ACTA CHEMICA SCANDINAVICA 25 (1971) 2467–2475

The Crystal and Molecular Structure of a *trans* Square-planar Complex of Tellurium Dibenzenethiosulphonate with Ethylenethiourea

KJELL ÅSE, KNUT MAARTMANN-MOE and JON ODDVAR SOLHEIM

Chemical Institute, University of Bergen, Bergen, Norway

The complex, *trans*-dibenzenethiosulphonatobis(ethylenethiourea)-tellurium(II), $Te(S{:}C{\cdot}NH{\cdot}[CH_2]_2{\cdot}NH)_2(S_2O_2C_6H_5)_2$, crystallizes in the space group $P\bar{1}$ (No. 2). The unit cell dimensions (standard deviations in parentheses) are, $a = 7.069(4)$ Å, $b = 10.580(7)$ Å, $c = 8.938(5)$ Å, $\alpha = 101.98(8)°$, $\beta = 91.00(8)°$, $\gamma = 94.54(8)°$, with one molecule per unit cell. The crystal and molecular structure has been determined by three-dimensional X-ray diffraction methods. The intensities of 1265 independent, non-zero reflections were collected, using integrating Weissenberg techniques. Refinement by full-matrix least squares methods resulted in a conventional R value of 0.081.

The tellurium atom, which is bonded to two ethylenethiourea sulphur atoms and to two benzenethiosulphonate sulphur atoms, lies in a centre of symmetry. The arrangement around tellurium is *trans* square-planar, with the following dimensions: Te – S(ethylenethiourea) = 2.713(5) Å, Te – S(benzenethiosulphonate) = 2.686(4) Å, ∠S – Te – S = 90.80(13)°. The benzenethiosulphonate S – S bond length is 2.016(5) Å.

A crystal structure determination of *trans*-dibenzenethiosulphonatobis-(ethylenethiourea)tellurium(II), $Te(S{:}C{\cdot}NH{\cdot}[CH_2]_2{\cdot}NH)_2(S_2O_2C_6H_5)_2$, has been undertaken as part of a series of structural studies on square-planar complexes of divalent tellurium. Preliminary results have been mentioned in a review.[1] Based on more data, the structure has now been further refined, and a full report is given here.

In 1961, Foss and Johannessen reported the preparation of five complexes of divalent tellurium thiosulphonates with thioureas, together with unit cell and space group data on the complexes.[2] Of the five complexes, four, including the subject of the present study, were yellow, and one was red. The structure of the closely related, yellow complex of tellurium dibenzenethiosulphonate

with trimethylenethiourea has recently been reported.[3] The red complex of tellurium dibenzenethiosulphonate with tetramethylthiourea is under study in this laboratory, and the structure will be reported in a subsequent article.

EXPERIMENTAL

The crystals of $Te(etu)_2(S_2O_2C_6H_5)_2$, where etu is ethylenethiourea, were prepared by Foss and Johannessen.[2]

For determination of unit cell dimensions, 2θ-values for 41 reflections were measured from zero-layer Weissenberg photographs about the a, b, and c axes, using $CuK\alpha_1$ radiation ($\lambda = 1.5405$ Å). Sodium chloride powder lines were superimposed on the films for reference ($a = 5.6405$ Å at 22°C).[4]

Intensity data were collected for the $hk0 - hk3$, $h0l$, and $0kl$ layers, using multiple-film integrating equi-inclination Weissenberg techniques with (Ni-filtered) $CuK\alpha$ radiation. The dimensions of the crystals are shown in Table 1. Out of 1386 accessible, inde-

Table 1. Distance (mm) from origin to faces for the three crystals used for collecting intensity data.

Distance to	Crystal rotating about the a axis	Crystal rotating about the b axis	Crystal rotating about the c axis
(010) and ($0\bar{1}0$)	0.043	0.025	0.028
($\bar{1}10$) and ($1\bar{1}0$)	0.065	0.055	0.052
(011) and ($0\bar{1}\bar{1}$)	0.096	0.074	0.113

pendent reflections, 1265 were strong enough to be estimated visually by comparison with a scale of timed exposures. The intensities of the remaining 121 reflections were set equal to the observable limit.

Estimated corrections for the splitting of α_1 and α_2 were applied for high-angle reflections. Lorentz, polarization, and absorption corrections were done ($\mu = 141$ cm^{-1}). A modified version of the absorption correction method described by Busing and Levy [5] was applied, using an $8 \times 6 \times 10$ grid for each of the crystals.

The scattering factor curves listed in *International Tables* (Ref. 4, p. 202) were used for structure factor calculations. Using the $\Delta f'$ and $\Delta f''$ values given by Cromer,[6] the tellurium and sulphur scattering curves were corrected for anomalous dispersion, by taking the amplitude of f as the corrected value.

The structure was refined by a least squares, full-matrix program which minimized the function

$$r = \sum W(|F_o| - K|F_c|)^2$$

where K is a scale factor. The weight is defined by $W = 1/\sigma^2(F_o)$, where $\sigma(F_o)$ is the estimated standard deviation in F_o. Non-observed reflections for which $K|F_c|$ is greater than the observable limit, are included in the refinement, with $|F_o|$ equal to the observable limit.

The calculations were carried out on an IBM 360/50 H computer. Most computer programs were made available by the Weizmann Institute of Science, Rehovoth, Israel, and modified for use on the IBM computer by Dr. Dove Rabinovich. A program calculating weighted least squares planes was written by Knut Maartmann-Moe; and two other programs, one for Fourier summations and another for extinction corrections, were written by Kjell Åse.

CRYSTAL DATA

The crystals occur as yellow, triclinic prisms bounded mainly by {010}, {1$\bar{1}$0}, and {011}. They are elongated in the *c*-axis direction, and attempts to cut them across this direction usually results in a bundle of thin needles parallel to *c*. The following unit cell dimensions, based on 41 high-angle 2θ values, were calculated by a least squares procedure.

$a = 7.069(4)$ Å; $b = 10.580(7)$ Å; $c = 8.938(5)$ Å;
$\alpha = 101.98\ (8)°$; $\beta = 91.00\ (8)°$; $\gamma = 94.54\ (8)°$.

Standard deviations are given in parentheses.

$V = 651.5(8)$ Å^3; $M = 678.38$; $F(000) = 338$; $Z = 1$.

Possible space groups: $P1$ (No. 1) and $P\bar{1}$ (No. 2).

STRUCTURE DETERMINATION

Space group $P\bar{1}$, which requires that the tellurium atom lies in a centre of symmetry, was assumed to be the most probable one. Starting with phases based on the tellurium contributions alone, the structure was solved through two-dimensional Fourier synthesis along the *a*, *b*, and *c* axis.

Three-dimensional least squares refinement on scale factors, positional parameters, and individual isotropic thermal parameters resulted in an *R* value of 0.119. Anisotropic thermal parameters for the tellurium and sulphur atoms were then introduced, and further refinement on all parameters except scale factors lowered the *R* value to 0.089.

Observed structure factors for strong, low-order reflections seemed to be smaller than the corresponding calculated structure factors, and a correction for extinction was therefore carried out, using the expression given by Zachariasen.[7] The absorption term in this expression was set equal to 1. With I_o on an absolute scale, the value of the extinction parameter, *C*, was found to be 18.3×10^{-6} for the crystal rotating about the *a* axis, 15.3×10^{-6} for the crystal rotating about the *b* axis, and 6.8×10^{-6} for the crystal rotating about the *c* axis.

The scale factors for each layer were then replaced by an overall scale factor, and the refinement on all parameters was continued until no shift was greater than 0.25 times the standard deviation. A three-dimensional difference Fourier summation at this point showed no peaks higher than 1.1 e/Å^3. The final *R* value, including non-observed reflections when $K|F_c|$ exceeds the observable limit, was 0.081. The successful refinement confirms the choice of space group $P\bar{1}$.

The final atomic coordinates are listed in Table 2, together with the final isotropic thermal parameters for the light atoms. The final anisotropic thermal parameters for the tellurium and sulphur atoms are listed in Table 3. The structure factors calculated from the final parameters are listed in Table 4, together with the observed values.

Table 2. Atomic coordinates in fractions of triclinic cell edges. Isotropic thermal parameters (Å²) in the form $\exp[-8\pi^2 U(\sin^2\theta/\lambda^2)]$. Standard deviations from the least squares refinement in parentheses.

	x	y	z	U
Te	0	0	0	
S(1)	−0.1581 (5)	−0.0770 (4)	0.2443 (6)	
S(2)	0.0990 (4)	0.2372 (3)	0.1708 (6)	
S(3)	0.3580 (4)	0.2276 (3)	0.2638 (6)	
O(1)	0.4282(13)	0.1000 (9)	0.2164(15)	0.0505(25)
O(2)	0.3501(15)	0.2825(11)	0.4220(18)	0.0653(32)
N(1)	0.0006(17)	−0.2094(13)	0.4239(21)	0.0592(35)
N(2)	0.2106(16)	−0.1101(11)	0.3053(19)	0.0506(30)
C(1)	0.5088(16)	0.3338(11)	0.1902(20)	0.0354(28)
C(2)	0.5359(19)	0.4592(13)	0.2669(23)	0.0494(35)
C(3)	0.6638(20)	0.5509(14)	0.2016(25)	0.0553(39)
C(4)	0.7561(19)	0.5007(14)	0.0669(22)	0.0504(36)
C(5)	0.7361(19)	0.3777(13)	0.0042(22)	0.0520(37)
C(6)	0.6157(18)	0.2855(13)	0.0617(22)	0.0459(34)
C(7)	0.0275(15)	−0.1368(11)	0.3286(20)	0.0331(27)
C(8)	0.1847(21)	−0.2479(15)	0.4869(25)	0.0591(41)
C(9)	0.3257(21)	−0.1657(15)	0.4188(25)	0.0577(41)

Table 3. Anisotropic thermal parameters (Å²) in the form $\exp[-2\pi^2(h^2a^{-2}U_{11}+\cdots+2hka^{-1}b^{-1}U_{12}+\cdots)]$. All values have been multiplied by 10^4. Standard deviations in parentheses.

	U_{11}	U_{22}	U_{33}	U_{12}	U_{23}	U_{13}
Te	304 (6)	416 (7)	366(13)	−25 (4)	174 (8)	−12 (8)
S(1)	374(15)	658(21)	487(37)	12(14)	237(27)	23(24)
S(2)	376(14)	501(17)	477(36)	−21(12)	204(22)	−58(23)
S(3)	377(14)	532(18)	383(33)	−66(13)	234(24)	−25(24)

RESULTS

Bond lengths and angles are listed in Table 5. The standard deviations are based on those of Table 2, neglecting coordinate covariances and standard deviations in unit cell dimensions. A drawing of the molecule, with selected bond lengths and angles, is presented in Fig. 1.

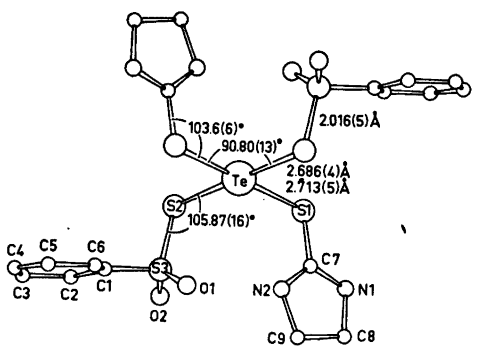

Fig. 1. The molecule as seen along the normal to a plane through Te, O(1), and the midpoint between S(1) and S(2′), where S(2′) is at $-x,-y,-z$ relative to S(2).

Table 4. Observed and calculated structure factors ($\times 10$). Unobserved reflections are indicated by a minus sign on $F(O)$ and are included at the threshold values.

H	K	L	F(O)	F(C)	H	K	L	F(O)	F(C)	H	K	L	F(O)	F(C)	H	K	L	F(O)	F(C)	H	K	L	F(O)	F(C)
0	1	C	750	716	8	4	0	72	77	0	6	1	163	156	2	-4	1	506	498	4	10	-1	64	-23
0	2	C	175	-126	8	5	0	155	158	0	7	1	263	243	2	-5	1	400	395	5	0	-1	150	168
0	3	C	75	52	9	0	0	90	101	0	8	1	309	325	2	-6	1	58	11	5	1	-1	237	233
0	4	0	602	640	1	-1	0	1275	1124	0	9	1	57	55	3	-1	1	389	391	5	2	-1	420	444
0	5	0	168	148	1	-2	0	472	552	0	10	1	-43	22	3	-2	1	883	897	5	3	-1	353	353
0	6	0	86	-75	1	-3	0	203	148	0	11	1	97	92	3	-3	1	531	501	5	4	-1	50	-32
0	7	C	54	20	1	-4	0	384	442	0	12	1	126	123	3	-4	1	275	261	5	5	-1	90	-43
0	8	C	318	304	1	-5	0	686	789	1	0	1	133	127	3	-5	1	315	344	5	6	-1	194	198
0	9	0	320	290	1	-6	0	253	264	1	1	1	548	641	3	-6	1	508	481	5	7	-1	315	257
0	10	C	93	99	1	-7	0	95	79	1	2	1	840	930	3	-7	1	146	131	5	8	-1	87	85
0	11	C	75	66	1	-8	0	96	104	1	3	1	647	741	4	-1	1	103	-81	5	9	-1	-41	0
0	12	C	107	110	1	-9	0	122	112	1	4	1	531	532	4	-2	1	398	439	5	10	-1	89	93
0	13	0	132	132	1-10		0	131	144	1	5	1	127	140	4	-3	1	595	642	6	0	-1	164	168
1	0	C	386	365	1-11		0	-42	19	1	6	1	237	226	4	-4	1	189	174	6	1	-1	184	194
1	1	C	576	562	1-12		0	56	59	1	7	1	238	235	4	-5	1	82	60	6	2	-1	150	140
1	2	C	211	218	1-13		0	75	80	1	8	1	-41	28	4	-6	1	267	286	6	3	-1	-43	38
1	3	0	401	407	2	-1	0	397	411	1	9	1	-42	-21	4	-7	1	396	415	6	4	-1	56	73
1	4	C	342	316	2	-2	0	326	304	1	10	1	88	85	4	-8	1	216	192	6	5	-1	122	112
1	5	C	64	56	2	-3	0	415	464	1	11	1	216	200	5	-1	1	51	-14	6	6	-1	176	153
1	6	C	81	81	2	-4	0	463	451	1	12	1	99	103	5	-2	1	146	126	6	7	-1	163	151
1	7	C	276	233	2	-5	0	357	379	2	0	1	599	592	5	-3	1	210	211	6	8	-1	101	91
1	8	C	413	402	2	-6	0	378	378	2	1	1	370	394	5	-4	1	333	359	6	9	-1	149	144
1	9	0	160	168	2	-7	0	292	280	2	2	1	291	285	5	-5	1	253	257	7	0	-1	62	54
1	10	C	78	68	2	-8	0	215	173	2	3	1	428	449	5	-6	1	233	213	7	1	-1	-47	11
1	11	0	123	118	2	-9	0	183	212	2	4	1	108	89	5	-7	1	230	226	7	2	-1	148	135
1	12	C	176	158	2-10		0	-43	21	2	5	1	50	-12	5	-8	1	195	194	7	3	-1	227	191
2	0	C	339	350	2-11		0	-42	22	2	6	1	152	170	6	-1	1	65	60	7	4	-1	86	66
2	1	C	428	478	2-12		0	52	49	2	7	1	176	199	6	-2	1	169	152	7	5	-1	60	64
2	2	C	234	203	2-13		0	66	78	2	8	1	174	181	6	-3	1	206	210	7	6	-1	109	126
2	3	0	236	250	3	-1	0	555	599	2	9	1	124	142	6	-4	1	82	81	7	7	-1	186	177
2	4	0	229	213	3	-2	0	214	179	2	10	1	174	144	6	-5	1	56	42	8	0	-1	-45	33
2	5	C	280	308	3	-3	0	113	95	2	11	1	115	124	6	-6	1	201	184	8	1	-1	109	108
2	6	C	254	250	3	-4	0	422	438	2	12	1	106	103	6	-7	1	234	206	8	2	-1	186	168
2	7	C	240	229	3	-5	C	589	603	3	0	1	58	-31	7	-1	1	66	55	8	3	-1	66	66
2	8	C	157	149	3	-6	C	407	419	3	1	1	99	83	7	-2	1	119	109	8	4	-1	-38	35
2	9	0	258	251	3	-7	0	106	113	3	2	1	446	469	7	-3	1	275	246	8	5	-1	92	121
2	10	C	190	171	3	-8	C	99	85	3	3	1	422	431	7	-4	1	172	154	1	-1	-1	1028	991
2	11	C	140	136	3	-9	C	189	169	3	4	1	42	32	7	-5	1	-49	19	1	-2	-1	401	357
2	12	C	92	87	3-10		0	175	162	3	5	1	-39	19	7	-6	1	76	-56	1	-3	-1	516	495
3	0	C	422	422	3-11		C	-40	41	3	6	1	149	133	7	-7	1	79	74	1	-4	-1	588	567
3	1	C	139	-134	3-12		0	-31	-9	3	7	1	379	410	8	-1	1	213	206	1	-5	-1	515	467
3	2	C	167	-128	4	-1	0	313	282	3	8	1	161	162	8	-2	1	55	40	1	-6	-1	105	107
3	3	0	263	279	4	-2	0	359	356	3	9	1	99	96	8	-3	1	77	81	1	-7	-1	191	196
3	4	0	424	452	4	-3	C	61	-25	3	10	1	113	128	8	-4	1	167	169	1	-8	-1	229	202
3	5	C	332	309	4	-4	0	115	-98	3	11	1	178	160	8	-5	1	102	95	1	-9	-1	230	212
3	6	C	179	189	4	-5	0	349	358	4	0	1	67	53	8	-6	1	-34	8	1-10		-1	114	120
3	7	C	458	456	4	-6	0	437	427	4	1	1	398	397	0	2	-1	391	355	1-11		-1	-42	15
3	8	C	330	321	4	-7	0	220	193	4	2	1	488	518	0	3	-1	142	-148	1-12		-1	72	74
3	9	0	145	120	4	-8	C	112	112	4	3	1	72	45	0	4	-1	251	248	2	-1	-1	350	353
3	10	C	61	70	4	-9	C	183	171	4	4	1	-38	5	0	5	-1	518	512	2	-2	-1	122	118
3	11	0	84	74	4-10		C	211	186	4	5	1	242	263	0	6	-1	403	390	2	-3	-1	74	-53
3	12	C	36	53	4-11		0	96	89	4	6	1	368	364	0	7	-1	81	57	2	-4	-1	365	387
4	0	C	46	56	4-12		0	-25	39	4	7	1	94	89	0	8	-1	127	138	2	-5	-1	381	357
4	1	C	61	20	5	-1	0	152	156	4	8	1	113	97	0	9	-1	277	289	2	-6	-1	364	317
4	2	C	632	665	5	-2	0	249	243	4	9	1	137	133	1	0	-1	603	613	2	-7	-1	278	299
4	3	0	540	545	5	-3	0	145	140	4	10	1	216	210	1	1	-1	180	142	2	-8	-1	291	304
4	4	C	157	160	5	-4	0	113	116	4	11	1	125	137	1	2	-1	597	-634	2	-9	-1	221	221
4	5	C	64	61	5	-5	0	42	-16	5	0	1	132	121	1	3	-1	60	39	2-10		-1	103	63
4	6	0	440	424	5	-6	0	108	109	5	1	1	199	195	1	4	-1	503	564	2-11		-1	101	110
4	7	C	239	247	5	-7	0	187	185	5	2	1	148	151	1	5	-1	416	453	2-12		-1	48	52
4	8	C	204	177	5	-8	C	204	186	5	3	1	204	200	1	6	-1	227	224	3	-1	-1	274	274
4	9	C	-45	11	5	-9	0	94	80	5	4	1	284	297	1	7	-1	253	243	3	-2	-1	42	33
4	10	0	63	67	5-10		0	134	137	5	5	1	256	278	1	8	-1	496	531	3	-3	-1	310	323
4	11	0	87	108	5-11		0	95	96	5	6	1	302	282	1	9	-1	305	307	3	-4	-1	225	182
5	0	0	295	267	6	-1	0	264	246	5	7	1	154	128	1	10	-1	94	74	3	-5	-1	169	144
5	1	C	550	551	6	-2	0	110	109	5	8	1	83	84	2	0	-1	159	153	3	-6	-1	59	54
5	2	0	303	343	6	-3	0	136	131	5	9	1	128	136	2	1	-1	59	55	3	-7	-1	183	186
5	3	C	218	228	6	-4	0	69	71	5	10	1	100	109	2	2	-1	308	350	3	-8	-1	264	262
5	4	C	146	147	6	-5	0	144	130	6	0	1	89	-37	2	3	-1	867	909	3	-9	-1	287	265
5	5	0	241	239	6	-6	0	169	159	6	1	1	255	264	2	4	-1	429	464	3-10		-1	135	123
5	6	C	205	208	6	-7	0	155	146	6	2	1	368	362	2	5	-1	221	254	3-11		-1	43	40
5	7	0	157	130	6	-8	0	-45	7	6	3	1	291	281	2	6	-1	275	269	3-12		-1	75	78
5	8	C	-46	27	6	-9	0	93	94	6	4	1	162	164	2	7	-1	468	504	4	-1	-1	440	476
5	9	0	98	91	6-10		0	62	55	6	5	1	286	230	2	8	-1	173	163	4	-2	-1	353	348
5	10	C	160	155	7	-1	0	140	151	6	6	1	152	158	2	9	-1	170	150	4	-3	-1	38	-8
6	0	0	294	317	7	-2	0	284	259	6	7	1	129	117	2	10	-1	-45	22	4	-4	-1	157	134
6	1	C	267	289	7	-3	C	282	244	6	8	1	41	54	3	0	-1	437	450	4	-5	-1	278	266
6	2	0	258	270	7	-4	0	114	104	7	0	1	274	248	3	1	-1	440	438	4	-6	-1	234	239
6	3	0	226	225	7	-5	0	60	67	7	1	1	305	287	3	2	-1	398	434	4	-7	-1	45	-16
6	4	0	200	203	7	-6	0	101	97	7	2	1	175	171	3	3	-1	205	250	4	-8	-1	124	126
6	5	C	154	128	7	-7	0	110	103	7	3	1	56	54	3	4	-1	636	652	4	-9	-1	163	133
6	6	0	95	81	7	-8	0	61	61	7	4	1	170	164	3	5	-1	428	462	4-10		-1	159	142
6	7	0	55	61	7	-9	0	34	-24	7	5	1	193	208	3	6	-1	151	139	4-11		-1	60	60
6	8	0	68	62	8	-1	0	-45	17	7	6	1	120	111	3	7	-1	66	73	5	-1	-1	490	520
6	9	0	83	101	8	-2	0	103	86	8	0	1	266	262	3	8	-1	277	259	5	-2	-1	499	522
7	0	0	98	94	8	-3	0	258	246	8	1	1	142	129	3	9	-1	115	112	5	-3	-1	204	190
7	1	0	308	279	8	-4	0	232	216	8	2	1	-42	37	3	10	-1	89	67	5	-4	-1	58	43
7	2	0	317	293	8	-5	0	71	80	8	3	1	131	132	4	0	-1	498	496	5	-5	-1	82	66
7	3	0	81	69	8	-6	0	55	65	8	4	1	146	160	4	1	-1	58	27	5	-6	-1	123	115
7	4	0	74	-38	8	-7	0	69	80	1	-1	1	94	-42	4	2	-1	133	149	5	-7	-1	135	137
7	5	0	99	87	9	-1	0	80	81	1	-2	1	938	1067	4	3	-1	591	619	5	-8	-1	-47	3
7	6	0	131	127	9	-2	0	57	66	1	-3	1	300	304	4	4	-1	490	528	5	-9	-1	57	53
7	7	0	73	86	0	1	1	234	-254	1	-4	1	56	29	4	5	-1	163	159	5-10		-1	142	143
8	0	C	188	178	0	2	1	891	1010	1	-5	1	256	247	4	6	-1	114	102	5-11		-1	93	100
8	1	C	175	169	0	3	1	1052	1176	2	-1	1	1264	1373	4	7	-1	200	196	6	-1	-1	284	264
8	2	C	-43	24	0	4	1	483	480	2	-2	1	209	237	4	8	-1	214	203	6	-2	-1	364	377
8	3	0	68	-25	0	5	1	85	73	2	-3	1	449	459	4	9	-1	-47	25	6	-3	-1	303	315

Table 4. Continued.

H	K	L	F(O)	F(C)	H	K	L	F(O)	F(C)	H	K	L	F(O)	F(C)	H	K	L	F(O)	F(C)	H	K	L	F(O)	F(C)
6	-4	-1	140	123	1	-12	2	74	84	2	2	-2	83	81	6	-2	-2	202	202	8	2	3	123	123
6	-5	-1	155	147	1	-13	2	47	46	2	3	-2	297	353	6	-3	-2	198	214	8	3	3	100	108
6	-6	-1	151	130	2	-1	2	1019	945	2	4	-2	808	772	6	-4	-2	190	195	1	-1	3	192	234
6	-7	-1	78	63	2	-2	2	747	719	2	5	-2	544	507	6	-5	-2	205	215	1	-2	3	531	642
6	-8	-1	43	26	2	-3	2	223	163	2	6	-2	154	131	6	-6	-2	154	144	1	-3	3	377	391
6	-9	-1	90	107	2	-4	2	164	-117	2	7	-2	190	191	6	-7	-2	67	72	1	-4	3	218	210
6	-10	-1	38	39	2	-5	2	226	206	2	8	-2	150	154	6	-8	-2	71	78	1	-5	3	289	293
7	-1	-1	297	272	2	-6	2	268	278	2	9	-2	190	191	7	-1	-2	101	92	1	-6	3	500	522
7	-2	-1	210	189	2	-7	2	219	188	2	10	-2	68	80	7	-2	-2	56	48	2	-1	3	156	-168
7	-3	-1	106	108	2	-8	2	48	42	2	11	-2	-41	30	7	-3	-2	81	78	2	-2	3	265	299
7	-4	-1	78	75	2	-9	2	181	211	2	12	-2	63	85	7	-4	-2	141	144	2	-3	3	273	-296
7	-5	-1	168	140	2	-10	2	308	330	3	0	-2	661	690	7	-5	-2	138	140	2	-4	3	322	312
7	-6	-1	199	152	2	-11	2	206	198	3	1	-2	653	627	7	-6	-2	104	117	2	-5	3	203	175
7	-7	-1	133	135	2	-12	2	64	65	3	2	-2	789	762	7	-7	-2	57	56	2	-6	3	425	433
7	-8	-1	61	75	2	-13	2	25	23	3	3	-2	317	289	8	-1	-2	85	99	2	-7	3	603	630
8	-1	-1	76	-42	3	-1	2	239	219	3	4	-2	183	174	8	-2	-2	174	178	3	-1	3	107	121
8	-2	-1	182	171	3	-2	2	447	436	3	5	-2	122	133	8	-3	-2	-41	26	3	-2	3	366	-385
8	-3	-1	170	160	3	-3	2	649	661	3	6	-2	181	186	8	-4	-2	54	-30	3	-3	3	429	466
8	-4	-1	78	72	3	-4	2	104	-74	3	7	-2	42	44	8	-5	-2	40	42	3	-4	3	340	387
8	-5	-1	-38	39	3	-5	2	152	-147	3	8	-2	128	112	8	-6	-2	89	105	3	-5	3	122	106
8	-6	-1	120	130	3	-6	2	304	299	3	9	-2	82	109	0	0	3	218	227	3	-6	3	63	-52
0	0	2	190	-232	3	-7	2	392	405	3	10	-2	180	172	0	1	3	467	544	3	-7	3	301	301
0	1	2	422	-393	3	-8	2	141	136	3	11	-2	149	157	0	2	3	505	582	3	-8	3	388	409
0	2	2	80	37	3	-9	2	41	41	3	12	-2	113	123	0	3	3	66	49	4	-1	3	233	229
0	3	2	654	629	3	-10	2	108	103	4	0	-2	546	523	0	4	3	241	-211	4	-2	3	358	342
0	4	2	380	355	3	-11	2	207	219	4	1	-2	382	406	0	5	3	207	204	4	-3	3	232	193
0	5	2	413	404	3	-12	2	86	90	4	2	-2	80	66	0	6	3	380	419	4	-4	3	257	244
0	6	2	401	434	3	-13	2	20	23	4	3	-2	159	144	0	7	3	225	229	4	-5	3	168	175
1	0	2	795	826	4	-1	2	376	352	4	4	-2	239	270	0	8	3	62	63	4	-6	3	99	84
1	1	2	377	421	4	-2	2	393	383	4	5	-2	276	283	0	9	3	125	117	4	-7	3	-64	26
1	2	2	425	434	4	-3	2	329	350	4	6	-2	-42	2	0	10	3	218	211	4	-8	3	203	185
1	3	2	332	347	4	-4	2	546	511	4	7	-2	-45	7	0	11	3	91	85	5	-1	3	274	264
1	4	2	484	466	4	-5	2	268	234	4	8	-2	197	208	0	12	3	-28	-5	5	-2	3	218	212
1	5	2	308	319	4	-6	2	77	45	4	9	-2	300	254	1	0	3	239	303	5	-3	3	264	250
1	6	2	407	402	4	-7	2	60	59	4	10	-2	169	168	1	1	3	390	376	5	-4	3	240	230
1	7	2	171	168	4	-8	2	166	177	4	11	-2	55	63	1	2	3	315	263	5	-5	3	-60	40
1	8	2	59	76	4	-9	2	65	60	5	0	-2	309	314	1	3	3	177	168	5	-6	3	71	52
2	0	2	113	-80	4	-10	2	70	66	5	1	-2	69	-65	1	4	3	153	129	5	-7	3	206	189
2	1	2	396	358	4	-11	2	79	81	5	2	-2	50	3	1	5	3	199	179	5	-8	3	198	168
2	2	2	639	646	4	-12	2	93	102	5	3	-2	335	345	1	6	3	270	279	6	-1	3	252	267
2	3	2	432	455	5	-1	2	242	239	5	4	-2	374	384	1	7	3	207	166	6	-2	3	118	102
2	4	2	244	253	5	-2	2	355	332	5	5	-2	59	38	1	8	3	236	249	6	-3	3	166	152
2	5	2	257	263	5	-3	2	375	336	5	6	-2	-46	37	1	9	3	178	173	6	-4	3	317	342
2	6	2	200	207	5	-4	2	342	307	5	7	-2	204	214	1	10	3	122	119	6	-5	3	266	293
2	7	2	174	176	5	-5	2	305	315	5	8	-2	250	256	1	11	3	56	67	6	-6	3	86	62
2	8	2	104	115	5	-6	2	208	188	5	9	-2	96	111	2	0	3	51	-43	6	-7	3	-71	17
3	0	2	368	357	5	-7	2	172	157	5	10	-2	-30	25	2	1	3	355	402	6	-8	3	123	113
3	1	2	644	672	5	-8	2	101	107	6	0	-2	44	-24	2	2	3	540	545	7	-1	3	247	229
3	2	2	531	552	5	-9	2	85	87	6	1	-2	127	127	2	3	3	232	207	7	-2	3	144	123
3	3	2	316	322	5	-10	2	64	54	6	2	-2	136	129	2	4	3	291	254	7	-3	3	103	73
3	4	2	120	118	5	-11	2	50	50	6	3	-2	159	148	2	5	3	346	342	7	-4	3	162	128
3	5	2	217	223	6	-1	2	124	112	6	4	-2	73	95	2	6	3	382	391	7	-5	3	262	276
3	6	2	240	258	6	-2	2	110	99	6	5	-2	160	161	2	7	3	265	289	7	-6	3	231	248
3	7	2	92	100	6	-3	2	289	276	6	6	-2	261	233	2	8	3	-63	16	7	-7	3	90	62
3	8	2	90	-83	6	-4	2	293	294	6	7	-2	290	262	2	9	3	104	68	8	-1	3	66	54
3	9	2	-43	40	6	-5	2	70	41	6	8	-2	92	110	2	10	3	112	92	8	-2	3	122	113
4	0	2	540	531	6	-6	2	93	95	6	9	-2	64	76	2	11	3	81	77	8	-3	3	104	84
4	1	2	368	362	6	-7	2	237	221	7	0	-2	108	105	3	0	3	481	503	8	-4	3	87	87
4	2	2	148	132	6	-8	2	250	222	7	1	-2	-45	35	3	1	3	642	707	8	-5	3	124	129
4	3	2	58	-36	6	-9	2	98	90	7	2	-2	159	147	3	2	3	349	320	8	-6	3	105	107
4	4	2	99	106	6	-10	2	36	49	7	3	-2	180	191	3	3	3	205	176	0	1	-3	168	237
4	5	2	314	333	7	-1	2	186	154	7	4	-2	206	208	3	4	3	219	229	0	2	-3	494	572
4	6	2	133	126	7	-2	2	91	-57	7	5	-2	235	203	3	5	3	454	410	0	3	-3	547	646
4	7	2	-46	21	7	-3	2	-46	30	7	6	-2	165	151	3	6	3	257	229	0	4	-3	468	530
4	8	2	83	113	7	-4	2	184	162	7	7	-2	93	102	3	7	3	-65	16	0	5	-3	331	308
4	9	2	182	181	7	-5	2	252	232	8	0	-2	82	72	3	8	3	86	73	0	6	-3	294	259
5	0	2	217	202	7	-6	2	88	80	8	1	-2	89	88	3	9	3	149	145	0	7	-3	390	347
5	1	2	54	38	7	-7	2	72	66	8	2	-2	198	200	3	10	3	115	97	0	8	-3	367	349
5	2	2	59	50	7	-8	2	135	153	8	3	-2	213	223	3	11	3	-19	-3	1	0	-3	344	345
5	3	2	103	123	7	-9	2	155	180	8	4	-2	135	129	4	0	3	445	463	1	1	-3	657	836
5	4	2	250	250	8	-1	2	149	164	1	-1	-2	476	-653	4	1	3	416	384	1	2	-3	784	983
5	5	2	113	118	8	-2	2	98	102	1	-2	-2	161	138	4	2	3	195	165	1	3	-3	734	860
5	6	2	208	194	8	-3	2	-41	-22	1	-3	-2	491	516	4	3	3	194	177	1	4	-3	105	-54
5	7	2	100	114	8	-4	2	-39	18	1	-4	-2	509	532	4	4	3	332	314	1	5	-3	158	164
5	8	2	156	170	8	-5	2	96	92	1	-5	-2	124	112	4	5	3	260	241	1	6	-3	410	415
6	0	2	203	154	8	-6	2	94	94	2	-1	-2	389	365	4	6	3	-68	2	1	7	-3	314	271
6	1	2	280	263	8	-7	2	60	72	2	-2	-2	71	65	4	7	3	113	85	1	8	-3	199	-152
6	2	2	-42	10	0	1	-2	520	521	2	-3	-2	300	326	4	8	3	185	175	1	9	-3	125	91
6	3	2	45	-6	0	2	-2	567	623	2	-4	-2	341	339	4	9	3	136	112	1	10	-3	179	179
6	4	2	166	157	0	3	-2	502	520	2	-5	-2	214	215	4	10	3	-31	14	2	0	-3	431	459
6	5	2	296	266	0	4	-2	377	354	2	-6	-2	65	61	5	0	3	411	425	2	1	-3	553	648
6	6	2	112	129	0	5	-2	451	406	2	-7	-2	146	167	5	1	3	338	350	2	2	-3	392	393
6	7	2	114	123	0	6	-2	678	660	3	-1	-2	370	351	5	2	3	276	264	2	3	-3	60	-42
7	0	2	299	258	0	7	-2	395	377	3	-2	-2	165	141	5	3	3	181	140	2	4	-3	328	282
7	1	2	104	91	0	8	-2	174	171	3	-3	-2	302	308	5	4	3	109	70	2	5	-3	295	295
7	2	2	-47	9	0	9	-2	43	22	3	-4	-2	208	210	5	5	3	-72	52	2	6	-3	220	208
7	3	2	140	134	0	10	-2	268	272	3	-5	-2	46	35	5	6	3	169	132	2	7	-3	60	18
7	4	2	233	242	0	11	-2	144	147	3	-6	-2	84	89	5	7	3	63	55	2	8	-3	195	163
7	5	2	202	199	0	12	-2	49	42	3	-7	-2	103	114	5	8	3	75	76	2	9	-3	323	295
7	6	2	66	71	0	13	-2	-27	32	4	-1	-2	323	313	5	9	3	82	87	2	10	-3	316	242
8	0	2	125	126	1	0	-2	264	250	4	-2	-2	276	263	6	0	3	326	326	2	11	-3	74	56
8	1	2	80	73	1	1	-2	1002	1081	4	-3	-2	228	236	6	1	3	246	207	3	0	-3	427	423
8	2	2	141	151	1	2	-2	580	608	4	-4	-2	458	509	6	2	3	-66	29	3	1	-3	272	246
8	3	2	191	206	1	3	-2	150	108	4	-5	-2	288	339	6	3	3	-70	26	3	2	-3	80	83
8	4	2	141	150	1	4	-2	328	274	4	-6	-2	-43	-3	6	4	3	192	167	3	3	-3	152	160
1	-1	2	102	-47	1	5	-2	970	962	4	-7	-2	96	-109	6	5	3	92	74	3	4	-3	357	292
1	-2	2	481	418	1	6	-2	489	481	4	-8	-2	176	191	6	6	3	-59	22	3	5	-3	308	257
1	-3	2	59	37	1	7	-2	105	-65	5	-1	-2	359	343	6	7	3	82	85	3	6	-3	105	75
1	-4	2	264	251	1	8	-2	38	60	5	-2	-2	152	156	7	0	3	77	55	3	7	-3	196	185
1	-5	2	248	205	1	9	-2	395	406	5	-3	-2	161	166	7	1	3	-69	-25	3	8	-3	370	303
1	-6	2	262	261	1	10	-2	183	181	5	-4	-2	284	297	7	2	3	85	78	3	9	-3	280	235
1	-7	2	256	286	1	11	-2	-42	33	5	-5	-2	321	344	7	3	3	243	233	3	10	-3	137	124
1	-8	2	290	278	1	12	-2	-36	-1	5	-6	-2	165	175	7	4	3	127	105	3	11	-3	86	81
1	-9	2	309	312	1	13	-2	61	81	5	-7	-2	98	117	7	5	3	69	51	4	0	-3	358	350
1	-10	2	240	243	2	0	-2	576	533	5	-8	-2	-44	-6	8	0	3	57	55	4	1	-3	342	317
1	-11	2	175	178	2	1	-2	687	656	6	-1	-2	172	181	8	1	3	61	55	4	2	-3	194	204

Table 4. Continued.

H	K	L	F(O)	F(C)	H	K	L	F(O)	F(C)	H	K	L	F(O)	F(C)	H	K	L	F(O)	F(C)	H	K	L	F(O)	F(C)
4	3	-3	87	-59	3	-9	-3	-62	24	3	0	9	132	109	0	12	2	58	65	0	11	-4	177	170
4	4	-3	58	22	3	-10	-3	55	40	3	0	10	121	124	0	1	4	510	550	0	12	-4	109	129
4	5	-3	238	259	3	-11	-3	41	42	4	0	4	178	164	0	2	4	405	438	0	13	-4	97	107
4	6	-3	355	322	4	-1	-3	188	174	4	0	5	120	111	0	3	4	263	255	0	1	-5	276	302
4	7	-3	241	187	4	-2	-3	232	235	4	0	6	264	289	0	4	4	332	346	0	2	-5	134	142
4	8	-3	274	217	4	-3	-3	316	321	4	0	7	156	166	0	5	4	144	135	0	3	-5	244	274
4	9	-3	291	243	4	-4	-3	312	308	4	0	8	-100	10	0	6	4	-66	-4	0	4	-5	160	157
4	10	-3	244	223	4	-5	-3	170	142	4	0	9	143	136	0	7	4	61	-52	0	5	-5	210	239
4	11	-3	93	83	4	-6	-3	80	68	5	0	4	324	315	0	8	4	67	82	0	6	-5	95	120
5	0	-3	264	271	4	-7	-3	230	245	5	0	5	140	110	0	9	4	182	167	0	7	-5	181	202
5	1	-3	208	208	4	-8	-3	193	181	5	0	6	-107	-28	0	10	4	123	125	0	8	-5	203	200
5	2	-3	-54	-2	4	-9	-3	-59	2	5	0	7	-102	72	0	11	4	57	63	0	9	-5	232	227
5	3	-3	199	200	4	-10	-3	-48	11	5	0	8	211	219	0	1	5	246	246	0	10	-5	212	198
5	4	-3	389	404	4	-11	-3	49	77	5	0	9	109	130	0	2	5	260	278	0	11	-5	309	246
5	5	-3	334	319	5	-1	-3	101	68	6	0	4	220	203	0	3	5	364	349	0	12	-5	160	141
5	6	-3	160	122	5	-2	-3	84	-53	6	0	5	-107	34	0	4	5	279	234	0	13	-5	57	60
5	7	-3	137	107	5	-3	-3	117	106	6	0	6	-97	56	0	5	5	250	222	0	1	-6	209	212
5	8	-3	309	245	5	-4	-3	256	254	6	0	7	192	175	0	6	5	205	199	0	2	-6	244	247
5	9	-3	299	273	5	-5	-3	260	276	6	0	8	124	139	0	7	5	72	90	0	3	-6	311	350
5	10	-3	-44	39	5	-6	-3	156	146	7	0	4	-99	41	0	8	5	-61	50	0	4	-6	248	289
6	0	-3	104	86	5	-7	-3	143	128	7	0	5	113	121	0	9	5	69	66	0	5	-6	210	223
6	1	-3	151	140	5	-8	-3	152	125	7	0	6	100	104	0	10	5	-39	40	0	6	-6	217	229
6	2	-3	152	206	5	-9	-3	120	131	8	0	4	96	75	0	1	6	132	116	0	7	-6	266	274
6	3	-3	382	364	5	-10	-3	-37	28	1	0	-4	69	25	0	2	6	146	130	0	8	-6	344	346
6	4	-3	361	314	6	-1	-3	254	256	1	0	-5	163	188	0	3	6	211	210	0	9	-6	230	196
6	5	-3	175	128	6	-2	-3	76	63	1	0	-6	237	261	0	4	6	71	54	0	10	-6	70	65
6	6	-3	-74	40	6	-3	-3	80	-39	1	0	-7	243	264	0	5	6	253	244	0	11	-6	121	98
6	7	-3	214	187	6	-4	-3	-69	26	1	0	-8	210	231	0	6	6	170	164	0	12	-6	144	140
6	8	-3	184	187	6	-5	-3	182	158	1	0	-9	127	117	0	7	6	151	164	0	1	-7	231	241
6	9	-3	44	44	6	-6	-3	167	156	1	0	-10	-90	43	0	8	6	117	136	0	2	-7	65	90
7	0	-3	263	244	6	-7	-3	102	102	1	0	-11	-58	54	0	9	6	95	93	0	3	-7	228	229
7	1	-3	97	115	6	-8	-3	83	84	2	0	-4	182	171	0	1	7	169	161	0	4	-7	392	433
7	2	-3	233	203	6	-9	-3	79	91	2	0	-5	-83	-5	0	2	7	-65	50	0	5	-7	352	398
7	3	-3	235	206	7	-1	-3	141	113	2	0	-6	329	338	0	3	7	118	106	0	6	-7	191	213
7	4	-3	194	158	7	-2	-3	70	69	2	0	-7	440	444	0	4	7	96	88	0	7	-7	169	131
7	5	-3	106	112	7	-3	-3	71	53	2	0	-8	-102	85	0	5	7	171	174	0	8	-7	236	191
7	6	-3	149	129	7	-4	-3	130	115	2	0	-9	-104	31	0	6	7	-67	45	0	9	-7	151	147
7	7	-3	113	104	7	-5	-3	92	73	2	0	-10	-87	67	0	7	7	54	63	0	10	-7	-67	44
8	0	-3	161	173	7	-6	-3	73	75	3	0	-4	-79	24	0	8	7	81	84	0	11	-7	-52	5
8	1	-3	116	121	7	-7	-3	-43	38	3	0	-5	200	208	0	1	8	83	93	0	12	-7	58	69
8	2	-3	92	102	8	-1	-3	180	195	3	0	-6	147	165	0	2	8	195	181	0	1	-8	374	360
8	3	-3	147	151	8	-2	-3	111	99	3	0	-7	297	300	0	3	8	200	199	0	2	-8	258	231
8	4	-3	153	153	8	-3	-3	-56	22	3	0	-8	109	133	0	4	8	139	127	0	3	-8	74	93
1	-1	-3	224	250	8	-4	-3	56	55	3	0	-9	103	103	0	5	8	-68	50	0	4	-8	135	125
1	-2	-3	433	454	8	-5	-3	87	117	3	0	-10	-77	61	0	6	8	-52	21	0	5	-8	357	359
1	-3	-3	200	113	0	0	1	463	484	4	0	-4	-90	82	0	7	8	37	46	0	6	-8	111	116
1	-4	-3	118	-56	0	0	4	751	756	4	0	-5	224	245	0	1	9	154	148	0	7	-8	-79	-19
1	-5	-3	-51	21	0	0	5	457	456	4	0	-6	269	263	0	2	9	203	190	0	8	-8	-91	37
1	-6	-3	280	292	0	0	6	92	92	4	0	-7	-110	67	0	3	9	151	137	0	9	-8	228	197
1	-7	-3	300	335	0	0	7	286	260	4	0	-8	110	115	0	4	9	69	60	0	10	-8	173	177
1	-8	-3	140	125	0	0	8	162	155	4	0	-9	186	192	0	5	9	-45	50	0	11	-8	80	83
1	-9	-3	-62	47	0	0	9	74	59	4	0	-10	111	116	0	1	10	160	159	0	1	-9	186	191
1	-10	-3	99	74	0	0	10	-90	50	5	0	-4	253	247	0	2	10	137	127	0	2	-9	289	272
1	-11	-3	123	136	0	0	11	94	111	5	0	-5	-99	28	0	3	10	53	51	0	3	-9	142	120
1	-12	-3	62	74	1	0	4	294	300	5	0	-6	107	123	0	1	-1	530	621	0	4	-9	181	-169
2	-1	-3	520	560	1	0	5	314	340	5	0	-7	121	115	0	10	-1	290	282	0	5	-9	73	76
2	-2	-3	301	268	1	0	6	534	542	5	0	-8	-96	60	0	11	-1	120	108	0	6	-9	221	228
2	-3	-3	454	483	1	0	7	146	156	5	0	-9	109	115	0	12	-1	56	64	0	7	-9	221	201
2	-4	-3	369	358	1	0	8	-97	29	6	0	-4	300	332	0	13	-1	113	110	0	8	-9	-81	51
2	-5	-3	190	158	1	0	9	191	167	6	0	-5	237	204	0	9	-3	-62	7	0	9	-9	115	97
2	-6	-3	75	-43	1	0	10	107	124	6	0	-6	-106	-53	0	10	-3	87	79	0	10	-9	242	210
2	-7	-3	188	161	1	0	11	-52	54	6	0	-7	-93	60	0	11	-3	122	130	0	1	-10	-72	-47
2	-8	-3	112	92	2	0	4	185	182	6	0	-8	117	142	0	12	-3	79	78	0	2	-10	109	95
2	-9	-3	62	55	2	0	5	661	699	7	0	-4	240	210	0	13	-3	-37	49	0	3	-10	186	215
2	-10	-3	-58	32	2	0	6	250	260	7	0	-5	145	145	0	1	-4	296	328	0	4	-10	109	111
2	-11	-3	70	80	2	0	7	94	-98	7	0	-6	-83	73	0	2	-4	347	356	0	5	-10	90	47
3	-1	-3	264	274	2	0	8	-100	78	7	0	-7	-61	65	0	3	-4	296	328	0	6	-10	169	143
3	-2	-3	449	461	2	0	9	207	214	8	0	-4	116	132	0	4	-4	133	141	0	7	-10	279	232
3	-3	-3	401	410	2	0	10	132	138	8	0	-5	-62	42	0	5	-4	261	287	0	8	-10	222	192
3	-4	-3	248	245	3	0	4	354	329	0	7	2	421	426	0	6	-4	116	113	0	1	-11	-57	19
3	-5	-3	152	120	3	0	5	329	296	0	8	2	193	219	0	7	-4	184	188	0	2	-11	72	64
3	-6	-3	306	349	3	0	6	116	86	0	9	2	-56	-65	0	8	-4	223	224	0	3	-11	210	190
3	-7	-3	113	105	3	0	7	208	205	0	10	2	99	99	0	9	-4	177	180	0	4	-11	214	228
3	-8	-3	107	57	3	0	8	-102	73	0	11	2	131	130	0	10	-4	98	92	0	5	-11	114	110
																				0	6	-11	86	57

The structure of this complex is similar to the structure of the corresponding trimethylenethiourea complex,[3] $Te(trtu)_2(S_2O_2C_6H_5)_2$. The tellurium atom is bonded to two ethylenethiourea sulphur atoms and two benzenethiosulphonate sulphur atoms. With the tellurium atom in a centre of symmetry, the TeS_4 group is *trans* square-planar. The S – Te – S angle deviates slightly from 90°. The Te – S bond lengths are close to 2.68 Å, which is a weighted average value of Te – S bond lengths in *trans* square-planar complexes of divalent tellurium, based on earlier investigations.[1]

The S – S bond length of the benzenethiosulphonate group, 2.016(5) Å, agrees with the S – S bond length in $Te(trtu)_2(S_2O_2C_6H_5)_2$,[3] which was found

Table 5. Bond lengths (Å) and angles (°). Standard deviations in parentheses.

TeS_4 coordination group

Te–S(1)	2.713(5)	∠S(1)–Te–S(2)	90.80(13)
Te–S(2)	2.686(4)		

Benzenethiosulphonate group

S(2)–S(3)	2.016(5)	∠Te –S(2)–S(3)	105.87(16)
S(3)–O(1)	1.458(10)	∠S(2)–S(3)–O(1)	112.5(5)
S(3)–O(2)	1.416(16)	∠S(2)–S(3)–O(2)	106.6(5)
S(3)–C(1)	1.724(15)	∠S(2)–S(3)–C(1)	105.6(6)
C(1)–C(2)	1.358(18)	∠O(1)–S(3)–O(2)	119.1(8)
C(2)–C(3)	1.488(24)	∠O(1)–S(3)–C(1)	106.4(7)
C(3)–C(4)	1.405(26)	∠O(2)–S(3)–C(1)	105.7(7)
C(4)–C(5)	1.301(19)	∠S(3)–C(1)–C(2)	118.7(13)
C(5)–C(6)	1.425(23)	∠S(3)–C(1)–C(6)	119.3(9)
C(6)–C(1)	1.414(23)	∠C(6)–C(1)–C(2)	121.7(13)
		∠C(1)–C(2)–C(3)	118.5(16)
		∠C(2)–C(3)–C(4)	117.6(13)
		∠C(3)–C(4)–C(5)	121.3(16)
		∠C(4)–C(5)–C(6)	123.4(17)
		∠C(5)–C(6)–C(1)	117.0(12)

Ethylenethiourea group

S(1)–C(7)	1.726(14)	∠Te –S(1)–C(7)	103.6(6)
C(7)–N(1)	1.267(24)	∠S(1)–C(7)–N(1)	122.1(10)
C(7)–N(2)	1.332(16)	∠S(1)–C(7)–N(2)	124.9(13)
N(1)–C(8)	1.526(22)	∠N(1)–C(7)–N(2)	113.0(14)
N(2)–C(9)	1.527(25)	∠C(7)–N(1)–C(8)	113.2(13)
C(8)–C(9)	1.491(25)	∠C(7)–N(2)–C(9)	107.6(15)
		∠N(1)–C(8)–C(9)	100.0(15)
		∠N(2)–C(9)–C(8)	105.1(13)

to be 2.018(4) Å. It is intermediate between the corresponding bond length in uncomplexed tellurium dibenzenethiosulphonate,[8] and in ionic sodium methanethiosulphonate monohydrate,[9] which are 2.080(2) and 1.98(1) Å, respectively, although it is closer to the latter value.

The atoms bonded to S(3) form an approximate tetrahedron, with greatest deviation in the O(1)–S(3)–O(2) angle, which is 119.1(8)°. With the sulphur coordinates given three times the weight of the carbon and nitrogen coordinates, the atoms of a least squares plane through S(3) and the benzene ring deviate 0.003–0.040 Å from the plane. The atoms of a least squares plane through the ethylenethiourea group deviate 0.000–0.092 Å from the plane.

The hydrogen atoms bonded to the ethylenethiourea nitrogen atoms appear to be engaged in hydrogen bonding to the benzenethiosulphonate oxygen atoms. This is illustrated in Fig. 2. The N(2)···O(1) distance, which occurs within the molecule, is 2.859(17) Å. The C(7)–N(2)···O(1) angle is 134.9(10)°, and the C(9)–N(2)···O(1) angle is 110.3(8)°. The other hydrogen bond occurs between neighbouring molecules. With O(2″) at $-x,-y,1-z$ relative to O(2), the N(1)···O(2″) distance is 2.984(19) Å. The C(7)–N(1)···O(2″) angle is 130.9(10)°, and the C(8)–N(1)···O(2″) angle is 115.1(12)°. O(1) and O(2″)

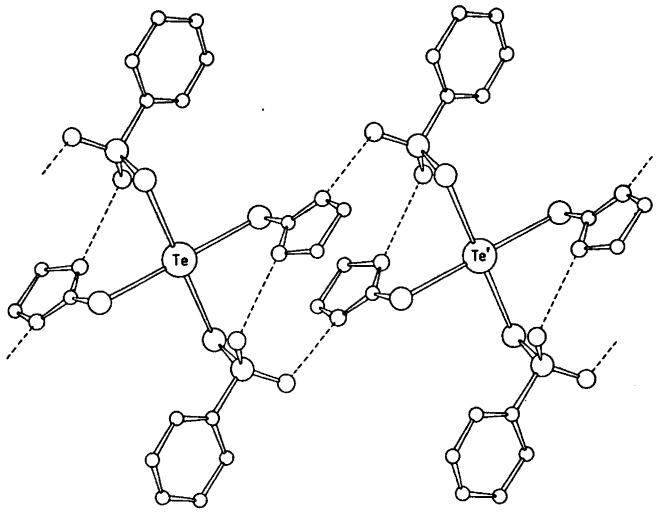

Fig. 2. Two of the molecules of the infinite chain along the *c* axis, as seen along the normal to the $(1\bar{1}0)$ plane. With Te at the origin, Te′ is at lattice point 0,0,1. Hydrogen bonds indicated by dashed lines.

are 0.754 and 0.534 Å, respectively, out of the least squares plane through the ethylenethiourea group referred to above. As is seen in Fig. 2, the molecules are linked together in infinite chains along the *c* axis by hydrogen bonds. This is in agreement with the fact that the crystals are easily cleaved along the *c*-axis direction.

We thank Professor Olav Foss for his interest in this work. One of us (K. Å.) is indebted to *Norges Almenvitenskapelige Forskningsråd* for financial support.

REFERENCES

1. Foss, O. In Andersen, P., Bastiansen, O. and Furberg, S. *Selected Topics in Structure Chemistry*, Universitetsforlaget, Oslo 1967, p. 145.
2. Foss, O. and Johannessen, I. J. *Acta Chem. Scand.* **15** (1961) 1943.
3. Åse, K. *Acta Chem. Scand.* **23** (1969) 3206.
4. *International Tables for X-ray Crystallography*, Kynoch Press, Birmingham 1962, Vol. III, p. 122.
5. Busing, W. R. and Levy, A. H. *Acta Cryst.* **10** (1957) 180.
6. Cromer, D. T. *Acta Cryst.* **18** (1965) 17.
7. Zachariasen, W. H. *Acta Cryst.* **16** (1963) 1139.
8. Åse, K. *Acta Chem. Scand.* **25** (1971) 838.
9. Foss, O. and Hordvik, A. *Acta Chem. Scand.* **18** (1964) 619.

Received December 2, 1970.