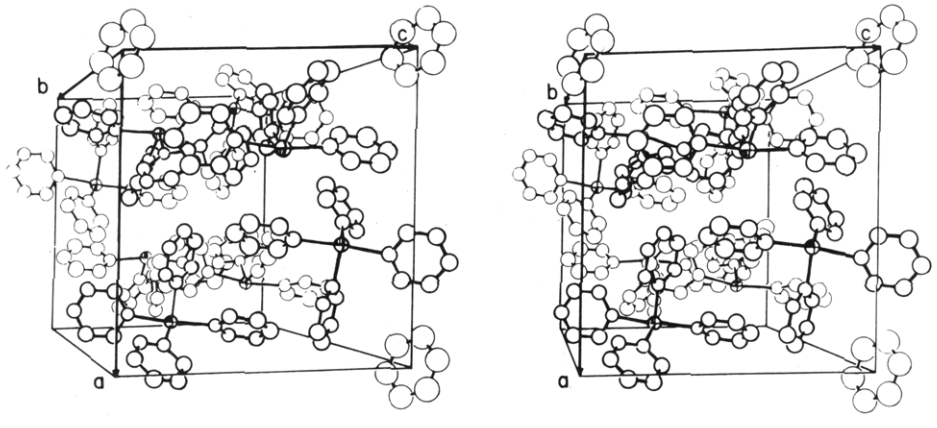

Figure 2. Stereoscopic unit cell drawing of $(C_6H_5)_4Te\cdot{}^1/_8C_6H_6$.

identical with those calculated for the axial distances in other trigonal-bipyramidal molecules such as $(CH_3)_2TeCl_2$[5] and $(C_6H_5)_2TeBr_2$.[16] These long distances are also in keeping with the strong trans influence observed for the phenyl group in several Te(II) complexes[32,33] and in the seven-coordinate Te(IV) compound tris(diethyldithiocarbamato)phenyltellurium(IV).[34] Various bonding models have been used to explain the axial elongation in the AB_4E molecules.[26,35]

Assuming that the R_4Te [and $(R{=})_2Te$][38] compounds require the ψ-tbp geometry, it is reasonable to suggest that the thermal stability of the R_nTeX_{4-n} (n = 2, 4) compounds depends, in part, on the stability of the long, axial $M^{\delta+}\cdots L^{\delta-}$ bonds.[36] Thus, ligand groups of low electronegativity, e.g., CH_3, would be expected to yield less stable structures than groups of higher electronegativity such as phenyls or halogens. Many R_2TeX_2 compounds are known and their thermal stability is well established.[4] In contrast, few R_4Te compounds are known. The thermal stability of these

(31) For comparison, a significantly short intramolecular Te(IV)–C distance is 2.945 (9) Å, in 2-biphenylyltellurium tribromide.[37]
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(36) Evidence for the polarization of the axial bond has been noted in $(CH_3)_2TeCl_2$.[11]
(37) Knobler, C.; McCullough, J. D. *Inorg. Chem.* **1977**, *16*, 612.
(38) The tellurium catecholate, $Te(C_6H_4O_2)_2$, has a ψ-tbp structure (Lindqvist, O. *Acta Chem. Scand.* **1967**, *21*, 1473) as does $Te(C_6H_{12}O_2)_2$ (Day, R. O.; Holmes, R. R. *Inorg. Chem.* **1981**, *20*, 3071).

Table I. Positional ($\times 10^4$) and Thermal Parameters for Atoms in $(C_6H_5)_4Te \cdot {}^1/_8(C_6H_6)$

atom	x	y	z	B, Å²	atom	x	y	z	B, Å²
Te1	2172 (1)	4014 (0)	2755 (1)	3.416 (2)	C313	5828 (10)	6926 (7)	1175 (12)	6.69 (4)
Te2	1055 (1)	6095 (0)	6663 (1)	3.454 (3)	C314	5496 (9)	6470 (7)	359 (11)	5.70 (3)
Te3	3795 (1)	8442 (0)	1505 (1)	4.278 (2)	C315	4687 (10)	6568 (7)	−183 (11)	5.96 (3)
Te4	3046 (1)	645 (0)	5845 (1)	4.154 (2)	C316	4203 (8)	7137 (6)	105 (10)	4.61 (3)
C111	3052 (8)	4759 (5)	2606 (9)	3.80 (2)	C321	2384 (8)	8250 (6)	1667 (9)	4.04 (2)
C112	2751 (9)	5363 (6)	2960 (10)	5.02 (3)	C322	1965 (8)	7690 (6)	1171 (9)	4.63 (3)
C113	3304 (10)	5880 (7)	2821 (12)	6.81 (4)	C323	1022 (9)	7607 (6)	1303 (10)	4.87 (3)
C114	4117 (10)	5777 (7)	2328 (11)	6.35 (3)	C324	523 (9)	8068 (6)	1931 (10)	5.36 (3)
C115	4427 (10)	5159 (7)	1990 (11)	6.60 (4)	C325	953 (10)	8630 (7)	2443 (11)	6.03 (3)
C116	3900 (9)	4626 (7)	2129 (11)	5.89 (3)	C326	1896 (9)	8730 (6)	2305 (10)	4.83 (3)
C121	2950 (7)	3170 (5)	2645 (8)	3.46 (2)	C331	3436 (8)	8479 (6)	−205 (9)	4.56 (3)
C122	3486 (8)	2950 (5)	1792 (9)	3.94 (3)	C332	2580 (9)	8398 (6)	−709 (11)	5.73 (3)
C123	3981 (8)	2379 (6)	1725 (9)	4.65 (3)	C333	2426 (10)	8552 (7)	−1706 (11)	6.12 (3)
C124	3893 (9)	2031 (6)	2519 (10)	5.06 (3)	C334	3141 (10)	8785 (7)	−2160 (11)	6.40 (3)
C125	3342 (9)	2252 (6)	3363 (10)	5.44 (3)	C335	4010 (10)	8866 (7)	−1675 (11)	6.18 (3)
C126	2888 (8)	2834 (6)	3437 (9)	4.69 (3)	C336	4165 (10)	8723 (7)	−667 (11)	5.95 (3)
C131	2027 (8)	3777 (5)	959 (9)	3.99 (3)	C341	3982 (8)	8212 (6)	3110 (10)	4.95 (3)
C132	1622 (9)	3185 (6)	540 (11)	5.59 (3)	C342	3651 (10)	7680 (7)	3408 (12)	7.25 (4)
C133	1392 (10)	3068 (7)	−576 (12)	6.69 (4)	C343	3773 (11)	7583 (8)	4432 (13)	7.89 (4)
C134	1539 (10)	3501 (7)	−1157 (12)	6.36 (4)	C344	4235 (10)	8030 (8)	5186 (12)	6.99 (4)
C135	1902 (10)	4075 (7)	−729 (12)	6.43 (4)	C345	4545 (10)	8560 (7)	4914 (12)	6.83 (4)
C136	2170 (8)	4222 (6)	357 (10)	4.81 (3)	C346	4438 (9)	8666 (6)	3870 (11)	5.65 (3)
C141	2636 (8)	4227 (5)	4461 (9)	4.13 (3)	C411	2349 (8)	1532 (6)	5874 (9)	4.21 (3)
C142	3564 (9)	4270 (6)	4810 (10)	5.07 (3)	C412	2921 (8)	2050 (6)	6009 (10)	4.98 (3)
C143	3815 (10)	4393 (7)	5907 (12)	6.24 (4)	C413	2451 (10)	2655 (7)	6059 (11)	5.99 (3)
C144	3105 (10)	4447 (7)	6607 (11)	6.09 (3)	C414	1519 (10)	2680 (7)	5992 (11)	6.06 (4)
C145	2189 (10)	4414 (6)	6295 (11)	6.26 (3)	C415	982 (10)	2149 (7)	5864 (11)	6.00 (3)
C146	1953 (8)	4305 (6)	5195 (10)	4.56 (3)	C416	1409 (9)	1547 (6)	5805 (10)	5.26 (3)
C211	2459 (7)	6342 (5)	6588 (8)	3.70 (2)	C422	1400 (8)	0 (6)	6617 (9)	5.64 (3)
C212	2978 (8)	5953 (6)	5886 (9)	4.51 (3)	C423	804 (9)	−514 (6)	6658 (10)	7.42 (3)
C213	3933 (10)	6090 (7)	5815 (11)	6.04 (3)	C424	916 (11)	−1068 (8)	5940 (12)	7.06 (4)
C214	4304 (8)	6634 (6)	6470 (10)	4.90 (3)	C425	1587 (10)	−1153 (7)	5227 (12)	6.76 (4)
C215	3745 (8)	7029 (6)	7174 (10)	4.96 (3)	C426	2184 (10)	−644 (7)	5169 (12)	5.75 (4)
C216	2814 (8)	6877 (6)	7232 (9)	4.59 (3)	C421	2069 (9)	−74 (7)	5877 (11)	4.51 (3)
C221	376 (8)	6968 (5)	7265 (9)	3.81 (2)	C431	3000 (8)	879 (6)	7610 (10)	4.97 (3)
C222	574 (8)	7301 (6)	8270 (9)	4.44 (3)	C432	3529 (10)	458 (7)	8051 (11)	6.45 (3)
C223	116 (9)	7865 (6)	8654 (10)	5.05 (3)	C433	3589 (11)	554 (8)	9199 (13)	7.79 (4)
C224	−530 (9)	8108 (6)	8017 (11)	5.68 (3)	C434	3153 (11)	1072 (8)	9800 (12)	7.08 (4)
C225	−720 (9)	7771 (6)	7011 (10)	5.10 (3)	C435	2681 (11)	1506 (8)	9355 (13)	8.08 (4)
C226	−269 (8)	7205 (6)	6601 (9)	4.42 (3)	C436	2586 (9)	1409 (6)	8227 (11)	5.75 (3)
C231	1355 (8)	6002 (5)	8355 (9)	4.01 (3)	C441	2778 (9)	463 (6)	4068 (10)	4.92 (3)
C232	566 (9)	5859 (6)	8846 (10)	5.48 (3)	C442	1946 (10)	504 (7)	3560 (12)	6.71 (4)
C233	631 (10)	5744 (7)	9878 (11)	6.05 (3)	C443	1865 (11)	391 (7)	2418 (13)	7.82 (4)
C234	1482 (10)	5755 (6)	10364 (11)	5.75 (3)	C444	2685 (12)	271 (8)	1942 (13)	7.50 (4)
C235	2263 (9)	5874 (6)	9885 (11)	5.70 (3)	C445	3500 (11)	216 (7)	2390 (12)	7.27 (4)
C236	2207 (8)	5993 (6)	8853 (10)	4.79 (3)	C446	3589 (10)	313 (7)	3523 (11)	6.14 (3)
C241	907 (8)	6326 (5)	5028 (9)	3.99 (3)	C1	−887 (12)	39 (9)	390 (14)	8.79 (5)
C242	1279 (9)	6848 (6)	4742 (10)	5.22 (3)	C2	−289 (13)	−457 (9)	524 (13)	8.59 (4)
C243	1171 (9)	6924 (7)	3688 (11)	6.34 (3)	C3	587 (13)	−490 (9)	158 (14)	8.94 (5)
C244	705 (10)	6465 (7)	2975 (11)	6.08 (3)					
C245	357 (9)	5932 (7)	3220 (11)	5.66 (3)					
C246	463 (8)	5863 (6)	4286 (9)	4.55 (3)					
C311	4515 (8)	7588 (6)	964 (9)	4.69 (3)					
C312	5331 (10)	7495 (7)	1517 (11)	6.62 (4)					

compounds increases in the series alkyl, phenyl, pentafluorophenyl, and 2,2′-biphenylylene, with the solid tetraalkyl- or dialkyldiaryl telluriums not yet isolated.[4] Tetraphenyltellurium decomposes just above 100 °C while the latter two decompose above 200 °C.[4] Similarly, the R_nTeX_{4-n} (n = 2, 4) compounds show greater thermal stability than the analogous selenium compounds where M is less electropositive, although in this case both steric and electronic factors may be important. To our knowledge, no R_4Se compounds have been prepared. If the solid-state geometry of $(C_6H_5)_4Te$ makes any contribution to the structure of the molecule in solution, the axial elongation might facilitate intramolecular and intermolecular processes. Recent solution studies of some organotellurium compounds show that $(C_6H_5)_4Te$ appears to decompose by an intramolecular process[3] and that several ψ-tbp tetraalkoxytellurium compounds undergo both intramolecular and intermolecular ligand reorganization.[40]

The four independent molecules in $(C_6H_5)_4Te$ are separated by normal van der Waals distances. The intermolecular Te–C (aromatic) distances fall between those observed in dibenzotellurophene[41] and those in trimethyltelluronium tetraphenylborate.[14] The Te–C (aromatic) intermolecular distances less than 4.0 Å are Te3–C445 [x, $1 - y$, z] at 3.80 (1) Å, Te2–C145 at 3.93 (1) Å and Te4–C346 [x, $y - 1$, z] at 3.94 (1) Å. These contacts are in the general direction of one of the two vacant octahedral sites around tellurium and involve conformationally, nearly the same carbon atom (n45 meta or 346 ortho) on the three

(39) See, for example: Zingaro, R. A.; Cooper, W. C. "Selenium"; Van Nostrand: New York, 1974. Klayman, D. L.; Gunther, W. H. H. "Organic Selenium Compounds: Their Chemistry and Biology", Wiley-Interscience: New York, 1973.

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Table II. Interatomic Distances (Å) and Angles (Deg)[44]

Distances[a]			
Te1-Te2′	4.803 (2)	Te3-C321	2.13 (1)
Te3-Te4′	5.757 (3)	Te3-C331	2.27 (1)
Te1-C111	2.12 (1)	Te3-C341	2.30 (1)
Te1-C121	2.12 (1)	Te4-C411	2.13 (1)
Te1-C131	2.27 (1)	Te4-C421	2.16 (1)
Te1-C141	2.31 (1)	Te4-C431	2.27 (1)
Te2-C211	2.13 (1)	Te4-C441	2.30 (1)
Te2-C221	2.14 (1)	C1-C2	1.41 (3)
Te2-C231	2.30 (1)	C2-C3	1.38 (3)
Te2-C241	2.31 (1)	C3-C1′	1.41 (3)
Te3-C311	2.12 (1)		
Angles			
C111-Te1-C121	109.4 (4)	C311-Te3-C321	110.0 (4)
C131-Te1-C141	167.9 (4)	C341-Te3-C331	167.9 (4)
C111-Te1-C131	87.1 (4)	C311-Te3-C331	88.2 (4)
C121-Te1-C131	87.2 (4)	C321-Te3-C331	87.9 (4)
C111-Te1-C141	85.9 (4)	C311-Te3-C341	85.8 (5)
C121-Te1-C141	85.8 (4)	C321-Te3-C341	84.2 (4)
C211-Te2-C221	104.8 (4)	C411-Te4-C421	110.0 (4)
C231-Te2-C241	170.8 (4)	C441-Te4-C431	168.3 (4)
C211-Te2-C231	88.5 (4)	C411-Te4-C431	86.5 (4)
C221-Te2-C231	87.7 (4)	C421-Te4-C431	86.8 (5)
C211-Te2-C241	84.4 (4)	C411-Te4-C441	85.6 (4)
C221-Te2-C241	88.5 (4)	C421-Te4-C441	87.8 (5)

[a] Primes indicate symmetry-related atoms.

different molecules. The contacts in the indium and gallium phenyls similarly involve either ortho or meta carbons,[13] but in the present case distances are not less than the van der Waals sums which are 3.76 Å after Bondi[42] and 3.90 Å after Pauling,[28c] using 1.70 Å for the half-thickness of an aromatic molecule[28c] in both sums. No evidence is seen for a π donor–acceptor interaction as observed in $(C_6H_5)_3SeNCS$.[43] Thus, tellurium in $(C_6H_5)_4Te$ appears to have a genuine fourfold configuration devoid of secondary bonding as defined by Alcock.[8] As in the case of $(CH_3)_3TeB(C_6H_5)_4$,[14] it is not clear whether the absence of secondary bonding is due to electronic or steric constraints or to a combination of the two. The Te···C contacts in the present case appear to be favored electrostatically and are taken as an indication of packing efficiency in the structure. We note that, within the limits of a error, the volume observed for $(C_6H_5)_4Te$ is exactly four-thirds that of the $(C_6H_5)_3Te^+$ ion as calculated from the unit-cell volume of $(C_6H_5)_3TeCl$.[29] An examination of the dihedral angles between the planes of the phenyl rings[44] of the independent molecules revealed no trends in the orientations of the rings which are assumed to be governed by the packing forces.

A stereoscopic drawing of the unit cell appears in Figure 2. The molecules pack with the C–Te–C axis in the general direction of the crystallographic *c* axis and the equatorial plane in the general direction of the *ab* plane. The closest Te–Te approach is 4.803 (1) Å. The benzene of crystallization appears normal[45] and is located at the cell origin. The presence or absence of solvent is expected to have little or no effect on the molecular geometry of $(C_6H_5)_4Te$. This is in contrast to the effect of solvent on the structures of the R_3TeX compounds.[7]

Registry No. $(C_6H_5)_4Te\cdot{}^1/_8(C_6H_6)$, 79768-49-3.

Supplementary Material Available: A listing of the observed and calculated structure factors and tables of the hydrogen atom positional and thermal parameters and of the least-squares planes of the phenyl rings (51 pages). Ordering information is given on any current masthead page.

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(44) The 16 independent phenyl rings appear normal. The mean value and its estimated variance[23] for the 96 C–C distances is 1.40 (0) Å and for the 96 C–C–C angles is 120 (0)°. The least-squares planes of the 16 rings and the average atom deviation for each plane are given as supplementary material. The rings are planar with the largest average atom deviation being 0.029 Å for the C11*n* (*n* = 1–6) plane. The C–C distances range from 1.32 (2) to 1.47 (2) Å and the C–C–C angles from 114 (1) to 127 (2)°.
(45) The average of the three independent C–C distances is 1.40 Å and that of the three angles is 120°.