ACTA CHEMICA SCANDINAVICA 25 (1971) 3808–3820

The Crystal and Molecular Structures of *trans* Square-planar Complexes of Tellurium Diselenocyanate with Trimethylenethiourea and Tetramethylthiourea

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The crystal and molecular structures of *trans*-diselenocyanatobis(trimethylenethiourea)tellurium(II), $Te(S{:}C{\cdot}\underline{NH{\cdot}[CH_2]_3{\cdot}NH})_2(SeCN)_2$ (I), and *trans*-diselenocyanatobis(tetramethylthiourea)tellurium(II), $Te(SC[N(CH_3)_2]_2)_2(SeCN)_2$ (II), have been determined by X-ray diffraction methods. Both complexes crystallize in space group $P2_1/c$ (No. 14) with $Z=2$, and with the tellurium atoms located in centres of symmetry. Cell dimensions and densities are: $a=4.782(3)$ Å, $b=15.362(5)$ Å, $c=13.203(5)$ Å, $\beta=106.54(5)°$, ϱ_o(flotation) = 2.05 g/cm³, $\varrho_c=2.04$ g/cm³ for I, and $a=8.804(5)$ Å, $b=6.363(6)$ Å, $c=19.749(8)$ Å, $\beta=98.80(5)°$, ϱ_o(flotation) = 1.86 g/cm³, $\varrho_c=1.83$ g/cm³ for II. Intensity data were collected using integrating Weissenberg techniques. Based on 924 independent, non-zero reflections for I, and 1119 for II, refinement by full-matrix, least squares methods resulted in conventional R-values of 0.073 and 0.076, respectively.

In both complexes the tellurium atom is bonded to two selenium atoms and two sulphur atoms in a *trans* square-planar arrangement, with the dimensions: Te–Se = 2.834(2) Å, Te–S = 2.670(5) Å, ∠Se–Te–S = 89.73(11)° in I; and Te–Se = 2.815(3) Å, Te–S = 2.728(4) Å, ∠Se–Te–S = 91.61(10)° in II.

The crystal structure of a centrosymmetric, *trans* square-planar complex of tellurium diselenocyanate with ethylenethiourea, $Te(etu)_2(SeCN)_2$, has been determined.[1] This article reports the crystal structures of two additional tellurium diselenocyanate complexes, $Te(trtu)_2(SeCN)_2$ and $Te(tmtu)_2(SeCN_2)$, where trtu = trimethylenethiourea and tmtu = tetramethylthiourea. As in the ethylenethiourea complex, the tellurium atoms in both compounds lie in crystallographic centres of symmetry, and the configuration around tellurium is square-planar *trans*.

EXPERIMENTAL

trans-Diselenocyanatobis(trimethylenethiourea)tellurium(II), $Te(trtu)_2(SeCN)_2$ (I), and *trans*-diselenocyanatobis(tetramethylthiourea)tellurium(II), $Te(tmtu)_2(SeCN)_2$ (II), were prepared from the dibromo complexes, $Te(trtu)_2Br_2$ [2] and $Te(tmtu)_2Br_2$,[3] and an

excess of potassium selenocyanate in methanol.[4] Crystallization from the gently warmed and filtered reaction mixtures took place on cooling. The crystals are light brown in colour, and are stable when dry, but liberate tellurium in contact with water as do other tellurium(II) complexes.

For determination of cell dimensions, 2θ-values were measured from zero-layer Weissenberg photographs around the a and b axes, taken with Cu$K\alpha_1$ radiation ($\lambda = 1.5405$ Å). Sodium chloride powder lines were superimposed on the films for reference ($a = 5.6394$ Å at 18°C).[5]

Intensity data were collected using multiple-film, integrating, equi-inclination Weissenberg techniques with (Ni-filtered) Cu$K\alpha$ radiation. The crystal dimensions of I, given as distances from a common origin to faces, had the following values for the crystal rotating about the a axis (zero layer): distances to (100) and $(\bar{1}00) = 0.054$ mm, to (011), $(0\bar{1}1)$, $(0\bar{1}\bar{1})$, and $(01\bar{1}) = 0.023$ mm. The crystal rotating about the a axis (upper layers) had the dimensions: distances to (100) and $(\bar{1}00) = 0.088$ mm, to (011), $(0\bar{1}1)$, $(0\bar{1}\bar{1})$, and $(01\bar{1}) = 0.025$ mm. The dimensions of the crystal rotating about the b axis were: distances to (100) and $(\bar{1}00) = 0.042$ mm, to (011), $(0\bar{1}1)$, $(0\bar{1}\bar{1})$, and $(01\bar{1}) = 0.032$ mm. The crystal of II rotating about the a axis had the dimensions: distances to (001) and $(00\bar{1}) = 0.054$ mm, to (101) and $(\bar{1}0\bar{1}) = 0.066$ mm, to $(10\bar{1})$ and $(\bar{1}01) = 0.089$ mm, to (010) and $(0\bar{1}0) = 0.044$ mm. The dimensions of the crystal rotating about the b axis were: distances to (100) and $(\bar{1}00) = 0.034$ mm, to (001) and $(00\bar{1}) = 0.026$ mm, to (010) and $(0\bar{1}0) = 0.087$ mm.

Intensities of the $0kl - 2kl$ and $h0l$ reflections of I, and the $0kl$, $1kl$, and $h0l - h3l$ reflections of II, were estimated visually by comparison with a scale of timed exposures. Out of 1174 accessible, independent reflections for I, and 1638 for II, 924 and 1119, respectively, were strong enough to be measured. The remaining reflections were assigned an intensity equal to the observable limit, and labelled as unobserved reflections.

The intensities were corrected for absorption, using a modified version of the absorption correction method described by Busing and Levy.[6] The corrections were based on the crystal dimensions quoted above, $8 \times 8 \times 8$ grids for all of the crystals, and $\mu = 205$ cm^{-1} for I and 175 cm^{-1} for II. Lorentz and polarization corrections were carried out, and the corrected intensities were reduced to relative observed structure factors. No extinction corrections were applied.

Calculated structure factors were based on the atomic scattering factor curves listed in *International Tables* (Ref. 5, p. 202). Using Cromer's values of $\Delta f'$ and $\Delta f''$,[7] the tellurium, selenium, and sulphur scattering curves were corrected for anomalous dispersion, by taking the amplitude of f as the corrected value.

The structures were refined by a least squares, full-matrix program minimizing the function

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

where K is a scale factor. The weight, W, is defined by $W = 1/[(Ka_1)^2 + \sigma^2(F_o)]$, where a_1 is a constant and $\sigma(F_o)$ is the estimated standard deviation of 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, using a program library 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 Mr. Knut Maartmann-Moe, of this Institute.

CRYSTAL DATA

The crystals of I occurred as monoclinic needles along a, bounded mainly by {011}. They exhibited a pronounced tendency of twinning. Using 28 high-angle 2θ-values, the cell dimensions were calculated by a least squares procedure. The standard deviations, which do not include uncertainties in film radii, are given in parentheses:

$a = 4.782(3)$ Å, $b = 15.362(5)$ Å, $c = 13.203(5)$ Å, $\beta = 106.54(5)°$, $V = 929.8(8)$ Å^3, $M = 569.93$, $F(000) = 540$, $Z = 2$, ϱ_o(flotation) = 2.05 g/cm^3, $\varrho_c = 2.04$ g/cm^3.

The crystals of II occurred as monoclinic needles or prisms along b. Different batches of crystals showed varying forms. Cell dimensions, calculated as for I, were based on 65 high-angle 2θ-values:

$a = 8.804(5)$ Å, $b = 6.363(6)$ Å, $c = 19.749(8)$ Å, $\beta = 98.80(5)°$, $V = 1093.3(13)$ Å^3, $M = 602.01$, $F(000) = 580$, $Z = 2$, ϱ_o(flotation) = 1.86 g/cm^3, $\varrho_c = 1.83$ g/cm^3.

For both compounds the systematic absences are $h0l$ when l is odd, and $0k0$ when k is odd. The uniquely determined space group is $P2_1/c$ (No. 14).

STRUCTURE DETERMINATION

The structures were solved through Fourier syntheses in the $0kl$ and $h0l$ projections. With the tellurium atoms in centres of symmetry, the initial phases were based on the tellurium contributions alone. As the tellurium atoms did not contribute to reflections with $k+l$ odd, the first Fourier maps in the $0kl$ projections had extra (false) mirror planes. Two relatively high peaks, related by a false mirror plane, occurred in each map. The coordinates of one of the peaks were chosen as selenium coordinates. On inclusion of $k+l$ odd reflections in subsequent Fourier summations, the rest of the atoms, except hydrogen, could be located.

Three-dimensional least squares refinement with individual isotropic thermal parameters resulted in conventional R values of 0.105 for I and 0.094 for II. Some strong, low-order reflections seemed to have markedly lower observed than calculated structure factors; 29 such reflections of I, and 31 of II, were therefore given zero weight at this stage. After introduction of overall scale factors, and anisotropic thermal parameters for the tellurium, selenium, and sulphur atoms, the refinement was continued until no shift was greater than 0.19 times the standard deviation for I, and 0.16 times the standard deviation for II. The value of the adjustable constant a_1 in the weighting scheme was 3.4 for I and 1.3 for II during the last refinement cycles. The final values of R, including the reflections with zero weight mentioned above, and with non-observed reflections included when $K|F_c|$ exceeded the observable limit, were 0.073 for I and 0.076 for II. The highest peaks in difference Fourier maps at this stage were 1.7 e/Å^2 in the $0kl$ projection of I, and 1.3 e/Å^2 in the $h0l$ projection of II.

The final atomic coordinates are listed in Table 1, together with isotropic thermal parameters for the carbon and nitrogen atoms, while Table 2 contains anisotropic thermal parameters for the heavier atoms. Observed and calculated structure factors are listed in Table 3 for I and Table 4 for II.

RESULTS

Bond lengths and angles are listed in Table 5 for the coordination groups, and in Table 6 for the ligands. The standard deviations are calculated from those of Table 1, without regard to coordinate covariances and standard deviations in cell dimensions. Drawings of the molecules are shown in Fig. 1 (trimethylenethiourea complex) and Fig. 2 (tetramethylthiourea complex).

Table 1. Atomic coordinates in fractions of monoclinic cell edges. Origin at a centre of symmetry. Isotropic thermal parameters (Å²) in the form $\exp[-8\pi^2 U(\sin^2\theta/\lambda^2)]$. Standard deviations from the least squares refinement are given in parentheses.

Diselenocyanatobis(trimethylenethiourea)tellurium(II)

	x	*y*	*z*	*U*
Te	0	0	0	
Se	0.4957(5)	0.02231(11)	0.17673(15)	
S	0.0846(13)	0.15877(27)	−0.06807(34)	
N(1)	0.221(5)	0.1004(12)	0.3290(15)	0.085(6)
N(2)	−0.140(4)	0.2058(8)	0.0883(10)	0.038(4)
N(3)	−0.013(4)	0.3139(9)	−0.0108(12)	0.050(4)
C(1)	0.331(5)	0.0695(11)	0.2707(14)	0.050(5)
C(2)	−0.046(4)	0.2312(9)	0.0079(12)	0.037(3)
C(3)	−0.242(5)	0.2649(11)	0.1584(14)	0.048(5)
C(4)	−0.117(6)	0.3521(16)	0.1575(21)	0.092(8)
C(5)	−0.095(5)	0.3850(14)	0.0523(17)	0.069(6)

Diselenocyanatobis(tetramethylthiourea)tellurium(II)

	x	*y*	*z*	*U*
Te	0	0	0	
Se	−0.13897(21)	0.37586(40)	0.03414(10)	
S	0.27479(38)	0.11362(68)	0.07433(18)	
N(1)	−0.2781(19)	0.2197(30)	0.1524(10)	0.101(6)
N(2)	0.2003(14)	−0.1763(26)	0.1685(7)	0.066(4)
N(3)	0.4347(15)	−0.2205(24)	0.1281(7)	0.066(4)
C(1)	−0.2242(19)	0.2864(32)	0.1067(10)	0.074(5)
C(2)	0.3060(18)	−0.1079(30)	0.1276(9)	0.064(5)
C(3)	0.0984(21)	−0.0304(33)	0.1904(10)	0.082(6)
C(4)	0.1756(21)	−0.3927(40)	0.1814(10)	0.080(6)
C(5)	0.5164(25)	−0.3516(40)	0.1884(12)	0.106(7)
C(6)	0.5217(21)	−0.2166(35)	0.0729(10)	0.084(6)

Table 2. 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 from the least squares refinement are given in parentheses.

Diselenocyanatobis(trimethylenethiourea)tellurium(II)

	U_{11}	U_{22}	U_{33}	U_{12}	U_{23}	U_{13}
Te	554(15)	351(6)	387(7)	11(9)	−43(7)	265(8)
Se	523(18)	551(11)	520(12)	2(11)	−39(8)	237(12)
S	965(50)	461(22)	519(26)	−6(27)	0(19)	430(30)

Diselenocyanatobis(tetramethylthiourea)tellurium(II)

	U_{11}	U_{22}	U_{33}	U_{12}	U_{23}	U_{13}
Te	570(7)	532(12)	486(6)	86(9)	32(9)	135(5)
Se	756(12)	671(18)	815(13)	82(11)	−38(12)	158(10)
S	492(18)	329(27)	623(21)	51(18)	26(19)	84(16)

Table 3. Observed and calculated structure factors (× 10) for *trans*-diselenocyanatobis(trimethylenethiourea)tellurium(II). Unobserved reflections are indicated by a minus sign on $F(O)$ and included at the threshold values. An asterisk denotes reflections given zero weight during the last refinement cycles.

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	2	0	1130	1281 *	0	12	5	238	260	0	5	11	555	556	1	2	2	704	716 *	1	8	7	480	448
0	4	0	1177	1359 *	0	13	5	270	265	0	6	11	-142	115	1	3	2	554	531	1	9	7	432	414
0	6	0	1383	1474 *	0	14	5	212	234	0	7	11	365	363	1	4	2	872	959 *	1	10	7	321	297
0	8	0	898	875	0	15	5	165	163	0	8	11	-137	-1	1	5	2	393	433	1	11	7	253	243
0	10	0	471	496	0	16	5	-123	64	0	9	11	354	358	1	6	2	957	1024 *	1	12	7	237	237
0	12	0	524	511	0	17	5	132	166	0	10	11	126	116	1	7	2	497	485	1	13	7	215	222
0	14	0	264	252	0	18	5	-86	-14	0	11	11	166	181	1	8	2	628	642	1	14	7	206	199
0	16	0	-139	46	0	0	6	1398	1382	0	12	11	130	135	1	9	2	343	349	1	15	7	196	203
0	18	0	134	140	0	1	6	197	198	0	13	11	138	175	1	10	2	440	432	1	16	7	84	86
0	1	1	1333	1481 *	0	2	6	1330	1261	0	14	11	-72	-24	1	11	2	293	276	1	0	8	705	720
0	2	1	243	-264	0	3	6	-106	-77	0	0	12	690	701	1	12	2	461	443	1	1	8	128	99
0	3	1	1126	1143 *	0	4	6	1401	1337	0	1	12	-144	-110	1	13	2	295	273	1	2	8	747	737
0	4	1	844	-920 *	0	5	6	292	-237	0	2	12	393	380	1	14	2	277	253	1	3	8	-128	94
0	5	1	1408	1498 *	0	6	6	700	682	0	3	12	-162	-84	1	15	2	164	162	1	4	8	840	846
0	6	1	726	-767	0	7	6	-123	17	0	4	12	434	466	1	16	2	140	100	1	5	8	161	136
0	7	1	922	958	0	8	6	783	796	0	5	12	-138	-36	1	17	2	-112	67	1	6	8	463	424
0	8	1	272	-277	0	9	6	134	-138	0	6	12	394	392	1	18	2	152	162	1	7	8	235	236
0	9	1	514	490	0	10	6	550	528	0	7	12	147	-162	1	19	2	-62	50	1	8	8	536	519
0	10	1	405	-421	0	11	6	215	-232	0	8	12	274	273	1	1	3	1579	1832 *	1	9	8	-136	118
0	11	1	365	361	0	12	6	250	260	0	9	12	119	-116	1	2	3	-80	50	1	10	8	396	354
0	12	1	431	-441	0	13	6	-143	-55	0	10	12	175	197	1	3	3	1137	1230 *	1	11	8	146	132
0	13	1	534	526	0	14	6	-138	104	0	11	12	-100	5	1	4	3	290	-322	1	12	8	176	183
0	14	1	164	-136	0	15	6	-129	1	0	12	12	136	168	1	5	3	1158	1295 *	1	13	8	128	110
0	15	1	162	156	0	16	6	163	181	0	13	12	-65	-52	1	6	3	210	-216	1	14	8	103	85
0	16	1	170	-186	0	17	6	-98	-39	0	1	13	178	209	1	7	3	876	901	1	15	8	-87	74
0	17	1	126	113	0	18	6	-72	56	0	2	13	164	-174	1	8	3	195	179	1	16	8	116	137
0	18	1	-108	-78	0	1	7	515	482	0	3	13	133	108	1	9	3	561	525	1	1	9	653	635
0	19	1	179	199	0	2	7	-115	-82	0	4	13	-131	-14	1	10	3	-127	-35	1	2	9	-134	-14
0	0	2	954	850	0	3	7	1078	1046	0	5	13	202	218	1	11	3	339	299	1	3	9	798	801
0	1	2	367	-245	0	4	7	361	-363	0	6	13	123	-132	1	12	3	168	-166	1	4	9	-135	-68
0	2	2	385	-385	0	5	7	358	331	0	7	13	185	222	1	13	3	457	418	1	5	9	508	436
0	3	2	75	70	0	6	7	356	-351	0	8	13	135	-141	1	14	3	-137	95	1	6	9	-136	-59
0	4	2	223	261	0	7	7	346	312	0	9	13	152	147	1	15	3	-131	92	1	7	9	398	354
0	5	2	750	-772	0	8	7	353	-362	0	10	13	90	-93	1	16	3	-120	-78	1	8	9	151	-152
0	6	2	771	775	0	9	7	575	559	0	11	13	92	134	1	17	3	-106	58	1	9	9	455	427
0	7	2	275	-329	0	10	7	321	-304	0	0	14	146	151	1	18	3	-85	-19	1	10	9	-128	-56
0	8	2	375	392	0	11	7	280	280	0	1	14	-119	-59	1	0	4	983	1008	1	11	9	183	149
0	9	2	463	-438	0	12	7	288	-293	0	2	14	-118	-30	1	1	4	-87	-50	1	12	9	127	-109
0	10	2	410	411	0	13	7	171	191	0	3	14	-116	62	1	2	4	609	628	1	13	9	125	113
0	11	2	520	-537	0	14	7	161	-158	0	4	14	-113	33	1	3	4	202	-198	1	14	9	-88	-57
0	12	2	455	458	0	15	7	241	245	0	5	14	-109	-15	1	4	4	789	838	1	15	9	95	103
0	13	2	-145	-143	0	16	7	-105	-68	0	6	14	136	150	1	5	4	710	-740	1	0	10	241	201
0	14	2	356	350	0	17	7	170	201	0	7	14	-98	-8	1	6	4	842	861	1	1	10	-139	-81
0	15	2	-144	-104	0	0	8	213	-175	0	8	14	87	102	1	7	4	275	-263	1	2	10	351	297
0	16	2	246	260	0	1	8	-124	-118	0	9	14	-74	-32	1	8	4	525	486	1	3	10	153	-153
0	17	2	-124	-138	0	2	8	-125	60	0	10	14	-53	80	1	9	4	324	-304	1	4	10	417	385
0	18	2	259	285	0	3	8	154	-156	0	1	15	129	150	1	10	4	428	415	1	5	10	152	-142
0	19	2	-81	-20	0	4	8	386	341	0	2	15	-96	15	1	11	4	527	-497	1	6	10	165	154
0	1	3	143	102	0	5	8	173	-164	0	3	15	-93	43	1	12	4	330	296	1	7	10	175	-163
0	2	3	688	655	0	6	8	-134	0	0	4	15	-89	86	1	13	4	168	-141	1	8	10	183	172
0	3	3	294	-247	0	7	8	-138	-126	0	5	15	-83	116	1	14	4	212	197	1	9	10	285	-251
0	4	3	122	132	0	8	8	200	197	0	6	15	-75	54	1	15	4	141	-100	1	10	10	270	231
0	5	3	116	-29	0	9	8	268	-271	0	7	15	100	150	1	16	4	152	151	1	11	10	110	-60
0	6	3	218	-188	0	10	8	381	362	0	0	16	168	243	1	17	4	131	-135	1	12	10	131	132
0	7	3	247	232	0	11	8	-143	14	0	1	16	-45	31	1	18	4	131	145	1	13	10	105	-125
0	8	3	432	422	0	12	8	221	225	0	2	16	116	193	1	1	5	109	52	1	14	10	109	139
0	9	3	451	425	0	13	8	-133	-92	1	0	0	899	1025 *	1	2	5	174	156	1	1	11	-136	9
0	10	3	-127	-43	0	14	8	221	260	1	1	0	198	169	1	3	5	216	160	1	2	11	152	-117
0	11	3	292	295	0	15	8	-109	-51	1	2	0	821	-867	1	4	5	174	-135	1	3	11	-135	47
0	12	3	-141	-46	0	16	8	265	309	1	3	0	527	-567	1	5	5	172	144	1	4	11	-133	-1
0	13	3	632	612	0	17	8	-64	3	1	4	0	322	-298	1	6	5	506	-479	1	5	11	-131	69
0	14	3	178	207	0	1	9	-134	-7	1	5	0	157	141	1	7	5	245	232	1	6	11	-128	-37
0	15	3	300	296	0	2	9	-134	-21	1	6	0	505	511	1	8	5	-124	-125	1	7	11	-124	51
0	16	3	-133	-8	0	3	9	202	164	1	7	0	158	-113	1	9	5	422	399	1	8	11	146	-138
0	17	3	289	333	0	4	9	192	192	1	8	0	284	287	1	10	5	362	-342	1	9	11	251	238
0	18	3	-102	7	0	5	9	-138	80	1	9	0	-109	30	1	11	5	247	217	1	10	11	-104	16
0	19	3	206	247	0	6	9	211	212	1	10	0	319	318	1	12	5	248	-242	1	11	11	114	109
0	0	4	642	608	0	7	9	-143	112	1	11	0	154	132	1	13	5	413	389	1	12	11	-80	16
0	1	4	372	362	0	8	9	-144	51	1	12	0	526	506	1	14	5	-130	-6	1	13	11	110	157
0	2	4	648	593	0	9	9	475	472	1	13	0	-139	-71	1	15	5	199	201	1	0	12	-127	85
0	3	4	149	172	0	10	9	237	245	1	14	0	427	405	1	16	5	119	-98	1	1	12	-127	6
0	4	4	667	623	0	11	9	197	208	1	15	0	-138	-45	1	17	5	219	245	1	2	12	-127	7
0	5	4	135	123	0	12	9	162	175	1	16	0	292	276	1	0	6	-107	36	1	3	12	-126	26
0	6	4	461	456	0	13	9	195	233	1	17	0	-117	25	1	1	6	187	223	1	4	12	138	128
0	7	4	844	836	0	14	9	-111	39	1	18	0	300	322	1	2	6	-110	8	1	5	12	170	161
0	8	4	402	395	0	15	9	195	227	1	19	0	-72	-14	1	3	6	-111	2	1	6	12	142	123
0	9	4	699	727	0	16	9	-72	97	1	1	1	160	93	1	4	6	127	65	1	7	12	-110	78
0	10	4	498	471	0	0	10	416	396	1	2	1	324	347	1	5	6	-117	-27	1	8	12	137	121
0	11	4	-137	117	0	1	10	-142	2	1	3	1	183	196	1	6	6	-121	14	1	9	12	-95	62
0	12	4	426	414	0	2	10	418	399	1	4	1	548	535	1	7	6	351	295	1	10	12	134	171
0	13	4	419	382	0	3	10	-141	133	1	5	1	797	826	1	8	6	252	214	1	11	12	111	132
0	14	4	269	312	0	4	10	532	541	1	6	1	533	563	1	9	6	232	245	1	1	13	264	260
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0	16	4	301	318	0	6	10	385	356	1	8	1	445	440	1	11	6	-138	-86	1	3	13	219	197
0	17	4	-115	38	0	7	10	249	252	1	9	1	318	291	1	12	6	333	310	1	4	13	168	177
0	18	4	196	206	0	8	10	277	281	1	10	1	413	408	1	13	6	161	137	1	5	13	229	232
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0	3	5	1718	1684	0	11	10	298	310	1	13	1	569	530	1	16	6	280	296	1	8	13	-82	84
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0	5	5	954	927	0	13	10	122	116	1	15	1	236	247	1	1	7	290	226	1	0	14	386	410
0	6	5	-109	70	0	14	10	157	189	1	16	1	143	154	1	2	7	267	232	1	1	14	-92	-30
0	7	5	848	824	0	15	10	-74	75	1	17	1	190	193	1	3	7	698	712	1	2	14	225	221
0	8	5	564	543	0	1	11	723	724	1	18	1	-96	61	1	4	7	220	211	1	3	14	-88	23
0	9	5	755	732	0	2	11	-145	-129	1	19	1	227	273	1	5	7	344	286	1	4	14	234	271
0	10	5	224	238	0	3	11	624	613	1	0	2	2466	2953 *	1	6	7	192	195	1	5	14	-78	41
0	11	5	325	323	0	4	11	239	246	1	1	2	232	194	1	7	7	328	302	1	6	14	197	219

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	7	14	-59	12	1	8	-6	339	327	1	1-13		503	488	2	12	3	-105	-15	2	1	-2	103	-87
1	1	15	183	214	1	9	-6	-126	-84	1	2-13		-135	8	2	13	3	387	387	2	2	-2	198	189
1	2	15	-59	-64	1	10	-6	500	477	1	3-13		315	273	2	14	3	-97	64	2	3	-2	310	315
1	1	-1	762	787 *	1	11	-6	319	-274	1	4-13		162	-187	2	15	3	200	228	2	4	-2	363	378
1	2	-1	746	-783 *	1	12	-6	365	304	1	5-13		358	361	2	16	3	-79	17	2	5	-2	537	519
1	3	-1	273	273	1	13	-6	-137	-129	1	6-13		154	-147	2	17	3	122	173	2	6	-2	120	96
1	4	-1	328	-308	1	14	-6	345	320	1	7-13		361	373	2	0	4	739	748	2	7	-2	161	141
1	5	-1	398	401	1	15	-6	-124	-100	1	8-13		256	-216	2	1	4	224	182	2	8	-2	307	298
1	6	-1	244	-269	1	16	-6	377	400	1	9-13		200	192	2	2	4	108	21	2	9	-2	254	230
1	7	-1	435	410	1	17	-6	-96	-50	1	10-13		169	-185	2	3	4	398	379	2	10	-2	425	384
1	8	-1	904	-916	1	18	-6	167	202	1	11-13		193	188	2	4	4	308	306	2	11	-2	549	523
1	9	-1	467	447	1	1	-7	480	460	1	12-13		98	-137	2	5	4	245	243	2	12	-2	408	392
1	10	-1	379	-360	1	2	-7	237	-189	1	0-14		553	583	2	6	4	425	374	2	13	-2	152	157
1	11	-1	337	324	1	3	-7	844	852	1	1-14		-124	3	2	7	4	405	395	2	14	-2	267	277
1	12	-1	220	-215	1	4	-7	339	-375	1	2-14		442	438	2	8	4	288	281	2	15	-2	-101	46
1	13	-1	667	608	1	5	-7	401	398	1	3-14		-121	-63	2	9	4	299	286	2	16	-2	289	332
1	14	-1	373	-364	1	6	-7	538	-531	1	4-14		371	353	2	10	4	265	279	2	17	-2	88	96
1	15	-1	242	236	1	7	-7	347	340	1	5-14		-115	18	2	11	4	166	182	2	18	-2	171	210
1	16	-1	-130	-91	1	8	-7	369	-350	1	6-14		500	484	2	12	4	278	288	2	1	-3	382	-332
1	17	-1	267	265	1	9	-7	766	773	1	7-14		-105	-79	2	13	4	217	223	2	2	-3	260	-238
1	18	-1	-99	-59	1	10	-7	478	-457	1	8-14		265	280	2	14	4	203	221	2	3	-3	423	395
1	19	-1	198	219	1	11	-7	331	311	1	9-14		-88	-48	2	15	4	133	140	2	4	-3	65	57
1	0	-2	1279	1598 *	1	12	-7	292	-306	1	10-14		139	145	2	16	4	119	153	2	5	-3	193	-159
1	1	-2	95	-80	1	13	-7	233	224	1	11-14		-52	-28	2	17	4	-54	53	2	6	-3	-71	4
1	2	-2	1353	1445 *	1	14	-7	157	-155	1	1-15		349	363	2	1	5	945	913 *	2	7	-3	203	196
1	3	-2	126	-172	1	15	-7	282	253	1	2-15		-105	-14	2	2	5	167	168	2	8	-3	293	-258
1	4	-2	1344	1391	1	16	-7	179	-173	1	3-15		261	258	2	3	5	684	650	2	9	-3	440	393
1	5	-2	113	-49	1	17	-7	217	229	1	4-15		-99	53	2	4	5	130	139	2	10	-3	-97	-69
1	6	-2	1175	1196	1	0	-8	912	962	1	5-15		265	282	2	5	5	641	635	2	11	-3	313	308
1	7	-2	744	-745	1	1	-8	-114	75	1	6-15		88	111	2	6	5	194	157	2	12	-3	141	-131
1	8	-2	609	641	1	2	-8	1053	1109	1	7-15		246	288	2	7	5	472	448	2	13	-3	336	350
1	9	-2	620	-644	1	3	-8	-117	-105	1	8-15		-70	12	2	8	5	328	335	2	14	-3	-105	-106
1	10	-2	577	528	1	4	-8	1291	1211	1	9-15		-51	134	2	9	5	353	357	2	15	-3	364	377
1	11	-2	-127	-103	1	5	-8	450	-411	1	0-16		176	185	2	10	5	181	200	2	16	-3	-91	-36
1	12	-2	436	404	1	6	-8	717	702	1	1-16		-82	-64	2	11	5	214	197	2	17	-3	279	317
1	13	-2	403	-369	1	7	-8	204	-204	1	2-16		99	120	2	12	5	112	71	2	18	-3	-59	29
1	14	-2	223	231	1	8	-8	498	477	1	3-16		-77	38	2	13	5	264	283	2	0	-4	362	359
1	15	-2	238	-221	1	9	-8	-136	-62	1	4-16		88	93	2	14	5	174	199	2	1	-4	261	-230
1	16	-2	225	192	1	10	-8	591	550	1	5-16		112	135	2	15	5	86	93	2	2	-4	486	430
1	17	-2	-116	-3	1	11	-8	365	-304	2	0	0	1515	1631 *	2	16	5	-63	15	2	3	-4	413	-399
1	18	-2	138	137	1	12	-8	214	199	2	1	0	111	159	2	2	6	719	723 *	2	4	-4	808	754
1	19	-2	-71	-38	1	13	-8	-129	-61	2	2	0	1191	1245 *	2	3	6	-96	-72	2	5	-4	203	-209
1	1	-3	1531	1686 *	1	14	-8	209	202	2	3	0	59	-40	2	4	6	689	686	2	6	-4	299	284
1	2	-3	493	-493	1	15	-8	-108	-39	2	4	0	1206	1162	2	5	6	263	-252	2	7	-4	675	-640
1	3	-3	1753	1891 *	1	16	-8	191	190	2	5	0	318	258	2	6	6	610	599	2	8	-4	550	532
1	4	-3	-75	81	1	17	-8	110	-119	2	6	0	1201	1236	2	7	6	-103	30	2	9	-4	454	-415
1	5	-3	1191	1202	1	1	-9	1027	1038	2	7	0	124	-97	2	8	6	405	384	2	10	-4	563	521
1	6	-3	526	499	1	2	-9	320	317	2	8	0	653	636	2	9	6	-104	23	2	11	-4	388	-379
1	7	-3	1105	1147	1	3	-9	900	922	2	9	0	-92	-80	2	10	6	263	291	2	12	-4	325	301
1	8	-3	174	-162	1	4	-9	-127	-73	2	10	0	424	407	2	11	6	151	-163	2	13	-4	267	-273
1	9	-3	878	834	1	5	-9	726	741	2	11	0	178	161	2	12	6	172	167	2	14	-4	249	227
1	10	-3	258	234	1	6	-9	162	150	2	12	0	339	320	2	13	6	-89	15	2	15	-4	229	-219
1	11	-3	349	325	1	7	-9	477	478	2	13	0	-107	-85	2	14	6	97	103	2	16	-4	295	310
1	12	-3	-136	53	1	8	-9	306	312	2	14	0	148	154	2	15	6	-67	-6	2	17	-4	-75	-77
1	13	-3	362	315	1	9	-9	574	556	2	15	0	-99	-31	2	16	6	49	78	2	18	-4	118	149
1	14	-3	-140	-56	1	10	-9	-137	74	2	16	0	90	83	2	2	7	-101	2	2	1	-5	1036	1073
1	15	-3	151	95	1	11	-9	233	230	2	17	0	-77	62	2	3	7	467	450	2	2	-5	273	-188
1	16	-3	-127	53	1	12	-9	-130	-15	2	18	0	72	87	2	4	7	169	-139	2	3	-5	1498	1574
1	17	-3	139	134	1	13	-9	285	211	2	1	1	1192	1118 *	2	5	7	343	324	2	4	-5	270	-218
1	18	-3	-94	77	1	14	-9	184	176	2	2	1	234	-266	2	6	7	313	-332	2	5	-5	818	793
1	19	-3	-67	50	1	15	-9	153	157	2	3	1	839	859	2	7	7	255	260	2	6	-5	492	-446
1	0	-4	1037	1110 *	1	16	-9	-78	-11	2	4	1	199	-189	2	8	7	138	-146	2	7	-5	631	582
1	1	-4	278	-255	1	0	10	569	562	2	5	1	867	839	2	9	7	308	312	2	8	-5	278	-265
1	2	-4	971	994	1	1	10	232	210	2	6	1	282	-254	2	10	7	222	-231	2	9	-5	904	858
1	3	-4	372	353	1	2	10	283	234	2	7	1	641	580	2	11	7	134	133	2	10	-5	291	-275
1	4	-4	1134	1123	1	3	10	250	231	2	8	1	589	-600	2	12	7	140	-173	2	11	-5	368	332
1	5	-4	740	712	1	4	10	458	449	2	9	1	440	412	2	13	7	133	174	2	12	-5	176	-177
1	6	-4	437	466	1	5	10	135	120	2	10	1	323	-306	2	14	7	-69	-45	2	13	-5	140	140
1	7	-4	205	249	1	6	10	394	365	2	11	1	296	266	2	15	7	66	78	2	14	-5	135	104
1	8	-4	660	678	1	7	10	382	372	2	12	1	206	-205	2	3	8	-104	-98	2	15	-5	195	196
1	9	-4	358	390	1	8	10	324	292	2	13	1	391	405	2	4	8	104	86	2	16	-5	104	-125
1	10	-4	583	547	1	9	10	306	286	2	14	1	218	-239	2	5	8	128	-107	2	17	-5	166	159
1	11	-4	673	643	1	10	10	365	314	2	15	1	119	110	2	6	8	-104	7	2	18	-5	-48	-48
1	12	-4	388	356	1	11	10	-129	65	2	16	1	-87	-58	2	7	8	-103	-60	2	0	-6	1059	1118
1	13	-4	250	245	1	12	10	242	227	2	17	1	91	121	2	8	8	159	160	2	1	-6	184	160
1	14	-4	182	192	1	13	10	175	157	2	18	1	-54	-51	2	9	8	-97	-78	2	2	-6	1274	1295
1	15	-4	-133	83	1	14	10	170	193	2	0	2	944	1015 *	2	10	8	139	168	2	3	-6	112	92
1	16	-4	308	276	1	15	10	128	144	2	1	2	-62	29	2	11	8	137	-164	2	4	-6	1280	1340
1	17	-4	123	116	1	1	11	-140	38	2	2	2	170	-163	2	12	8	125	169	2	5	-6	-82	29
1	18	-4	119	133	1	2	11	278	264	2	3	2	510	-511	2	13	8	-69	-29	2	6	-6	823	763
1	1	-5	291	-213	1	3	11	-138	-28	2	4	2	123	57	2	14	8	110	136	2	7	-6	188	150
1	2	-5	-85	27	1	4	11	196	-149	2	5	2	272	-242	2	5	9	-102	-3	2	8	-6	553	502
1	3	-5	803	791	1	5	11	149	161	2	6	2	419	399	2	6	9	-100	62	2	9	-6	321	295
1	4	-5	354	406	1	6	11	-138	43	2	7	2	404	-400	2	7	9	-98	70	2	10	-6	586	563
1	5	-5	166	-73	1	7	11	274	223	2	8	2	279	272	2	8	9	116	120	2	11	-6	-106	-24
1	6	-5	360	358	1	8	11	165	142	2	9	2	338	-313	2	9	9	155	170	2	12	-6	225	190
1	7	-5	188	134	1	9	11	245	193	2	10	2	268	256	2	10	9	-84	101	2	13	-6	116	128
1	8	-5	275	229	1	10	11	-126	35	2	11	2	181	-182	2	11	9	108	133	2	14	-6	221	207
1	9	-5	558	512	1	11	11	205	212	2	12	2	382	369	2	1	-1	860	1015 *	2	15	-6	-91	75
1	10	-5	314	280	1	12	11	-109	-9	2	13	2	181	-193	2	2	-1	260	-292	2	16	-6	184	207
1	11	-5	370	337	1	13	11	251	264	2	14	2	256	279	2	3	-1	983	959	2	17	-6	-65	-22
1	12	-5	194	207	1	14	11	-81	70	2	15	2	140	-140	2	4	-1	370	365	2	1	-7	670	625
1	13	-5	294	310	1	0	12	408	376	2	16	2	139	173	2	5	-1	715	673	2	2	-7	369	372
1	14	-5	-136	97	1	1	12	-141	86	2	17	2	-70	-62	2	6	-1	734	740	2	3	-7	703	681
1	15	-5	405	396	1	2	12	-140	10	2	18	2	147	210	2	7	-1	744	754	2	4	-7	249	195
1	16	-5	-118	60	1	3	12	241	-206	2	1	3	195	-190	2	8	-1	186	168	2	5	-7	506	457
1	17	-5	334	325	1	4	12	-138	102	2	2	3	-74	54	2	9	-1	616	589	2	6	-7	389	387
1	18	-5	-82	58	1	5	12	193	-175	2	3	3	288	-214	2	10	-1	526	534	2	7	-7	304	298
1	0	-6	295	-264	1	6	12	301	277	2	4	3	-78	-39	2	11	-1	303	273	2	8	-7	496	497
1	1	-6	-93	-26	1	7	12	132	-128	2	5	3	266	259	2	12	-1	322	310	2	9	-7	652	619
1	2	-6	135	-60	1	8	12	180	183	2	6	3	-86	40	2	13	-1	339	351	2	10	-7	262	250
1	3	-6	154	-139	1	9	12	121	-114	2	7	3	279	267	2	14	-1	-107	113	2	11	-7	259	249
1	4	-6	409	376	1	10	12	140	148	2	8	3	-95	111	2	15	-1	124	104	2	12	-7	148	123
1	5	-6	-104	-47	1	11	12	210	-196	2	9	3	172	157	2	16	-1	121	121	2	13	-7	247	230
1	6	-6	-109	-13	1	12	12	271	288	2	10	3	-103	66	2	17	-1	135	164	2	14	-7	237	262
1	7	-6	326	-296	1	13	12	95	-116	2	11	3	210	227	2	18	-1	74	93	2	15	-7	215	229

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)
2	16	-7	-74	36	2	13	-9	309	321	2	13	-11	228	262	2	4	-14	-93	1	3	0	8	497	379
2	17	-7	140	179	2	14	-9	-82	-16	2	14	-11	-59	-38	2	5	-14	110	107	3	0	10	111	119
2	0	-8	87	29	2	15	-9	251	273	2	0	-12	800	775	2	6	-14	183	186	4	0	2	109	104
2	1	-8	284	231	2	16	-9	104	-125	2	1	-12	-109	101	2	7	-14	-81	-62	4	0	4	145	176
2	2	-8	168	-115	2	0	-10	969	886	2	2	-12	529	515	2	8	-14	146	144	4	0	6	368	439
2	3	-8	222	184	2	1	-10	115	116	2	3	-12	-107	-10	2	9	-14	-68	-32	4	0	8	-57	37
2	4	-8	274	254	2	2	-10	425	394	2	4	-12	435	414	2	10	-14	116	118	5	0	2	143	210
2	5	-8	-95	-59	2	3	-10	332	-301	2	5	-12	139	147	2	1	-15	110	136	5	0	4	107	148
2	6	-8	218	170	2	4	-10	516	468	2	6	-12	656	648	2	2	-15	117	-127	2	0	-2	233	137
2	7	-8	290	263	2	5	-10	343	-336	2	7	-12	113	115	2	3	-15	140	142	3	0	-2	929	808
2	8	-8	247	206	2	6	-10	533	513	2	8	-12	322	341	2	4	-15	-78	-25	3	0	-4	596	519
2	9	-8	235	207	2	7	-10	231	-230	2	9	-12	139	145	2	5	-15	175	168	3	0	-6	123	-93
2	10	-8	418	401	2	8	-10	338	345	2	10	-12	137	164	2	6	-15	-70	-78	3	0	-8	1399	1176
2	11	-8	-105	-37	2	9	-10	276	-256	2	11	-12	-79	88	2	7	-15	218	236	3	0	-10	611	521
2	12	-8	256	253	2	10	-10	283	270	2	12	-12	226	261	2	8	-15	179	-220	3	0	-12	293	261
2	13	-8	128	106	2	11	-10	358	-361	2	13	-12	-57	53	2	0	-16	308	329	3	0	-14	634	596
2	14	-8	240	274	2	12	-10	317	332	2	1	-13	321	311	2	1	-16	124	-127	3	0	-16	90	96
2	15	-8	112	102	2	13	-10	160	-186	2	2	-13	-105	29	2	2	-16	236	283	4	0	-2	193	-23
2	16	-8	236	259	2	14	-10	202	230	2	3	-13	146	128	2	3	-16	94	-101	4	0	-4	266	227
2	1	-9	136	95	2	15	-10	57	-67	2	4	-13	124	98	2	4	-16	245	288	4	0	-6	864	823
2	2	-9	211	193	2	1	-11	917	883	2	5	-13	238	227	2	5	-16	-53	-2	4	0	-8	163	157
2	3	-9	-97	60	2	2	-11	192	162	2	6	-13	205	202	2	6	-16	172	237	4	0	-10	475	479
2	4	-9	520	-459	2	3	-11	665	628	2	7	-13	271	306	3	0	0	131	-92	4	0	-12	521	565
2	5	-9	251	207	2	4	-11	184	-178	2	8	-13	-88	81	4	0	0	606	599	4	0	-14	-65	30
2	6	-9	270	-239	2	5	-11	667	667	2	9	-13	123	119	5	0	0	96	-73	5	0	-2	284	335
2	7	-9	294	260	2	6	-11	106	-90	2	10	-13	159	175	2	0	6	1099	855	5	0	-4	234	273
2	8	-9	-106	-81	2	7	-11	612	613	2	11	-13	164	165	2	0	8	-96	40	5	0	-6	90	93
2	9	-9	280	282	2	8	-11	-103	-99	2	12	-13	94	105	2	0	10	198	165	5	0	-8	397	486
2	10	-9	182	-196	2	9	-11	311	306	2	0	-14	160	157	2	0	12	264	255	5	0	-10	168	255
2	11	-9	240	266	2	10	-11	135	-130	2	1	-14	-96	-80	3	0	2	845	788	5	0	-12	75	110
2	12	-9	229	-229	2	11	-11	237	246	2	2	-14	-96	43	3	0	4	890	810	6	0	-4	76	148
					2	12	-11	82	-97	2	3	-14	-94	13	3	0	6	-102	77	6	0	-6	132	254

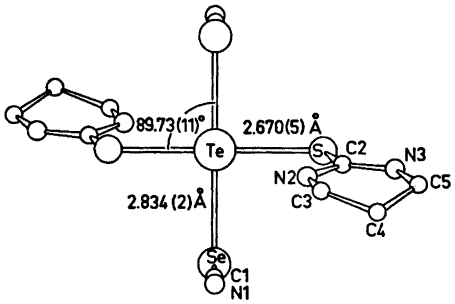

Fig. 1. The *trans*-diselenocyanatobis(trimethylenethiourea)tellurium(II) molecule as seen along the normal to the plane of the $TeSe_2S_2$ coordination group.

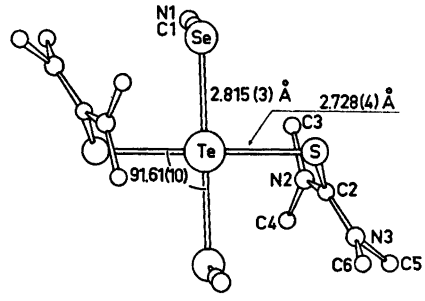

Fig. 2. The *trans*-diselenocyanatobis(tetramethylthiourea)tellurium(II) molecule as seen along the normal to the plane of the $TeSe_2S_2$ coordination group.

Both compounds exhibit *trans* square-planar coordination, with the tellurium atom bonded to two selenium atoms and two sulphur atoms.

Including the present compounds, the crystal structures of four centrosymmetric, square-planar tellurium(II) complexes containing Te – Se bonds have been determined so far. Three are tellurium diselenocyanate complexes, $TeL_2(SeCN)_2$, where L = ethylenethiourea,[1] trimethylenethiourea, and tetramethylthiourea. Each of these yield one Te – Se bond length. The fourth compound is tetrakis(selenourea)tellurium(II) dichloride,[8] $Te(su)_4Cl_2$, where su = selenourea. The latter yields two crystallographically independent Te – Se bond lengths. The bond length data are summarized in Table 7, together with bond angles at tellurium and bond angles at selenium. The former angles are very close to 90° in all compounds, and the latter angles range from 91.7° to 100.9°.

Table 4. Observed and calculated structure factors ($\times 10$) for *trans*-diselenocyanatobis(tetramethylthiourea)tellurium(II). Unobserved reflections are indicated by a minus sign on $F(O)$ and included at the threshold values. An asterisk denotes reflections given zero weight during the last refinement cycles.

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	2	0	290	324	1	4	-1	-238	-112	1	7	5	-217	39	3	0	16	427	430	7	0	-14	224	188
0	4	0	328	-277	1	4	-2	-239	-28	1	7	6	-211	-83	3	0	18	250	265	7	0	-16	-116	54
0	6	0	168	136	1	4	-3	-243	-6	1	7	7	-203	71	3	0	20	118	127	7	0	-18	-101	15
0	8	0	187	236	1	4	-4	350	344	1	7	8	-193	-49	3	0	22	-70	23	7	0	-20	-81	46
0	4	1	-112	-54	1	4	-5	-253	-75	1	7	9	-180	113	3	0	-2	73	62	8	0	0	416	372
0	4	2	100	-106	1	4	-6	662	613	1	7	10	-162	46	3	0	-4	653	-511	8	0	2	334	324
0	4	3	163	-170	1	4	-7	-267	24	1	7	11	-141	118	3	0	-6	410	-419	8	0	4	253	247
0	4	4	149	158	1	4	-8	807	717	1	7	12	-114	101	3	0	-8	746	704	8	0	6	241	203
0	4	5	-120	-44	1	4	-9	-286	103	1	7	-1	-232	136	3	0	-10	876	825	8	0	8	214	236
0	4	6	425	444	1	4	-10	925	842	1	7	-2	-231	-20	3	0	-12	879	803	8	0	10	191	211
0	4	7	-127	27	1	4	-11	-298	-35	1	7	-3	-229	148	3	0	-14	796	745	8	0	12	119	143
0	4	8	602	620	1	4	-12	678	612	1	7	-4	-226	-86	3	0	-16	500	467	8	0	14	-65	66
0	4	9	-136	54	1	4	-13	-306	-47	1	7	-5	-222	186	3	0	-18	328	318	8	0	-2	482	506
0	4	10	495	484	1	4	-14	365	343	1	7	-6	-217	-150	3	0	-20	240	285	8	0	-4	468	465
0	4	11	-142	66	1	4	-15	-289	-12	1	7	-7	-211	194	3	0	-22	247	253	8	0	-6	-123	103
0	4	12	377	356	1	4	-16	-276	182	1	7	-8	-202	-144	3	0	-24	140	177	8	0	-8	123	-86
0	4	13	-145	-13	1	4	-17	-260	-23	1	7	-9	-193	150	4	0	0	556	493	8	0	-10	-122	-22
0	4	14	355	320	1	4	-18	-238	78	1	7	-10	-177	-31	4	0	2	83	55	8	0	-12	-119	50
0	4	15	-135	-9	1	4	-19	-214	24	1	7	-11	-159	114	4	0	4	545	-537	8	0	-14	133	116
0	4	16	208	213	1	4	-20	-186	52	1	7	-12	-136	73	4	0	6	135	-121	8	0	-16	167	155
0	4	17	-120	-16	1	5	0	-270	-92	1	8	0	-133	114	4	0	8	431	403	8	0	-18	169	164
0	4	18	236	243	1	5	1	514	561	1	8	1	-131	53	4	0	10	511	477	8	0	-20	128	140
0	4	19	-97	-45	1	5	2	-271	-86	1	8	2	-126	75	4	0	12	621	617	9	0	0	117	81
0	4	20	175	214	1	5	3	656	715	1	8	3	-119	1	4	0	14	511	528	9	0	2	228	199
0	5	1	439	441	1	5	4	-276	-109	1	8	-1	-133	29	4	0	16	255	271	9	0	4	210	193
0	5	2	136	140	1	5	5	595	669	1	8	-2	130	162	4	0	18	181	186	9	0	6	229	266
0	5	3	441	403	1	5	6	-280	3	1	8	-3	-125	6	4	0	20	110	114	9	0	8	232	268
0	5	4	307	285	1	5	7	331	348	1	8	-4	117	154	4	0	-2	421	375	9	0	10	129	152
0	5	5	528	602	1	5	8	-284	69	0	0	2	1900	1992 *	4	0	-4	547	531	9	0	-2	-118	3
0	5	6	242	206	1	5	9	284	214	0	0	4	560	558	4	0	-6	518	486	9	0	-4	118	123
0	5	7	426	461	1	5	10	-283	123	0	0	6	1156	1108	4	0	-8	314	362	9	0	-6	149	144
0	5	8	-135	65	1	5	11	-279	133	0	0	8	133	146	4	0	-10	692	765	9	0	-8	122	130
0	5	9	210	200	1	5	12	-274	135	0	0	10	292	286	4	0	-12	978	944	9	0	-10	-111	79
0	5	10	-137	58	1	5	13	-259	91	0	0	12	369	278	4	0	-14	812	781	9	0	-12	-105	7
0	5	11	-136	103	1	5	14	-243	81	0	0	14	203	166	4	0	-16	660	617	9	0	-14	95	74
0	5	12	-135	2	1	5	15	-225	166	0	0	16	242	234	4	0	-18	406	353	9	0	-16	123	140
0	5	13	-125	10	1	5	16	-204	17	0	0	18	-120	59	4	0	-20	177	145	9	0	-18	96	156
0	5	14	-122	-12	1	5	17	-181	146	0	0	20	-112	26	4	0	-22	98	78	10	0	0	-98	80
0	5	15	-113	17	1	5	18	-153	-40	0	0	22	117	122	4	0	-24	-65	59	10	0	2	93	111
0	5	16	-104	16	1	5	19	-116	76	0	0	24	116	155	5	0	0	92	69	10	0	4	118	130
0	5	17	-93	85	1	5	-1	432	400	1	0	0	1052	1293 *	5	0	2	123	-54	10	0	6	120	150
0	5	18	-80	-17	1	5	-2	-271	-148	1	0	2	921	1080 *	5	0	4	154	-144	10	0	8	56	67
0	5	19	76	108	1	5	-3	-273	135	1	0	4	2003	2134 *	5	0	6	150	147	10	0	-2	-100	-30
0	6	1	-131	75	1	5	-4	275	-196	1	0	6	1555	1551	5	0	8	290	244	10	0	-4	-101	-46
0	6	2	156	155	1	5	-5	-277	126	1	0	8	1189	1148	5	0	10	233	189	10	0	-6	-99	36
0	6	3	-131	35	1	5	-6	312	-274	1	0	10	1077	1124	5	0	12	280	236	10	0	-8	107	121
0	6	4	248	245	1	5	-7	-282	174	1	0	12	596	581	5	0	14	128	113	10	0	-10	104	101
0	6	5	-130	-76	1	5	-8	-285	-120	1	0	14	133	123	5	0	16	121	110	10	0	-12	134	101
0	6	6	241	268	1	5	-9	-287	158	1	0	16	-119	-57	5	0	18	107	192	10	0	-14	110	118
0	6	7	212	-162	1	5	-10	-287	15	1	0	18	-119	-55	5	0	20	119	167	11	0	0	-63	69
0	6	8	172	152	1	5	-11	286	236	1	0	20	-109	130	5	0	-2	542	518	11	0	-2	68	71
0	6	9	267	-278	1	5	-12	-284	54	1	0	22	-91	169	5	0	-4	1005	1094	11	0	-4	-69	49
0	6	10	115	167	1	5	-13	-277	161	1	0	24	-62	99	5	0	-6	1094	1120	11	0	-6	-67	22
0	6	11	181	-170	1	5	-14	-261	127	1	0	-2	1634	1811 *	5	0	-8	957	1007	11	0	-8	-60	55
0	6	12	136	131	1	5	-15	-244	31	1	0	-4	1050	1122 *	5	0	-10	744	767	0	1	1	709	706
0	6	13	-100	-43	1	5	-16	-225	87	1	0	-6	892	771	5	0	-12	543	483	0	1	2	143	-126
0	6	14	90	75	1	5	-17	-203	38	1	0	-8	189	-134	5	0	-14	321	280	0	1	3	291	153
0	6	15	-75	25	1	5	-18	-178	39	1	0	-10	438	-321	5	0	-16	328	309	0	1	4	1245	-1135
0	6	16	74	80	1	5	-19	-147	85	1	0	-12	-101	1	5	0	-18	359	320	0	1	5	156	156
0	7	1	-111	63	1	6	0	309	298	1	0	-14	-111	5	5	0	-20	123	152	0	1	6	603	-580
0	7	2	-111	125	1	6	1	276	236	1	0	-16	340	295	5	0	-22	-65	62	0	1	7	488	489
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0	7	7	112	90	1	6	6	-268	155	2	0	0	108	-66	6	0	8	-123	-59	0	1	12	-125	-66
0	7	8	-96	12	1	6	7	-264	-207	2	0	2	798	946 *	6	0	10	-126	22	0	1	13	823	859
0	7	9	116	136	1	6	8	-259	137	2	0	4	2069	2257 *	6	0	12	-121	2	0	1	14	167	-136
0	7	10	-83	-62	1	6	9	-252	-203	2	0	6	1260	1215	6	0	14	-110	10	0	1	15	687	695
0	7	11	136	160	1	6	10	-244	115	2	0	8	1228	1225	6	0	16	135	147	0	1	16	-145	-21
0	7	12	-62	-24	1	6	11	-233	-53	2	0	10	1198	1221	6	0	18	116	159	0	1	17	411	413
0	8	1	-96	17	1	6	12	-215	100	2	0	12	404	380	6	0	-2	523	535	0	1	18	-145	119
0	8	2	160	154	1	6	13	-197	4	2	0	14	296	308	6	0	-4	682	673	0	1	19	226	214
0	8	3	-81	25	1	6	14	-176	106	2	0	16	326	307	6	0	-6	895	973	0	1	20	-135	49
0	8	4	95	102	1	6	15	-152	-25	2	0	18	170	168	6	0	-8	831	840	0	1	21	125	129
1	4	0	-237	147	1	6	16	-120	127	2	0	20	123	150	6	0	-10	512	498	0	1	22	-114	39
1	4	1	-235	-84	1	6	-1	277	321	2	0	22	-83	76	6	0	-12	353	346	0	1	23	99	120
1	4	2	308	318	1	6	-2	-276	167	2	0	-2	119	89	6	0	-14	220	164	0	1	24	-80	65
1	4	3	-246	104	1	6	-3	275	245	2	0	-4	153	-136	6	0	-16	-123	21	1	1	0	1003	1103 *
1	4	4	251	156	1	6	-4	-274	106	2	0	-6	453	366	6	0	-18	-113	42	1	1	1	193	-183
1	4	5	-257	-12	1	6	-5	-273	143	2	0	-8	282	257	6	0	-20	140	103	1	1	2	481	-417
1	4	6	-264	35	1	6	-6	-271	171	2	0	-10	-93	11	6	0	-22	107	126	1	1	3	586	-479
1	4	7	-271	-35	1	6	-7	-268	-24	2	0	-12	224	200	7	0	0	733	748	1	1	4	517	-534
1	4	8	-280	-11	1	6	-8	-265	224	2	0	-14	400	385	7	0	2	619	621	1	1	5	280	246
1	4	9	-286	89	1	6	-9	-260	-45	2	0	-16	449	417	7	0	4	414	414	1	1	6	408	378
1	4	10	-291	83	1	6	-10	-253	188	2	0	-18	388	391	7	0	6	218	222	1	1	7	331	288
1	4	11	-295	-35	1	6	-11	-245	26	2	0	-20	384	413	7	0	8	123	63	1	1	8	-104	-54
1	4	12	-298	218	1	6	-12	-233	182	2	0	-22	307	330	7	0	10	-120	-16	1	1	9	582	508
1	4	13	-292	-108	1	6	-13	-214	32	2	0	-24	132	173	7	0	12	-108	45	1	1	10	548	-499
1	4	14	300	340	1	6	-14	-195	155	3	0	0	294	-299	7	0	14	113	127	1	1	11	691	636
1	4	15	-271	-15	1	6	-15	-173	8	3	0	2	620	541	7	0	16	93	107	1	1	12	423	-385
1	4	16	301	354	1	6	-16	-147	87	3	0	4	885	871	7	0	-2	751	715	1	1	13	499	491
1	4	17	-238	7	1	7	0	-232	42	3	0	6	744	762	7	0	-4	359	367	1	1	14	278	-280
1	4	18	215	283	1	7	1	-231	79	3	0	8	858	864	7	0	-6	236	223	1	1	15	404	394
1	4	19	-190	7	1	7	2	-230	21	3	0	10	454	444	7	0	-8	393	364	1	1	16	145	-143
1	4	20	-160	176	1	7	3	-227	25	3	0	12	533	546	7	0	-10	246	232	1	1	17	282	288
1	4	21	-120	8	1	7	4	-223	-53	3	0	14	716	702	7	0	-12	193	176	1	1	18	-144	13

Table 4. Continued.

H	K	L	F(o)	F(c)
1	1	19	253	266
1	1	20	-131	62
1	1	21	213	252
1	1	22	-108	57
1	1	23	121	178
1	1	-1	724	628 *
1	1	-2	642	651
1	1	-3	1146	1158
1	1	-4	420	373
1	1	-5	1554	1473
1	1	-6	1137	958
1	1	-7	1051	1013
1	1	-8	553	468
1	1	-9	835	865
1	1	-10	-111	102
1	1	-11	915	859
1	1	-12	215	-208
1	1	-13	634	556
1	1	-14	449	-422
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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)
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3	2-20	151	162	6	2 16	99	113	9	2 -3	184	-198	2	3 4	472	448	4	3 -1	102	117
3	2-21	91	-100	6	2 17	-53	-40	9	2 -4	200	204	2	3 5	781	802	4	3 -2	247	-206
3	2-22	134	152	6	2 -1	362	335	9	2 -5	107	-99	2	3 6	334	343	4	3 -3	238	217
3	2-23	91	-103	6	2 -2	297	294	9	2 -6	184	179	2	3 7	660	680	4	3 -4	201	-209
3	2-24	115	127	6	2 -3	-82	43	9	2 -7	-83	-23	2	3 8	202	-204	4	3 -5	329	311
4	2 0	356	327	6	2 -4	337	334	9	2 -8	135	139	2	3 9	589	564	4	3 -6	136	-124
4	2 1	158	-165	6	2 -5	207	-211	9	2 -9	128	110	2	3 10	341	-303	4	3 -7	636	651
4	2 2	425	411	6	2 -6	331	322	9	2-10	124	122	2	3 11	556	535	4	3 -8	195	-176
4	2 3	454	-352	6	2 -7	298	-284	9	2-11	130	125	2	3 12	208	-198	4	3 -9	687	697
4	2 4	623	642	6	2 -8	447	415	9	2-12	111	119	2	3 13	461	460	4	3-10	346	-320
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4	2 6	455	435	6	2-10	387	394	9	2-14	112	120	2	3 15	264	271	4	3-12	303	-276
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4	2 -8	553	572	7	2 9	171	176	10	2-13	62	86	2	3-16	189	-173	5	3 11	132	126
4	2 -9	262	256	7	2 10	155	148	0	3 1	545	844 *	2	3-17	365	357	5	3 12	-120	13
4	2-10	418	404	7	2 11	114	127	0	3 2	267	-291	2	3-18	130	-130	5	3 13	196	200
4	2-11	-84	-37	7	2 12	137	148	0	3 3	904	996 *	2	3-19	209	217	5	3 14	-109	39
4	2-12	344	324	7	2 13	-69	22	0	3 4	727	-821 *	2	3-20	-101	-43	5	3 15	171	188
4	2-13	193	-167	7	2 14	90	96	0	3 5	900	998 *	2	3-21	152	133	5	3 16	-91	24
4	2-14	358	331	7	2 15	-53	-39	0	3 6	520	-505	2	3-22	-79	28	5	3 17	125	140
4	2-15	-93	-58	7	2 -1	145	116	0	3 7	502	534	2	3-23	111	141	5	3 -1	393	372
4	2-16	306	254	7	2 -2	293	273	0	3 8	225	-220	3	3 0	478	433	5	3 -2	458	-403
4	2-17	-91	-26	7	2 -3	-89	-7	0	3 9	442	446	3	3 1	139	15	5	3 -3	479	468
4	2-18	256	249	7	2 -4	331	326	0	3 10	117	-92	3	3 2	422	395	5	3 -4	337	-330
4	2-19	93	-78	7	2 -5	228	-197	0	3 11	239	233	3	3 3	223	220	5	3 -5	403	375
4	2-20	165	168	7	2 -6	260	261	0	3 12	-114	23	3	3 4	253	243	5	3 -6	209	-203
4	2-21	-73	-60	7	2 -7	262	-283	0	3 13	138	-34	3	3 5	413	363	5	3 -7	526	513
4	2-22	132	132	7	2 -8	256	244	0	3 14	-121	-85	3	3 6	-101	-4	5	3 -8	-116	84
4	2-23	57	-72	7	2 -9	388	-366	0	3 15	-122	73	3	3 7	592	548	5	3 -9	579	591
5	2 0	341	320	7	2-10	300	293	0	3 16	-121	-96	3	3 8	-112	36	5	3-10	171	140
5	2 1	336	310	7	2-11	305	-292	0	3 17	139	130	3	3 9	602	622	5	3-11	457	445
5	2 2	373	381	7	2-12	262	261	0	3 18	-114	-27	3	3 10	201	169	5	3-12	-126	61
5	2 3	301	255	7	2-13	-91	-38	0	3 19	162	173	3	3 11	514	494	5	3-13	407	393
5	2 4	371	366	7	2-14	205	195	0	3 20	-99	32	3	3 12	-123	87	5	3-14	-126	1
5	2 5	256	256	7	2-15	-86	67	0	3 21	153	184	3	3 13	345	353	5	3-15	249	270
5	2 6	314	290	7	2-16	175	167	0	3 22	-75	76	3	3 14	-122	-3	5	3-16	-119	16
5	2 7	-88	44	7	2-17	-75	65	0	3 23	-56	99	3	3 15	227	218	5	3-17	126	115
5	2 8	327	315	7	2-18	161	152	1	3 0	70	46	3	3 16	-114	-85	5	3-18	-106	60
5	2 9	308	-247	7	2-19	-60	52	1	3 1	1044	1252 *	3	3 17	179	163	5	3-19	97	77
5	2 10	323	279	7	2-20	98	110	1	3 2	137	157	3	3 18	-99	-101	5	3-20	-86	64
5	2 11	349	-325	8	2 0	255	241	1	3 3	1108	1266 *	3	3 19	136	127	5	3-21	77	77
5	2 12	234	228	8	2 1	254	-238	1	3 4	199	200	3	3 20	-75	-73	6	3 0	1640	-1224
5	2 13	236	-229	8	2 2	226	197	1	3 5	849	895	3	3 21	68	87	6	3 1	400	389
5	2 14	183	173	8	2 3	-90	-79	1	3 6	105	65	3	3 -1	209	168	6	3 2	-120	-80
5	2 15	104	-102	8	2 4	157	158	1	3 7	720	675	3	3 -2	185	176	6	3 3	190	194
5	2 16	134	120	8	2 5	87	68	1	3 8	204	-195	3	3 -3	316	298	6	3 4	150	-147
5	2 17	-69	-29	8	2 6	161	152	1	3 9	503	503	3	3 -4	140	-145	6	3 5	131	90
5	2 18	100	107	8	2 7	150	162	1	3 10	312	-282	3	3 -5	297	305	6	3 6	203	-179
5	2 -1	203	207	8	2 8	106	109	1	3 11	292	280	3	3 -6	335	-312	6	3 7	125	120
5	2 -2	489	454	8	2 9	129	121	1	3 12	367	-372	3	3 -7	385	371	6	3 8	139	-130
5	2 -3	216	186	8	2 10	99	108	1	3 13	263	250	3	3 -8	580	-585	6	3 9	-123	97
5	2 -4	500	523	8	2 11	-64	31	1	3 14	301	-293	3	3 -9	251	221	6	3 10	-121	-67
5	2 -5	358	358	8	2 12	90	103	1	3 15	232	223	3	3-10	389	-387	6	3 11	122	101
5	2 -6	415	433	8	2 13	-48	-4	1	3 16	-120	-57	3	3-11	344	345	6	3 12	-109	34
5	2 -7	305	298	8	2 -1	219	-223	1	3 17	143	144	3	3-12	-120	-19	6	3 13	118	125
5	2 -8	353	357	8	2 -2	206	220	1	3 18	-112	19	3	3-13	487	485	6	3 14	-92	60
5	2 -9	179	143	8	2 -3	174	-147	1	3 19	133	119	3	3-14	-123	-11	6	3 15	87	79
5	2-10	242	243	8	2 -4	201	210	1	3 20	-95	33	3	3-15	368	384	6	3 -1	476	466
5	2-11	-88	-45	8	2 -5	164	-159	1	3 21	-83	64	3	3-16	-128	-32	6	3 -2	211	-211
5	2-12	370	351	8	2 -6	253	235	1	3 -1	626	793 *	3	3-17	346	369	6	3 -3	379	372
5	2-13	359	-323	8	2 -7	-91	-53	1	3 -2	61	93	3	3-18	-115	2	6	3 -4	195	-173
5	2-14	405	369	8	2 -8	257	248	1	3 -3	295	322	3	3-19	272	293	6	3 -5	578	539
5	2-15	354	-321	8	2 -9	-89	-24	1	3 -4	540	548	3	3-20	-99	2	6	3 -6	-120	-80
5	2-16	255	240	8	2-10	175	178	1	3 -5	235	230	3	3-21	137	160	6	3 -7	377	370
5	2-17	163	-168	8	2-11	-87	-107	1	3 -6	571	603	3	3-22	-76	2	6	3 -8	-123	14
5	2-18	207	154	8	2-12	153	147	1	3 -7	292	274	3	3-23	91	102	6	3 -9	342	295
5	2-19	89	-88	8	2-13	-83	-61	1	3 -8	382	370	4	3 0	170	-173	6	3-10	133	133
5	2-20	180	185	8	2-14	181	173	1	3 -9	241	248	4	3 1	129	-61	6	3-11	268	241
5	2-21	-65	1	8	2-15	-74	21	1	3-10	166	136	4	3 2	158	-162	6	3-12	234	213
5	2-22	127	138	8	2-16	129	143	1	3-11	228	205	4	3 3	207	204	6	3-13	148	169
6	2 0	347	323	8	2-17	80	82	1	3-12	189	-176	4	3 4	123	-93	6	3-14	202	172
6	2 1	430	422	8	2-18	89	111	1	3-13	188	187	4	3 5	370	330	6	3-15	183	173
6	2 2	332	341	8	2-19	69	101	1	3-14	208	-211	4	3 6	184	149	6	3-16	-112	31
6	2 3	450	472	9	2 0	142	136	1	3-15	199	208	4	3 7	266	261	6	3-17	148	146
6	2 4	229	213	9	2 1	105	-90	1	3-16	136	-133	4	3 8	420	406	6	3-18	-95	-53
6	2 5	271	217	9	2 2	114	114	1	3-17	207	180	4	3 9	311	296	6	3-19	-85	71
6	2 6	339	316	9	2 3	-79	7	1	3-18	123	-103	4	3 10	281	285	6	3-20	-71	-27
6	2 7	58	-68	9	2 4	137	138	1	3-19	145	139	4	3 11	255	228	7	3 0	-123	24
6	2 8	324	322	9	2 5	-74	5	1	3-20	-101	-11	4	3 12	-125	34	7	3 1	300	290
6	2 9	110	-111	9	2 6	121	129	1	3-21	166	189	4	3 13	212	189	7	3 2	198	-161
6	2 10	161	136	9	2 7	-67	-21	1	3-22	-78	25	4	3 14	-119	-39	7	3 3	269	270
6	2 11	-90	-73	9	2 8	75	87	1	3-23	128	172	4	3 15	219	231	7	3 4	231	-264
6	2 12	140	119	9	2 9	-54	-42	2	3 0	575	614	4	3 16	-106	-67	7	3 5	236	248
6	2 13	-82	-11	9	2 10	69	84	2	3 1	663	637	4	3 17	197	220	7	3 6	201	-196
6	2 14	138	136	9	2 -1	234	-237	2	3 2	364	323	4	3 18	-86	-63	7	3 7	209	225

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)
7	3	8	-116	-80	7	3-13	-117	69	8	3	11	-71	57	9	3	1	139	159	9	3-12	-34	-27
7	3	9	112	126	7	3-14	-113	62	8	3	-1	220	219	9	3	2	-99	77	9	3-13	113	137
7	3	10	-105	-19	7	3-15	-106	61	8	3	-2	-120	90	9	3	3	132	149	9	3-14	65	-74
7	3	11	-98	82	7	3-16	-98	52	8	3	-3	127	97	9	3	4	-93	90	9	3-15	82	131
7	3	12	-89	11	7	3-17	99	103	8	3	-4	134	138	9	3	5	104	117	10	3	0	-74	58
7	3	13	-75	41	7	3-18	-78	-2	8	3	-5	126	92	9	3	6	-82	19	10	3	1	-71	43
7	3	-1	270	278	7	3-19	101	122	8	3	-6	163	180	9	3	7	91	89	10	3	2	-67	67
7	3	-2	130	125	8	3	0	-119	-56	8	3	-7	125	151	9	3	8	-64	-54	10	3	3	-59	47
7	3	-3	392	417	8	3	1	258	268	8	3	-8	130	115	9	3	-1	128	153	10	3	-1	-77	44
7	3	-4	123	117	8	3	2	-117	-90	8	3	-9	128	141	9	3	-2	-106	-3	10	3	-2	-76	19
7	3	-5	412	431	8	3	3	227	263	8	3-10		-113	-1	9	3	-3	176	137	10	3	-3	-79	61
7	3	-6	-122	58	8	3	4	-113	-59	8	3-11		117	110	9	3	-4	-106	-39	10	3	-4	-79	-25
7	3	-7	296	271	8	3	5	234	266	8	3-12		-106	-84	9	3	-5	-105	18	10	3	-5	76	96
7	3	-8	-123	-1	8	3	6	-108	-10	8	3-13		102	93	9	3	-6	-104	-13	10	3	-6	-76	-13
7	3	-9	144	140	8	3	7	165	181	8	3-14		95	-103	9	3	-7	-102	13	10	3	-7	-74	14
7	3	-10	-123	28	8	3	8	-98	1	8	3-15		-86	68	9	3	-8	-100	43	10	3	-8	-70	-37
7	3	-11	-122	91	8	3	9	95	93	8	3-16		-76	-47	9	3	-9	-97	75	10	3	-9	65	70
7	3	-12	-120	69	8	3	10	-81	-26	8	3-17		64	72	9	3	-10	-94	17	10	3	-10	66	-59
										9	3	0	-104	25	9	3	-11	90	102	10	3	-11	50	74

Table 5. Bond lengths (Å) and angles (°) in the coordination groups. Standard deviations are given in parentheses.

	Trimethylenethiourea complex	Tetramethylthiourea complex
Te – Se	2.834(2)	2.815(3)
Te – S	2.670(5)	2.728(4)
∠Se – Te – S	89.73(11)	91.61(10)
∠Te – Se – C(1)	100.9(6)	99.8(7)
∠Te – S – C(2)	106.2(6)	98.9(6)

Table 6. Bond lengths (Å) and angles (°) in the ligands. Standard deviations are given in parentheses.

Diselenocyanatobis(trimethylenethiourea)tellurium(II)

Se – C(1)	1.799(22)	∠Se – C(1) – N(1)	178.5(17)
C(1) – N(1)	1.152(31)	∠S – C(2) – N(2)	122.4(11)
S – C(2)	1.729(18)	∠S – C(2) – N(3)	115.6(15)
C(2) – N(2)	1.324(24)	∠C(2) – N(2) – C(3)	124.8(13)
C(2) – N(3)	1.311(19)	∠C(2) – N(3) – C(5)	122.7(17)
N(2) – C(3)	1.477(24)	∠N(2) – C(3) – C(4)	110.3(19)
N(3) – C(5)	1.491(27)	∠N(3) – C(5) – C(4)	111.5(17)
C(3) – C(4)	1.468(30)	∠N(2) – C(2) – N(3)	121.5(16)
C(5) – C(4)	1.511(37)	∠C(3) – C(4) – C(5)	116.7(20)

Diselenocyanatobis(tetramethylthiourea)tellurium(II)

Se – C(1)	1.809(20)	∠Se – C(1) – N(1)	176.9(19)
C(1) – N(1)	1.162(27)	∠S – C(2) – N(2)	122.8(13)
S – C(2)	1.755(19)	∠S – C(2) – N(3)	119.3(13)
C(2) – N(2)	1.392(23)	∠N(2) – C(2) – N(3)	117.9(16)
C(2) – N(3)	1.339(22)	∠C(2) – N(2) – C(3)	119.2(17)
N(2) – C(3)	1.405(25)	∠C(2) – N(2) – C(4)	122.8(16)
N(2) – C(4)	1.424(30)	∠C(3) – N(2) – C(4)	117.4(15)
N(3) – C(5)	1.539(26)	∠C(2) – N(3) – C(5)	126.2(15)
N(3) – C(6)	1.425(25)	∠C(2) – N(3) – C(6)	122.5(15)
		∠C(5) – N(3) – C(6)	111.0(15)

Table 7. Te–Se bond lengths in centrosymmetric, square-planar tellurium(II) complexes.

Compound[a]	Te–Se	∠ X–Te–Se[b]	∠ Te–Se–C	Ref.
$Te(etu)_2(SeCN)_2$	2.809(3) Å	89.9(2)°	95.9(9)°	1
$Te(trtu)_2(SeCN)_2$	2.834(2)	89.7(1)°	100.9(6)°	Present
$Te(tmtu)_2(SeCN)_2$	2.815(3)	91.6(1)°	99.8(7)°	Present
$Te(su)_4Cl_2$	2.814(3)	90.3(1)°	91.7(7)°	8
	2.809(4)		98.0(8)°	

[a] etu = ethylenethiourea, trtu = trimethylenethiourea, tmtu = tetramethylthiourea, su = selenourea.
[b] Or the supplementary angles.

Four of the five Te–Se bond lengths, *i.e.*, all except the length in $Te(trtu)_2(SeCN)_2$, are equal within the error. The extremes of the four nearly equal lengths are 2.809(3) and 2.815(3) Å; the difference between the extremes is 1.4 times the standard deviation of the difference. The weighted average of the four is 2.812(2) Å, with an average deviation of 0.003 Å. This length for a Te–Se bond, 2.81 Å, is 0.13 Å larger than the average Te–S bond length,[9] 2.68 Å, in centrosymmetric, square-planar tellurium(II) complexes. This is the same difference as between the covalent single-bond radii of the ligand atoms, 1.17 Å for selenium and 1.04 Å for sulphur.

The Te–Se bond length in $Te(trtu)_2(SeCN)_2$, 2.834(2) Å, is significantly larger than the other four. Also, the Te–S bond length in $Te(tmtu)_2(SeCN)_2$, 2.728(4) Å, is significantly larger than the average, 2.68 Å, for Te–S bonds. The reasons are not clear; however, bond length variations like these do hardly appear surprising. The bonds are longer and weaker than covalent single bonds, and lattice effects, and ligand properties other than the nature of the coordinating atom, may be expected to influence their length.

In $Te(tmtu)_2(SeCN)_2$ a non-bonded contact occurs between a tetramethylthiourea methyl group and the tellurium atom of the same molecule: Te · · · C(3) = 3.732 Å, which is markedly shorter than the sum of the van der Waals radii[10] of tellurium, 2.20 Å, and methyl, 2.00 Å. This contact is probably repulsive, and may relate to the observed lengthening of the Te–S(tmtu) bond.

Looking at Te–S(tmtu) bond lengths in other centrosymmetric tellurium(II) complexes, the bond is 2.724(6) Å in the dibenzenethiosulphonate complex, $Te(tmtu)_2(S_2O_2C_6H_5)_2$, but there the S–Te–S bond angle, 79.51(15)°, deviates markedly from 90°.[11] The Te–S(benzenethiosulphonate) bond is 2.657(4) Å.[11] In the cationic complexes, *trans*-dithioureabis(tetramethylthiourea)tellurium(II) chloride and bromide, $[Te(tu)_2(tmtu)_2]X_2$, Te–S(tmtu) = 2.688(3) Å, Te–S(tu) = 2.710(3) Å, ∠ S–Te–S = 91.37(10)° in the chloride, and Te–S(tmtu) = 2.679(3) Å, Te–S(tu) = 2.706(3) Å, ∠ S–Te–S = 91.45(9)° in the bromide.[12]

Bond lengths and angles in the ligands of the present complexes (Table 6) are in the normal range. With the sulphur coordinates given four times the weight of the carbon and nitrogen coordinates, and with C(4) excluded, a

least-squares plane through the trimethylenethiourea group of $Te(trtu)_2(SeCN)_2$ was calculated. The distances of the atoms from the plane range from 0.005 to 0.059 Å. The distance between C(4) and the plane is 0.482 Å. The angle between the least-squares plane and the plane through the $TeSe_2S_2$ coordination group is 75.7°.

In calculations of least-squares planes through groups of atoms in $Te(tmtu)_2(SeCN)_2$, the coordinates of all atoms were assigned equal weights. The atoms of a least-squares plane through the thiourea part of the tetramethylthiourea group deviate 0.003 – 0.009 Å from the plane. This plane makes an angle of 77.3° with the plane through the $TeSe_2S_2$ coordination group, 29.9° with a least-squares plane through N(2) and the carbon atoms bonded to N(2), and 25.7° with a least-squares plane through N(3) and the carbon atoms bonded to N(3).

A DIMORPH OF THE TRIMETHYLENETHIOUREA COMPLEX

The dithiocyanato complex, $Te(trtu)_2(SCN)_2$, crystallizes in the space group $C2/c$ (No. 15) with four formula units per unit cell, and $a = 13.27$ Å, $b = 14.43$ Å, $c = 9.76$ Å, $\beta = 108.5°$.[2] On seeding the diselenocyanato reaction mixture with crystals of the dithiocyanato complex, the isomorphous diselenocyanato complex, $Te(trtu)_2(SeCN)_2$, a dimorph of I, crystallized: $a = 13.33$ Å, $b = 14.60$ Å, $c = 9.92$ Å, $\beta = 108.5°$. As in the case of the dithiocyanato complex,[2] the systematic absences, and weak *hkl* reflections when *l* is odd, indicate that the tellurium atoms lie in symmetry centres of the space group $C2/c$ (No. 15). The crystals of both compounds occur as prisms {110}.

It was not possible, by seeding with crystals of I, to obtain isomorphous crystals of the dithiocyanato complex.

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Received March 29, 1971.