CONTRIBUTION NO. 3006 FROM THE DEPARTMENT OF CHEMISTRY,
UNIVERSITY OF CALIFORNIA, LOS ANGELES, CALIFORNIA 90024

Crystal and Molecular Structure of 1-Thia-4-telluracyclohexane 4,4-Dibromide, $C_4H_8STeBr_2$

BY CAROLYN KNOBLER AND J. D. McCULLOUGH*

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The structure of 1-thia-4-telluracyclohexane 4,4-dibromide, $C_4H_8STeBr_2$, has been determined from three-dimensional X-ray data collected on an automated diffractometer with Mo Kα radiation. The space group is $P2_1/c$ with four molecules in the unit cell for which $a = 11.898$ (1) Å, $b = 6.672$ (1) Å, $c = 12.256$ (2) Å, and $\beta = 112.68$ (1)°. The measured density is 2.76 g cm^{-3} and that calculated from the X-ray data is 2.779 (2) g cm^{-3}. Least-squares refinement based on 1468 observed reflections led to a final value of the conventional R index of 5.4%. The molecule approximates mirror symmetry with the six-membered ring in the chair form. The bonding about tellurium is octahedral. There are two Te–C bonds with distances of 2.14 (1) and 2.16 (1) Å which make a C–Te–C angle of 99.4 (6)°. Approximately perpendicular to the C–Te–C plane, tellurium forms axial bonds to bromine atoms at 2.657 (2) and 2.689 (2) Å with a Br–Te–Br angle of 176.63 (6)°. The octahedron about tellurium is completed through weak intermolecular bonding with a bromine atom in a neighboring molecule at 3.591 (2) Å and with a sulfur atom in a third molecule at 3.588 (4) Å. These weakly bonded atoms make bond angles with opposing carbon atoms of 172.4 (4)° for C(2)–Te···Br(2)′ and 170.2 (4)° for C(3)–Te···S″. Except for three angles involving the sulfur atom, the remaining bond angles about tellurium are within 6° of the ideal 90° value. Observed distances and angles within the six-membered ring are as follows: S–C, 1.79 (1), 1.81 (1) Å; C–C, 1.52 (2), 1.53 (2) Å; C–H(av), 0.93 (20) Å; C–S–C, 100.6 (7)°; S–C–C, 114 (1), 116 (1)°; Te–C–C, 115 (1), 117 (1)°.

Introduction

One of the interesting features of the structures of organoselenium and organotellurium dihalides in the solid state is the intermolecular bonding involving the heavy atoms. Tendencies toward this type of bonding increase, as one would expect, with the atomic numbers of the atoms involved. Thus, in general, intermolecular bonding is more pronounced in tellurium compounds than in those of selenium and decreases as one goes from iodides to bromides to chlorides with a given chalcogen. These effects are usually of sufficient importance to override the normal tendency toward isomorphism of closely related compounds; thus only a few isomorphous pairs have been noted to date. An exception to this trend is the pair 1-thia-4-selenacyclohexane 4,4-dibromide ($C_4H_8SSeBr_2$) and the corresponding tellurium compound, $C_4H_8STeBr_2$. The structure of the selenium compound has been reported earlier.[1] The structure of the tellurium compound was undertaken in order to make a detailed comparison of the secondary (intermolecular) bonding tendencies of the two chalcogens under closely similar circumstances.

Experimental Section

Crystals of 1-thia-4-telluracyclohexane 4,4-dibromide were prepared as previously reported[2] and specimens suitable for the X-ray studies were grown from ethylene chloride. The crystals are small, well-formed, pale yellow prisms, slightly elongated on the b axis of the monoclinic unit. Preliminary precession and Weissenberg photographs showed systematic absences for $0k0$ with k odd and for $h0l$ with l odd, which are characteristic of the space group $P2_1/c$. The pronounced similarities of these photographs with those of 1-thia-4-selenacyclohexane 4,4-dibromide strongly suggested an isomorphous relationship. The crystal selected for data collection was 0.05 × 0.12 × 0.07 nm along the a, b, and c axes, respectively. It was aligned on a Picker FACS-1 four-circle automatic diffractometer with the crystallographic b axis collinear with φ. A set of lattice parameters was calculated by a least-squares refinement of the angles obtained at 22° from the centering of 44 reflections in the 2θ range from 18 to 54°. The results, based on Mo Kα radiation (λ 0.71069 Å), are $a = 11.898$ (1) Å, $b = 6.672$ (1) Å, $c = 12.256$ (2) Å, and $\beta = 112.68$ (1)°. The density observed by flotation is 2.76 g cm^{-3}; that calculated from the X-ray data with $Z = 4$ is 2.779 (2) g cm^{-3}.

The intensity data were collected by use of the θ–2θ scan procedure with Mo Kα radiation in conjunction with a graphite crystal monochromator set at a 2θ angle of 12.066°. The X-ray takeoff angle was 2.6° and the pulse height analyzer was set at a 95% window for Mo Kα radiation. The scan rate was 1°/min with a scan range from 0.60° below the Kα_1 peak to 0.60° above the Kα_2 peak. Background counts (10 sec) were taken at each end of the scan range. The automatic attenuator mechanism was set to keep the count rate below 10,000 counts/sec. The intensities of three standard reflections (040, 700, and 670) were measured every 50 reflections and these showed no appreciable drift or significant fluctuations with time. The absorption coefficient (μ = 130 cm^{-1}) and the crystal dimensions indicated values of μR in the range from ~0.33 to ~0.45 and transmission factors in the range ~0.58 to ~0.47. It was estimated that the neglect of absorption effects could have produced errors in the relative F_o values of no more than ~5% in the extreme cases; no corrections for absorption were made. The data reduction and processing were accomplished by use of UCFACS[3] as modified by J. D. Bell and M. R. Murphy to suit local conditions. This program checks for errors, corrects for background and Lorentz and polarization effects, and calculates intensities, structure factors, and their standard deviations according to the equations

$$I = C_s + 4.5 - (t_s/2t_b)(B_1 + B_2 + 9)$$

$$\sigma(I) = [C_s + 9 + (t_s/2t_b)^2(B_1 + B_2 + 18) + (0.04I)^2]^{1/2}$$

$$F_o = k[I/(Lp)]^{1/2}$$

$$\sigma(F_o) = (k/2)[\sigma(I)/I(Lp)]^{1/2}$$

C_s is the total scan count, B_1 and B_2 are the individual background counts, t_s is the scan time (sec), and t_b is the time (10 sec) each background is counted.

The intensities of a total of 2504 reflections were measured. These included 180 space group abscences, 96 duplicate $0kl$, $0k\bar{l}$ pairs, and 150 periodic checks of the standard reflections. The resulting 2078 unique reflections represent all of those accessible within the range $2\theta \leq 55°$ for Mo Kα radiation or all for which $(\sin\theta)/\lambda \leq 0.650$ Å^{-1}. Among these, 610 reflections had values of $F_o \leq 1.95\sigma F_o$ and were considered to be unobserved. The number of unique, observed reflections was thus 1468. An analysis of the F_o values of the 70 observed pairs of equivalent

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(1) L. Battelle, C. Knobler, and J. D. McCullough, *Inorg. Chem.*, **6**, 958 (1967).

(2) J. D. McCullough, *ibid.*, **4**, 862 (1965).

(3) E. N. Duesler and K. N. Raymond, *ibid.*, **10**, 1486 (1971).

$0kl$ reflections showed an average deviation of 1.1% from their respective mean values and a maximum deviation of 3.2%.

Determination and Refinement of the Structure

A satisfactory trial structure was obtained by the application of heavy-atom methods to Patterson and Fourier summations.[4] Refinement was carried out by the use of full-matrix least-squares procedures with anomalous dispersion corrections ($\Delta f'$ and $\Delta f''$) applied to the structure factors for Te, Br, and S. Near the end of the refinement, with anisotropic temperature factors on all nonhydrogen atoms, the value of R converged to 0.056. At this point a difference Fourier summation was prepared for possible location of the hydrogen atoms; also a set of hydrogen positions was calculated by use of HPOSN. The calculated positions of five of the hydrogen atoms agreed well with maxima on the difference Fourier, two agreed fairly well, and one, H(3B), did not show on the Fourier. Three more cycles of least-squares were then computed in which the positional (but not the thermal) parameters of the eight hydrogen atoms were allowed to vary, along with the positional and anisotropic thermal parameters of the eight heavier atoms. In these cycles, the hydrogen atoms were assigned fixed isotropic thermal parameters of 4.0 Å^2. The value of R decreased slightly to 0.054. A set of structure factors[5] for all measured reflections was calculated on the basis of the final positional and thermal parameters given in Tables I and II. The atomic scattering factors used for Te were based on the averages of the Sb^0 and I^0 values of Doyle and Turner,[6] those for Br and S were the neutral atom values given in Table 3.3.1A of ref 7, the diamond values of McWeeny[8] were used for carbon, and the factors for hydrogen were from Stewart, Davidson, and Simpson.[9] The real and imaginary anomalous dispersion corrections given for Mo Kα radiation in Table 3.3.2C of ref 7 were applied to the scattering factors for Te, Br, and S. An analysis of the values of $||F_o| - |F_c||$ for the 610 "unobserved" reflections showed 90.0% to be less than $\sigma(F_o)$, 7.7% between $\sigma(F_o)$ and $2\sigma(F_o)$, 2.1% between $2\sigma(F_o)$ and $3\sigma(F_o)$, and none greater than $3.4\sigma(F_o)$. In the final least-squares cycle, the largest shift of a parameter for a nonhydrogen atom was 0.02σ for positional parameters and 0.05σ for thermal parameters. The average shift in the 24 positional parameters of the hydrogen atoms was 0.4σ with two showing shifts slightly larger than σ. The final "goodness of fit," defined as $[\Sigma w(|F_o| - |F_c|)^2/(N_o - N_v)]^{1/2}$, was 1.48. In this expression, N_o = 1468, the number of observed reflections, and N_v = 97, the number of variable parameters.

TABLE I

ATOMIC POSITIONAL PARAMETERS IN $C_4H_8STeBr_2$

Atom	x	y	z
Te	0.28937 (7)[a]	0.38205 (13)	0.19695 (7)
Br(1)	0.1404 (1)	0.6761 (2)	0.0815 (1)
Br(2)	0.4437 (1)	0.0974 (2)	0.3254 (1)
S	0.1572 (3)	0.3855 (6)	0.4228 (3)
C(1)	0.1465 (12)	0.1672 (21)	0.3309 (11)
C(2)	0.1403 (11)	0.2165 (21)	0.2076 (11)
C(3)	0.3373 (12)	0.5588 (21)	0.3561 (12)
C(4)	0.3119 (12)	0.4587 (24)	0.4568 (13)
H(1A)[b]	0.072 (9)	0.147 (18)	0.272 (10)
H(1B)	0.211 (10)	0.052 (19)	0.369 (9)
H(2A)	0.062 (10)	0.300 (19)	0.156 (10)
H(2B)	0.142 (10)	0.159 (18)	0.166 (10)
H(3A)	0.269 (10)	0.696 (19)	0.314 (10)
H(3B)	0.398 (10)	0.543 (18)	0.360 (10)
H(4A)	0.368 (10)	0.350 (18)	0.463 (10)
H(4B)	0.326 (10)	0.513 (19)	0.526 (9)

[a] The numbers given in parentheses here and in succeeding tables are the estimated standard deviations in the least significant digits. [b] Hydrogen atoms are numbered to correspond to the carbon atoms to which they are bonded.

TABLE II

ATOMIC THERMAL PARAMETERS IN $C_4H_8STeBr_2$[a]

Atom	β_{11}	β_{22}	β_{33}	β_{12}	β_{13}	β_{23}
Te	048 (1)	113 (1)	058 (1)	−007 (2)	059 (1)	009 (2)
Br(1)	080 (1)	148 (3)	088 (1)	006 (3)	034 (2)	051 (3)
Br(2)	081 (1)	207 (4)	131 (1)	107 (3)	108 (2)	087 (4)
S	061 (2)	232 (9)	068 (2)	−028 (8)	069 (3)	−065 (8)
C(1)	080 (10)	172 (33)	045 (9)	−006 (33)	040 (14)	−005 (30)
C(2)	060 (8)	157 (31)	067 (9)	−031 (29)	073 (12)	−014 (30)
C(3)	072 (10)	135 (29)	062 (9)	−062 (29)	047 (10)	−052 (29)
C(4)	063 (10)	188 (35)	092 (12)	−059 (33)	053 (16)	−007 (37)

[a] All parameters have been multiplied by 10^4. The anisotropic temperature factor expression is of the form: $\exp[-(\beta_{11}h^2 + \beta_{22}k^2 + \beta_{33}l^2 + \beta_{12}hk + \beta_{13}hl + \beta_{23}kl)]$. The hydrogen atoms were assigned fixed isotropic thermal parameters of 4.0 Å^2.

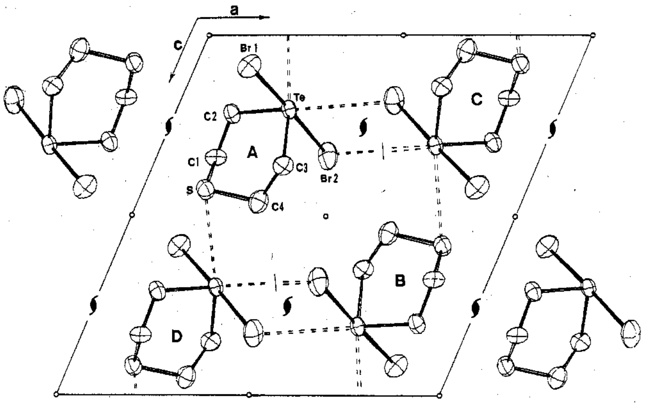

Figure 1.—View of the structure of $C_4H_8STeBr_2$ down the b axis. Coordinates of positions: A = x, y, z; B = $1 - x, 1 - y, 1 - z$; C = $1 - x, {}^1/_2 + y, {}^1/_2 - z$; D = $x, {}^1/_2 - y, {}^1/_2 + z$.

Description and Discussion of the Structure

A view of the crystal structure of $C_4H_8STeBr_2$ down the b axis is shown in Figure 1 and views of the molecule and of the coordination about tellurium are shown in Figures 2 and 3, respectively. Ideally, the free $C_4H_8STeBr_2$ molecule would probably have mirror symmetry. In the crystal, small deviations from this symmetry are observed which are presumed to be the result of intermolecular "secondary" bonds which tellurium forms in accordance with its tendency toward octahedral coordination. The result is a bonding arrangement about tellurium of some interest. There are two normal bonds to carbon atoms with observed distances of 2.14 (1) and 2.16 (1) Å. The angle between these bonds is 99.4 (6)°. Two axial bonds (approximately perpendicular to the C–Te–C plane) are formed with bromine atoms at 2.657 (2) and 2.689 (2) Å, and these

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(4) Fourier summations were computed by use of UCLAFOUR written by Gantzel and Hope and the least-squares refinement was carried out by using CADLS, the centric, anomalous dispersion modification (by Hope and Frank) of the full-matrix program UCLALS4 by Gantzel, Sparks, Long, and Trueblood. This program minimizes $\Sigma w(kF_o - |F_c|)^2$, where k is a scale factor. The weights, w, were taken as $1/\sigma^2(F_o)$. The esd values for the atomic parameters were obtained from the final least-squares inverse matrix and those for bond distances and angles were derived by use of a modification of ORFFE by Busing, Martin, and Levy. Thermal ellipsoid plots were prepared by use of Johnson's ORTEP and tentative hydrogen positions were computed by use of HPOSN by Hope. The C–H distances were taken initially as 1.0 Å and the H–C–H angles as 109.5°. The index, R, was defined as $\Sigma||F_o| - |F_c||/\Sigma|F_o|$.

(5) A listing of structure factor amplitudes for the observed reflections will appear immediately following these pages in the microfilm edition of this volume of the journal. Single copies may be obtained from the Business Operations Office, Books and Journals Division, American Chemical Society, 1155 Sixteenth Street, N.W., Washington, D. C. 20036, by referring to code number INORG-72-3026. Remit check or money order for $3.00 for photocopy or $2.00 for microfiche.

(6) P. A. Doyle and P. S. Turner, *Acta Crystallogr., Sect. A*, **24**, 392 (1968).

(7) "International Tables for X-Ray Crystallography," Vol. III, Kynoch Press, Birmingham, England, 1962.

(8) R. McWeeny, *Acta Crystallogr.*, **7**, 180 (1954).

(9) R. F. Stewart, E. R. Davidson, and W. T. Simpson, *J. Chem. Phys.*, **42**, 3175 (1965).

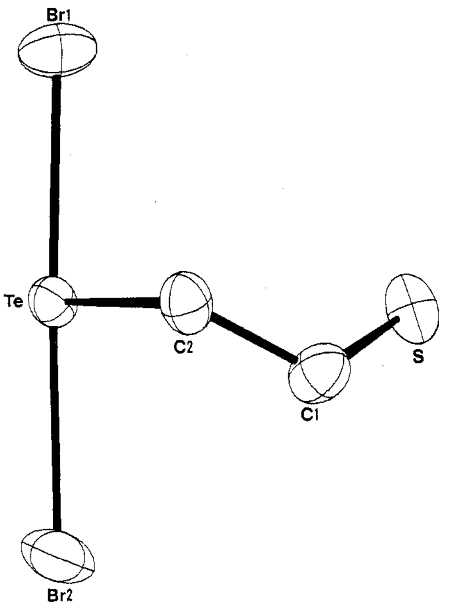

Figure 2.—View of the $C_4H_8STeBr_2$ molecule normal to the approximate mirror of symmetry. The eclipsed carbon atoms C(3) and C(4) are omitted for clarity.

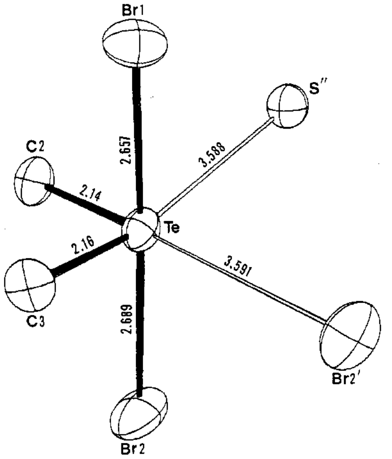

Figure 3.—View of the coordination about tellurium. A complete listing of the angles involved is given in Table III.

make an angle of 176.63 (6)° with each other. The octahedron is completed through intermolecular bonding of Te with a Br(2) atom in a neighboring molecule at 3.591 (2) Å and a sulfur atom in a third molecule at 3.588 (4) Å. For comparison, the sums of the van der Waals radii are 4.15 Å for Te + Br and 4.05 Å for Te + S. The bond angles which these secondary bonded atoms make with opposing carbon atoms are C(2)–Te···Br(2)′ = 172.4° and C(3)–Te···S″ = 170.2°. Except for three angles involving the sulfur atom, the remaining bond angles about tellurium are within 6° of the ideal 90° value. A complete listing of the bond distances and bond angles about tellurium is given in Table III, which also includes the corresponding observations on the selenium atom in $C_4H_8SSeBr_2$ for comparison. As observed in all other $R_2(Se,Te)X_2$ compounds which have been studied, the axial chalcogen–halogen bonds are somewhat longer (0.15 and 0.18 Å in the present case) than the sum of the normal, single-bond radii (2.51 Å for Te–Br)[10] and correspond to a bond order of $\sim {}^1/_2$.

TABLE III

DISTANCES AND ANGLES ABOUT TELLURIUM IN $C_4H_8STeBr_2$ COMPARED WITH THOSE ABOUT SELENIUM IN $C_4H_8SSeBr_2$

Atoms[a]	$C_4H_8STeBr_2$	$C_4H_8SSeBr_2$[b]
	Distances, Å	
(VI)–C(2)	2.14 (1)	2.01 (3)
(VI)–C(3)	2.16 (1)	2.02 (3)
(VI)–Br(1)	2.657 (2)	2.545 (6)
(VI)–Br(2)	2.689 (2)	2.548 (6)
(VI)···Br(2)′	3.591 (2)	3.567 (4)
(VI)···S″	3.588 (4)	3.629 (7)
	Angles, Deg	
C(2)–(VI)–C(3)	99.4 (6)	105 (1)
C(2)–(VI)–Br(1)	90.9 (3)	93.1 (7)
C(2)–(VI)–Br(2)	89.7 (3)	91.3 (7)
C(3)–(VI)–Br(1)	88.1 (3)	89.2 (7)
C(3)–(VI)–Br(2)	88.5 (3)	91.7 (7)
Br(1)–(VI)–Br(2)	176.63 (6)	175.1 (1)
C(2)–(VI)···Br(2)′	172.4 (4)	169.3 (7)
C(2)–(VI)···S″	74.1 (4)	71.7 (7)
C(3)–(VI)···Br(2)′	85.2 (4)	84.4 (8)
C(3)–(VI)···S″	170.2 (4)	170.1 (6)
Br(1)–(VI)···Br(2)′	95.28 (5)	91.4 (2)
Br(1)–(VI)···S″	84.68 (7)	81.6 (2)
Br(2)–(VI)···Br(2)′	84.43 (4)	83.9 (1)
Br(2)–(VI)···S″	98.68 (8)	97.8 (2)
Br(2)′···(VI)···S″	102.04 (8)	99.4 (1)

[a] Definition of symbols: (VI) represents Te or Se as required; Br(2)′ represents Br(2)(C,000), *i.e.*, the Br(2) atom in symmetry position C of the origin cell; S″ represents S(D,00$\bar{1}$), *i.e.*, the S atom in symmetry position D in the cell located one unit in the negative direction along the *c* axis; unprimed atom symbols represent atoms in symmetry position A of the origin cell; and (VI)···S″ represents a weak or secondary bond between the indicated atoms. The symmetry positions A, B, C, and D are defined in Figure 1. [b] Distances, angles, and esd values in the selenium compound were recalculated by use of ORFFE.

TABLE IV

DISTANCES AND ANGLES ABOUT S AND Br(2)[a] IN $C_4H_8STeBr_2$ COMPARED WITH THOSE IN $C_4H_8SSeBr_2$

Atoms[b]	$C_4H_8STeBr_2$	$C_4H_8SSeBr_2$
	Distances, Å	
S–C(1)	1.81 (1)	1.83 (3)
S–C(4)	1.79 (1)	1.79 (3)
S···(VI)′	3.588 (4)	3.629 (7)
Br(2)–(VI)	2.689 (2)	2.545 (6)
Br(2)···(VI)″	3.591 (2)	3.567 (5)
	Angles, Deg	
C(1)–S–C(4)	100.6 (7)	97 (1)
C(1)–S···(VI)′	94.7 (4)	97.0 (8)
C(4)–S···(VI)′	83.0 (5)	82.0 (8)
(VI)–Br(2)···(VI)″	131.47 (7)	132.7 (1)

[a] Br(1) is not involved in secondary bonding. [b] (VI)′ represents (VI)(D,000) and (VI)″ represents (VI)(C,0$\bar{1}$0). See footnote *a* in Table III for meaning of symbols.

The intermolecular bonding system is shown by means of dotted lines in Figure 1. The Te···Br(2)′ bonds spiral down 2_1 screw axes parallel to the *b* axis and these helices are bonded together by Te···S″ bonds in the general direction of the *c* axis. The result is a system of sheets two molecules thick in the direction of the *a* axis and of infinite extent along *b* and *c*. Although the secondary bonds are very weak (bond orders from ~0.005 to ~0.02), it is clear that they are strong enough to be a determining factor in the crystal structure and that they are somewhat stronger in the tellurium compound than they are in $C_4H_8SSeBr_2$. In fact, the Te···S distance is actually 0.04 Å shorter than the Se···S distance and the Te···Br(2) distance

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[10] L. Pauling, "The Nature of the Chemical Bond," 3rd ed, Cornell University Press, Ithaca, N. Y., 1960, p 224.

is only 0.025 Å longer than the Se···Br(2) distance, even though the Te radius is 0.20 Å larger than that of Se. In the formation of the secondary bonds, the configuration about sulfur also follows a normal pattern, that of a trigonal pyramid, as shown in Table IV. In contrast, however, the angle of 131.47° observed at Br(2) is somewhat removed from the angles of ~90 or ~180° usually found at central atoms in polyhalide ions.

In comparing the tellurium and selenium compounds, another item is of interest, namely, the orientation of the Br–(VI)–Br angle with respect to the ring system. In the selenium compound, the bromine atoms are bent away from C(2) and C(3) as shown by the four C–Se–Br angles (Table III), which average 91.3°. In contrast, the four C–Te–Br angles average 89.3°, indicating that the bromine atoms in the tellurium compound are bent slightly toward the carbon atoms. The reason for this difference may be found in the intramolecular Br–C distances given in Table V. If one assumes a trigonal-bipyramidal configuration about the chalcogen atom in the free, uncrowded molecule, the normal tendency would probably be for the bromine atoms to be bent toward the carbon atoms because of repulsion by the unshared electron pair on the chalcogen. However, due to shorter Se–Br and Se–C distances (as compared to their tellurium counterparts), crowding results in the selenium compound and the bromine atoms are pushed out. In the tellurium compound, the intramolecular, nonbonded Br–C separations are enough larger to permit the lone-pair repulsion to be effective.

TABLE V
SOME NONBONDED DISTANCES IN $C_4H_8STeBr_2$ COMPARED WITH THOSE IN $C_4H_8SSeBr_2$

Atoms[a]	$C_4H_8STeBr_2$	$C_4H_8SSeBr_2$
	Intramolecular Distances, Å	
Br(1)–C(2)	3.43 (1)	3.33 (3)
Br(1)–C(3)	3.37 (1)	3.23 (3)
Br(2)–C(2)	3.42 (1)	3.28 (3)
Br(2)–C(3)	3.40 (1)	3.30 (3)
Br(2)–C(1)	3.59 (1)	3.48 (3)
Br(2)–C(4)	3.58 (1)	3.45 (3)
(VI)–S	3.673 (4)	3.529 (7)
	Intermolecular Distances, Å	
(VI)–Br(2)(C,000)	3.591 (2)	3.567 (4)
(VI)–S(D,00$\bar{1}$)	3.588 (4)	3.629 (7)
(VI)–C(4)(D,00$\bar{1}$)	3.81 (2)	3.82 (3)
Br(1)–Br(1)(B,$\bar{1}$0$\bar{1}$)	3.941 (3)	3.935 (7)
Br(1)–S(D,01$\bar{1}$)	3.561 (5)	3.51 (1)
Br(1)–S(C,$\bar{1}$00)	3.788 (5)	3.78 (1)
Br(1)–C(1)(D,00$\bar{1}$)	3.85 (1)	3.78 (3)
Br(1)–C(2)(A,010)	3.92 (1)	3.84 (3)
Br(1)–C(4)(D,01$\bar{1}$)	3.85 (1)	3.81 (3)
Br(2)–C(3)(A,0$\bar{1}$0)	3.88 (1)	3.78 (3)
S–C(2)(D,000)	3.64 (1)	3.56 (3)

[a] See footnote *a* in Table III for meaning of symbols.

The bond distances, bond angles, and torsion angles in the 1,4-thiatellurane moiety in $C_4H_8STeBr_2$ are listed in Table VI. With the possible exception of the C–S–C–C torsion angles, the present values are in excellent agreement with those found in $C_4H_8STeI_2$.[11] In the dibromide, these angles are each 74 (1)° while the four values in the two independent molecules in the diiodide range from 75 to 77°. It should be noted that, unlike the situation in $C_4H_8STeBr_2$, the sulfur atoms in $C_4H_8STeI_2$ are not involved in secondary bonding and this may be responsible for the small difference in the torsion angles involving the S–C bonds.

TABLE VI
DISTANCES AND ANGLES IN THE 1,4-THIATELLURANE MOIETY IN $C_4H_8STeBr_2$

	Distances, Å		
Te–C(2)	2.14 (1)	Te–C(3)	2.16 (1)
S–C(1)	1.81 (1)	S–C(4)	1.79 (1)
C(1)–C(2)	1.52 (2)	C(3)–C(4)	1.53 (2)
C–H (range)	0.64 (20)–1.20 (20)	C–H (av)	0.93
	Bond Angles, Deg		
C(2)–Te–C(3)	99.4 (6)	C(1)–S–C(4)	100.6 (7)
Te–C(2)–C(1)	117 (1)	S–C(1)–C(2)	114 (1)
Te–C(3)–C(4)	115 (1)	S–C(4)–C(3)	116 (1)
	Torsion Angles, Deg		
Te–C(2)–C(1)–S	59 (1)	C(3)–Te–C(2)–C(1)	31.9 (8)
Te–C(3)–C(4)–S	58 (1)	C(1)–S–C(4)–C(3)	74 (1)
C(2)–Te–C(3)–C(4)	30.4 (8)	C(4)–S–C(1)–C(2)	74 (1)

Because of the influence of secondary bonding, comparisons of Te–Br distances in various R_2TeBr_2 compounds are not very significant. However, the value of 2.682 (3) Å observed in $(C_6H_5)_2TeBr_2$[12] is bracketed by the values of 2.657 (2) and 2.689 (2) Å observed in the present study. The level of secondary bonding in $(C_6H_5)_2TeBr_2$ is very low; the shortest nonbonded Te···Br contacts are two equivalent ones at 3.90 Å. The fact that aromatic C–Te bonds are involved in one compound and not in the other is probably also of significance.

TABLE VII
ROOT-MEAN-SQUARE AMPLITUDES OF VIBRATION (Å)

Atom	Min	Intermed	Max	Atom	Min	Intermed	Max
Te	0.147	0.165	0.197	C(1)	0.170	0.197	0.226
Br(1)	0.173	0.216	0.268	C(2)	0.159	0.188	0.218
Br(2)	0.167	0.233	0.303	C(3)	0.147	0.209	0.225
S	0.170	0.193	0.248	C(4)	0.170	0.227	0.248

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