

The Molecular Structure of Chlorotris[*N*-(2-hydroxyethyl)-*N*-methylthiocarbamato]tellurium(IV) Dihydrate

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The structure of the title compound, $[\text{TeCl}\{\text{HOCH}_2\text{CH}_2(\text{CH}_3)\text{NCS}_2\}_3] \cdot 2\text{H}_2\text{O}$ has been determined by X-ray crystallographic methods. The crystals are monoclinic, space group $P2_1/c$, with $a = 6.389(1)$ Å, $b = 17.707(4)$ Å, $c = 21.943(3)$ Å, $\beta = 98.95(1)^\circ$ and $Z = 4$. Based on 3231 observed reflections collected with a CAD-4 diffractometer, the full-matrix least squares refinement gave a final R -value of 0.021.

Tellurium is bonded to the six sulfur atoms in the molecule and to chlorine. The resulting structure is distorted pentagonal, bipyramidal with chlorine in an axial position. The Te–S bond lengths vary from 2.493(1) Å to 2.835(1) Å, while Te–Cl is 2.772(1) Å. The angle $S_{ax}-\text{Te}-\text{Cl}_{ax} = 174.87(3)^\circ$. There is extensive hydrogen bonding in the crystals.

Seven-coordinate tellurium(IV) complexes have been found to have distorted^{1–3} pentagonal bipyramidal structures. The main reason for the distortion is the small bite of the three dialkylthiocarbamate ligands found in such complexes. The lone pair of electrons in the valency shell of the tellurium atom is found largely inert in the sense that it does not occupy a position in the coordination polyhedron. The present study is an extension of our work on highly coordinated tellurium complexes with dithiocarbamate- and halogenide ions as ligands.³

EXPERIMENTAL

Yellow crystals of chlorotris[*N*-(2-hydroxyethyl)-*N*-methyl-dithiocarbamato]tellurium(IV) dihydrate were prepared according to Aravamudan *et al.*⁴ Recrystallization from a 1:1 ethanol–benzene mixture gave prisms and plates suitable for X-ray work. The crystal used for data collection had approximate dimensions $0.06 \times 0.032 \times 0.17$ mm.

X-Ray data. Intensity data and data for measurement of unit cell dimensions were obtained on an Enraf-Nonius CAD-4 diffractometer. Unit cell parameters were determined by least-squares refinement of the setting angles of 25 high-order reflections. The values are $a = 6.389(1)$ Å, $b = 17.707(4)$ Å, $c = 21.943(3)$ Å, $\beta = 98.95(1)^\circ$ and $Z = 4$. From systematic absences; $0k0$, $k = 2n + 1$ and $h0l$, $l = 2n + 1$, the space group is $P2_1/c$ (No. 14). $D_m(\text{floatation}) = 1.74$ g/cm³; $D_x = 1.76$ g/cm³.

Reflection intensities were measured using an omega scan with scan width $(1.00 + 0.35 \tan \theta)^\circ$, a graphite monochromator and $\text{MoK}\alpha$ radiation. The scan rate varied from 0.50 to 2.50° min⁻¹. Out of 4892 unique reflections with $2\theta \leq 50^\circ$, 3231 had intensities larger than $3\sigma(I)$ and were treated as observed. For further details about data collection and least squares refinement, see Ref. 5. The intensity data were corrected for absorption ($\mu = 18.7$ cm⁻¹; transmission factor range 0.792–0.896).

STRUCTURE DETERMINATION

The structure of $[\text{TeCl}\{\text{HOCH}_2\text{CH}_2(\text{CH}_3)\text{NCS}_2\}_3] \cdot 2\text{H}_2\text{O}$ was solved by conventional heavy atom methods and refined by means of least-squares full-matrix programs.⁶ The positions of the hydrogen atoms were found from a difference map and the structure was then further refined with anisotropic temperature factors for all atoms except hydrogen, using the weighting scheme described previously with $p = 0.02$.⁵ The final conventional R -factor was 0.021, and $R_w = 0.024$. No peaks above 0.4 e Å⁻³ were found in the final difference map. The scattering factors for all nonhydrogen atoms were corrected for anomalous dispersion.

Final atomic coordinates are listed in Table 1. Tables of observed and calculated structure factors

Table 1. Final atomic coordinates with standard deviations.

	x	y	z
Te	0.24627(3)	0.24627(1)	0.20825(1)
S1	0.1777(1)	0.09252(5)	0.21178(4)
S2	0.5270(1)	0.16795(5)	0.16224(4)
S3	0.1322(1)	0.39051(5)	0.23253(4)
S4	0.5058(1)	0.34568(5)	0.17652(3)
S5	-0.0100(1)	0.22984(5)	0.30187(4)
S6	0.4568(1)	0.24029(5)	0.31377(4)
C1	-0.0138(2)	0.26079(6)	0.09539(4)
O1	0.2586(4)	-0.0869(2)	0.0575(1)
O2	0.2711(4)	0.5372(2)	0.0558(1)
O3	0.3928(4)	0.3470(2)	0.4728(1)
O4	-0.0532(5)	0.4397(2)	0.0654(1)
O5	0.0663(5)	0.0995(2)	0.0353(1)
N1	0.4539(4)	0.0210(2)	0.1531(1)
N2	0.3694(4)	0.4870(1)	0.1812(1)
N3	0.2511(5)	0.2130(2)	0.4069(1)
C1	0.3897(5)	0.0860(2)	0.1734(1)
C2	0.6299(6)	0.0183(2)	0.1174(2)
C3	0.3467(6)	-0.0503(2)	0.1630(2)
C4	0.1722(6)	-0.0698(2)	0.1112(2)
C5	0.3359(5)	0.4161(2)	0.1954(1)
C6	0.2260(6)	0.5463(2)	0.1957(2)
C7	0.5354(5)	0.5084(2)	0.1450(2)
C8	0.4634(6)	0.4996(2)	0.0765(2)
C9	0.2275(5)	0.2268(2)	0.3473(1)
C10	0.0639(7)	0.1973(3)	0.4365(2)
C11	0.4533(6)	0.2163(3)	0.4484(2)
C12	0.4538(6)	0.2754(2)	0.4976(2)
H1	0.582(6)	0.035(2)	0.074(2)
H2	0.657(6)	0.032(2)	0.109(2)
H3	0.741(6)	0.043(2)	0.138(2)
H4	0.449(4)	-0.088(2)	0.166(1)
H5	0.274(5)	-0.043(2)	0.201(1)
H6	0.081(4)	-0.025(2)	0.101(1)
H7	0.094(5)	-0.111(2)	0.124(1)
H8	0.172(6)	-0.090(2)	0.030(2)
H9	0.077(7)	0.536(3)	0.174(2)
H10	0.283(6)	0.590(2)	0.187(2)
H11	0.216(6)	0.544(2)	0.237(2)
H12	0.654(5)	0.479(2)	0.159(1)
H13	0.574(5)	0.561(2)	0.152(1)
H14	0.439(5)	0.441(2)	0.068(1)
H15	0.420(6)	0.016(2)	0.443(2)
H16	0.161(9)	0.510(3)	0.063(3)
H17	0.018(9)	0.242(3)	0.449(2)
H18	0.097(8)	0.179(3)	0.479(2)
H19	-0.036(6)	0.174(2)	0.413(2)
H20	0.479(6)	0.165(2)	0.467(2)
H21	0.559(5)	0.229(2)	0.427(2)
H22	0.361(6)	0.256(2)	0.525(2)
H23	0.598(5)	0.274(2)	0.521(2)
H24	0.495(6)	0.368(2)	0.463(2)

Table 1. Continued.

H25	-0.127(7)	0.437(3)	0.028(2)
H26	-0.049(8)	0.399(2)	0.071(2)
H27	0.035(10)	0.144(3)	0.057(3)
H28	0.153(5)	0.102(2)	0.019(1)

Table 2. Bond lengths (Å) with standard deviations.

Te—C1	2.772(1)	C5—N2	1.319(4)
Te—S1	2.755(1)	C9—N3	1.315(4)
Te—S2	2.593(1)	N1—C2	1.469(5)
Te—S3	2.731(1)	N1—C3	1.468(4)
Te—S4	2.587(1)	N2—C6	1.462(4)
Te—S5	2.835(1)	N2—C7	1.469(4)
Te—S6	2.493(1)	N3—C10	1.474(5)
S1—C1	1.708(3)	N3—C11	1.462(5)
S2—C1	1.733(3)	C3—C4	1.504(5)
S3—C5	1.701(3)	C7—C8	1.510(5)
S4—C5	1.745(3)	C11—C12	1.502(6)
S5—C9	1.682(3)	C4—O1	1.410(5)
S6—C9	1.756(3)	C8—O2	1.409(5)
C1—N1	1.322(4)	C12—O3	1.410(5)

Table 3. Bond angles (°) with standard deviations.

Cl—Te—S1	92.34(3)	Te—S3—C5	84.7(1)
Cl—Te—S2	93.23(3)	Te—S4—C5	88.5(1)
Cl—Te—S3	86.94(3)	S3—C5—S4	118.3(2)
Cl—Te—S4	90.94(3)	S3—C5—N2	122.1(2)
Cl—Te—S5	108.90(3)	S4—C5—N2	119.6(2)
Cl—Te—S6	174.87(3)	Te—S5—C9	82.2(1)
S1—Te—S2	66.82(2)	Te—S6—C9	91.8(1)
S1—Te—S3	150.25(3)	S5—C9—S6	118.8(2)
S1—Te—S4	142.18(3)	S5—C9—N3	123.3(2)
S1—Te—S5	76.47(2)	S6—C9—N3	117.9(2)
S1—Te—S6	89.84(3)	C1—N1—C2	120.8(3)
S2—Te—S3	142.92(3)	C1—N1—C3	121.5(3)
S2—Te—S4	75.38(3)	C2—N1—C3	117.7(3)
S2—Te—S5	137.74(3)	C5—N2—C7	122.1(3)
S2—Te—S6	91.90(3)	C5—N2—C6	120.1(3)
S3—Te—S4	67.55(2)	C7—N2—C6	117.5(3)
S3—Te—S5	75.68(2)	C9—N3—C11	124.5(3)
S3—Te—S6	88.87(3)	C9—N1—C10	119.9(4)
S4—Te—S5	137.04(3)	C11—N3—C10	115.6(4)
S4—Te—S6	90.18(3)	N1—C3—C4	113.2(3)
S5—Te—S6	67.12(2)	O1—C4—C3	109.9(3)
Te—S1—C1	85.1(1)	N2—C7—C8	112.2(3)
Te—S2—C1	89.8(1)	O2—C8—C7	112.8(3)
S1—C1—S2	117.9(2)	N3—C11—C12	112.3(4)
S1—C1—N1	122.7(2)	O3—C12—C11	112.3(3)
S2—C1—N1	119.4(2)		

Table 4. Hydrogen bonds (Å) and their bond angles (°) with standard deviations.

A—H...B	A—H	A...B	H...B	Bond angle	Translation of B
O4—H26...Cl	0.78(6)	3.236(4)	2.46(6)	177(3)	None
O5—H27...Cl	0.97(7)	3.220(4)	2.27(7)	170(3)	None
O3—H24...O1	0.82(5)	2.690(4)	1.88(5)	180(2)	1 - x, -1/2 + y, 1/2 - z
O1—H8...O5	0.75(4)	2.683(4)	1.93(4)	177(3)	-x, -y, -z
O2—H16...O4	0.88(7)	2.731(5)	1.86(7)	169(3)	None
O4—H25...O2	0.88(6)	2.834(5)	1.98(6)	165(2)	-x, 1 - y, -z
O5—H28...O3	0.71(4)	2.832(5)	2.16(6)	161(2)	x, 1/2 - y, 1/2 + z

and of atomic temperature factors are available from one of the authors (S.H.) upon request.

RESULTS AND DISCUSSION

Interatomic distances and angles are listed in Tables 2–5, while molecular least squares planes are listed in Table 6. The complex molecule as seen along a^* is shown in Fig. 1. while the molecular packing is shown in Fig. 2.

The crystals of [TeCl{HOCH₂CH₂(CH₃)NCS₂}₃].2H₂O contain monomeric molecules where the central tellurium atom is coordinated to the chlorine atom and to the six sulfur atoms of the three bidentate dithiocarbamate ligands. Tellurium is thus seven-coordinate, and the complex molecule has an approximate pentagonal bipyra-

midal structure with chlorine in an axial position. If the the -CH₂OH groups of the bidentate ligands are ignored, the molecular symmetry is nearly C_{2v} , with the mirror plane containing Te, Cl and the unique bidentate ligand spanning both an axial and an equatorial position.

Seven-coordination has been discussed by several authors.^{7–10} Calculations indicate that the pentagonal bipyramid (PB), the monocapped octahedron (CO), and the monocapped trigonal prism,

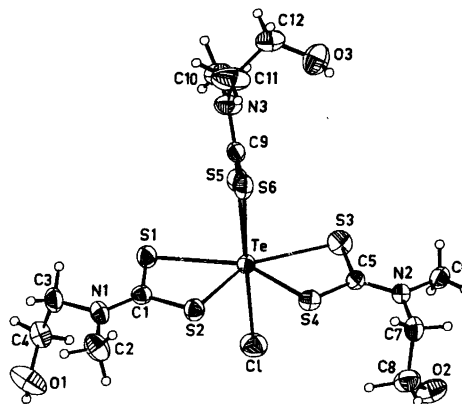
Fig. 1. The complex molecule as seen along a^* .

Table 5. Short, nonbonded intramolecular distances (Å) with standard deviations.

S1—S2	2.948(1)
S3—S4	2.958(1)
S5—S6	2.959(1)
S2—S4	3.167(1)
S1—S5	3.460(1)
S3—S5	3.415(1)

Table 6. Least squares mean planes. S5 is 1.021 Å above plane 2.

No. of plane	Atoms included	Interplanar angles (°)	RMS deviation from planes (Å)
1	Te, S5, S6, Cl	1–2 89.0 2–4 11.6	0.035
2	Te, S1, S2, S3, S4	1–3 -85.4 2–5 87.1	0.016
3	S1, S2, C1, N1, C2, C3	1–4 78.2 3–4 16.3	0.029
4	S3, S4, C5, N2, C6, C7	1–5 4.1 3–5 -87.0	0.027
5	S5, S6, C9, N3, C10, C11	2–3 6.9 4–5 76.8	0.046

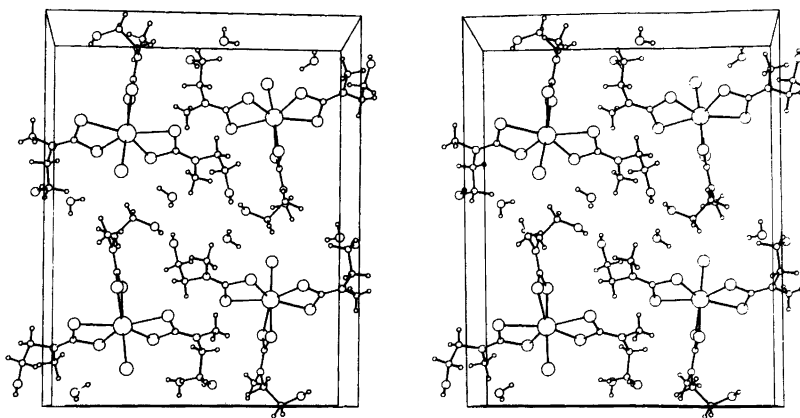


Fig. 2. The packing in the unit cell as seen along a^* (stereo). The b -axis is horizontal, while c is vertical.

(CTP), are the preferred structures and that they differ little in energy. Some of the seven-coordinate complexes with PB structures have been found to be non-rigid at room or higher temperatures with exchange of the unique ligand and the equatorial ones. A polytypal rearrangement involving a CO transition state has been suggested for this exchange.^{10,11} NMR studies in this laboratory undertaken on $[\text{Te}(\text{Me}_2\text{NCS}_2)_3\text{Ph}]$ and on $[\text{Te}(\text{Et}_2\text{NCS}_2)\text{Ph}]$ ¹ with a distorted PB structure, show only one methyl or methylene signal (respectively 3.45 and 3.95 p.p.m. relative to TMS) at room temperature, indicating that also seven-coordinate tellurium(IV) complexes with a PB structure may be non-rigid.¹²

Keper's studies indicate that for ML_3X (L = bidentate), a small normalized bite* in L ; $b \leq 1.1$, favor the PB. In the present work $b = 1.1$ in agreement with this. It was also found that the energy minimum was particularly shallow in the direction of a swing of the unique ligand up from the equatorial plane.⁷ For a PB structure of the ML_3X type, the monodentate ligand is invariably found in an axial position and this agrees with calculation.⁹ For the above type seven-coordinate complexes, the type of structure found in the present investigation (PB with near C_2 symmetry) predominates. The structural variations can be rationalized in terms of a rotation in the approximate mirror plane of the unique bidentate ligand about the central atom. One

* The normalized bite is defined as the distance between the two donor atoms of the chelate divided by the metal ligand bond length.

should here have in mind that most bidentate ligands have so small bites that they cannot span an axial and an equatorial position in a perfect PB. Thus distortion invariably results.^{1,3}

In Fig. 3, two extremes of the rotation of the bidentate ligand are shown. Fig. 3a represents the present investigation and has the unique ligand moved up from the equatorial plane towards the axial position so that the $\text{Cl}_{\text{ax}}-\text{Te}-\text{S}_{\text{ax}}$ angle is close to 180° [actual value $174.87(3)^\circ$]. Because of the small bite, the equatorial sulfur atom of the unique ligand is moved 1.02 \AA up above the equatorial plane. This atom is thus moved towards the capping position in a monocapped octahedron. The other extreme, Fig. 3b, is represented by the structure of tris-(diethyldithiocarbamato)phenyltellurium (IV).¹ There, the axial sulfur atom of the unique ligand is pushed so far away from the true axial position that the equatorial sulfur atom in the unique ligand becomes positioned almost exactly in the equatorial plane. In this case, the $\text{Ph}_{\text{ax}}-\text{Te}-\text{S}_{\text{ax}}$ angle is only 144.6° . Due to the large crowding in the equatorial girdle in the latter case, the structures of most of the seven-coordinate ML_3X complexes are closer to that outlined in Fig. 3a than that in Fig. 3b.^{8,10,13-21}

In $[\text{TeCl}\{\text{HOCH}_2\text{CH}_2(\text{CH}_3)\text{NCS}_2\}_3]$, (I), the $\text{Te}-\text{S}$ bond length varies between $2.493(1)$ and $2.835(1) \text{ \AA}$ with an average of 2.67 \AA . The average equatorial $\text{Te}-\text{S}$ bond length is 2.70 \AA . This latter value may be compared to 2.72 \AA found in $[\text{TeCl}(\text{Et}_2\text{NCS}_2)_3]$, (II),² and to 2.71 \AA found in $[\text{Te}(\text{Et}_2\text{NCS}_2)_3\text{Ph}]$ (III).¹ The axial $\text{Te}-\text{S}$ bond

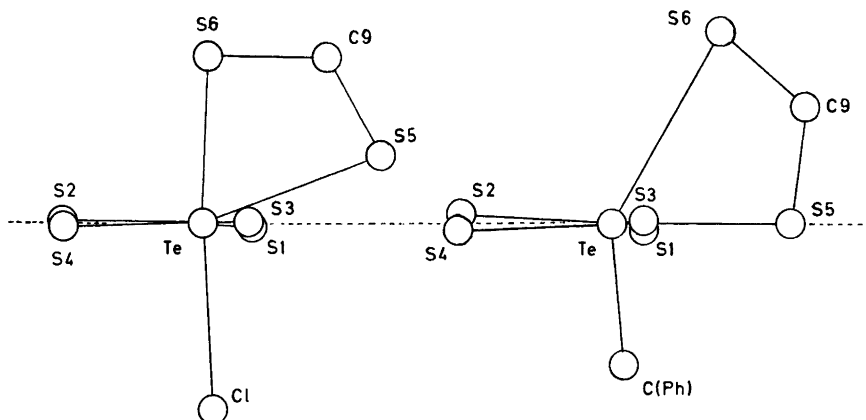


Fig. 3. The coordination of [TeCl{HOCH₂CH₂(Me)NCS₂}₃] (3a), and [Te(Et₂NCS₂)₃Ph] (3b), projected into the quasi-mirror plane. Atom names in Fig. 3b are changed to correspond to those in 3a. In 3a Te–S₆ and Te–Cl form angles with the normal to the equatorial plane of *ca.* 2 and 3°, respectively, while Te–S₅ forms an angle with the equatorial plane of *ca.* 21°.

length of 2.493(1) Å is significantly shorter than the equatorial ones and comparable to the corresponding bond length in II, 2.512(4) Å.² In III, the axial Te–S bond is much longer than the other Te–S bonds, 3.23 Å, probably due to the great *trans* effect of the phenyl ligand. More moderate *trans* effects are found in transition metal complexes with PB symmetry.^{15,21} The lengthening of the Te–S_{ax} bond in III leads to a shortening of the Te–S_{eq} bond in the same ligand. In I and II the opposite effect leads to a lengthening of the Te–S_{eq} bond in the unique ligand so that it becomes significantly longer than the Te–S_{ax} bond and this is a feature found in most such complexes having monodentate ligands with small *trans* effects (Table 7).

In the equatorial plane of I, the two almost coplanar dithiocarbamate ligands have similar Te–S bond lengths. In each ligand, the sulfur atom adjacent to the equatorial sulfur atom of the unique dithiocarbamate ligand is *ca.* 0.16 Å further away from the central tellurium atom than the other. Comparable differences are found in II and in the tin compounds Sn(Et₂NCS₂)₃X with X=Me and *n*-butyl.^{19,20} Such a ligand to central atom bond length variation is found in most ML₃X (L=bidentate, X=monodentate) compounds where X has a small *trans* effect, but the differences in bond lengths are usually much smaller for M=transition metal or if L has hard donor atoms like oxygen (Table 7 and Ref. 18). The above bond length varia-

Table 7. Bond lengths (Å) and angles (°) in selected ML₃X compounds where L is a uninegative, bidentate dithiocarbamate ligand and X is a monodentate ligand.^a

Compound	M–S1	M–S2	M–S3	M–S4	M–S5	M–S6	M–X	∠X–M–S6	∠X–M–S5
TeCl(Et ₂ NCS ₂) ₃ ²	2.765(3)	2.594(4)	2.773(3)	2.605(3)	2.874(4)	2.512(4)	2.686(4)	179.1(1)	114.1(1)
TeCl(HOCH ₂ CH ₂ (Me)-NCS ₂) ₃ .2H ₂ O	2.755(1)	2.593(1)	2.731(1)	2.587(1)	2.835(1)	2.493(1)	2.772(1)	174.87(3)	108.90(3)
Te(Et ₂ NCS ₂) ₃ Ph ¹	2.701(3)	2.797(3)	2.657(3)	2.816(3)	2.606(3)	3.228(4)	2.12(1)	144.6(2)	84.2(2)
Sn(Et ₂ NCS ₂) ₃ <i>n</i> -Bu ²⁰	2.820(8)	2.619(8)	2.741(8)	2.674(3)	2.763(8)	2.491(8)	2.15(3)	166.3(5)	97.2(5)
TiCl(Me ₂ NCS ₂) ₃ ¹⁴	2.516(3)	2.473(3)	2.533(3)	2.496(3)	2.577(3)	2.477(3)	2.305(3)	165.0(1)	95.1(1)
RuI(Me ₂ NCS ₂) ₃ ·I ₂ ¹⁶	2.459(7)	2.405(6)	2.459(7)	2.405(6)	2.371(9)	2.337(8)	2.752(4)	174.2(3)	102.0(2)
Re(CO)(Et ₂ NCS ₂) ₂ ²¹	2.481(2)	2.474(2)	2.487(2)	2.489(2)	2.433(2)	2.518(2)	1.852(6)	173.2(2)	102.5(2)

^a The atoms in the table correspond to those in Fig. 1. S₆ and X are axial.

tion is probably due to steric effects. Thus the lone pair of electrons on the central tellurium atom in the present investigation is probably stereochemically inert and does not occupy a position in the coordination polyhedron. The fact that seven-coordinate Sn(IV) PB complexes with no lone pairs in the valency shell of tin have structures very similar to I and II strongly supports this.^{19,20}

The S—Te—S bond angles in the equatorial "plane" in I average 67.2° and 75.9° for the intra- and interligand ones respectively. Interligand S---S contacts in the plane are S2—S4 = 3.167(1) Å, S1—S5 = 3.460(1) Å and S3—S5 = 3.415(1) Å. Here S5 belongs to the unique ligand, and strain in the equatorial girdle is relieved by the puckering at this atom (Fig. 3a) and also by the great length of the Te—S5 bond [2.835(1) Å]. By comparison, III, with the corresponding atom truly equatorial and a Te—S bond length of only 2.606(3) Å, has two interligand angles involving that atom about 5° larger than I. This increase is compensated for by a decrease in the other equatorial S—Te—S angles. To relieve the strain due to the decrease in the third interligand equatorial angle, the two Te—S bonds making up

that angle increase in length from *ca.* 2.59 Å in I to *ca.* 2.80 Å in III.

The structures of [TeCl{HOCH₂CH₂(CH₃)NCS₂}₃ · 2H₂O, (I), the corresponding bromide,³ and of TeCl(Et₂NCS₂)₃, (II), are very similar. Looking at the structures of I and II, the most accurately determined, the corresponding bond lengths and angles do not differ much except that Te—S5 in I is 0.04 Å longer than the corresponding bond in II and that Te—Cl in I is 0.09 Å longer than in II. The latter effect may be due the fact that Cl is involved in hydrogen bonding to the two water molecules in I, and that this may occur at the expense of the Te—Cl bond. The Te—Cl bond is unusually long, 2.772(1) Å, and may be compared to 2.5–2.6 Å found for such a bond in octahedral tellurium complexes. In addition to hydrogen bonding, the *trans* effect of the dithiocarbamate ligand probably contributes to this bond lengthening. The axial Te—S bond *trans* to Te—Cl is therefore a bit shorter in I than in II (Table 7) but the difference is hardly significant. Also the unique ligand is moved *ca.* 5° higher up from the equatorial plane in II, relative to I, making the Cl—Te—S_{ax} sequence almost

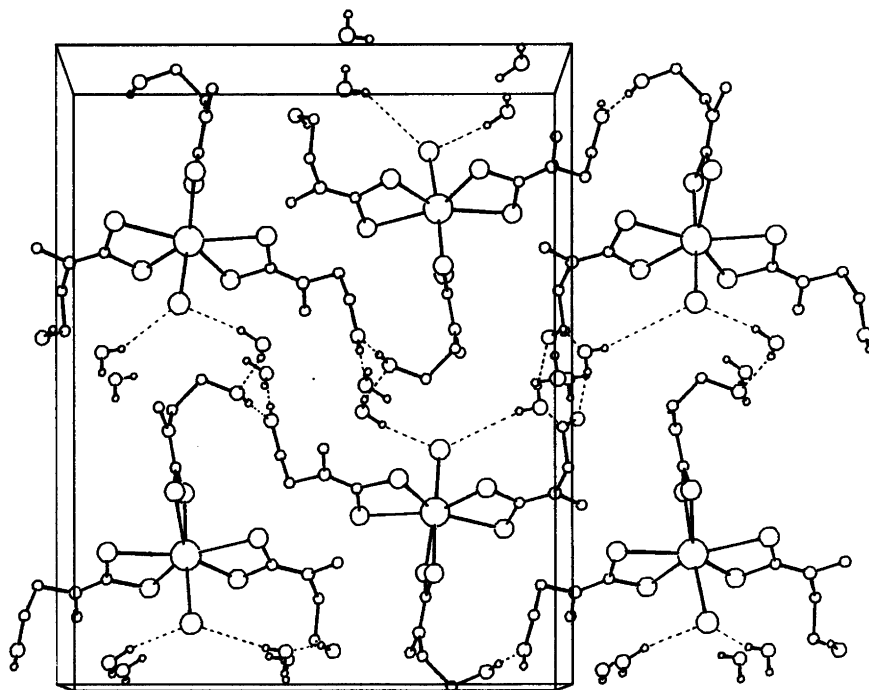


Fig. 4. Hydrogen bonding in the unit cell. The hydrogen bonds are indicated by dotted lines. Methyl and methylene hydrogen atoms are not included.

linear in II (Table 7). A common feature for highly coordinated Te(IV) complexes is the inertness of the lone pair of electrons and the long ligand to central atom bond lengths. This latter effect indicates that the lone pair may have an antibonding influence. Also stereochemical crowding and polycenter bonding may be contributing to the lengthening of these bonds.²²⁻²⁴

The dithiocarbamate ligands are roughly planar out to the carbon atoms bonded to nitrogen (Table 6). The bond lengths and angles within the dithiocarbamate groups are normal with the asymmetry in the C-S bonds reflecting the asymmetry in the corresponding S-Te bonds such that each sulfur atom preserves a bond order of two. The average C-S, C-N and N-C bond lengths are 1.721, 1.319 and 1.467 Å, respectively. The partial double bonding in the >NCS₂ group and the sp² hybridization on N and C in that group reflect the mesomeric shift of electron density from nitrogen to sulfur.

Molecular packing. The packing of the molecules in the unit cell is shown in Fig. 2. The hydroxyl groups of the dithiocarbamate ligands, the chlorine atoms and the water molecules are knit together in a three-dimensional network by hydrogen bonds, indicated in Fig. 4. The O---H-O and Cl---H-O bonds have normal lengths and angles (Table 4). All hydrogen bonds are intermolecular, and both water molecules are H-bonded to the same chlorine atom in the asymmetric unit.

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