ACTA CHEMICA SCANDINAVICA 25 (1971) 2457–2466

The Crystal and Molecular Structures of *trans* Square-planar Complexes of Tellurium Dithiocyanate and Diselenocyanate with Ethylenethiourea

KJELL ÅSE, KJELL BØYUM, OLAV FOSS and KJARTAN MARØY

Chemical Institute, University of Bergen, Bergen, Norway

The crystal and molecular structures of *trans*-dithiocyanato- and *trans*-diselenocyanato-bis(ethylenethiourea)tellurium(II), $Te(etu)_2(SCN)_2$ (I) and $Te(etu)_2(SeCN)_2$ (II), have been determined by X-ray methods, and refined by least squares for the $0kl-2kl$ and $h0l$ reflections. The crystals of the two compounds are isomorphous, space group $P2_1/c$ (No. 14) with $Z=2$, and unit cells, $a=6.00$ Å, $b=12.47$ Å, $c=10.92$ Å, $\beta=99.6°$ for I, and $a=6.24$ Å, $b=12.62$ Å, $c=10.83$ Å, $\beta=101.7°$ for II. The tellurium atoms lie in centres of symmetry.

The dimensions of the *trans* square-planar coordination groups are: Te–S(thiocyanate) = 2.684(7) Å, Te–S(etu) = 2.651(6) Å, ∠S–Te–S = 90.1(2)° in I, and Te–Se(selenocyanate) = 2.809(3) Å, Te–S(etu) = 2.676(6) Å, ∠Se–Te–S = 89.9(2)° in II. The thio- and selenocyanate ligands coordinate through the sulphur and selenium atoms, and not through the nitrogen atoms.

Whereas sulphur dithiocyanate, selenium dithiocyanate, and selenium diselenocyanate, $S(SCN)_2$, $Se(SCN)_2$, and $Se(SeCN)_2$, are known and their crystal structures have been determined,[1–3] neither tellurium dithiocyanate, $Te(SCN)_2$, nor tellurium diselenocyanate, $Te(SeCN)_2$, have been isolated so far, except possibly a polymeric form of the former.[4] Complexes of tellurium dithiocyanate [5–8] and tellurium diselenocyanate [9] with thioureas have been prepared, not from the parent compounds, but from other tellurium(II) complexes through displacements.

A complex, $Te(etu)_2(SCN)_2$, isolated earlier,[7] crystallizes in the space group $P2_1/c$ with four molecules per unit cell. The corresponding diselenocyanato complex, $Te(etu)_2(SeCN)_2$, was prepared later,[9] through reaction of the dibromo complex, $Te(etu)_2Br_2$, with potassium selenocyanate in methanol. It crystallizes in the space group $P2_1/c$ with two molecules per unit cell. The isomorphous dithiocyanato complex then crystallized from a filtered solution

of $Te(etu)_2Br_2$ and potassium thiocyanate in methanol, on seeding with crystals of the diselenocyanato complex.

The crystal structure analyses, reported here, were carried out in 1965–1966. The results have been mentioned in a review.[10]

CRYSTAL DATA

The crystals of *trans*-dithiocyanatobis(ethylenethiourea)tellurium(II), $Te(etu)_2(SCN)_2$ (I), and *trans*-diselenocyanatobis(ethylenethiourea)tellurium(II), $Te(etu)_2(SeCN)_2$ (II), are isomorphous. They are yellow and brownish-red, respectively, and occur as short prisms extended along the *a* axis, bounded by {010}, {011}, and {100}. The space group is $P2_1/c$ (No. 14), and there are two molecules per unit cell; the tellurium atoms are required to lie in centres of symmetry.

Unit cell dimensions were determined from *0kl* and *h0l* Weissenberg photographs, where sodium chloride powder lines had been superimposed for reference, $a_{NaCl} = 5.6394$ Å. The derived values, $a = 6.00$ Å, $b = 12.47$ Å, $c = 10.92$ Å, $\beta = 99.6°$ for I, and $a = 6.24$ Å, $b = 12.62$ Å, $c = 10.83$ Å, $\beta = 101.7°$ for II, are estimated to be reliable to within 0.3 %.

The *trans* form of $Te(etu)_2(SCN)_2$ obtained on seeding, considered here, appears to be unstable at room temperature, relative to the spontaneously crystallizing form. In the preparations of the former, crystals of the latter occurred in varying amounts; crystals of the former adhering to crystals of the latter had in some cases after a few days become opaque, and on oscillation photographs gave powder lines, and only faint layer lines of the original *trans* form. It was not possible, through seeding with the spontaneously crystallizing form of the dithiocyanato complex, to obtain isomorphous crystals of the diselenocyanato complex.

EXPERIMENTAL

Intensities of the *0kl*, *1kl*, *2kl*, and *h0l* reflections were estimated visually from multiple-film integrated equi-inclination Weissenberg photographs, taken with Ni-filtered Cu$K\alpha$ radiation. For the weakest *0kl* reflections of I, a non-integrated film set was used. Out of 865 accessible, independent reflections for I, and 867 for II, 607 and 645, respectively, were strong enough to be measured. The crystals used for collecting intensity data had cross-sections 0.05×0.05 mm for the *a*-axis photographs and 0.08×0.07 mm for the *b*-axis photographs of I, and 0.06×0.09 mm for the *a*-axis photographs and 0.09×0.13 mm for the *b*-axis photographs of II ($\mu = 200$ cm^{-1} for I, and 228 cm^{-1} for II). No corrections for absorption were made.

Lorentz-polarization corrections, and reduction to relative observed structure factors, were carried out on the IBM 650 computer, using Shiono's program,[11] and so were Fourier summations and structure factor calculations[12] in the early stages. Least squares refinement was carried out on an IBM 1620 computer, using Mair's program,[13] and Mair's weighting scheme No. 3,

$$W = 1/[1 + (KF_o - b)^2/a^2]$$

where K is the scale factor, and a and b were put equal to 40 and 25, respectively, for structure factors based on half the cell content.

The calculated structure factors were based on the scattering curves listed in *International Tables* (Ref. 14, pp. 202, 206, 211). The Freeman-Watson curve for selenium (Ref. 14, p. 206) was used. The tellurium and selenium scattering curves were corrected for anomalous dispersion, using the $\Delta f'$ and $\Delta f''$ values given by Cromer,[15] by taking the amplitude of f as the corrected value.

STRUCTURE ANALYSIS

With the tellurium atoms located in centres of symmetry, the structures were solved in a fairly straight-forward way in the $0kl$ and $h0l$ projections through Fourier summations of reflections with positive signs. Atoms in centres of symmetry in this space group do not contribute to reflections with $k+l$ odd. The first Fourier summation of each $0kl$ zone was therefore based on the strongest reflections with $k+l$ even. The resulting maps, although having false (extra) symmetry because of the omission of the $k+l$ odd reflections, permitted correct sets of sulphur and selenium coordinates to be picked out. In the $h0l$ projection of II, which was worked out before the $h0l$ projection of I, it turned out on inclusion of the contributions of all atoms, that one of the strongest reflections, 102, had negative sign. This reflection was put negative in the first Fourier summation of the $h0l$ reflections of I. The projections were refined by least squares.

Three-dimensional least squares refinement was started, using the coordinates derived from the projections. At first, only the coordinates of the heavy atoms, tellurium, sulphur, and selenium, were allowed to vary. Anisotropic thermal parameters for the heavy atoms were introduced at an early stage, and, finally, anisotropic thermal parameters for all atoms. In the case of I, five strong low-order reflections, 011, 020, 120, 140, and $\bar{2}11$,

Table 1. Atomic coordinates, in fractions of monoclinic cell edges. Origin at a centre of symmetry.

Dithiocyanatobis(ethylenethiourea)tellurium(II)

	x	y	z
Te	0	0	0
S_1	0.3546	0.1223	−0.0310
C_1	0.2720	0.2323	0.0370
N_1	0.2216	0.3052	0.0868
S_2	0.1542	−0.0108	0.2418
C_2	−0.0350	0.0702	0.2953
N_2	−0.1772	0.0361	0.3631
C_3	−0.3266	0.1200	0.4045
C_4	−0.2567	0.2173	0.3321
N_3	−0.0656	0.1751	0.2732

Diselenocyanatobis(ethylenethiourea)tellurium(II)

	x	y	z
Te	0	0	0
Se	0.3651	0.1203	−0.0293
C_1	0.2826	0.2409	0.0395
N_1	0.2231	0.3125	0.0865
S	0.1533	−0.0063	0.2493
C_2	−0.0419	0.0750	0.2929
N_2	−0.1845	0.0427	0.3606
C_3	−0.3166	0.1269	0.3939
C_4	−0.2505	0.2229	0.3259
N_3	−0.0581	0.1818	0.2705

had markedly lower observed than calculated values, and were omitted from the last stages of refinement. The last refinement cycles gave insignificant coordinate shifts also for the carbon and nitrgen atoms. The final value of the conventioned R factor, with non-observed reflections included when $|F_c|$ exceeds the observable limit, and with the above-mentioned five strong reflections of I omitted, was 0.070 for I, and 0.065 for II.

The final atomic coordinates are listed in Table 1, thermal parameters in Table 2, and observed and calculated structure factors in Tables 3 and 4.

Table 2. 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.

Dithiocyanatobis(ethylenethiourea)tellurium(II)

	U_{11}	U_{22}	U_{33}	U_{12}	U_{23}	U_{13}
Te	392	300	464	33	− 39	124
S_1	520	485	1179	− 18	−145	417
C_1	286	510	842	−272	− 9	− 73
N_1	715	483	854	130	− 37	18
S_2	807	757	571	303	− 43	50
C_2	549	406	497	186	− 82	40
N_2	734	425	773	−224	51	67
C_3	402	481	971	91	− 71	190
C_4	587	543	648	156	162	195
N_3	929	433	561	224	− 22	264

Diselenocyanatobis(ethylenethiourea)tellurium(II)

	U_{11}	U_{22}	U_{33}	U_{12}	U_{23}	U_{13}
Te	366	236	421	25	− 34	118
Se	583	410	865	− 63	−127	334
C_1	965	315	542	30	− 35	− 38
N_1	609	569	912	139	−219	−128
S	552	537	465	203	− 55	66
C_2	316	336	367	66	− 85	33
N_2	530	441	608	−178	− 20	112
C_3	535	480	837	− 1	− 89	435
C_4	462	363	598	−126	− 5	302
N_3	525	391	444	66	− 40	235

RESULTS

Bond lengths and angles in the coordination groups, from the atomic coordinates of Table 1, are listed in Table 5. Views of the molecules are shown in Figs. 1 and 2.

Tellurium(II) is in each complex coordinated to four ligand atoms in a square-planar *trans* arrangement: to two ethylenethiourea sulphur atoms and two thiocyanate sulphur atoms in I, and to two ethylenethiourea sulphur atoms and two selenocyanate selenium atoms in II. The thiocyanate and selenocyanate ligands coordinate to tellurium(II) through the sulphur and selenium atoms, and not through the nitrogen atoms. Tellurium(II) is a class B [16] or soft [17] complex former.

Table 3. Observed and calculated structure factors ($\times 5$) for *trans*-dithiocyanatobis-(ethylenethiourea)tellurium(II). 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	0	2	339	347	0	7	12	-14	-9	-1	1	1	271	312	1	5	5	154	159	1	9	3	223	221
0	0	4	616	631	0	8	0	411	409	-1	1	2	282	312	1	5	6	-69	45	1	9	4	-75	-39
0	0	6	158	155	0	8	1	30	37	-1	1	3	73	73	1	5	7	220	202	1	9	5	149	139
0	0	8	285	273	0	8	2	348	349	-1	1	4	-92	-30	1	5	8	-76	30	1	9	6	66	-61
0	0	10	89	84	0	8	3	28	-37	-1	1	5	347	348	1	5	9	85	80	1	9	7	142	141
0	0	12	99	102	0	8	4	329	329	-1	1	6	-56	0	1	5	10	-72	-5	1	9	8	-70	35
0	1	1	428	456	0	8	5	55	53	-1	1	7	149	140	1	5	11	83	83	1	9	9	80	91
0	1	2	180	154	0	8	6	158	164	-1	1	8	-70	-55	1	5	12	-48	12	1	9	10	-51	-1
0	1	3	660	702	0	8	7	-26	13	-1	1	9	231	205	-1	5	1	424	471	1	9	11	-30	62
0	1	4	129	-119	0	8	8	172	175	-1	1	10	-77	13	-1	5	2	103	93	-1	9	1	248	251
0	1	5	412	418	0	8	9	-24	15	-1	1	11	74	76	-1	5	3	294	311	-1	9	2	-70	53
0	1	6	79	70	0	8	10	38	56	-1	1	12	-67	-23	-1	5	4	-56	33	-1	9	3	81	60
0	1	7	237	234	0	8	11	-17	-6	-1	1	13	92	99	-1	5	5	465	501	-1	9	4	-74	42
0	1	8	-24	13	0	9	1	340	332	1	2	0	463	625	-1	5	6	-66	14	-1	9	5	238	222
0	1	9	174	169	0	9	2	85	75	1	2	1	373	-388	-1	5	7	186	185	-1	9	6	-77	12
0	1	10	-26	23	0	9	3	262	270	1	2	2	328	339	-1	5	8	-75	12	-1	9	7	-76	59
0	1	11	87	85	0	9	4	78	73	1	2	3	-42	-7	-1	5	9	220	215	-1	9	8	-73	-16
0	1	12	-22	-4	0	9	5	263	262	1	2	4	441	461	-1	5	10	-74	36	-1	9	9	146	143
0	1	13	65	78	0	9	6	-26	-4	1	2	5	140	-113	-1	5	11	84	90	-1	9	10	-59	6
0	2	0	452	554	0	9	7	113	121	1	2	6	247	238	-1	5	12	-57	8	-1	9	11	45	57
0	2	1	181	-179	0	9	8	-25	21	1	2	7	-68	-54	-1	5	13	61	73	1	10	0	226	209
0	2	2	154	133	0	9	9	123	132	1	2	8	248	236	1	6	0	427	432	1	10	1	70	-55
0	2	3	165	152	0	9	10	-19	12	1	2	9	-76	-4	1	6	1	112	101	1	10	2	166	156
0	2	4	491	465	0	9	11	28	44	1	2	10	76	66	1	6	2	226	233	1	10	3	117	-98
0	2	5	135	117	0	10	0	287	258	1	2	11	-70	-6	1	6	3	141	130	1	10	4	185	178
0	2	6	193	188	0	10	1	53	56	1	2	12	83	97	1	6	4	335	344	1	10	5	-76	27
0	2	7	73	54	0	10	2	181	179	1	2	13	-40	12	1	6	5	67	53	1	10	6	105	101
0	2	8	294	292	0	10	3	59	-68	-1	2	1	158	153	1	6	6	153	142	1	10	7	-70	-42
0	2	9	36	41	0	10	4	240	227	-1	2	2	223	238	1	6	7	-75	-14	1	10	8	122	128
0	2	10	83	94	0	10	5	101	106	-1	2	3	131	102	1	6	8	242	220	1	10	9	-55	16
0	2	11	-42	-2	0	10	6	114	110	-1	2	4	315	335	1	6	9	-74	46	-1	10	1	188	184
0	2	12	93	97	0	10	7	-25	9	-1	2	5	-51	4	1	6	10	-68	58	-1	10	2	207	190
0	2	13	-16	13	0	10	8	135	129	-1	2	6	220	220	1	6	11	-58	0	-1	10	3	-76	-32
0	3	1	340	366	0	10	9	-20	28	-1	2	7	-64	-33	1	6	12	73	87	-1	10	4	204	196
0	3	2	237	237	0	10	10	54	72	-1	2	8	211	201	-1	6	1	133	-107	-1	10	5	-77	31
0	3	3	234	217	0	11	1	159	145	-1	2	9	-75	-12	-1	6	2	258	264	-1	10	6	132	131
0	3	4	173	145	0	11	2	34	33	-1	2	10	150	150	-1	6	3	117	-105	-1	10	7	-73	-9
0	3	5	309	289	0	11	3	124	112	-1	2	11	-73	-29	-1	6	4	2121	324	-1	10	8	97	99
0	3	6	114	87	0	11	4	32	38	-1	2	12	81	78	-1	6	5	126	108	-1	10	9	-61	-16
0	3	7	143	123	0	11	5	146	132	-1	2	13	-52	7	-1	6	6	182	184	-1	10	10	70	64
0	3	8	-24	7	0	11	6	-24	17	1	3	0	66	77	-1	6	7	73	67	1	11	0	-76	-10
0	3	9	200	207	0	11	7	131	136	1	3	1	195	207	-1	6	8	178	176	1	11	1	161	151
0	3	10	37	37	0	11	8	34	40	1	3	2	-40	-20	-1	6	9	-76	26	1	11	2	85	-75
0	3	11	92	93	0	11	9	78	87	1	3	3	440	468	-1	6	10	118	111	1	11	3	186	188
0	3	12	-21	10	0	12	0	131	110	1	3	4	163	-143	-1	6	11	-65	0	1	11	4	-76	-17
0	3	13	80	91	0	12	1	34	40	1	3	5	177	165	-1	6	12	68	78	1	11	5	135	126
0	4	0	418	472	0	12	2	55	64	1	3	6	78	-73	1	7	0	144	137	1	11	6	-70	-30
0	4	1	36	21	0	12	3	-25	-5	1	3	7	234	220	1	7	1	175	168	1	11	7	117	118
0	4	2	62	63	0	12	4	179	175	1	3	8	-74	-9	1	7	2	83	66	1	11	8	-56	16
0	4	3	175	-163	0	12	5	40	34	1	3	9	133	131	1	7	3	317	310	1	11	9	58	50
0	4	4	334	345	0	12	6	72	82	1	3	10	-74	3	1	7	4	96	96	-1	11	1	258	258
0	4	5	87	76	0	12	7	-20	11	1	3	11	111	95	1	7	5	232	223	-1	11	2	-77	42
0	4	6	183	179	0	12	8	85	98	1	3	12	-56	-2	1	7	6	74	58	-1	11	3	179	179
0	4	7	-23	5	0	12	9	-11	15	-1	3	1	597	796	1	7	7	191	182	-1	11	4	-76	24
0	4	8	260	243	0	13	1	152	136	-1	3	2	-37	47	1	7	8	-76	30	-1	11	5	156	155
0	4	9	39	46	0	13	2	-24	-14	-1	3	3	337	378	1	7	9	127	122	-1	11	6	-72	-2
0	4	10	59	69	0	13	3	107	101	-1	3	4	48	-30	1	7	10	-64	3	-1	11	7	113	121
0	4	11	-23	-15	0	13	4	-22	-9	-1	3	5	543	589	1	7	11	87	91	-1	11	8	-61	0
0	4	12	93	106	0	13	5	76	74	-1	3	6	85	78	-1	7	1	361	377	-1	11	9	90	98
0	4	13	-14	17	0	13	6	-19	-1	-1	3	7	138	128	-1	7	2	70	62	1	12	0	234	224
0	5	1	206	202	0	13	7	92	78	-1	3	8	-72	-44	-1	7	3	103	101	1	12	1	-76	33
0	5	2	-16	20	0	14	0	123	116	-1	3	9	246	229	-1	7	4	87	86	1	12	2	170	167
0	5	3	294	286	0	14	1	-22	5	-1	3	10	-76	-3	-1	7	5	239	234	1	12	3	-73	-19
0	5	4	145	-130	0	14	2	87	91	-1	3	11	73	55	-1	7	6	-72	24	1	12	4	150	153
0	5	5	271	258	0	14	3	37	-34	-1	3	12	-64	1	-1	7	7	93	87	1	12	5	-68	13
0	5	6	77	-68	0	14	4	106	110	-1	3	13	104	107	-1	7	8	-77	-23	1	12	6	62	59
0	5	7	164	156	0	14	5	-17	-7	1	4	0	508	642	-1	7	9	160	157	1	12	7	-55	-11
0	5	8	-25	-9	0	14	6	61	82	1	4	1	47	-54	-1	7	10	-70	58	1	12	8	77	77
0	5	9	183	170	0	15	1	99	109	1	4	2	254	269	-1	7	11	60	60	-1	12	1	-76	12
0	5	10	-25	-7	0	15	2	-17	-4	1	4	3	61	-57	-1	7	12	-46	6	-1	12	2	152	144
0	5	11	74	79	0	15	3	85	95	1	4	4	341	340	1	8	0	172	160	-1	12	3	-74	1
0	5	12	-19	0	0	15	4	-13	-13	1	4	5	122	122	1	8	1	-65	24	-1	12	4	198	203
0	5	13	41	63	1	0	2	386	-343	1	4	6	116	112	1	8	2	224	233	-1	12	5	-70	27
0	6	0	416	456	1	0	4	486	500	1	4	7	-71	-37	1	8	3	-69	-11	-1	12	6	152	155
0	6	1	73	-52	1	0	6	190	181	1	4	8	185	158	1	8	4	242	231	-1	12	7	-59	17
0	6	2	145	144	1	0	8	303	276	1	4	9	-77	16	1	8	5	74	64	-1	12	8	94	99
0	6	3	40	-47	1	0	10	100	93	1	4	10	-73	55	1	8	6	165	166	1	13	0	-71	25
0	6	4	355	360	1	0	12	85	99	1	4	11	-66	-18	1	8	7	-76	-3	1	13	1	121	116
0	6	5	-22	18	-1	0	2	325	317	1	4	12	92	91	1	8	8	160	158	1	13	2	-70	13
0	6	6	112	96	-1	0	4	373	369	-1	4	1	103	100	1	8	9	-68	4	1	13	3	127	114
0	6	7	129	-110	-1	0	6	154	139	-1	4	2	519	560	1	8	10	59	60	1	13	4	-63	34
0	6	8	234	220	-1	0	8	197	181	-1	4	3	86	-77	1	8	11	-44	5	1	13	5	72	75
0	6	9	-25	-21	-1	0	10	144	133	-1	4	4	404	442	-1	8	1	-64	-6	1	13	6	-52	-4
0	6	10	51	71	-1	0	12	82	75	-1	4	5	-57	-3	-1	8	2	164	162	1	13	7	82	94
0	6	11	-21	-14	1	1	1	296	301	-1	4	6	325	322	-1	8	3	67	-61	-1	13	1	205	199
0	6	12	85	93	1	1	2	319	-323	-1	4	7	-68	-27	-1	8	4	169	159	-1	13	2	70	20
0	7	1	452	463	1	1	3	608	678	-1	4	8	298	285	-1	8	5	-73	0	-1	13	3	171	179
0	7	2	-20	-13	1	1	4	194	-183	-1	4	9	-76	43	-1	8	6	142	136	-1	13	4	-66	-10
0	7	3	236	243	1	1	5	152	136	-1	4	10	143	138	-1	8	7	-77	0	-1	13	5	143	153
0	7	4	116	-98	1	1	6	-60	36	-1	4	11	-71	-6	-1	8	8	138	133	-1	13	6	-56	42
0	7	5	263	288	1	1	7	306	291	-1	4	12	75	85	-1	8	9	-72	27	-1	13	7	92	100
0	7	6	-25	-1	1	1	8	-73	-18	-1	4	13	-16	9	-1	8	10	89	84	1	14	0	125	124
0	7	7	137	137	1	1	9	125	115	1	5	0	138	138	-1	8	11	-53	0	1	14	1	-62	26
0	7	8	-26	-9	1	1	10	-76	11	1	5	1	298	323	-1	8	12	59	70	1	14	2	113	121
0	7	9	135	132	1	1	11	127	125	1	5	2	70	62	1	9	0	-70	22	1	14	3	-57	10
0	7	10	-23	24	1	1	12	-59	0	1	5	3	380	423	1	9	1	158	154	1	14	4	109	115
0	7	11	59	72	1	1	13	42	52	1	5	4	-59	17	1	9	2	71	-63	1	14	5	-46	31

Table 3. 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)
1	14	6	55	73	-2	2	11	-39	-12	-2	5	10	-40	14	2	9	1	104	95	2	13	2	-35	-32
-1	14	1	-63	-3	-2	2	12	69	75	-2	5	11	69	87	2	9	2	-40	-43	2	13	3	132	139
-1	14	2	118	113	-2	2	13	-28	17	-2	5	12	-31	7	2	9	3	174	166	2	13	4	-31	8
-1	14	3	-59	-8	2	3	0	178	184	-2	5	13	45	66	2	9	4	-42	26	2	13	5	90	104
-1	14	4	104	103	2	3	1	220	212	2	6	0	258	265	2	9	5	84	96	-2	13	1	115	113
-1	14	5	-50	21	2	3	2	-23	-18	2	6	1	137	-133	2	9	6	-41	-12	-2	13	2	64	70
-1	14	6	98	104	2	3	3	553	545	2	6	2	299	291	2	9	7	116	120	-2	13	3	109	108
1	15	0	-50	26	2	3	4	40	-44	2	6	3	38	-29	2	9	8	-35	37	-2	13	4	-34	5
1	15	1	87	86	2	3	5	172	164	2	6	4	229	219	2	9	9	46	58	-2	13	5	90	95
1	15	2	-47	14	2	3	6	-37	17	2	6	5	39	-29	-2	9	1	308	293	-2	13	6	37	39
1	15	3	100	109	2	3	7	288	278	2	6	6	186	184	-2	9	2	65	-46	-2	13	7	61	77
1	15	4	-34	31	2	3	8	-42	5	2	6	7	-42	21	-2	9	3	142	133	2	14	0	96	105
-1	15	1	107	100	2	3	9	71	86	2	6	8	123	135	-2	9	4	41	-28	2	14	1	-31	-35
-1	15	2	-48	7	2	3	10	-38	-15	2	6	9	-38	27	-2	9	5	259	258	2	14	2	109	120
-1	15	3	62	64	2	3	11	82	91	2	6	10	59	61	-2	9	6	-42	23	2	14	3	-27	-2
2	0	2	122	59	2	3	12	-24	1	2	6	11	-26	0	-2	9	7	124	125	2	14	4	62	76
2	0	4	324	327	-2	3	1	440	480	-2	6	1	172	165	-2	9	8	-39	16	-2	14	1	42	49
2	0	6	169	153	-2	3	2	86	-94	-2	6	2	381	379	-2	9	9	129	137	-2	14	2	113	121
2	0	8	140	140	-2	3	3	114	129	-2	6	3	86	79	-2	9	10	-31	29	-2	14	3	45	45
2	0	10	90	88	-2	3	4	248	-223	-2	6	4	246	232	-2	9	11	70	88	-2	14	4	81	89
2	0	12	51	62	-2	3	5	432	420	-2	6	5	-36	21	2	10	0	155	155	-2	14	5	-24	25
-2	0	2	367	393	-2	3	6	-33	-16	-2	6	6	277	271	2	10	1	133	129	-2	14	6	70	98
-2	0	4	420	405	-2	3	7	147	120	-2	6	7	100	84	2	10	2	211	206	2	15	0	-23	-10
-2	0	6	444	426	-2	3	8	-39	-22	-2	6	8	129	125	2	10	3	-42	37	2	15	1	63	78
-2	0	8	205	198	-2	3	9	185	187	-2	6	9	41	40	2	10	4	133	131	-2	15	1	102	115
-2	0	10	233	248	-2	3	10	-41	4	-2	6	10	130	132	2	10	5	-40	33	-2	15	2	28	35
-2	0	12	40	50	-2	3	11	52	53	-2	6	11	-35	-2	2	10	6	116	127	-2	15	3	86	106
2	1	0	164	179	-2	3	12	-34	8	-2	6	12	42	54	2	10	7	-35	-11	1	0	0	720	685
2	1	1	260	274	-2	3	13	60	82	2	7	0	-33	26	2	10	8	71	91	2	0	0	85	71
2	1	2	58	49	2	4	0	214	226	2	7	1	144	135	2	10	9	-23	9	3	0	0	382	373
2	1	3	395	365	2	4	1	-24	-21	2	7	2	128	-117	-2	10	1	-41	-15	4	0	0	198	163
2	1	4	151	156	2	4	2	332	367	2	7	3	266	251	-2	10	2	220	199	5	0	0	202	189
2	1	5	42	10	2	4	3	80	70	2	7	4	-38	-3	-2	10	3	49	-47	6	0	0	158	180
2	1	6	62	58	2	4	4	308	283	2	7	5	98	104	-2	10	4	164	157	7	0	0	44	72
2	1	7	230	260	2	4	5	-35	38	2	7	6	-42	-37	-2	10	5	-42	-33	3	0	2	576	563
2	1	8	-41	-16	2	4	6	275	250	2	7	7	133	143	-2	10	6	171	172	3	0	4	313	306
2	1	9	51	57	2	4	7	41	-51	2	7	8	-39	9	-2	10	7	-39	36	3	0	6	229	238
2	1	10	-39	2	2	4	8	151	166	2	7	9	68	74	-2	10	8	98	109	3	0	8	87	98
2	1	11	110	112	2	4	9	-41	19	2	7	10	-30	-11	-2	10	9	-32	-7	3	0	10	94	101
2	1	12	-26	-6	2	4	10	86	105	2	7	11	46	66	-2	10	10	80	89	-3	0	2	504	461
-2	1	1	423	546	2	4	11	-31	-9	-2	7	1	362	352	2	11	0	59	51	-3	0	4	259	222
-2	1	2	61	-36	2	4	12	42	65	-2	7	2	207	192	2	11	1	164	156	-3	0	6	360	335
-2	1	3	305	284	-2	4	1	66	64	-2	7	3	270	263	2	11	2	-41	-3	-3	0	8	-59	39
-2	1	4	126	-107	-2	4	2	469	453	-2	7	4	63	55	2	11	3	208	214	-3	0	10	191	194
-2	1	5	416	408	-2	4	3	-26	23	-2	7	5	347	337	2	11	4	53	58	-3	0	12	-48	40
-2	1	6	-31	24	-2	4	4	184	171	-2	7	6	113	103	2	11	5	108	114	4	0	2	237	225
-2	1	7	282	254	-2	4	5	-31	0	-2	7	7	162	155	2	11	6	-35	-11	4	0	4	123	123
-2	1	8	46	-59	-2	4	6	168	162	-2	7	8	46	-39	2	11	7	88	102	4	0	6	139	146
-2	1	9	224	219	-2	4	7	-37	-33	-2	7	9	166	175	2	11	8	-25	21	4	0	8	58	58
-2	1	10	46	40	-2	4	8	90	88	-2	7	10	-37	24	-2	11	1	212	193	4	0	10	70	78
-2	1	11	93	109	-2	4	9	-42	-1	-2	7	11	72	85	-2	11	2	-42	-38	-4	0	2	223	204
-2	1	12	-36	6	-2	4	10	132	143	-2	7	12	-23	-3	-2	11	3	169	169	-4	0	4	82	77
-2	1	13	86	100	-2	4	11	-38	6	2	8	0	150	143	-2	11	4	-41	-27	-4	0	6	238	227
2	2	0	419	454	-2	4	12	52	59	2	8	1	64	-58	-2	11	5	121	113	-4	0	8	68	61
2	2	1	161	159	-2	4	13	-24	-5	2	8	2	276	250	-2	11	6	-38	-19	-4	0	10	144	134
2	2	2	431	397	2	5	0	-26	3	2	8	3	-39	3	-2	11	7	83	91	-4	0	12	88	83
2	2	3	130	162	2	5	1	325	321	2	8	4	88	89	-2	11	8	-32	-17	5	0	2	110	109
2	2	4	295	278	2	5	2	88	-98	2	8	5	-41	-5	-2	11	9	69	77	5	0	4	109	98
2	2	5	72	-50	2	5	3	394	402	2	8	6	125	120	2	12	0	173	184	5	0	6	64	54
2	2	6	261	231	2	5	4	-34	0	2	8	7	-41	-27	2	12	1	-40	-5	5	0	8	51	51
2	2	7	-39	6	2	5	5	196	180	2	8	8	69	73	2	12	2	159	156	-5	0	2	227	227
2	2	8	107	101	2	5	6	-39	24	2	8	9	-33	0	2	12	3	-38	-10	-5	0	4	243	229
2	2	9	-41	4	2	5	7	231	218	2	8	10	46	65	2	12	4	117	122	-5	0	6	251	264
2	2	10	77	91	2	5	8	-42	22	-2	8	1	46	56	2	12	5	-34	3	-5	0	8	183	200
2	2	11	-34	-2	2	5	9	65	75	-2	8	2	298	279	2	12	6	93	102	-5	0	10	106	119
2	2	12	49	65	2	5	10	-36	2	-2	8	3	-37	12	2	12	7	-24	-2	6	0	2	93	109
-2	2	1	274	-288	2	5	11	79	104	-2	8	4	198	178	-2	12	1	-40	-15	6	0	4	101	122
-2	2	2	536	556	-2	5	1	426	408	-2	8	5	-40	12	-2	12	2	151	140	-6	0	2	118	139
-2	2	3	156	-138	-2	5	2	108	111	-2	8	6	258	256	-2	12	3	-39	-8	-6	0	4	112	123
-2	2	4	227	228	-2	5	3	93	78	-2	8	7	-42	12	-2	12	4	73	78	-6	0	6	59	67
-2	2	5	96	-84	-2	5	4	153	119	-2	8	8	161	169	-2	12	5	-37	-12	-6	0	8	71	80
-2	2	6	342	333	-2	5	5	286	259	-2	8	9	-38	17	-2	12	6	111	113	-6	0	10	39	55
-2	2	7	35	-21	-2	5	6	104	91	-2	8	10	120	130	-2	12	7	-31	19	7	0	2	37	47
-2	2	8	132	132	-2	5	7	136	136	-2	8	11	-28	18	-2	12	8	37	45	-7	0	2	46	59
-2	2	9	-41	25	-2	5	8	-41	-15	-2	8	12	44	70	2	13	0	-37	5	-7	0	4	50	73
-2	2	10	177	166	-2	5	9	134	131	2	9	0	90	96	2	13	1	83	95	-7	0	6	38	64

The Te – S bond lengths are close to 2.68 Å, which is the weighted average of earlier values for the length of Te – S bonds in centrosymmetric, square-planar complexes of tellurium(II).[10] With single covalent bond radii for ligand atoms, this corresponds to a bonding radius of 1.64 Å for tellurium(II). So does the Te – Se bond length in the diselenocyanato complex, 2.81 Å.

The S – Te – S and Se – Te – S bond angles are 90° within the error. The bond angles at the sulphur and selenium atoms are in the range 96 to 100°.

The ethylenethiourea carbon and nitrogen coordinates give bond lengths, 1.29 to 1.44 Å for $C_2 - N_2$ and $C_2 - N_3$, 1.44 to 1.50 Å for $N_2 - C_3$ and $N_3 - C_4$,

Table 4. Observed and calculated structure factors (× 5) for *trans*-diselenocyanatobis-(ethylenethiourea)tellurium(II). 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	0	2	634	607	0	8	0	616	643	-1	1	2	403	415	1	5	11	80	92	1	9	10	-49	-3
0	0	4	859	838	0	8	1	43	44	-1	1	3	174	-123	1	5	12	-44	18	-1	9	1	185	169
0	0	6	232	233	0	8	2	504	518	-1	1	4	-43	0	-1	5	1	650	688	-1	9	2	79	64
0	0	8	313	316	0	8	3	58	-54	-1	1	5	219	191	-1	5	2	55	41	-1	9	3	73	-41
0	0	10	70	55	0	8	4	504	479	-1	1	6	57	-33	-1	5	3	496	505	-1	9	4	74	76
0	0	12	87	67	0	8	5	-50	36	-1	1	7	64	53	-1	5	4	56	40	-1	9	5	153	139
0	1	1	618	707	0	8	6	201	209	-1	1	8	112	-109	-1	5	5	632	649	-1	9	6	-78	-34
0	1	2	272	227	0	8	7	-53	1	-1	1	9	152	156	-1	5	6	-66	29	-1	9	7	-77	-7
0	1	3	898	915	0	8	8	200	201	-1	1	10	-78	-37	-1	5	7	284	284	-1	9	8	-74	-27
0	1	4	37	-22	0	8	9	-49	-12	-1	1	11	74	66	-1	5	8	85	75	-1	9	9	123	132
0	1	5	459	462	0	8	10	42	42	-1	1	12	-66	-53	-1	5	9	276	280	-1	9	10	-59	-34
0	1	6	175	167	0	8	11	34	-13	1	2	0	550	609	-1	5	10	-75	61	-1	9	11	-44	38
0	1	7	305	301	0	9	1	525	512	1	2	1	622	-634	-1	5	11	97	114	1	10	0	243	233
0	1	8	85	78	0	9	2	105	93	1	2	2	354	359	-1	5	12	-56	25	1	10	1	177	-165
0	1	9	142	141	0	9	3	426	416	1	2	3	228	-215	1	6	0	485	492	1	10	2	162	148
0	1	10	55	63	0	9	4	127	122	1	2	4	472	438	1	6	1	277	263	1	10	3	211	-200
0	1	11	94	108	0	9	5	313	316	1	2	5	322	-308	1	6	2	283	289	1	10	4	220	210
0	1	12	-43	13	0	9	6	-53	10	1	2	6	277	267	1	6	3	356	338	1	10	5	77	-62
0	1	13	56	60	0	9	7	169	178	1	2	7	153	-156	1	6	4	377	357	1	10	6	104	103
0	2	0	509	601	0	9	8	56	63	1	2	8	233	223	1	6	5	179	173	1	10	7	71	-73
0	2	1	165	-141	0	9	9	119	132	1	2	9	-78	-53	1	6	6	180	177	1	10	8	136	156
0	2	2	191	169	0	9	10	-38	7	1	2	10	89	85	1	6	7	94	87	1	10	9	-54	-2
0	2	3	348	315	0	9	11	42	51	1	2	11	-68	-9	1	6	8	237	235	1	10	10	61	75
0	2	4	526	506	0	10	0	354	361	1	2	12	83	101	1	6	9	75	65	-1	10	1	272	264
0	2	5	306	287	0	10	1	92	71	-1	2	1	310	297	1	6	10	73	65	-1	10	2	119	113
0	2	6	213	197	0	10	2	206	197	-1	2	2	208	211	1	6	11	-56	16	-1	10	3	-76	-14
0	2	7	197	200	0	10	3	-51	2	-1	2	3	187	155	1	6	12	71	97	-1	10	4	205	195
0	2	8	332	328	0	10	4	316	326	-1	2	4	365	357	-1	6	1	292	-265	-1	10	5	-78	19
0	2	9	108	111	0	10	5	172	176	-1	2	5	-52	-32	-1	6	2	293	298	-1	10	6	94	84
0	2	10	88	89	0	10	6	123	126	-1	2	6	161	162	-1	6	3	155	-152	-1	10	7	-74	-56
0	2	11	-49	31	0	10	7	68	72	-1	2	7	98	-87	-1	6	4	422	439	-1	10	8	85	97
0	2	12	108	122	0	10	8	186	186	-1	2	8	244	230	-1	6	5	147	122	-1	10	9	61	-45
0	2	13	-31	29	0	10	9	64	73	-1	2	9	-76	-70	-1	6	6	172	183	-1	10	10	50	50
0	3	1	230	202	0	10	10	68	82	-1	2	10	123	123	-1	6	7	105	107	-1	10	11	-26	-15
0	3	2	315	302	0	11	1	127	126	-1	2	11	83	-78	-1	6	8	252	231	1	11	0	92	-86
0	3	3	140	112	0	11	2	71	64	-1	2	12	86	95	-1	6	9	77	71	1	11	1	170	160
0	3	4	269	257	0	11	3	106	100	1	3	0	127	-109	-1	6	10	97	104	1	11	2	174	-152
0	3	5	216	186	0	11	4	116	118	1	3	1	273	288	-1	6	11	-65	30	1	11	3	234	225
0	3	6	200	178	0	11	5	139	135	1	3	2	208	-205	-1	6	12	90	113	1	11	4	94	-87
0	3	7	152	143	0	11	6	75	81	1	3	3	532	501	1	7	0	247	251	1	11	5	112	115
0	3	8	110	108	0	11	7	163	177	1	3	4	320	-318	1	7	1	112	105	1	11	6	100	-98
0	3	9	139	204	0	11	8	77	91	1	3	5	135	119	1	7	2	233	229	1	11	7	129	131
0	3	10	78	86	0	11	9	94	103	1	3	6	161	-169	1	7	3	378	343	1	11	8	-55	-14
0	3	11	110	131	0	12	0	91	78	1	3	7	229	216	1	7	5	225	220	1	11	9	-62	28
0	3	12	-61	29	0	12	1	61	51	1	3	8	-76	-58	1	7	5	244	241	-1	11	1	333	337
0	3	13	73	54	0	12	2	-53	-3	1	3	9	83	78	1	7	6	147	134	-1	11	2	78	72
0	4	0	211	201	0	12	3	-51	23	1	3	10	-75	-28	1	7	7	255	243	-1	11	3	247	234
0	4	1	34	2	0	12	4	162	168	1	3	11	88	101	1	7	8	86	86	-1	11	4	-77	26
0	4	2	250	-200	0	12	5	51	35	1	3	12	-53	-12	1	7	9	125	140	-1	11	5	228	205
0	4	3	163	-139	0	12	6	53	58	-1	3	1	824	966	1	7	10	-63	7	-1	11	6	-74	-12
0	4	4	262	234	0	12	7	-41	34	-1	3	2	113	132	1	7	11	107	124	-1	11	7	147	156
0	4	5	95	88	0	12	8	94	116	-1	3	3	524	554	-1	7	1	339	340	-1	11	8	-62	-15
0	4	6	96	95	0	13	1	71	67	-1	3	4	-48	20	-1	7	2	60	-63	-1	11	9	105	119
0	4	7	-48	12	0	13	2	55	-53	-1	3	5	692	726	-1	7	3	67	-29	1	11	10	-36	-8
0	4	8	249	245	0	13	3	64	66	-1	3	6	-60	21	-1	7	4	109	-102	1	12	0	320	319
0	4	9	63	49	0	13	4	51	-41	-1	3	7	229	210	-1	7	5	208	184	1	12	1	-76	2
0	4	10	68	69	0	13	5	48	48	-1	3	8	89	-99	-1	7	6	-73	27	1	12	2	191	193
0	4	11	-46	-8	0	13	6	-39	-29	-1	3	9	281	277	-1	7	7	76	54	1	12	3	-75	-55
0	4	12	115	143	0	13	7	79	85	-1	3	10	-77	-42	-1	7	8	-78	22	1	12	4	175	163
0	4	13	25	25	0	14	0	107	116	-1	3	11	73	72	-1	7	9	170	170	1	12	5	-69	-27
0	5	1	46	-11	0	14	1	-45	-3	-1	3	12	-63	-10	-1	7	10	85	94	1	12	6	-63	33
0	5	2	45	-33	0	14	2	58	53	1	4	0	750	833	-1	7	11	60	57	1	12	7	-55	-23
0	5	3	131	121	0	14	3	63	-64	1	4	1	100	-107	-1	7	12	-44	33	1	12	8	61	69
0	5	4	228	-218	0	14	4	108	110	1	4	2	374	377	1	8	0	76	49	-1	12	1	-77	18
0	5	5	152	141	0	14	5	44	-45	1	4	3	84	-73	1	8	1	80	80	-1	12	2	238	240
0	5	6	153	-148	0	14	6	63	70	1	4	4	366	353	1	8	2	197	183	-1	12	3	-76	36
0	5	7	166	158	0	15	1	134	144	1	4	5	82	78	1	8	3	-70	29	-1	12	4	334	332
0	5	8	56	-60	0	15	2	-35	-17	1	4	6	89	71	1	8	4	261	245	-1	12	5	-71	34
0	5	9	150	155	0	15	3	109	126	1	4	7	-73	-52	1	8	5	93	97	-1	12	6	225	228
0	5	10	53	-52	0	15	4	-29	-31	1	4	8	122	109	1	8	6	198	199	-1	12	7	-61	13
0	5	11	93	110	0	16	0	166	212	1	4	9	-77	3	1	8	7	-77	17	-1	12	8	162	160
0	5	12	-36	-4	1	0	2	545	-455	1	4	10	-73	31	1	8	8	205	201	-1	12	9	-39	20
0	6	0	331	411	1	0	4	565	493	1	4	11	-64	-20	1	8	9	-68	10	1	13	0	-73	19
0	6	1	119	-124	1	0	6	249	240	1	4	12	61	76	1	8	10	70	100	1	13	1	174	180
0	6	2	122	106	1	0	8	313	323	-1	4	1	143	133	1	8	11	-41	23	1	13	2	-71	27
0	6	3	131	-131	1	0	10	132	144	-1	4	2	676	750	-1	8	1	-65	-25	1	13	3	162	171
0	6	4	363	342	1	0	12	101	123	-1	4	3	82	-69	-1	8	2	-66	7	1	13	4	65	64
0	6	5	143	136	-1	0	2	68	19	-1	4	4	644	706	-1	8	3	80	-74	1	13	5	77	74
0	6	6	61	43	-1	0	4	184	149	-1	4	5	-58	20	-1	8	4	75	53	1	13	6	-53	9
0	6	7	205	-202	-1	0	6	118	-89	-1	4	6	491	482	-1	8	5	-73	-9	1	13	7	96	113
0	6	8	239	244	-1	0	8	150	132	-1	4	7	-69	-21	-1	8	6	-76	26	-1	13	1	293	299
0	6	9	76	-85	-1	0	10	87	75	-1	4	8	417	429	-1	8	7	-78	4	-1	13	2	-72	20
0	6	10	55	56	-1	0	12	101	101	-1	4	9	-77	44	-1	8	8	109	110	-1	13	3	255	255
0	6	11	-42	-35	1	1	0	218	-258	-1	4	10	144	149	-1	8	9	-73	36	-1	13	4	-68	-2
0	6	12	96	122	1	1	1	184	171	-1	4	11	-71	-23	-1	8	10	65	57	-1	13	5	235	251
0	7	1	507	519	1	1	2	527	-497	-1	4	12	113	123	-1	8	11	-53	-1	-1	13	6	58	56
0	7	2	92	-84	1	1	3	698	650	1	5	0	247	253	-1	8	12	70	100	-1	13	7	138	142
0	7	3	363	337	1	1	4	325	-323	1	5	1	407	439	1	9	0	70	-57	-1	13	8	-37	16
0	7	4	170	-154	1	1	5	127	124	1	5	2	192	187	1	9	1	76	69	1	14	0	173	187
0	7	5	334	344	1	1	6	62	-48	1	5	3	523	506	1	9	2	149	-141	1	14	1	79	88
0	7	6	108	-102	1	1	7	397	373	1	5	4	134	127	1	9	3	214	208	1	14	2	153	156
0	7	7	166	168	1	1	8	-74	-61	1	5	5	146	149	1	9	4	98	-89	1	14	3	72	65
0	7	8	53	-53	1	1	9	129	132	1	5	6	117	111	1	9	5	140	138	1	14	4	163	168
0	7	9	102	121	1	1	10	-76	7	1	5	7	213	203	1	9	6	87	-91	1	14	5	58	63
0	7	10	-46	-15	1	1	11	147	181	1	5	8	-78	53	1	9	7	204	207	-1	14	1	-65	-36
	7	11	70	76	1	1	12	-56	-1	1	5	9	-76	33	1	9	8	-70	40	-1	14	2	153	157
	7	12	26	-25	-1	1	1	150	117	1	5	10	-71	5	1	9	9	93	106	-1	14	3	-61	-26

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)
-1	14	4	151	156	2	3	0	348	374	2	6	3	145	-144	2	9	8	-77	33	-2	13	2	108	101
-1	14	5	53	46	2	3	1	208	220	2	6	4	220	216	2	9	9	-64	33	-2	13	3	92	73
-1	14	6	125	134	2	3	2	171	150	2	6	5	108	-108	-2	9	1	364	353	-2	13	4	-79	14
-1	14	7	-29	25	2	3	3	643	625	2	6	6	222	228	-2	9	2	140	-146	-2	13	5	105	98
1	15	0	68	79	2	3	4	69	46	2	6	7	-93	16	-2	9	3	201	192	-2	13	6	67	52
1	15	1	90	98	2	3	5	244	248	2	6	8	122	131	-2	9	4	-92	-52	-2	13	7	-57	33
1	15	2	63	66	2	3	6	84	77	2	6	9	-84	22	-2	9	5	425	386	2	14	0	138	125
1	15	3	137	153	2	3	7	345	350	2	6	10	93	88	-2	9	6	-93	1	2	14	1	88	-78
1	15	4	67	77	2	3	8	-93	-2	2	6	11	-53	18	-2	9	7	186	188	2	14	2	158	155
-1	15	1	119	124	2	3	9	113	117	-2	6	1	365	380	-2	9	8	-89	35	2	14	3	-63	-44
-1	15	2	-51	-28	2	3	10	-84	-17	-2	6	2	334	348	-2	9	9	262	231	2	14	4	97	104
-1	15	3	55	63	2	3	11	112	116	-2	6	3	227	233	-2	9	10	-70	44	-2	14	1	95	103
-1	15	4	-42	-18	2	3	12	-47	-2	-2	6	4	269	250	-2	9	11	92	116	-2	14	2	146	147
-1	15	5	67	82	-2	3	1	429	485	-2	6	5	152	137	2	10	0	207	213	-2	14	3	86	83
2	0	2	56	34	-2	3	2	273	-299	-2	6	6	287	268	2	10	1	254	248	-2	14	4	99	96
2	0	4	228	216	-2	3	3	-52	22	-2	6	7	151	128	2	10	2	220	214	-2	14	5	64	59
2	0	6	87	71	-2	3	4	353	-347	-2	6	8	163	133	2	10	3	115	100	-2	14	6	92	110
2	0	8	67	64	-2	3	5	381	374	-2	6	9	-93	46	2	10	4	141	134	2	15	0	61	-67
2	0	10	93	87	-2	3	6	90	-85	-2	6	10	125	115	2	10	5	92	70	2	15	1	72	81
2	0	12	38	46	-2	3	7	-82	9	-2	6	11	-78	-36	2	10	6	123	127	2	15	2	68	-76
-2	0	2	475	487	-2	3	8	-89	-47	-2	6	12	62	62	2	10	7	-79	1	2	15	3	88	100
-2	0	4	588	611	-2	3	9	162	164	2	7	0	167	-166	2	10	8	83	83	-2	15	1	135	142
-2	0	6	554	563	-2	3	10	-93	-4	2	7	1	82	72	2	10	9	-50	-5	-2	15	2	79	88
-2	0	8	353	356	-2	3	11	-88	-2	2	7	2	259	-247	-2	10	1	118	-118	-2	15	3	116	132
-2	0	10	317	316	-2	3	12	-77	26	2	7	3	244	241	-2	10	2	255	247	-2	15	4	49	54
-2	0	12	58	98	2	4	0	229	252	2	7	4	98	-99	-2	10	3	162	-148	1	0	0	463	473
2	1	0	344	384	2	4	1	-55	33	2	7	5	-92	53	-2	10	4	210	201	2	0	0	80	70
2	1	1	248	253	2	4	2	490	505	2	7	6	-93	-60	-2	10	5	93	-84	3	0	0	533	527
2	1	2	208	196	2	4	3	116	116	2	7	7	129	128	-2	10	6	246	224	4	0	0	-42	6
2	1	3	321	292	2	4	4	385	386	2	7	8	-89	-2	-2	10	7	-89	0	5	0	0	312	296
2	1	4	235	245	2	4	5	-80	57	2	7	9	80	58	-2	10	8	143	136	6	0	0	218	221
2	1	5	90	-72	2	4	6	374	383	2	7	10	-66	-11	-2	10	9	-73	-6	7	0	0	43	50
2	1	6	97	89	2	4	7	-92	-29	2	7	11	58	74	-2	10	10	111	117	3	0	2	845	764
2	1	7	219	217	2	4	8	211	220	-2	7	1	432	432	2	11	0	163	153	3	0	4	486	443
2	1	8	-33	-22	2	4	9	-90	25	-2	7	2	353	353	2	11	1	188	180	3	0	6	340	330
2	1	9	-93	16	2	4	10	133	157	-2	7	3	288	284	2	11	2	-93	73	3	0	8	118	126
2	1	10	-87	-6	2	4	11	-66	-7	-2	7	4	179	176	2	11	3	303	289	3	0	10	124	129
2	1	11	105	112	-2	4	1	-52	48	-2	7	5	438	422	2	11	4	100	95	-3	0	2	567	574
2	1	12	-54	-18	-2	4	2	376	385	-2	7	6	156	152	2	11	5	149	139	-3	0	4	276	261
-2	1	1	488	616	-2	4	3	-58	-29	-2	7	7	187	178	2	11	6	-79	1	-3	0	6	336	328
-2	1	2	239	-234	-2	4	4	64	38	-2	7	8	-93	-31	2	11	7	139	146	-3	0	8	60	-29
-2	1	3	365	346	-2	4	5	-70	-20	-2	7	9	277	262	2	11	8	-55	25	-3	0	10	164	178
-2	1	4	237	-236	-2	4	6	-78	-7	-2	7	10	-84	20	-2	11	1	231	217	-3	0	12	-41	-20
-2	1	5	556	555	-2	4	7	84	-59	-2	7	11	89	91	-2	11	2	156	-129	4	0	2	139	127
-2	1	6	-70	-32	-2	4	8	-90	14	-2	7	12	-53	-14	-2	11	3	170	161	4	0	4	63	65
-2	1	7	350	346	-2	4	9	-93	14	2	8	0	147	136	-2	11	4	123	-117	4	0	6	132	122
-2	1	8	-86	-67	-2	4	10	93	82	2	8	1	93	-82	-2	11	5	112	108	4	0	8	63	71
-2	1	9	342	329	-2	4	11	-86	-12	2	8	2	250	240	-2	11	6	-87	-59	4	0	10	74	91
-2	1	10	-53	63	-2	4	12	-73	46	2	8	3	-88	-44	-2	11	7	82	65	-4	0	2	59	50
-2	1	11	156	136	2	5	0	113	-109	2	8	4	-92	0	-2	11	8	-73	-33	-4	0	4	104	-90
-2	1	12	-80	8	2	5	1	327	345	2	8	5	-93	-36	-2	11	9	87	93	-4	0	6	200	201
2	2	0	405	443	2	5	2	171	-193	2	8	6	104	87	-2	11	10	-40	30	-4	0	8	-51	-15
2	2	1	381	360	2	5	3	479	495	2	8	7	-90	-43	2	12	0	211	200	-4	0	10	205	198
2	2	2	418	415	2	5	4	78	-55	2	8	8	-84	38	2	12	1	-90	18	-4	0	12	87	96
2	2	3	350	337	2	5	5	268	258	2	8	9	-73	-5	2	12	2	210	209	5	0	2	142	141
2	2	4	255	247	2	5	6	-89	12	2	8	10	66	69	2	12	3	-87	30	5	0	4	119	123
2	2	5	-75	7	2	5	7	297	290	-2	8	1	81	89	2	12	4	185	181	5	0	6	55	38
2	2	6	267	254	2	5	8	-93	26	-2	8	2	327	331	2	12	5	-76	24	5	0	8	53	72
2	2	7	-89	36	2	5	9	108	115	-2	8	3	-84	48	2	12	6	160	169	-5	0	2	375	375
2	2	8	93	68	2	5	10	-78	18	-2	8	4	307	290	2	12	7	-55	22	-5	0	4	365	344
2	2	9	-93	-2	2	5	11	115	134	-2	8	5	-90	52	-2	12	1	-92	-68	-5	0	6	418	432
2	2	10	111	120	-2	5	1	416	429	-2	8	6	373	366	-2	12	2	117	122	-5	0	8	258	259
2	2	11	-73	-10	-2	5	2	198	201	-2	8	7	-93	24	-2	12	3	-90	-49	-5	0	10	164	163
2	2	12	51	50	-2	5	3	-64	5	-2	8	8	283	263	-2	12	4	-88	44	-5	0	12	92	99
-2	2	1	485	-544	-2	5	4	248	226	-2	8	9	-87	41	-2	12	5	-84	-25	6	0	2	124	126
-2	2	2	520	564	-2	5	5	231	213	-2	8	10	167	174	-2	12	6	97	80	6	0	4	182	186
-2	2	3	370	-355	-2	5	6	116	115	-2	8	11	-64	18	-2	12	7	-71	-18	6	0	6	53	71
-2	2	4	290	275	-2	5	7	-87	20	-2	8	12	82	106	-2	12	8	-61	15	-6	0	2	118	143
-2	2	5	247	-238	-2	5	8	-92	-16	2	9	0	139	131	-2	12	9	-43	-3	-6	0	4	75	88
-2	2	6	338	340	-2	5	9	93	93	2	9	1	-89	66	2	13	0	-84	-13	-6	0	6	-48	21
-2	2	7	102	-94	-2	5	10	-90	10	2	9	2	-90	32	2	13	1	118	114	-6	0	8	-43	62
-2	2	8	163	155	-2	5	11	-82	42	2	9	3	161	153	2	13	2	-81	-24	-6	0	10	36	19
-2	2	9	-92	22	-2	5	12	-69	0	2	9	4	-93	60	2	13	3	202	201	7	0	2	39	10
-2	2	10	200	195	2	6	0	261	273	2	9	5	-93	54	2	13	4	-71	20	-7	0	2	42	43
-2	2	11	-89	2	2	6	1	331	-328	2	9	6	-92	-7	2	13	5	136	145	-7	0	4	72	87
-2	2	12	88	90	2	6	2	314	314	2	9	7	111	102	2	13	6	-51	0	-7	0	6	60	71
															-2	13	1	165	158	-7	0	8	95	98

1.54 and 1.52 Å for C_3-C_4, and bond angles, 124 to 127° for $S_2-C_2-N_2$ and $S_2-C_2-N_3$, 110 and 112° for $N_2-C_2-N_3$, 107 to 115° for $C_2-N_2-C_3$ and $C_2-N_3-C_4$, and 100 to 104° for $N_2-C_3-C_4$ and $N_3-C_4-C_3$, with rather large standard deviations (0.024 – 0.031 Å and 1.5 – 1.8°). The ethylene-thiourea groups are planar within the error; the deviations of the atoms from the least-squares planes of the groups, with the sulphur coordinates given four times the weight of the carbon and nitrogen coordinates, are 0.001 – 0.035 Å in I, and 0.006 – 0.049 Å in II. In both compounds, the least-squares

Table 5. Bond lengths and angles in the coordination groups. Standard deviations, in parentheses, do not include uncertainties in unit cell dimensions.

	Dithiocyanato complex	Diselenocyanato complex
∠S–Te–S	90.1(2)°	
∠Se–Te–S		89.9(2)°
Thio- or selenocyanato ligand		
Te–S	2.684(7) Å	
Te–Se		2.809(3) Å
S–C	1.673(21)	
Se–C		1.814(21)
∠Te–S–C	96.3(8)°	
∠Te–Se–C		95.9(9)°
Ethylenethiourea ligand		
Te–S	2.651(6) Å	2.676(6) Å
S–C	1.694(22)	1.730(22)
∠Te–S–C	99.9(8)°	97.5(8)°

planes of the ethylenethiourea groups make angles of 89.7° with the planes of the TeS_4 or TeS_2Se_2 coordination groups.

In the thio- and selenocyanate groups, the C–N bond length is 1.13 and 1.14 Å, respectively, each ±0.03 Å, and the S–C–N and Se–C–N bond angles, 178 and 176°, each ±2°.

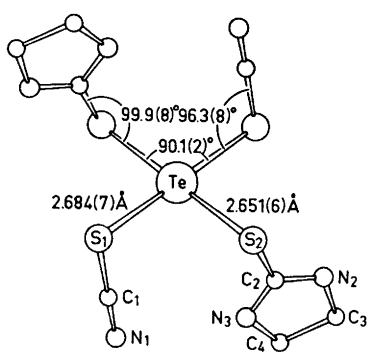

Fig. 1. The *trans*-dithiocyanatobis-(ethylenethiourea)tellurium(II) molecule as seen along the normal to a plane through Te, C_2, and the midpoint between S_1' and S_2, where S_1' is at $-x,-y,-z$ relative to S_1.

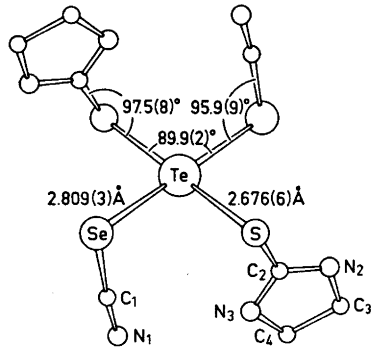

Fig. 2. The *trans*-diselenocyanatobis-(ethylenethiourea)tellurium(II) molecule as seen along the normal to a plane through Te, C_2, and the midpoint between Se′ and S, where Se′ is at $-x,-y,-z$ relative to Se.

REFERENCES

1. Fehér, F. and Linke, K.-H. *Z. anorg. allgem. Chem.* **327** (1964) 151.
2. Ohlberg, S. M. and Vaughan, P. A. *J. Am. Chem. Soc.* **76** (1954) 2649.
3. Aksnes, O. and Foss, O. *Acta Chem. Scand.* **8** (1954) 1787.
4. Montignie, E. *Ann. Pharm. Franc.* **2** (1944) 151.
5. Foss, O. and Hauge, S. *Acta Chem. Scand.* **13** (1959) 1252.
6. Foss, O. and Hauge, S. *Acta Chem. Scand.* **15** (1961) 1615.
7. Foss, O. and Fossen, S. *Acta Chem. Scand.* **15** (1961) 1618.
8. Foss, O. and Marøy, K. *Acta Chem. Scand.* **15** (1961) 1945.
9. Foss, O. *Unpublished work* (1965).
10. Foss, O. In Andersen, P., Bastiansen, O. and Furberg, S. *Selected Topics in Structure Chemistry*, Universitetsforlaget, Oslo 1967, p. 145.
11. Shiono, R. *Intensity Correction Program for IBM 650*, Technical Report No. 16, University of Pittsburgh 1960.
12. Shiono, R. *IBM 650 Programs for Crystallographic Computing*, Technical Report Nos. 9 and 2, University of Pittsburgh 1959 and 1957.
13. Mair, G. A. *Structure Factor and Least Square Programs for the IBM 1620*, National Research Council, Ottawa 1963.
14. *International Tables for X-ray Crystallography*, Kynoch Press, Birmingham 1962, Vol. III.
15. Cromer, D. T. *Acta Cryst.* **18** (1965) 17.
16. Ahrland, S., Chatt, J. and Davies, N. R. *Quart. Rev. (London)* **12** (1958) 265.
17. Pearson, R. G. *J. Am. Chem. Soc.* **85** (1963) 3533.

Received December 2, 1970.