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The Crystal and Molecular Structures of *trans*-Dithioureabis(tetramethylthiourea)tellurium(II) Chloride and Bromide

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The structures of the isomorphous chloride and bromide salts of the *trans*-dithioureabis(tetramethylthiourea)tellurium(II) cation, $[Te\{SC(NH_2)_2\}_2\{SC(N(CH_3)_2)_2\}_2]^{2+}$, have been determined by single-crystal X-ray diffraction methods. Both salts crystallize in the monoclinic space group $P2_1/c$ (No. 14), with unit cell dimensions of $a=8.841(3)$ Å, $b=14.401(6)$ Å, $c=9.919(4)$ Å, and $\beta=94.09(8)°$ for the chloride salt, and $a=8.776(2)$ Å, $b=15.024(4)$ Å, $c=10.026(3)$ Å, and $\beta=93.97(6)°$ for the bromide salt. The unit cell contains two molecules in both cases, and the position of the tellurium(II) ion must coincide with a center of symmetry.

For the chloride salt, the intensities of 1512 reflections were visually estimated from integrated, multiple films, and the structure was refined by full-matrix least-squares methods to a value of the conventional R factor of 0.080. For the bromide salt, the intensities of 1452 reflections were measured on an automated diffractometer by counter methods, and the structure was refined to a conventional R factor of 0.051.

The monomeric complex cations exhibit *trans* square planar coordination, with $Te-S_1$(thiourea) = 2.710(3) Å, $Te-S_2$(tetramethylthiourea) = 2.688(3) Å, and $\angle S_1-Te-S_2=91.37(10°)$ for the chloride salt, and $Te-S_1=2.706(3)$ Å, $Te-S_2=2.679(3)$ Å, and $\angle S_1-Te-S_2=91.45(9)°$ for the bromide salt.

The present work is a part of a series of studies of the syntheses and structures of compounds of divalent tellurium which has been undertaken in this laboratory. The structures of complexes involving tetramethylthiourea as a ligand coordinated to divalent tellurium are of interest in this regard because of the lack of success which has been experienced in attempting to synthesize the $[Te(tmtu)_4]^{2+}$ cation (tmtu = tetramethylthiourea). This cation has not been isolated, despite the fact that salts of $[Te(tu)_4]^{2+}$ (tu = thiourea),[1]

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$[Te(etu)_4]^{2+}$ (etu = ethylenethiourea),[2] and $[Te(trtu)_4]^{2+}$ (trtu = trimethylenethiourea)[3] are easily obtained. This difficulty is presumably associated with the steric requirements of the bulky $-N(CH_3)_2$ groups. The present study was undertaken to provide data on the nature of the Te–S(tmtu) bond, and to ascertain whether the configuration of the tetramethylthiourea group precludes formation of the tetrakis(tetramethylthiourea)tellurium(II) cation.

EXPERIMENTAL

Crystals of *trans*-dithioureabis(tetramethylthiourea)tellurium(II) chloride and bromide $([Te\{SC(NH_2)_2\}_2\{SC(N(CH_3)_2)_2\}_2]X_2$, where $X = Cl^-$, Br^-) were supplied by Professor Olav Foss. The syntheses and crystal data for these compounds have been reported by Foss and Johannessen.[4] These authors found that both compounds crystallize in the monoclinic, centrosymmetric space group $P2_1/c$ (No. 14), with two molecules in the unit cell. This requires the tellurium(II) ion to occupy a center of symmetry.

The unit cell dimensions of these two substances were redetermined for the purposes of this study. For the chloride salt, values of 2θ for 89 high-order reflections ($CuK\alpha_1$ radiation, $\lambda = 1.5405$ Å) were measured from zero-layer Weissenberg films taken about the *a*, *b*, and *c* axes, at an ambient temperature of 21°C. These films were calibrated by substituting a specially prepared sample of NaCl powder for the single crystal, and recording the powder lines on the same film. The corrected values of 2θ, based on $a_{NaCl} = 5.6403$ Å at 21°C, were used as input data for a least squares calculation of the cell parameters. The results of this calculation, with standard deviations in the least significant digits in parentheses, were $a = 8.841(3)$ Å, $b = 14.401(6)$ Å, $c = 9.919(4)$ Å, and $\beta = 94.09(8)°$.

For the bromide salt, values of the setting angles of the diffractometer arcs were carefully measured for 20 high-order reflections ($MoK\alpha_1$ radiation, $\lambda = 0.70926$ Å) at 22°C, and the results used as input for a least squares cell dimension calculation. The cell constants obtained were $a = 8.776(2)$ Å, $b = 15.024(4)$ Å, $c = 10.026(3)$ Å, and $\beta = 93.97(6)°$. For both compounds, the earlier results [4] agree well with the cell dimensions reported in the present work.

The intensity data for $[Te(tu)_2(tmtu)_2]Cl_2$ were collected by means of the multiple-film, integrating, equi-inclination Weissenberg technique, employing Ni-filtered $CuK\alpha$ radiation. The small, yellow-orange crystal used was mounted with the *c* axis coincident with the spindle axis of the camera, and layers $hk0 - hk5$ were successively collected. Care was taken to use the same exposure times on all layers, so that the layers would initially be nearly on a common scale.

Intensities were estimated from the films by visual comparison with a graduated scale of timed exposures of approximately the same size and shape as the integrated reflections. Of 1661 reflections accessible to the Weissenberg technique in these six layers, 1512 were strong enough to be observable on the film. Intensities of unobserved reflections were set equal to the threshold value on the visual scale, and labelled as unobserved. Lorentz and polarization corrections were applied to the raw intensities, as well as an empirical correction for the high-angle $\alpha_1 - \alpha_2$ splitting.

The crystal employed for the data collection was investigated by optical goniometry, and was found to be bounded by {100}, {010}, {001}, and {011}. Interfacial distances were carefully measured, and an absorption correction was carried out. The crystal dimensions, given as the distance in mm from the face concerned to the point taken as the center of the crystal, were 0.0475 mm ((100) and ($\bar{1}$00)), 0.070 mm ((010) and (0$\bar{1}$0)), 0.080 mm ((00$\bar{1}$)) and 0.080 mm ((011) and (0$\bar{1}$1)). The absorption correction was based on a Gaussian grid technique,[5] and with $\mu = 149$ cm^{-1}, the above crystal dimensions, and a $6 \times 8 \times 8$ grid, resulted in transmission factors between 0.2 and 0.4.

A small, reddish-orange crystal of the bromide salt was found suitable for intensity data collection, and the short prism was mounted on the Siemens automatic four-circle diffractometer, with the *a* axis nearly coincident with the Φ axis of the instrument. The values of the setting angles were determined for 20 accurately centered reflections of high order (Nb-filtered $MoK\alpha$ radiation, $\lambda = 0.70926$ Å), as mentioned earlier, and the

results were used to generate the steering data tape. This was accomplished by means of a least squares procedure programmed by Mr. K. Maartmann-Moe of this institute. The instrument was operated in the $\theta-2\theta$ mode, with a five-value scan, in which the peak is scanned twice and the background measured on either side of the peak. The scan range was 0.40° for the bottom half of the scan, and $(0.40+0.15 \tan \theta_{max})$ degrees for the upper half of the scan, where θ_{max} is the calculated peak maximum. The minimum rate of scan was set at 2.5°/min, and was automatically increased for strong reflections. A series of automatically coupled calibrated attenuators was employed to make coincidence losses negligible for strong reflections. A circular aperture of diameter 3.0 mm was used in front of the scintillation counter. Two reference reflections were measured every 50 reflections, as a check on the quality and orientation of the crystal, and no overall trend in the intensities of these reflections was observed. The data collected comprised a unique quarter of the sphere of reflection, with $\theta < 24.0°$. Within this zone were 2085 reflections, of which 1452 had measured intensities greater than twice the standard deviation in the intensity, where the standard deviation is defined as the square root of the total number of counts during the five-value measurement. For those reflections which were unobserved by this definition, the measured intensity was replaced by twice the standard deviation, with a label to indicate that these reflections were unobserved.

Lorentz and polarization corrections were applied. The crystal dimensions, given as the distance in mm from the face concerned to the point taken as the crystal center, were 0.058 mm ((1$\bar{0}$0) and ($\bar{1}$00)), 0.033 mm ((010) and (0$\bar{1}$0)), and 0.065 mm ((011), (0$\bar{1}\bar{1}$), (01$\bar{1}$), and (0$\bar{1}$1)). An absorption correction program based on the Gaussian grid technique,[5] and modified for diffractometer data by Mr. K. Åse of this institute, was applied to the data. With a $4 \times 6 \times 6$ grid and $\mu = 47$ cm^{-1} for Mo$K\alpha$ radiation, values of the transmission coefficient ranged from 0.55 to 0.75.

The main body of programs used in this study was made available to this institute by the Weizmann Institute of Science, Rehovoth, Israel, and modified for use on the University of Bergen's IBM 360/50H computer by Dr. D. Rabinovich. This program library includes the programs FILM (preliminary data treatment), DAT2 (*Lp* correction, absorption correction, data reduction), BDLS (structure factor calculation and full-matrix refinement), DIAN (calculation of distances and angles), and INTA (calculation of interatomic contacts). In addition, local programs employed, all written by Mr. K. Åse of this institute, included ASEN (calculation of Fourier maps), ZACH (extinction correction after that of Zachariasen [6]), DAT1 (*Lp* correction and data reduction for diffractometer data), and ABCD (absorption correction for diffractometer data).

SOLUTION AND REFINEMENT

The structure of the chloride salt was first to be solved. The procedure followed was to perform a structure factor calculation with the atoms at known positions, followed by a Fourier map to locate more atoms. On the basis of the required crystallographic symmetry, the tellurium ion was placed in the center of symmetry at (0,0,0), and the phases for the first cycle of the solution procedure were obtained from the tellurium ion alone. This ion contributes only to reflections with $k+l$ even, and the resultant Fourier map contains false symmetry. One of the two symmetry-related highest peaks was taken to be the chloride ion. Phases from the tellurium and chloride ions permitted location of the sulfur atoms, and this procedure continued until all non-hydrogen atoms had been located. No attempt has been made in this work to locate hydrogen atoms, and no account of them has been taken in the calculations.

When all the atoms had been located, the program BDLS was used to refine only the scale factors of the six Weissenberg layers. The raw data were then resubmitted, and the corrected scale factors for each layer were applied

by the data reduction program DAT2. A subsequent cycle of refinement on the six scale factors showed that the six layers were then all within 2 % of being on the same scale. Refinement of the structure was begun at this point. Atomic scattering factors for atomic tellurium, sulfur, carbon, and nitrogen, and for the chloride ion, were taken from the compilation in *International Tables for X-Ray Crystallography*.[7] Anomalous dispersion corrections $\Delta f'$ and $\Delta f''$ for tellurium in Cu$K\alpha$ radiation were taken from the compilation of Cromer,[8] and were included by letting f equal the magnitude of the complex scattering factor. No correction for anomalous dispersion was applied for the other atoms.

After two cycles of refinement by the program BDLS with all atoms allowed only isotropic thermal parameters and all data considered as one group, the R factor had dropped to 0.11. The program BDLS minimizes the function

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

where K is the scale factor and W is the weight. The weight W is evaluated as $W = 1/(K^2a_1^2 + a_2^2F_o^2/4W_o)$, where W_o is an individual constant reflecting the reliability of measurement of the particular reflection, and a_1 and a_2 are adjustable constants.

At this point, the most intense reflections in the structure factor list were examined for evidence of extinction. A majority of these reflections were found to have $|F_o| - |F_c| < 0$, and a correction for extinction was deemed necessary. Accordingly, program ZACH was applied to the observed structure factors. This program uses the formula due to Zachariasen [6]

$$F_o' = KF_o(1 + \beta CI_o)$$

where F_o is the observed structure factor, F_o' the structure factor corrected for secondary extinction, I_o the observed intensity, K and C adjustable scale factors, and $\beta = 2(1 + \cos^4 2\theta)/(1 + \cos^2 2\theta)^2$. The absorption ratio has been set equal to unity in the expression for β.

Refinement was recommenced, with anisotropic thermal parameters for tellurium, chloride, and the two sulfur atoms. The final weighting scheme was now introduced, with $a_1 = 0.8$ and $a_2 = 0.2$ in the expression for W given earlier. After four cycles of full-matrix refinement with group scale factors and anisotropic thermal parameters being refined in alternate cycles, no atomic positional shifts were greater than 10 % of the standard deviation in the position, and the refinement was terminated. The final value of R was 0.080. A difference Fourier map taken after the final refinement cycle showed no peaks higher than 0.5 electrons/Å^3, and no depressions lower than the same value, outside the heavy atom positions. Heavy atoms still were associated with areas of density up to 1.0 electrons/Å^3. The structure factor list generated by the final cycle of refinement is found in Table 1. Atomic positions and isotropic thermal parameters are listed in Table 3, and the anisotropic thermal parameters for the heavy atoms in Table 4.

Solution of the structure of the bromide salt was accomplished in much the same manner, with the added advantage that the atomic placements from the chloride salt served as a guide. All atoms were rapidly located, and three cycles of refinement brought the R factor down to the final value of 0.052,

Table 1. Observed and calculated structure factors ($\times 10$) for $[Te(tu)_2(tmtu)_2]Cl_2$. Unobserved reflections are indicated by a minus sign on $F(O)$.

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	C	1374	1644	5	16	0	178	200	1	11	1	446	46	7	10	1	-58	-38	4	13	-1	405	392
0	4	0	114	-21	6	0	0	649	666	1	12	1	122	10	7	11	1	96	59	4	14	-1	214	188
0	6	0	400	388	6	1	0	-49	50	1	13	1	552	588	7	12	1	120	-113	4	15	-1	251	251
0	8	0	368	336	6	2	0	894	864	1	14	1	287	-254	7	13	1	173	163	4	16	-1	97	79
0	10	0	329	255	6	3	0	-51	-41	1	15	1	398	375	7	14	1	43	46	4	17	-1	178	207
0	12	C	516	537	6	4	0	485	449	1	16	1	120	117	8	1	1	288	267	5	-1	-1	401	348
0	14	C	174	140	6	5	0	126	-117	1	17	1	205	190	8	2	1	106	83	5	-2	-1	139	-126
0	16	0	195	173	6	6	0	329	326	2	1	1	338	-288	8	3	1	275	279	5	-3	-1	689	626
0	18	C	356	439	6	7	0	344	-356	2	2	1	1670	-1906	8	4	1	-55	-6	5	-4	-1	365	-338
1	0	0	1242	1211	6	8	0	444	467	2	3	1	711	668	8	5	1	233	240	5	-5	-1	840	791
1	1	0	313	335	6	9	0	-62	-55	2	4	1	327	-290	8	6	1	113	129	5	-6	-1	119	-105
1	2	C	219	155	6	10	0	397	374	2	5	1	809	829	8	7	1	314	309	5	-7	-1	564	560
1	3	0	349	446	6	11	0	176	185	2	6	1	86	-27	8	8	1	69	72	5	-8	-1	141	133
1	4	C	520	500	6	12	0	198	164	2	7	1	850	866	8	9	1	518	525	5	-9	-1	350	345
1	5	0	511	435	6	13	0	57	62	2	8	1	-43	-8	8	10	1	65	-78	5	-10	-1	71	67
1	6	0	1020	1075	6	14	0	256	255	2	9	1	804	857	8	11	1	345	371	5	-11	-1	470	500
1	7	C	265	-220	6	15	0	-38	20	2	10	1	171	154	8	12	1	64	-86	5	-12	-1	88	76
1	8	0	784	824	7	0	0	493	502	2	11	1	540	584	9	1	1	268	234	5	-13	-1	457	467
1	9	0	-45	45	7	1	0	-53	-52	2	12	1	-54	-37	9	2	1	67	75	5	-14	-1	193	154
1	10	0	392	399	7	2	0	710	713	2	13	1	411	416	9	3	1	315	313	5	-15	-1	295	315
1	11	C	388	391	7	3	0	-54	4	2	14	1	163	-153	9	4	1	182	-169	5	-16	-1	108	-107
1	12	0	662	719	7	4	0	490	493	2	15	1	301	294	9	5	1	314	314	6	-1	-1	586	535
1	13	C	-58	39	7	5	0	-56	13	2	16	1	271	252	9	6	1	145	-132	6	-2	-1	614	600
1	14	C	272	275	7	6	0	243	237	2	17	1	266	270	9	7	1	404	399	6	-3	-1	626	614
1	15	C	246	-224	7	7	0	77	-71	2	18	1	67	71	9	8	1	-46	-40	6	-4	-1	210	179
1	16	0	150	160	7	8	0	215	190	3	1	1	1452	1470	9	9	1	332	353	6	-5	-1	478	455
1	17	0	117	-105	7	9	0	112	95	3	2	1	458	-411	10	1	1	432	437	6	-6	-1	111	95
1	18	C	322	373	7	10	0	278	272	3	3	1	856	837	10	2	1	-47	42	6	-7	-1	476	490
2	0	C	961	826	7	11	0	125	119	3	4	1	283	246	10	3	1	293	306	6	-8	-1	-58	35
2	1	C	60	-87	7	12	0	190	170	3	5	1	495	497	10	4	1	49	-51	6	-9	-1	425	421
2	2	0	135	70	7	13	0	-45	23	3	6	1	105	-94	10	5	1	232	252	6	-10	-1	-62	-31
2	3	0	120	78	7	14	0	252	288	3	7	1	425	447	10	6	1	72	-58	6	-11	-1	280	269
2	4	C	791	748	8	0	0	115	-19	3	8	1	281	-284	10	7	1	159	180	6	-12	-1	-61	-27
2	5	0	125	107	8	1	0	130	125	3	9	1	738	783	11	1	1	145	161	6	-13	-1	263	252
2	6	C	936	1008	8	2	0	339	350	3	10	1	86	58	11	2	1	68	86	6	-14	-1	58	-55
2	7	0	641	-622	8	3	0	164	149	3	11	1	290	286	11	3	1	151	203	6	-15	-1	216	257
2	8	C	551	544	8	4	0	491	485	3	12	1	66	3	1	-1	-1	397	367	7	-1	-1	682	684
2	9	0	-48	10	8	5	0	112	93	3	13	1	66	25	1	-2	-1	40	-18	7	-2	-1	89	69
2	10	0	520	520	8	6	0	395	388	3	14	1	206	-171	1	-3	-1	533	398	7	-3	-1	521	545
2	11	C	170	140	8	7	0	144	125	3	15	1	252	232	1	-4	-1	230	-129	7	-4	-1	184	-185
2	12	0	828	867	8	8	0	336	331	3	16	1	161	169	1	-5	-1	784	811	7	-5	-1	242	253
2	13	C	132	-114	8	9	0	-58	-29	3	17	1	294	309	1	-6	-1	770	-730	7	-6	-1	55	-47
2	14	0	432	449	8	10	0	354	365	4	1	1	863	817	1	-7	-1	1090	1089	7	-7	-1	195	193
2	15	0	89	-89	8	11	0	116	-96	4	2	1	145	81	1	-8	-1	545	-525	7	-8	-1	88	80
2	16	C	136	131	8	12	0	222	263	4	3	1	1043	1012	1	-9	-1	478	471	7	-9	-1	456	466
2	17	0	69	66	8	13	0	72	-82	4	4	1	550	533	1	-10	-1	273	240	7	-10	-1	-60	39
2	18	C	142	162	9	0	0	243	219	4	5	1	475	439	1	-11	-1	640	657	7	-11	-1	284	273
3	0	0	1756	1753	9	1	0	86	-78	4	6	1	188	150	1	-12	-1	389	391	7	-12	-1	-51	4
3	1	0	142	-157	9	2	0	378	364	4	7	1	390	390	1	-13	-1	436	465	7	-13	-1	94	84
3	2	0	1126	1113	9	3	0	192	-173	4	8	1	145	-138	1	-14	-1	-59	-38	7	-14	-1	53	53
3	3	0	521	-455	9	4	0	327	304	4	9	1	605	627	1	-15	-1	168	163	8	-1	-1	272	281
3	4	C	1000	1009	9	5	0	198	-182	4	10	1	262	246	1	-16	-1	-57	16	8	-2	-1	264	-266
3	5	0	270	217	9	6	0	313	303	4	11	1	148	166	1	-17	-1	300	307	8	-3	-1	529	515
3	6	0	819	830	9	7	0	100	79	4	12	1	196	187	2	-1	-1	1511	1544	8	-4	-1	267	-256
3	7	C	329	-311	9	8	0	364	334	4	13	1	235	194	2	-2	-1	633	-539	8	-5	-1	312	317
3	8	0	182	154	9	9	0	54	50	4	14	1	242	-207	2	-3	-1	156	-54	8	-6	-1	64	-60
3	9	C	116	-92	9	10	0	262	279	4	15	1	341	350	2	-4	-1	98	-40	8	-7	-1	344	333
3	10	C	89	12	9	11	0	76	-79	4	16	1	98	-96	2	-5	-1	565	486	8	-8	-1	-58	-2
3	11	C	161	170	10	0	0	515	489	4	17	1	246	311	2	-6	-1	259	212	8	-9	-1	537	504
3	12	C	413	436	10	1	0	-51	-7	5	1	1	395	-329	2	-7	-1	940	980	8	-10	-1	-52	3
3	13	0	-61	-35	10	2	0	387	385	5	2	1	100	-85	2	-8	-1	163	158	8	-11	-1	240	246
3	14	C	423	429	10	3	0	55	-66	5	3	1	663	644	2	-9	-1	654	699	8	-12	-1	46	44
3	15	0	82	67	10	4	0	206	207	5	4	1	131	129	2	-10	-1	162	154	8	-13	-1	117	159
3	16	0	244	224	10	5	0	144	-130	5	5	1	606	632	2	-11	-1	716	811	9	-1	-1	245	229
3	17	C	184	171	10	6	0	175	178	5	6	1	200	-165	2	-12	-1	108	108	9	-2	-1	-56	-22
4	0	0	932	891	10	7	0	-38	34	5	7	1	431	425	2	-13	-1	293	318	9	-3	-1	382	370
4	1	0	558	-556	10	8	0	142	173	5	8	1	202	-162	2	-14	-1	73	-68	9	-4	-1	97	72
4	2	0	917	870	11	0	0	241	267	5	9	1	726	798	2	-15	-1	135	106	9	-5	-1	278	267
4	3	C	472	-437	11	1	0	80	75	5	10	1	142	118	2	-16	-1	68	-55	9	-6	-1	201	196
4	4	C	548	536	11	2	0	226	252	5	11	1	476	486	2	-17	-1	256	275	9	-7	-1	235	236
4	5	C	725	682	11	3	0	88	99	5	12	1	87	51	3	-1	-1	1458	1445	9	-8	-1	64	58
4	6	0	482	441	11	4	0	146	203	5	13	1	377	344	3	-2	-1	111	-92	9	-9	-1	381	400
4	7	0	224	202	0	2	1	476	-444	5	14	1	93	-90	3	-3	-1	716	677	9	-10	-1	-37	-29
4	8	0	449	425	0	3	1	941	1043	5	15	1	338	345	3	-4	-1	247	199	9	-11	-1	202	251
4	9	0	163	166	0	4	1	600	577	5	16	1	77	-67	3	-5	-1	650	659	10	-1	-1	242	250
4	10	0	357	360	0	5	1	1413	1449	6	1	1	362	326	3	-6	-1	547	474	10	-2	-1	-49	-10
4	11	0	-59	-13	0	6	1	297	-237	6	2	1	83	-59	3	-7	-1	834	828	10	-3	-1	414	438
4	12	0	416	359	0	7	1	825	802	6	3	1	862	866	3	-8	-1	381	352	10	-4	-1	159	125
4	13	C	218	-205	0	8	1	137	-148	6	4	1	291	-266	3	-9	-1	190	144	10	-5	-1	304	327
4	14	0	346	340	0	9	1	164	-80	6	5	1	646	682	3	-10	-1	234	-213	10	-6	-1	69	66
4	15	C	-58	-22	0	10	1	264	252	6	6	1	196	-158	3	-11	-1	311	314	10	-7	-1	150	151
4	16	C	261	260	0	11	1	262	257	6	7	1	334	334	3	-12	-1	364	-370	11	-1	-1	251	269
4	17	0	89	105	0	12	1	52	35	6	8	1	133	-117	3	-13	-1	333	332	11	-2	-1	88	-109
5	0	0	498	477	0	13	1	427	438	6	9	1	398	404	3	-14	-1	91	-70	11	-3	-1	285	338
5	1	0	118	-100	0	14	1	329	-320	6	10	1	-61	-13	3	-15	-1	238	214	11	-4	-1	57	-64
5	2	C	447	425	0	15	1	310	294	6	11	1	179	162	3	-16	-1	-53	-3	0	2	2	1094	1216
5	3	0	98	-101	0	16	1	-57	-37	6	12	1	-59	29	3	-17	-1	267	307	0	3	2	342	-336
5	4	0	250	259	0	17	1	235	231	6	13	1	240	246	4	-1	-1	447	403	0	4	2	850	979
5	5	C	289	256	0	18	1	37	30	6	14	1	50	52	4	-2	-1	219	-201	0	5	2	551	582
5	6	0	467	438	1	1	1	822	814	6	15	1	258	323	4	-3	-1	575	622	0	6	2	723	795
5	7	C	159	-134	1	2	1	513	-495	7	1	1	543	530	4	-4	-1	662	-682	0	7	2	90	-57
5	8	C	714	760	1	3	1	902	945	7	2	1	113	-104	4	-5	-1	833	907	0	9	2	590	582
5	9	0	-59	1	1	4	1	904	915	7	3	1	709	706	4	-6	-1	105	-54	0	9	2	107	54
5	10	C	804	882	1	5	1	1100	1174	7	4	1	-52	8	4	-7	-1	642	646	0	10	2	347	362
5	11	0	-62	10	1	6	1	667	642	7	5	1	369	408	4	-8	-1	149	125	0	11	2	226	-187
5	12	C	401	375	1	7	1	704	683	7	6	1	243	231	4	-9	-1	208	199	0	12	2	236	197
5	13	C	204	-173	1	8	1	192	-144	7	7	1	230	255	4	-10	-1	95	-84	0	13	2	295	-295
5	14	0	190	183	1	9	1	224	242	7	8	1	224	191	4	-11	-1	416	443	0	14	2	290	280
5	15	0	84	-63	1	10	1	93	65	7	9	1	294	278	4	-12	-1	-59	-3	0	15	2	90	70

Table 1. Continued.

H	K	L	F(O)	F(C)
0	16	2	358	344
0	17	2	198	185
0	18	2	242	281
1	0	2	1607	1591
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1	2	2	1140	1335
1	3	2	386	354
1	4	2	296	265
1	5	2	915	917
1	6	2	422	367
1	7	2	94	67
1	8	2	791	817
1	9	2	-50	-7
1	10	2	891	950
1	11	2	57	40
1	12	2	244	223
1	13	2	253	-221
1	14	2	228	207
1	15	2	135	-100
1	16	2	352	324
1	17	2	87	68
1	18	2	168	205
2	0	2	629	-514
2	1	2	188	142
2	2	2	922	928
2	3	2	377	278
2	4	2	613	658
2	5	2	-39	-39
2	6	2	396	394
2	7	2	699	-657
2	8	2	807	850
2	9	2	255	-225
2	10	2	825	870
2	11	2	344	335
2	12	2	300	278
2	13	2	190	165
2	14	2	335	318
2	15	2	-67	26
2	16	2	397	359
2	17	2	45	48
3	0	2	448	360
3	1	2	64	-15
3	2	2	1194	1280
3	3	2	170	127
3	4	2	952	1022
3	5	2	387	-339
3	6	2	364	254
3	7	2	449	-396
3	8	2	364	263
3	9	2	-57	8
3	10	2	917	523
3	11	2	158	107
3	12	2	162	166
3	13	2	-67	-7
3	14	2	384	386
3	15	2	-65	-28
3	16	2	372	343
4	0	2	211	138
4	1	2	317	286
4	2	2	984	1002
4	3	2	592	511
4	4	2	944	1026
4	5	2	363	304
4	6	2	508	501
4	7	2	362	316
4	8	2	417	391
4	9	2	86	-67
4	10	2	361	341
4	11	2	128	-55
4	12	2	146	120
4	13	2	77	-49
4	14	2	462	421
4	15	2	-60	-22
4	16	2	327	334
5	0	2	244	-148
5	1	2	221	-161
5	2	2	561	512
5	3	2	164	-103
5	4	2	613	575
5	5	2	116	-86
5	6	2	341	294
5	7	2	295	274
5	8	2	603	590
5	9	2	-64	-16
5	10	2	610	634
5	11	2	268	-238
5	12	2	333	320
5	13	2	-68	23
5	14	2	397	372
5	15	2	137	137
5	16	2	237	297
6	0	2	662	620
6	1	2	-55	54
6	2	2	670	627
6	3	2	155	-123
6	4	2	478	435
6	5	2	475	-453
6	6	2	255	216
6	7	2	-63	15
6	8	2	516	487
6	9	2	89	-85
6	10	2	589	556
6	11	2	153	-146
6	12	2	175	161
6	13	2	91	80
6	14	2	140	138
6	15	2	122	121
7	0	2	742	735
7	1	2	293	251
7	2	2	705	691
7	3	2	334	298
7	4	2	485	437
7	5	2	-61	-58
7	6	2	252	224
7	7	2	202	169
7	8	2	344	319
7	9	2	-67	29
7	10	2	239	179
7	11	2	60	-50
7	12	2	124	114
7	13	2	58	49
7	14	2	147	182
8	0	2	266	235
8	1	2	165	132
8	2	2	213	185
8	3	2	205	183
8	4	2	327	320
8	5	2	-64	-44
8	6	2	338	314
8	7	2	102	81
8	8	2	362	340
8	9	2	-59	7
8	10	2	363	350
8	11	2	69	-54
8	12	2	267	316
9	0	2	240	222
9	1	2	98	89
9	2	2	248	210
9	3	2	82	-40
9	4	2	405	371
9	5	2	245	-212
9	6	2	386	342
9	7	2	71	-67
9	8	2	270	261
9	9	2	116	-99
9	10	2	194	223
10	0	2	471	482
10	1	2	-52	-21
10	2	2	356	349
10	3	2	70	-60
10	4	2	301	298
10	5	2	-44	-28
10	6	2	220	230
10	7	2	92	83
11	0	2	233	302
1	0	-2	501	426
1	-1	-2	270	-274
1	-2	-2	780	821
1	-3	-2	776	-811
1	-4	-2	965	1074
1	-5	-2	153	83
1	-6	-2	678	741
1	-7	-2	471	-426
1	-8	-2	325	278
1	-9	-2	208	-162
1	-10	-2	442	421
1	-11	-2	249	221
1	-12	-2	597	615
1	-13	-2	126	120
1	-14	-2	497	463
1	-15	-2	214	184
1	-16	-2	231	243
1	-17	-2	220	200
1	-18	-2	164	173
2	0	-2	623	638
2	-1	-2	237	170
2	-2	-2	337	367
2	-3	-2	570	519
2	-4	-2	830	1018
2	-5	-2	706	675
2	-6	-2	1069	1217
2	-7	-2	372	-318
2	-8	-2	544	546
2	-9	-2	59	-31
2	-10	-2	389	368
2	-11	-2	118	64
2	-12	-2	584	622
2	-13	-2	73	-67
2	-14	-2	475	433
2	-15	-2	140	-99
2	-16	-2	228	197
3	0	-2	954	1046
3	-1	-2	735	681
3	-2	-2	588	579
3	-3	-2	618	637
3	-4	-2	597	621
3	-5	-2	231	193
3	-6	-2	760	815
3	-7	-2	374	-291
3	-8	-2	596	600
3	-9	-2	-56	13
3	-10	-2	280	257
3	-11	-2	141	128
3	-12	-2	471	456
3	-13	-2	75	-60
3	-14	-2	265	221
3	-15	-2	209	-186
3	-16	-2	213	201
3	-17	-2	97	-106
4	0	-2	1565	1689
4	-1	-2	119	86
4	-2	-2	683	649
4	-3	-2	224	-237
4	-4	-2	466	409
4	-5	-2	299	-268
4	-6	-2	478	451
4	-7	-2	172	-139
4	-8	-2	460	444
4	-9	-2	-60	-1
4	-10	-2	461	474
4	-11	-2	-64	42
4	-12	-2	408	410
4	-13	-2	188	166
4	-14	-2	137	82
4	-15	-2	162	132
4	-16	-2	235	213
4	-17	-2	50	50
5	0	-2	715	724
5	-1	-2	98	-79
5	-2	-2	382	355
5	-3	-2	285	-202
5	-4	-2	575	524
5	-5	-2	128	-85
5	-6	-2	686	717
5	-7	-2	234	191
5	-8	-2	599	672
5	-9	-2	-64	-10
5	-10	-2	389	382
5	-11	-2	266	-247
5	-12	-2	458	447
5	-13	-2	86	58
5	-14	-2	282	236
5	-15	-2	146	135
5	-16	-2	179	200
6	0	-2	487	433
6	-1	-2	329	317
6	-2	-2	310	278
6	-3	-2	323	269
6	-4	-2	587	576
6	-5	-2	126	97
6	-6	-2	564	586
6	-7	-2	406	408
6	-8	-2	441	432
6	-9	-2	-68	-11
6	-10	-2	318	310
6	-11	-2	337	-288
6	-12	-2	455	405
6	-13	-2	87	-66
6	-14	-2	297	286
7	0	-2	465	453
7	-1	-2	108	83
7	-2	-2	543	541
7	-3	-2	-59	2
7	-4	-2	738	767
7	-5	-2	297	-285
7	-6	-2	402	425
7	-7	-2	111	96
7	-8	-2	165	154
7	-9	-2	133	96
7	-10	-2	143	127
7	-11	-2	270	-232
7	-12	-2	229	209
7	-13	-2	145	131
7	-14	-2	227	240
8	0	-2	348	321
8	-1	-2	187	159
8	-2	-2	449	449
8	-3	-2	106	80
8	-4	-2	437	443
8	-5	-2	289	-299
8	-6	-2	271	272
8	-7	-2	150	-122
8	-8	-2	369	375
8	-9	-2	162	-130
8	-10	-2	344	322
8	-11	-2	-50	12
8	-12	-2	219	224
9	0	-2	165	145
9	-1	-2	140	120
9	-2	-2	226	215
9	-3	-2	142	155
9	-4	-2	252	247
9	-5	-2	-42	-13
9	-6	-2	241	250
9	-7	-2	187	160
9	-8	-2	454	455
9	-9	-2	-48	42
9	-10	-2	425	455
9	-11	-2	64	-65
10	0	-2	263	269
10	-1	-2	-56	14
10	-2	-2	417	454
10	-3	-2	93	64
10	-4	-2	362	368
10	-5	-2	61	25
10	-6	-2	152	146
10	-7	-2	143	124
10	-8	-2	181	220
11	0	-2	197	207
11	-1	-2	79	-64
11	-2	-2	298	349
11	-3	-2	132	-128
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0	4	3	302	297
0	5	3	206	233
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0	7	3	203	175
0	8	3	298	-320
0	9	3	623	649
0	10	3	247	238
0	11	3	323	319
0	12	3	168	150
0	13	3	295	299
0	14	3	160	-128
0	15	3	331	312
0	16	3	58	-53
0	17	3	302	319
1	1	3	499	480
1	2	3	179	211
1	3	3	811	925
1	4	3	264	298
1	5	3	862	877
1	6	3	86	36
1	7	3	485	528
1	8	3	155	98
1	9	3	706	753
1	10	3	227	222
1	11	3	392	408
1	12	3	110	-89
1	13	3	398	421
1	14	3	238	-207
1	15	3	433	420
1	16	3	209	-189
1	17	3	109	110
2	1	3	312	314
2	2	3	57	-37
2	3	3	1070	1083
2	4	3	335	-330
2	5	3	736	730
2	6	3	63	39
2	7	3	378	365
2	8	3	109	-104
2	9	3	564	608
2	10	3	91	-55
2	11	3	365	402
2	12	3	85	86
2	13	3	455	473
2	14	3	200	197
2	15	3	432	451
2	16	3	72	69
2	17	3	129	124
3	1	3	650	597
3	2	3	434	-418
3	3	3	1025	1069
3	4	3	614	-623
3	5	3	506	541
3	6	3	-47	-34
3	7	3	292	308
3	8	3	282	276
3	9	3	457	466
3	10	3	132	-93
3	11	3	233	220
3	12	3	273	-230
3	13	3	270	239
3	14	3	217	181
3	15	3	372	366
3	16	3	87	67
3	17	3	196	245
4	1	3	1075	1140
4	2	3	422	421
4	3	3	589	562
4	4	3	78	-41
4	5	3	258	210
4	6	3	339	324
4	7	3	388	382
4	8	3	365	367
4	9	3	588	653
4	10	3	144	-122
4	11	3	393	398
4	12	3	283	-256
4	13	3	209	166
4	14	3	-62	-5
4	15	3	267	250
4	16	3	113	-115
5	1	3	371	366
5	2	3	342	261
5	3	3	404	394
5	4	3	254	-254
5	5	3	313	327
5	6	3	101	-82
5	7	3	572	621
5	8	3	137	125
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5	10	3	-65	7
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5	12	3	75	71
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6	1	3	499	510
6	2	3	147	126
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6	4	3	388	-376
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6	6	3	347	-350
6	7	3	337	358
6	8	3	-63	-19
6	9	3	238	224
6	10	3	66	-53
6	11	3	361	354
6	12	3	66	39
6	13	3	270	275
6	14	3	163	158
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7	2	3	271	265
7	3	3	442	463
7	4	3	-58	-46
7	5	3	471	486
7	6	3	136	96
7	7	3	362	354
7	8	3	225	177
7	9	3	-63	5
7	10	3	103	-58
7	11	3	198	182
7	12	3	-47	-47
7	13	3	241	285
8	1	3	277	260
8	2	3	-60	-36
8	3	3	193	156
8	4	3	-61	7
8	5	3	368	353
8	6	3	200	163
8	7	3	433	433
8	8	3	246	200
8	9	3	223	184
8	10	3	81	-62
8	11	3	251	290
9	1	3	327	318
9	2	3	142	-126
9	3	3	157	112
9	4	3	254	-217
9	5	3	278	261
9	6	3	169	-131
9	7	3	303	329
9	8	3	64	-40
9	9	3	214	234
10	1	3	390	434
10	2	3	-45	28
10	3	3	255	251
10	4	3	-41	12
10	5	3	241	238
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1	-2	-3	777	-774
1	-3	-3	577	574
1	-4	-3	138	-159
1	-5	-3	380	357
1	-6	-3	144	-92
1	-7	-3	405	417
1	-8	-3	241	-218
1	-9	-3	821	889
1	-10	-3	184	156
1	-11	-3	490	496
1	-12	-3	184	163
1	-13	-3	203	173
1	-14	-3	73	-11
1	-15	-3	229	196
1	-16	-3	226	190
1	-17	-3	315	308
2	-1	-3	767	727
2	-2	-3	839	-793
2	-3	-3	418	396
2	-4	-3	278	266
2	-5	-3	636	646
2	-6	-3	327	283
2	-7	-3	864	858
2	-8	-3	165	115
2	-9	-3	704	709
2	-10	-3	61	-9
2	-11	-3	487	501
2	-12	-3	229	-231
2	-13	-3	476	500
2	-14	-3	207	-190
2	-15	-3	279	263
2	-16	-3	163	151
2	-17	-3	186	206
3	-1	-3	786	761
3	-2	-3	65	-76
3	-3	-3	593	581
3	-4	-3	319	271
3	-5	-3	782	809
3	-6	-3	259	255
3	-7	-3	514	483
3	-8	-3	107	56
3	-9	-3	170	157
3	-10	-3	57	28
3	-11	-3	418	423
3	-12	-3	93	-51
3	-13	-3	556	553
3	-14	-3	236	-176
3	-15	-3	281	247
3	-16	-3	128	112
3	-17	-3	183	193
4	-1	-3	1052	1124
4	-2	-3	334	-277
4	-3	-3	764	695
4	-4	-3	-46	26
4	-5	-3	893	876
4	-6	-3	283	-273
4	-7	-3	402	378
4	-8	-3	146	-137
4	-9	-3	163	-99
4	-10	-3	156	132
4	-11	-3	353	336
4	-12	-3	221	191
4	-13	-3	494	492
4	-14	-3	-64	18
4	-15	-3	246	223

Table 1. Continued.

H	K	L	F(O)	F(C)	H	K	L	F(O)	F(C)	H	K	L	F(O)	F(C)	H	K	L	F(O)	F(C)	H	K	L	F(O)	F(C)
4	-16	-3	65	54	1	13	4	237	-210	8	8	4	349	349	6	-6	-4	703	771	3	5	5	547	543
5	-1	-3	564	575	1	14	4	440	399	8	9	4	-52	9	6	-7	-4	-67	-33	3	6	5	-50	36
5	-2	-3	355	280	1	15	4	-67	43	8	10	4	201	222	6	-8	-4	300	248	3	7	5	297	223
5	-3	-3	163	134	1	16	4	320	325	9	0	4	296	272	6	-9	-4	213	154	3	8	5	67	60
5	-4	-3	93	87	2	0	4	1110	1074	9	1	4	135	-91	6	-10	-4	268	198	3	9	5	106	-45
5	-5	-3	532	535	2	1	4	229	-199	9	2	4	216	171	6	-11	-4	168	137	3	10	5	148	-144
5	-6	-3	310	-299	2	2	4	681	678	9	3	4	142	-133	6	-12	-4	457	446	3	11	5	285	249
5	-7	-3	793	859	2	3	4	332	-340	9	4	4	224	211	6	-13	-4	99	-72	3	12	5	148	116
5	-8	-3	245	-226	2	4	4	446	423	9	5	4	81	-66	6	-14	-4	258	288	3	13	5	379	364
5	-9	-3	424	411	2	5	4	385	-356	9	6	4	313	328	7	0	-4	848	939	3	14	5	170	160
5	-10	-3	-64	-2	2	6	4	420	361	9	7	4	198	-211	7	-1	-4	162	98	3	15	5	263	286
5	-11	-3	518	517	2	7	4	275	246	9	8	4	169	197	7	-2	-4	659	606	4	1	5	390	348
5	-12	-3	220	149	2	8	4	780	807	10	0	4	294	299	7	-3	-4	152	106	4	2	5	85	-28
5	-13	-3	470	453	2	9	4	-59	-7	10	1	4	-43	-5	7	-4	-4	404	392	4	3	5	394	399
5	-14	-3	-59	-23	2	10	4	698	715	10	2	4	276	301	7	-5	-4	134	95	4	4	5	-53	11
5	-15	-3	125	107	2	11	4	-64	-49	10	3	4	-40	5	7	-6	-4	481	476	4	5	5	537	577
5	-16	-3	59	-47	2	12	4	264	231	10	4	4	223	279	7	-7	-4	216	-182	4	6	5	212	183
6	-1	-3	764	803	2	13	4	113	89	1	0	-4	318	316	7	-8	-4	239	199	4	7	5	504	532
6	-2	-3	218	197	2	14	4	247	203	1	-1	-4	411	-482	7	-9	-4	87	-40	4	8	5	271	275
6	-3	-3	115	50	2	15	4	79	71	1	-2	-4	906	1007	7	-10	-4	121	60	4	9	5	261	224
6	-4	-3	-56	31	2	16	4	244	257	1	-3	-4	84	-52	7	-11	-4	130	115	4	10	5	189	-150
6	-5	-3	294	286	3	0	4	709	674	1	-4	-4	1064	1100	7	-12	-4	267	282	4	11	5	369	338
6	-6	-3	118	107	3	1	4	255	221	1	-5	-4	135	-91	8	0	-4	561	619	4	12	5	216	-182
6	-7	-3	513	528	3	2	4	711	722	1	-6	-4	697	692	8	-1	-4	-65	-28	4	13	5	321	314
6	-8	-3	278	273	3	3	4	190	171	1	-7	-4	422	-379	8	-2	-4	207	178	4	14	5	-59	-10
6	-9	-3	357	398	3	4	4	667	706	1	-8	-4	411	404	8	-3	-4	264	-234	4	15	5	172	213
6	-10	-3	-68	32	3	5	4	415	-390	1	-9	-4	125	-73	8	-4	-4	165	127	5	1	5	525	578
6	-11	-3	575	552	3	6	4	401	382	1	-10	-4	418	412	8	-5	-4	247	-196	5	2	5	-53	16
6	-12	-3	101	-62	3	7	4	155	-98	1	-11	-4	339	298	8	-6	-4	469	453	5	3	5	168	90
6	-13	-3	316	301	3	8	4	499	506	1	-12	-4	223	191	8	-7	-4	117	-98	5	4	5	-55	3
6	-14	-3	81	-67	3	9	4	88	-64	1	-13	-4	93	61	8	-8	-4	426	397	5	5	5	332	308
6	-15	-3	92	68	3	10	4	304	253	1	-14	-4	406	416	8	-9	-4	-60	14	5	6	5	66	57
7	-1	-3	809	864	3	11	4	-67	61	1	-15	-4	-48	-37	8	-10	-4	306	311	5	7	5	513	550
7	-2	-3	-56	0	3	12	4	199	158	1	-16	-4	324	312	8	-11	-4	-45	22	5	8	5	-64	16
7	-3	-3	482	458	3	13	4	262	210	2	0	-4	196	-89	8	-12	-4	228	318	5	9	5	510	484
7	-4	-3	128	-86	3	14	4	230	174	2	-1	-4	151	-64	9	0	-4	318	329	5	10	5	154	-139
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7	-6	-3	113	63	3	16	4	232	272	2	-3	-4	316	313	9	-2	-4	199	163	5	12	5	-57	-40
7	-7	-3	360	366	4	0	4	663	672	2	-4	-4	389	374	9	-3	-4	-65	-9	5	13	5	256	267
7	-8	-3	197	172	4	1	4	364	305	2	-5	-4	97	72	9	-4	-4	256	224	6	1	5	561	621
7	-9	-3	104	57	4	2	4	419	368	2	-6	-4	609	641	9	-5	-4	-62	40	6	2	5	123	-92
7	-10	-3	155	-131	4	3	4	401	362	2	-7	-4	478	-463	9	-6	-4	376	378	6	3	5	332	347
7	-11	-3	240	210	4	4	4	590	629	2	-8	-4	805	928	9	-7	-4	158	143	6	4	5	-57	-22
7	-12	-3	87	-73	4	5	4	100	-73	2	-9	-4	104	-64	9	-8	-4	314	345	6	5	5	302	292
7	-13	-3	205	205	4	6	4	583	580	2	-10	-4	715	760	9	-9	-4	102	98	6	6	5	155	-145
7	-14	-3	113	133	4	7	4	153	127	2	-11	-4	335	336	9	-10	-4	191	260	6	7	5	341	314
8	-1	-3	417	399	4	8	4	421	411	2	-12	-4	367	355	10	0	-4	420	453	6	8	5	143	-127
8	-2	-3	-59	-25	4	9	4	119	90	2	-13	-4	118	-102	10	-1	-4	65	55	6	9	5	231	177
8	-3	-3	270	272	4	10	4	327	300	2	-14	-4	344	327	10	-2	-4	338	341	6	10	5	-59	39
8	-4	-3	350	-322	4	11	4	113	-101	2	-15	-4	186	-174	10	-3	-4	-51	18	6	11	5	235	218
8	-5	-3	380	387	4	12	4	398	385	2	-16	-4	253	247	10	-4	-4	309	344	6	12	5	135	156
8	-6	-3	104	-63	4	13	4	-71	-38	3	0	-4	1056	1026	10	-5	-4	79	70	6	13	5	172	195
8	-7	-3	416	408	4	14	4	294	289	3	-1	-4	307	-241	10	-6	-4	232	273	7	1	5	486	489
8	-8	-3	-62	56	4	15	4	130	-140	3	-2	-4	851	910	10	-7	-4	130	162	7	2	5	-59	25
8	-9	-3	243	211	4	16	4	134	166	3	-3	-4	165	86	0	1	5	1022	1174	7	3	5	389	321
8	-10	-3	163	-186	5	0	4	367	358	3	-4	-4	339	322	0	2	5	154	181	7	4	5	181	158
8	-11	-3	330	330	5	1	4	245	197	3	-5	-4	522	540	0	3	5	962	1010	7	5	5	367	338
9	-1	-3	105	100	5	2	4	218	179	3	-6	-4	410	382	0	4	5	75	-62	7	6	5	-61	-33
9	-2	-3	270	211	5	3	4	117	73	3	-7	-4	67	36	0	5	5	194	186	7	7	5	221	179
9	-3	-3	254	229	5	4	4	553	542	3	-8	-4	496	475	0	6	5	350	329	7	8	5	96	-61
9	-4	-3	-60	-13	5	5	4	-63	-9	3	-9	-4	74	72	0	7	5	231	165	7	9	5	148	143
9	-5	-3	424	394	5	6	4	682	710	3	-10	-4	593	624	0	8	5	249	242	7	10	5	53	58
9	-6	-3	57	28	5	7	4	152	101	3	-11	-4	208	187	0	9	5	634	646	7	11	5	211	243
9	-7	-3	406	373	5	8	4	463	458	3	-12	-4	156	214	0	10	5	54	-71	8	1	5	163	146
9	-8	-3	181	167	5	9	4	87	-89	3	-13	-4	278	-212	0	11	5	331	315	8	2	5	-58	43
9	-9	-3	273	262	5	10	4	267	218	3	-14	-4	171	149	0	12	5	101	-77	8	3	5	258	224
10	-1	-3	470	445	5	11	4	90	-62	3	-15	-4	118	-95	0	13	5	78	-22	8	4	5	218	182
10	-2	-3	236	230	5	12	4	494	456	3	-16	-4	261	279	0	14	5	77	77	8	5	5	355	347
10	-3	-3	424	430	5	13	4	117	101	4	0	-4	718	802	0	15	5	338	315	8	6	5	84	68
10	-4	-3	-48	21	5	14	4	302	330	4	-1	-4	628	-652	0	16	5	52	-41	8	7	5	330	327
10	-5	-3	234	234	6	0	4	555	560	4	-2	-4	826	875	1	1	5	324	309	8	8	5	67	-74
10	-6	-3	-42	16	6	1	4	199	-186	4	-3	-4	584	-523	1	2	5	738	760	8	9	5	233	270
10	-7	-3	153	156	6	2	4	361	332	4	-4	-4	622	637	1	3	5	651	647	9	1	5	208	213
10	-8	-3	55	51	6	3	4	387	-396	4	-5	-4	318	278	1	4	5	86	39	9	2	5	201	-210
11	-1	-3	255	326	6	4	4	430	462	4	-6	-4	691	759	1	5	5	258	224	9	3	5	233	257
11	-2	-3	-31	11	6	5	4	232	-193	4	-7	-4	125	-111	1	6	5	194	-170	9	4	5	-44	-14
11	-3	-3	212	251	6	6	4	509	514	4	-8	-4	394	387	1	7	5	541	565	9	5	5	232	237
0	1	4	205	-184	6	7	4	-68	-2	4	-9	-4	-65	8	1	8	5	-49	23	9	6	5	-37	-32
0	2	4	995	1064	6	8	4	296	236	4	-10	-4	233	168	1	9	5	732	784	9	7	5	151	160
0	3	4	59	-6	6	9	4	-72	14	4	-11	-4	99	74	1	10	5	95	-57	10	1	5	223	316
0	4	4	1269	1256	6	10	4	147	84	4	-12	-4	237	174	1	11	5	493	530	10	2	5	63	-86
0	5	4	-38	22	6	11	4	94	-72	4	-13	-4	144	-104	1	12	5	-61	1	1	-1	-5	596	627
0	6	4	473	460	6	12	4	319	309	4	-14	-4	245	218	1	13	5	271	253	1	-2	-5	371	-403
0	7	4	193	186	6	13	4	92	87	4	-15	-4	58	58	1	14	5	88	63	1	-3	-5	1014	1102
0	8	4	292	259	6	14	4	154	209	4	-16	-4	209	243	1	15	5	296	291	1	-4	-5	277	-279
0	9	4	78	-50	7	0	4	693	767	5	0	-4	417	323	1	16	5	157	-167	1	-5	-5	495	472
0	10	4	286	272	7	1	4	99	81	5	-1	-4	287	-221	2	1	5	465	448	1	-6	-5	91	27
0	11	4	103	99	7	2	4	394	352	5	-2	-4	315	254	2	2	5	393	351	1	-7	-5	393	409
0	12	4	224	165	7	3	4	-64	37	5	-3	-4	378	-331	2	3	5	565	568	1	-8	-5	-48	6
0	13	4	-70	6	7	4	4	281	266	5	-4	-4	388	361	2	4	5	208	-177	1	-9	-5	617	642
0	14	4	457	431	7	5	4	157	134	5	-5	-4	146	115	2	5	5	626	659	1	-10	-5	189	-174
0	15	4	-68	24	7	6	4	434	432	5	-6	-4	734	781	2	6	5	296	-304	1	-11	-5	260	239
0	16	4	364	363	7	7	4	109	77	5	-7	-4	234	-181	2	7	5	593	617	1	-12	-5	205	-177
1	0	4	216	-141	7	8	4	294	277	5	-8	-4	450	450	2	8	5	85	-49	1	-13	-5	234	188
1	1	4	250	-252	7	9	4	-66	-6	5	-9	-4	114	-85	2	9	5	457	465	1	-14	-5	237	184
1	2	4	472	500	7	10	4	209	190	5	-10	-4	388	366	2	10	5	126	-117	1	-15	-5	438	438
1	3	4	187	160	7	11	4	65	-78	5	-11	-4	111	80	2	11	5	444	461	1	-16	-5	136	116
1	4	4	772	807	7	12	4	203	234	5	-12	-4	607	557	2	12	5	70	60	2	-1	-5	310	-239
1	5	4	169	139	8	0	4	404	390	5	-13	-4	92	-80	2	13	5	339	323	2	-2	-5	170	166
1	6	4	639	641	8	1	4	31	54	5	-14	-4	408	384	2	14	5	176	146	2	-3	-5	838	863
1	7	4	475	447	8	2	4	233	194	6	0	-4	376	376	2	15	5	284	282	2	-4	-5	68	29
1	8	4	749	835	8	3	4	168	119	6	-1	-4	-58	-5	2	16	5	91	-96	2	-5	-5	617	610
1	9	4	69	33	8	4	4	192	153	6	-2	-4	295	259	3	1	5	855	847	2	-6	-5	75	72
1	10	4	564	580	8	5	4	233	203	6	-3	-4	164	131	3	2	5	243	207	2	-7	-5	457	461
1	11	4	362	-362	8	6	4	421	400	6	-4	-4	513	535	3	3	5	821	837	2	-8	-5	199	-174
1	12	4	284	259	8	7	4	-62	-4	6	-5	-4	326	306	3	4	5	161	-129	2	-9	-5	713	775

Table 1. 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)
2-10 -5	73	-71	3-15 -5	392	408	5 -5 -5	283	256	6-11 -5	303	273	8 -5 -5	493	477
2-11 -5	453	455	3-16 -5	106	-108	5 -6 -5	154	-112	6-12 -5	85	-87	8 -6 -5	247	-206
2-12 -5	88	-54	4 -1 -5	803	796	5 -7 -5	432	437	6-13 -5	238	234	8 -7 -5	376	353
2-13 -5	406	384	4 -2 -5	129	80	5 -8 -5	243	-216	6-14 -5	98	-104	8 -8 -5	186	-145
2-14 -5	62	60	4 -3 -5	913	868	5 -9 -5	746	777	7 -1 -5	610	602	8 -9 -5	162	156
2-15 -5	431	450	4 -4 -5	348	297	5-10 -5	177	191	7 -2 -5	228	-195	8-10 -5	-42	50
2-16 -5	99	85	4 -5 -5	393	341	5-11 -5	499	470	7 -3 -5	477	482	8-11 -5	220	260
3 -1 -5	510	470	4 -6 -5	240	-219	5-12 -5	63	56	7 -4 -5	130	119	9 -1 -5	270	250
3 -2 -5	109	89	4 -7 -5	294	305	5-13 -5	237	209	7 -5 -5	500	491	9 -2 -5	161	142
3 -3 -5	1074	1133	4 -8 -5	482	-507	5-14 -5	81	-75	7 -6 -5	137	125	9 -3 -5	228	207
3 -4 -5	462	451	4 -9 -5	517	538	5-15 -5	171	203	7 -7 -5	300	288	9 -4 -5	147	140
3 -5 -5	689	696	4-10 -5	137	116	6 -1 -5	415	400	7 -8 -5	131	-97	9 -5 -5	324	318
3 -6 -5	163	172	4-11 -5	206	188	6 -2 -5	167	-182	7 -9 -5	113	94	9 -6 -5	-49	-17
3 -7 -5	183	124	4-12 -5	217	164	6 -3 -5	493	469	7-10 -5	-56	-25	9 -7 -5	361	362
3 -8 -5	130	-70	4-13 -5	215	161	6 -4 -5	438	423	7-11 -5	187	159	9 -8 -5	-39	-22
3 -9 -5	433	415	4-14 -5	83	-66	6 -5 -5	498	489	7-12 -5	-41	-12	9 -9 -5	221	263
3-10 -5	254	243	4-15 -5	253	247	6 -6 -5	308	309	7-13 -5	207	267	10 -1 -5	401	434
3-11 -5	259	242	5 -1 -5	443	420	6 -7 -5	413	416	8 -1 -5	285	253	10 -2 -5	90	73
3-12 -5	78	62	5 -2 -5	406	-307	6 -8 -5	-64	17	8 -2 -5	119	-97	10 -3 -5	206	214
3-13 -5	263	241	5 -3 -5	262	253	6 -9 -5	415	401	8 -3 -5	272	229	10 -4 -5	92	82
3-14 -5	145	-123	5 -4 -5	66	-34	6-10 -5	-64	46	8 -4 -5	-60	-35	10 -5 -5	202	232
												10 -6 -5	77	84

with unobserved reflections included if the value of $K|F_c|$ was greater than the observable limit. Scattering factor curves were taken from the same sources as for the chloride structure. The tellurium curve was corrected for anomalous dispersion as described earlier, using values appropriate for Mo$K\alpha$ radiation. None of the other scattering curves were corrected. The weight, W, in this refinement was set equal to $1/\sigma^2(F_o)$, where $\sigma(F_o)$, the standard deviation in the observed structure factor, is evaluated from considerations of counting statistics. Tellurium, sulfur, and bromide were given anisotropic thermal parameters at the start of this refinement. An examination of the observed and calculated structure factors of the strongest reflections after the third refinement cycle indicated that extinction was probably not an important problem for this crystal, and the refinement was terminated. The calculated structure factors are listed with the observed values in Table 2. Atomic positions and isotropic thermal parameters are listed in Table 5, and anisotropic thermal parameters for the heavy atoms in Table 6.

RESULTS

Bond lengths and angles for $[Te(tu)_2(tmtu)_2]Cl_2$ are found in Table 7, and those for the bromide salt in Table 8. The standard deviations given in these tables are calculated from those of Tables 3 and 5, without regard to coordinate covariances or standard deviations in the cell dimensions. Fig. 1 shows the cations from the two salts, seen from above the nearly square coordination plane.

As pointed out earlier, the tellurium(II) ion is crystallographically required to occupy a center of symmetry. Thus, the configuration about the tellurium ion must be *trans*, and the TeS_4 unit must be planar. As expected, the coordination is approximately square planar, as the angle S_1-Te-S_2, found to be 91.37(10)° in the chloride and 91.45(9)° in the bromide, deviates slightly from 90°. The tellurium – sulfur bond distances are quite interesting, in that in this complex the $Te-S_1$ (thiourea) bond is significantly longer than the average length for this type of bond found previously. In thirteen previous studies of square planar complexes of tellurium(II) involving Te – S bonds, the average Te – S bond length has been found to be 2.682 Å, with an average deviation

Table 2. Observed and calculated structure factors ($\times 10$) for $[Te(tu)_2(tmtu)_2]Br_2$. Unobserved reflections are indicated by a minus sign on $F(O)$.

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	1979	1825	0	9	6	299	277	1	9	2	-136	-61	1	3	9	251	282	2	12	4	-148	34
0	4	0	678	-654	0	10	6	170	210	1	10	2	1009	997	1	4	9	-137	60	2	13	4	-150	67
0	6	0	323	333	0	11	6	-147	149	1	11	2	-144	18	1	5	9	523	555	2	14	4	-156	63
0	8	0	852	833	0	12	6	288	303	1	12	2	-148	-1	1	6	9	365	355	2	15	4	-159	113
0	10	0	416	366	0	13	6	-152	10	1	13	2	-150	-137	1	7	9	365	391	2	1	5	232	246
0	12	0	-150	121	0	14	6	325	261	1	14	2	-151	-22	1	8	9	-144	46	2	2	5	740	724
0	14	0	-152	43	0	1	7	566	567	1	15	2	-153	-62	1	9	9	185	202	2	3	5	711	723
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Table 2. Continued.

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3	16	2	166	203
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3	9	3	423	451
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3	12	3	361	-351
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3	15	3	224	265
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3	6	4	318	323
3	7	4	342	-336
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3	9	6	-139	68
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5	8	0	917	905
5	9	0	-151	-62
5	10	0	792	837
5	11	0	-150	9
5	12	0	199	216
5	13	0	195	-133
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5	0	2	206	-176
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5	5	2	-134	126
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5	3	3	287	269
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5	13	3	171	140
5	14	3	-159	41
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5	7	5	551	581
5	8	5	-144	82
5	9	5	526	528
5	10	5	161	-227
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6	3	0	-146	119
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6	8	1	-152	-97
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6	5	2	380	-356
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6	7	2	-144	2
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6	9	2	-148	-84
6	10	2	532	553
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6	3	3	494	514
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6	6	3	479	-480
6	7	3	263	253
6	8	3	193	-113
6	9	3	-151	136
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6	7	4	159	117
6	8	4	221	234
6	9	4	-148	-57
6	10	4	-151	62
6	11	4	208	-180
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6	4	5	-141	-29
6	5	5	-145	164
6	6	5	283	-234
6	7	5	332	361
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6	8	7	-151	-48
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6	3	8	-144	9
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7	1	0	-138	58
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7	3	0	-148	84
7	4	0	581	590
7	5	0	-150	-27
7	6	0	216	241
7	7	0	-153	-171
7	8	0	-154	49
7	9	0	-155	133
7	10	0	-157	179
7	11	0	221	225
7	12	0	250	228
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7	3	1	621	610
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7	6	1	360	364
7	7	1	173	202
7	8	1	210	210
7	9	1	278	280
7	10	1	-154	-109
7	11	1	-156	39
7	12	1	-157	-113
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7	1	2	345	301
7	2	2	668	650
7	3	2	395	398
7	4	2	326	315
7	5	2	-141	-96
7	6	2	230	201
7	7	2	-146	43
7	8	2	352	346
7	9	2	-150	111
7	10	2	244	211
7	11	2	-155	40
7	1	3	439	451
7	2	3	207	213
7	3	3	524	546
7	4	3	-138	-53
7	5	3	566	528
7	6	3	-143	105
7	7	3	240	251
7	8	3	182	176
7	9	3	-151	-64
7	10	3	-152	-11
7	11	3	170	162
7	0	4	824	806
7	1	4	-136	27

Table 2. 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	2	4	371	330	9	4	2	338	371	7	-1	-1	746	751	6	-12	-2	431	413	5	-4	-3	205	169
7	3	4	-138	7	9	5	2	218	-181	7	-2	-1	-147	41	6	-13	-2	-158	-38	5	-5	-3	284	302
7	4	4	-142	152	9	6	2	311	280	7	-3	-1	327	366	6	-1	-3	956	970	5	-6	-3	548	-539
7	5	4	176	119	9	1	3	338	321	7	-4	-1	200	-207	6	-2	-3	152	148	5	-7	-3	838	817
7	6	4	340	361	9	2	3	-145	-107	7	-5	-1	-152	86	6	-3	-3	-136	-63	5	-8	-3	246	-224
7	7	4	192	154	9	3	3	-148	81	7	-6	-1	-134	-77	6	-4	-3	-137	21	5	-9	-3	519	539
7	8	4	327	370	9	4	3	189	-195	7	-7	-1	263	283	6	-5	-3	-139	14	5-10	-3		-152	124
7	9	4	-150	-1	9	5	3	-152	139	7	-8	-1	-153	48	6	-6	-3	-147	91	5-11	-3		386	368
7	10	4	226	182	9	0	4	192	216	7	-9	-1	464	477	6	-7	-3	557	536	5-12	-3		194	171
7	1	5	403	412	9	1	4	-147	-27	7	-10	-1	-156	79	6	-8	-3	340	322	5-13	-3		357	341
7	2	5	195	142	9	2	4	-152	125	7	-11	-1	240	216	6	-9	-3	501	477	5-14	-3		202	-141
7	3	5	322	327	9	3	4	-147	-87	7	-12	-1	-158	1	6	-10	-3	-153	35	5	0	-4	135	-6
7	4	5	-142	143	10	0	0	427	427	7	0	-2	249	272	6	-11	-3	297	346	5	-1	-4	300	-271
7	5	5	364	328	10	1	0	-150	-11	7	-1	-2	175	160	6	-12	-3	-160	-21	5	-2	-4	256	229
7	6	5	157	-121	10	-1	-1	-164	172	7	-2	-2	464	463	6	-13	-3	180	148	5	-3	-4	328	-356
7	7	5	-150	184	10	0	-2	274	277	7	-3	-2	-141	48	6	0	-4	190	215	5	-4	-4	554	532
7	8	5	-150	-51	9	-1	-1	166	152	7	-4	-2	837	855	6	-1	-4	155	145	5	-5	-4	181	136
7	9	5	-153	85	9	-2	-1	-159	-51	7	-5	-2	318	-315	6	-2	-4	305	291	5	-6	-4	742	741
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7	1	6	-146	-150	9	-4	-1	-161	55	7	-7	-2	-150	-85	6	-4	-4	574	581	5	-8	-4	177	163
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7	3	6	170	-146	9	-6	-1	188	238	7	-9	-2	-157	144	6	-6	-4	749	737	5-10		-4	181	189
7	4	6	311	324	9	-7	-1	193	131	7	-10	-2	-156	70	6	-7	-4	-145	-106	5-11		-4	-154	110
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8	1	5	-145	65	8	0	-4	585	602	7	-2	-8	382	408	5	-4	-1	296	-265	5	-6	-9	183	-123
8	2	5	-146	53	8	-1	-4	-140	-12	7	-3	-8	155	-118	5	-5	-1	909	882	5	-7	-9	240	199
8	3	5	224	227	8	-2	-4	-143	164	7	-4	-8	448	439	5	-6	-1	261	-293	5	0	-10	470	446
8	4	5	154	162	8	-3	-4	202	-228	7	-5	-8	168	151	5	-7	-1	430	397	5	-1	-10	-148	-12
8	5	5	378	337	8	-4	-4	-149	-78	6	-1	-1	531	550	5	-8	-1	-149	56	5	-2	-10	219	224
8	6	5	-150	65	8	-5	-4	171	-176	6	-2	-1	801	817	5	-9	-1	-151	41	5	-3	-10	233	-226
8	0	6	260	199	8	-6	-4	341	350	6	-3	-1	495	520	5	-10	-1	-156	239	4	-1	-1	-129	96
8	1	6	-146	-48	8	-7	-4	-153	-57	6	-4	-1	228	232	5	-11	-1	513	494	4	-2	-1	419	-463
8	2	6	181	173	8	-8	-4	448	435	6	-5	-1	318	332	5	-12	-1	-157	104	4	-3	-1	772	819
8	3	6	-148	-64	8	-9	-4	-158	8	6	-6	-1	157	-133	5	-13	-1	567	547	4	-4	-1	676	-687
9	0	0	247	216	8	-1	-5	-144	136	6	-7	-1	485	483	5	-14	-1	-157	36	4	-5	-1	1058	1071
9	1	0	-147	-117	8	-2	-5	-143	37	6	-8	-1	-151	0	5	0	-2	684	699	4	-6	-1	-141	88
9	2	0	333	322	8	-3	-5	200	199	6	-9	-1	430	396	5	-1	-2	283	-260	4	-7	-1	500	529
9	3	0	258	-238	8	-4	-5	-144	-11	6	-10	-1	187	180	5	-2	-2	303	307	4	-8	-1	-147	174
9	4	0	220	228	8	-5	-5	463	453	6	-11	-1	186	216	5	-3	-2	501	-448	4	-9	-1	-148	-65
9	5	0	-164	-89	8	-6	-5	210	-235	6	-12	-1	-155	25	5	-4	-2	394	376	4	-10	-1	270	-252
9	6	0	248	224	8	-7	-5	306	269	6	-13	-1	-159	132	5	-5	-2	-140	169	4	-11	-1	406	460
9	7	0	172	78	8	-8	-5	-159	-163	6	0	-2	188	148	5	-6	-2	598	641	4	-12	-1	-153	-88
9	1	1	255	222	8	0	-6	292	277	6	-1	-2	205	202	5	-7	-2	413	399	4	-13	-1	478	502
9	2	1	-148	124	8	-1	-6	237	-253	6	-2	-2	278	246	5	-8	-2	673	696	4	-14	-1	290	254
9	3	1	226	236	8	-2	-6	273	276	6	-3	-2	153	107	5	-9	-2	-150	-91	4	-15	-1	-162	161
9	4	1	-155	-126	8	-3	-6	237	-232	6	-4	-2	726	747	5	-10	-2	363	363	4	0	-2	2024	2016
9	5	1	261	248	8	-4	-6	217	217	6	-5	-2	196	184	5	-11	-2	429	-430	4	-1	-2	-125	81
9	6	1	200	-176	8	-5	-6	-149	5	6	-6	-2	535	547	5	-12	-2	303	281	4	-2	-2	706	712
9	7	1	292	319	8	-6	-6	296	276	6	-7	-2	438	456	5	-13	-2	-156	25	4	-3	-2	289	-302
9	0	2	-145	112	8	-1	-7	342	347	6	-8	-2	218	201	5	-14	-2	222	226	4	-4	-2	-133	-52
9	1	2	-145	44	8	-2	-7	-146	12	6	-9	-2	-153	30	5	-1	-3	602	629	4	-5	-2	219	-223
9	2	2	185	204	8	-3	-7	215	245	6	-10	-2	-156	197	5	-2	-3	663	614	4	-6	-2	401	373
9	3	2	-146	-13	8	-4	-7	-148	-5	6	-11	-2	313	-308	5	-3	-3	-129	-6	4	-7	-2	157	-121

Table 2. Continued.

H K L	F(O)	F(C)	H K L	F(O)	F(C)	H K L	F(O)	F(C)	H K L	F(O)	F(C)	H K L	F(O)	F(C)
4 -8 -2	720	738	3 -3 -1	607	606	3 -4 -8	746	747	2-14 -5	-156	68	1 -7 -3	593	629
4 -9 -2	-148	-42	3 -4 -1	-137	136	3 -5 -8	-138	0	2-15 -5	317	336	1 -8 -3	206	-199
4-10 -2	493	509	3 -5 -1	476	497	3 -6 -8	462	439	2 0 -6	927	900	1 -9 -3	1153	1187
4-11 -2	-151	-18	3 -6 -1	861	872	3 -7 -8	-142	146	2 -1 -6	-125	-70	1-10 -3	-142	-42
4-12 -2	-153	119	3 -7 -1	969	940	3 -8 -8	-145	54	2 -2 -6	588	538	1-11 -3	406	370
4-13 -2	169	115	3 -8 -1	476	497	3 -9 -8	-147	30	2 -3 -6	277	-284	1-12 -3	-150	105
4-14 -2	-157	-13	3 -9 -1	228	257	3-10 -8	-151	98	2 -4 -6	-129	71	1-13 -3	-154	-80
4-15 -2	-162	155	3-10 -1	419	-446	3-11 -8	-154	-100	2 -5 -6	164	-171	1-14 -3	-155	29
4 -1 -3	870	875	3-11 -1	175	177	3 -1 -9	708	712	2 -6 -6	159	-107	1-15 -3	221	153
4 -2 -3	125	81	3-12 -1	413	-458	3 -2 -9	-140	-58	2 -7 -6	374	399	1-16 -3	187	168
4 -3 -3	869	828	3-13 -1	167	184	3 -3 -9	145	97	2 -8 -6	827	792	1 0 -4	-125	83
4 -4 -3	-129	62	3-14 -1	-153	88	3 -4 -9	-141	-124	2 -9 -6	191	135	1 -1 -4	230	-206
4 -5 -3	1043	1066	3-15 -1	175	190	3 -5 -9	-142	103	2-10 -6	848	850	1 -2 -4	923	925
4 -6 -3	541	-537	3-16 -1	-158	111	3 -6 -9	194	217	2-11 -6	213	-195	1 -3 -4	182	236
4 -7 -3	305	288	3 0 -2	1160	1187	3 -7 -9	365	365	2-12 -6	-150	102	1 -4 -4	1369	1336
4 -8 -3	204	-230	3 -1 -2	976	975	3 -8 -9	373	323	2-13 -6	-154	7	1 -5 -4	292	-293
4 -9 -3	259	-249	3 -2 -2	592	623	3 -9 -9	409	374	2-14 -6	-158	104	1 -6 -4	824	785
4-10 -3	198	238	3 -3 -2	874	908	3 0-10	355	379	2 -1 -7	-131	106	1 -7 -4	724	-715
4-11 -3	332	287	3 -4 -2	373	374	3 -1-10	280	279	2 -2 -7	631	656	1 -8 -4	188	171
4-12 -3	230	256	3 -5 -2	-129	-78	3 -2-10	258	252	2 -3 -7	593	581	1 -9 -4	-138	0
4-13 -3	569	574	3 -6 -2	721	747	3 -3-10	371	364	2 -4 -7	-131	-19	1-10 -4	333	323
4-14 -3	-158	-98	3 -7 -2	588	-591	3 -4-10	232	249	2 -5 -7	612	633	1-11 -4	530	532
4-15 -3	-163	148	3 -8 -2	759	776	3 -5-10	-144	-46	2 -6 -7	382	-405	1-12 -4	389	388
4 0 -4	766	814	3 -9 -2	146	156	3 -6-10	439	454	2 -7 -7	346	358	1-13 -4	-153	13
4 -1 -4	883	-912	3-10 -2	296	303	3 -7-10	-149	-64	2 -8 -7	-142	132	1-14 -4	344	345
4 -2 -4	803	805	3-11 -2	400	428	3 -1-11	284	273	2 -9 -7	251	247	1-15 -4	279	-271
4 -3 -4	847	-842	3-12 -2	221	212	3 -2-11	-149	-155	2-10 -7	228	229	1-16 -4	203	178
4 -4 -4	858	840	3-13 -2	-150	-76	3 -3-11	175	203	2-11 -7	460	439	1 -1 -5	511	494
4 -5 -4	408	399	3-14 -2	-156	141	2 -1 -1	1968	2033	2-12 -7	164	126	1 -2 -5	882	-910
4 -6 -4	788	793	3-15 -2	307	-312	2 -2 -1	614	-569	2-13 -7	295	332	1 -3 -5	1085	1111
4 -7 -4	208	209	3-16 -2	176	156	2 -3 -1	420	-419	2 0 -8	-136	97	1 -4 -5	284	-281
4 -8 -4	457	453	3 -1 -3	455	473	2 -4 -1	-138	-58	2 -1 -8	-135	-100	1 -5 -5	613	597
4 -9 -4	203	-190	3 -2 -3	201	-241	2 -5 -1	-138	-111	2 -2 -8	196	194	1 -6 -5	478	462
4-10 -4	-150	133	3 -3 -3	848	865	2 -6 -1	244	208	2 -3 -8	265	-235	1 -7 -5	381	402
4-11 -4	174	-153	3 -4 -3	235	230	2 -7 -1	1169	1224	2 -4 -8	497	490	1 -8 -5	-135	-9
4-12 -4	193	146	3 -5 -3	1124	1130	2 -8 -1	220	211	2 -5 -8	282	247	1 -9 -5	549	560
4-13 -4	-159	-14	3 -6 -3	401	415	2 -9 -1	920	966	2 -6 -8	648	652	1-10 -5	430	-437
4-14 -4	225	157	3 -7 -3	247	239	2-10 -1	185	138	2 -7 -8	400	396	1-11 -5	313	280
4 -1 -5	910	918	3 -8 -3	-137	139	2-11 -1	544	586	2 -8 -8	376	391	1-12 -5	309	-327
4 -2 -5	336	315	3 -9 -3	159	-169	2-12 -1	164	156	2 -9 -8	-148	-67	1-13 -5	-155	148
4 -3 -5	639	629	3-10 -3	-144	-143	2-13 -1	-150	59	2-10 -8	288	262	1-14 -5	255	274
4 -4 -5	310	307	3-11 -3	391	389	2-14 -1	-151	-30	2-11 -8	379	-377	1-15 -5	380	344
4 -5 -5	234	216	3-12 -3	-149	-13	2-15 -1	-156	154	2-12 -8	349	348	1 0 -6	837	848
4 -6 -5	388	-382	3-13 -3	701	722	2-16 -1	-157	-47	2 -1 -9	599	597	1 -1 -6	522	495
4 -7 -5	409	408	3-14 -3	-151	-24	2 0 -2	185	164	2 -2 -9	242	227	1 -2 -6	600	625
4 -8 -5	614	-611	3-15 -3	196	170	2 -1 -2	481	480	2 -3 -9	-139	3	1 -3 -6	218	240
4 -9 -5	648	657	3 0 -4	1599	1559	2 -2 -2	302	351	2 -4 -9	-140	-11	1 -4 -6	323	295
4-10 -5	221	217	3 -1 -4	404	-387	2 -3 -2	834	792	2 -5 -9	199	103	1 -5 -6	761	-780
4-11 -5	201	159	3 -2 -4	963	952	2 -4 -2	1240	1283	2 -6 -9	253	-214	1 -6 -6	189	161
4-12 -5	227	198	3 -3 -4	-122	-85	2 -5 -2	554	513	2 -7 -9	471	507	1 -7 -6	486	-488
4-13 -5	-156	-1	3 -4 -4	131	-112	2 -6 -2	1272	1286	2 -8 -9	-147	-27	1 -8 -6	889	907
4-14 -5	-161	-172	3 -5 -4	521	546	2 -7 -2	494	-508	2 -9 -9	564	556	1 -9 -6	-141	65
4 0 -6	-129	31	3 -6 -4	304	325	2 -8 -2	205	234	2-10 -9	-152	62	1-10 -6	643	660
4 -1 -6	181	-177	3 -7 -4	233	235	2 -9 -2	-140	51	2 0-10	-141	62	1-11 -6	-147	92
4 -2 -6	661	664	3 -8 -4	747	740	2-10 -2	212	200	2 -1-10	-140	-23	1-12 -6	-148	12
4 -3 -6	197	-162	3 -9 -4	-139	25	2-11 -2	347	331	2 -2-10	206	172	1-13 -6	-151	59
4 -4 -6	1020	1047	3-10 -4	576	594	2-12 -2	749	739	2 -3-10	-143	-4	1-14 -6	-157	58
4 -5 -6	168	-121	3-11 -4	-146	133	2-13 -2	-153	-127	2 -4-10	389	400	1 -1 -7	180	133
4 -6 -6	260	255	3-12 -4	-149	16	2-14 -2	502	502	2 -5-10	158	-74	1 -2 -7	328	302
4 -7 -6	-141	-39	3-13 -4	-153	-93	2-15 -2	285	-251	2 -6-10	539	529	1 -3 -7	798	776
4 -8 -6	-142	19	3-14 -4	-153	-33	2-16 -2	-157	52	2 -7-10	-148	-88	1 -4 -7	490	-469
4 -9 -6	176	-164	3-15 -4	-155	-68	2 -1 -3	818	770	2 -8-10	-152	127	1 -5 -7	851	853
4-10 -6	256	216	3 -1 -5	323	349	2 -2 -3	1312	-1277	2 -1-11	355	355	1 -6 -7	380	-348
4-11 -6	-149	-69	3 -2 -5	331	361	2 -3 -3	329	297	2 -2-11	267	-295	1 -7 -7	360	323
4-12 -6	327	323	3 -3 -5	1210	1215	2 -4 -3	206	191	2 -3-11	-148	6	1 -8 -7	-141	72
4-13 -6	-156	35	3 -4 -5	454	468	2 -5 -3	570	589	2 -4-11	-146	-37	1 -9 -7	-143	-89
4 -1 -7	764	768	3 -5 -5	906	915	2 -6 -3	792	790	1 -1 -1	538	556	1-10 -7	-146	-190
4 -2 -7	300	-282	3 -6 -5	-130	-71	2 -7 -3	807	782	1 -2 -1	634	574	1-11 -7	255	297
4 -3 -7	416	400	3 -7 -5	-134	58	2 -8 -3	251	243	1 -3 -1	324	210	1-12 -7	-150	9
4 -4 -7	449	-440	3 -8 -5	250	-227	2 -9 -3	707	694	1 -4 -1	-140	-44	1-13 -7	506	497
4 -5 -7	-138	29	3 -9 -5	230	171	2-10 -3	341	-347	1 -5 -1	457	502	1 0 -8	1146	1168
4 -6 -7	-141	-42	3-10 -5	462	501	2-11 -3	424	393	1 -6 -1	1215	-1238	1 -1 -8	-134	-40
4 -7 -7	399	394	3-11 -5	294	297	2-12 -3	286	-303	1 -7 -1	1201	1185	1 -2 -8	576	551
4 -8 -7	188	164	3-12 -5	239	251	2-13 -3	448	462	1 -8 -1	655	-655	1 -3 -8	361	-384
4 -9 -7	567	567	3-13 -5	283	254	2-14 -3	160	20	1 -9 -1	599	630	1 -4 -8	151	-59
4-10 -7	-149	-60	3-14 -5	244	-222	2-15 -3	294	267	1-10 -1	466	461	1 -5 -8	-136	-131
4-11 -7	171	166	3 0 -6	417	409	2-16 -3	191	195	1-11 -1	482	492	1 -6 -8	316	314
4-12 -7	-156	-70	3 -1 -6	363	-401	2 0 -4	319	322	1-12 -1	478	525	1 -7 -8	-141	171
4 0 -8	315	363	3 -2 -6	750	762	2 -1 -4	182	177	1-13 -1	249	311	1 -8 -8	455	443
4 -1 -8	384	390	3 -3 -6	184	-188	2 -2 -4	512	536	1-14 -1	204	-250	1 -9 -8	-145	-43
4 -2 -8	508	499	3 -4 -6	881	900	2 -3 -4	604	612	1-15 -1	-158	168	1-10 -8	309	280
4 -3 -8	253	256	3 -5 -6	521	489	2 -4 -4	-155	39	1-16 -1	162	-142	1-11 -8	242	-228
4 -4 -8	652	644	3 -6 -6	235	242	2 -5 -4	131	-115	1-17 -1	254	254	1-12 -8	-155	153
4 -5 -8	282	-289	3 -7 -6	694	666	2 -6 -4	511	489	1 0 -2	159	-179	1 -1 -9	442	452
4 -6 -8	296	282	3 -8 -6	346	344	2 -7 -4	670	-680	1 -1 -2	434	-468	1 -2 -9	259	258
4 -7 -8	275	-266	3 -9 -6	-142	11	2 -8 -4	1072	1051	1 -2 -2	857	787	1 -3 -9	330	319
4 -8 -8	-146	80	3-10 -6	383	358	2 -9 -4	-139	35	1 -3 -2	1039	-991	1 -4 -9	-141	-53
4 -9 -8	-150	86	3-11 -6	399	-369	2-10 -4	771	778	1 -4 -2	1570	1562	1 -5 -9	531	536
4-10 -8	-152	144	3-12 -6	-154	96	2-11 -4	548	550	1 -5 -2	265	222	1 -6 -9	379	-370
4 -1 -9	468	424	3-13 -6	-154	-43	2-12 -4	235	221	1 -6 -2	815	854	1 -7 -9	292	301
4 -2 -9	155	-158	3 -1 -7	695	709	2-13 -4	-155	-96	1 -7 -2	202	-161	1 -8 -9	-147	-124
4 -3 -9	464	488	3 -2 -7	682	671	2-14 -4	191	182	1 -8 -2	177	-171	1 -9 -9	160	119
4 -4 -9	-144	-134	3 -3 -7	477	473	2-15 -4	367	-361	1 -9 -2	418	-390	1-10 -9	187	225
4 -5 -9	440	454	3 -4 -7	249	226	2 -1 -5	643	-602	1-10 -2	-145	176	1 0-10	282	290
4 -6 -9	153	163	3 -5 -7	-137	105	2 -2 -5	-123	20	1-11 -2	-148	-5	1 -1-10	322	-315
4 -7 -9	207	193	3 -6 -7	-140	-156	2 -3 -5	1055	1093	1-12 -2	841	817	1 -2-10	298	303
4 -8 -9	185	236	3 -7 -7	535	533	2 -4 -5	151	108	1-13 -2	192	176	1 -3-10	251	-244
4 0-10	716	712	3 -8 -7	-141	81	2 -5 -5	966	966	1-14 -2	542	558	1 -4-10	435	452
4 -1-10	161	153	3 -9 -7	672	653	2 -6 -5	202	248	1-15 -2	185	253	1 -5-10	152	109
4 -2-10	437	425	3-10 -7	-147	96	2 -7 -5	217	203	1-16 -2	-158	73	1 -6-10	549	544
4 -3-10	-146	89	3-11 -7	181	230	2 -8 -5	217	-196	1 -1 -3	1835	1950	1 -7-10	-151	102
4 -4-10	-146	70	3-12 -7	-154	10	2 -9 -5	348	362	1 -2 -3	895	-885	1 -8-10	168	156
4 -5-10	221	-186	3 0 -8	173	115	2-10 -5	-146	-124	1 -3 -3	136	150	1 -1-11	601	577
4 -6-10	231	314	3 -1 -8	240	228	2-11 -5	543	560	1 -4 -3	138	-179	1 -2-11	-148	-74
3 -1 -1	1515	1506	3 -2 -8	444	425	2-12 -5	-150	-50	1 -5 -3	-127	-33	1 -3-11	164	200
3 -2 -1	591	-623	3 -3 -8	137	49	2-13 -5	541	527	1 -6 -3	-129	70	1 -4-11	-149	59

Table 3. Atomic coordinates in fractions of the monoclinic cell edges for $[Te(tu)_2(tmtu)_2]Cl_2$ Isotropic thermal parameters (Å²) in the form $\exp[-8\pi^2U(\sin^2\theta/\lambda^2)]$. Standard deviations in the least significant digits in parentheses.

	x	y	z	U
Te	0	0	0	
S_1	0.0687(4)	0.1637(2)	0.1247(5)	
C_1	0.0002(12)	0.1589(8)	0.2856(17)	0.0293(26)
N_1	0.0149(13)	0.0836(8)	0.3605(15)	0.0485(31)
N_2	−0.0668(12)	0.2353(7)	0.3293(15)	0.0411(28)
S_2	0.2936(3)	−0.0499(2)	0.0146(5)	
C_2	0.3484(13)	−0.0272(8)	−0.1487(17)	0.0313(27)
N_3	0.4151(11)	−0.0951(7)	−0.2129(14)	0.0359(25)
C_{Me1}	0.4026(15)	−0.1938(9)	−0.1795(18)	0.0458(35)
C_{Me2}	0.5294(18)	−0.0771(11)	−0.3145(21)	0.0604(45)
N_4	0.3294(11)	0.0565(7)	−0.2014(14)	0.0341(24)
C_{Me3}	0.3001(20)	0.0734(12)	−0.3504(24)	0.0686(51)
C_{Me4}	0.3178(15)	0.1393(9)	−0.1239(18)	0.0438(34)
Cl^-	0.1913(4)	−0.1098(2)	0.3883(5)	

Table 4. Anisotropic thermal parameters (Å²) for $[Te(tu)_2(tmtu)_2]Cl_2$, in the form $\exp[-2\pi^2(h^2a^{*2}U_{11}+\cdots+2hka^*b^*U_{12}+\cdots)]$. Standard deviations in the least significant digits in parentheses. All values multiplied by 10^4.

	U_{11}	U_{22}	U_{33}	U_{12}	U_{23}	U_{13}
Te	227(4)	224(4)	255(13)	9(4)	−1(5)	50(5)
S_1	455(17)	267(13)	262(42)	−30(22)	−29(16)	99(18)
S_2	226(12)	440(17)	319(42)	37(12)	38(18)	39(15)
Cl^-	593(20)	289(14)	434(44)	1(13)	−92(17)	129(20)

Table 5. Atomic coordinates in fractions of the monoclinic cell edges for $[Te(tu)_2(tmtu)_2]Br_2$. Isotropic thermal parameters (Å²) in the form $\exp[-8\pi^2U(\sin^2\theta/\lambda^2)]$. Standard deviations in the least significant digits in parentheses.

	x	y	z	U
Te	0	0	0	
S_1	0.0671(3)	0.1586(2)	0.1179(2)	
C_1	0.0029(11)	0.1545(7)	0.2769(9)	0.0334(24)
N_1	0.0155(10)	0.0805(6)	0.3495(8)	0.0482(24)
N_2	−0.0523(9)	0.2275(6)	0.3285(7)	0.0402(21)
S_2	0.2958(3)	−0.0456(2)	0.0116(2)	
C_2	0.3514(10)	−0.0241(6)	−0.1498(9)	0.0329(24)
N_3	0.4156(9)	−0.0903(6)	−0.2145(8)	0.0412(22)
C_{Me1}	0.4000(13)	−0.1842(8)	−0.1788(11)	0.0557(32)
C_{Me2}	0.5315(13)	−0.0724(8)	−0.3139(11)	0.0572(33)
N_4	0.3321(9)	0.0552(6)	−0.2044(7)	0.0380(21)
C_{Me3}	0.3071(13)	0.0692(8)	−0.3522(11)	0.0575(33)
C_{Me4}	0.3207(12)	0.1372(8)	−0.1278(10)	0.0524(32)
Br^-	0.1947(1)	−0.1152(1)	0.3864(1)	

of 0.010 Å[9]. The values of 2.710(3) Å and 2.706(3) Å found in this study for the chloride and bromide salts, respectively, deviate significantly from this average value. The lengths of the $Te-S_2$(tetramethylthiourea) bonds in this work have been found to be 2.688(3) Å and 2.679(3) Å for the chloride and bromide.

Table 6. Anisotropic thermal parameters ($Å^2$) for $[Te(tu)_2(tmtu)_2]Br_2$, in the form $\exp[-2\pi^2(h^2a^{*2}U_{11}+\cdots+2hka^*b^*U_{12}+\cdots)]$. Standard deviations in the least significant digits in parentheses. All values multiplied by 10^4.

	U_{11}	U_{22}	U_{33}	U_{12}	U_{23}	U_{13}
Te	304(5)	379(6)	231(4)	12(6)	−3(5)	40(3)
S_1	581(19)	391(18)	308(14)	−13(15)	−18(13)	134(13)
S_2	294(15)	576(19)	345(14)	48(14)	53(14)	40(11)
Br^-	739(9)	369(7)	458(7)	−17(7)	−59(6)	126(6)

Table 7. Bond lengths (Å) and angles (°) for $[Te(tu)_2(tmtu)_2]Cl_2$. Standard deviations in the least significant digits are given in parentheses.

$Te-S_1(tu)$	= 2.710(3)	S_1-Te-S_2	= 91.37(10)
$Te-S_2(tmtu)$	= 2.688(3)		
S_1-C_1	= 1.748(17)	$Te-S_1-C_1$	= 107.5(4)
C_1-N_1	= 1.315(18)	$S_1-C_1-N_1$	= 121.4(10)
C_1-N_2	= 1.337(16)	$S_1-C_1-N_2$	= 117.0(10)
		$N_1-C_1-N_2$	= 121.6(15)
S_2-C_2	= 1.754(17)	$Te-S_2-C_2$	= 103.3(4)
C_2-N_3	= 1.328(17)	$S_2-C_2-N_3$	= 117.8(10)
C_2-N_4	= 1.319(16)	$S_2-C_2-N_4$	= 120.1(11)
N_3-C_{Me1}	= 1.464(17)	$N_3-C_2-N_4$	= 122.1(15)
N_3-C_{Me2}	= 1.500(22)	$C_2-N_3-C_{Me1}$	= 124.3(13)
N_4-C_{Me3}	= 1.502(27)	$C_2-N_3-C_{Me2}$	= 122.5(11)
N_4-C_{Me4}	= 1.427(19)	$C_{Me1}-N_3-C_{Me2}$	= 112.7(11)
		$C_2-N_4-C_{Me3}$	= 123.1(13)
		$C_2-N_4-C_{Me4}$	= 124.2(14)
		$C_{Me3}-N_4-C_{Me4}$	= 112.4(12)

Table 8. Bond lengths (Å) and angles (°) for $[Te(tu)_2(tmtu)_2]Br_2$. Standard deviations in the least significant digits are given in parentheses.

$Te-S_1(tu)$	= 2.706(3)	S_1-Te-S_2	= 91.45(9)
$Te-S_2(tmtu)$	= 2.679(3)		
S_1-C_1	= 1.728(9)	$Te-S_1-C_1$	= 107.3(4)
C_1-N_1	= 1.329(13)	$S_1-C_1-N_1$	= 121.0(8)
C_1-N_2	= 1.318(13)	$S_1-C_1-N_2$	= 119.0(7)
		$N_1-C_1-N_2$	= 120.0(8)
S_2-C_2	= 1.751(9)	$Te-S_2-C_2$	= 104.1(3)
C_2-N_3	= 1.334(12)	$S_2-C_2-N_3$	= 117.7(7)
C_2-N_4	= 1.316(13)	$S_2-C_2-N_4$	= 121.0(7)
N_3-C_{Me1}	= 1.462(15)	$N_3-C_2-N_4$	= 121.3(8)
N_3-C_{Me2}	= 1.497(14)	$C_2-N_3-C_{Me1}$	= 123.4(8)
N_4-C_{Me3}	= 1.498(13)	$C_2-N_3-C_{Me2}$	= 121.2(8)
N_4-C_{Me4}	= 1.458(14)	$C_{Me1}-N_3-C_{Me2}$	= 114.6(8)
		$C_2-N_4-C_{Me3}$	= 123.0(8)
		$C_2-N_4-C_{Me4}$	= 123.8(8)
		$C_{Me3}-N_4-C_{Me4}$	= 113.0(8)

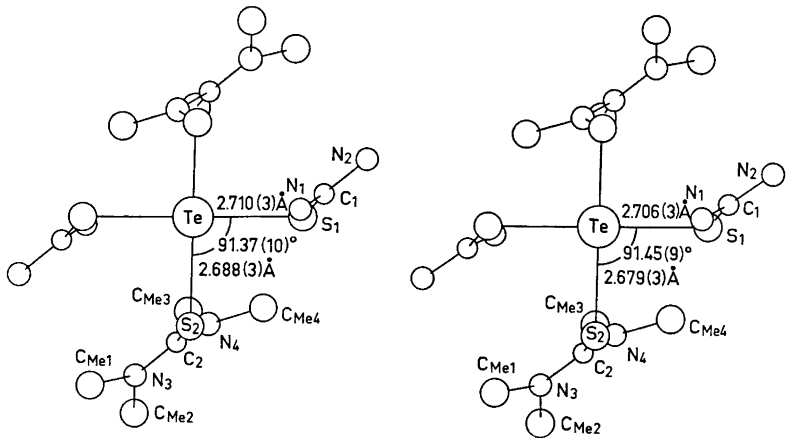

Fig. 1. The cation $[Te(tu)_2(tmtu)_2]^{2+}$ from the chloride salt (left) and the bromide salt (right), seen in projection from directly above the TeS_4 plane.

These values agree well with the average Te–S bond length just quoted. However, the Te–S(tetramethylthiourea) bond length in *trans*-diselenocyanatobis(tetramethylthiourea)tellurium(II) has been found to be 2.728(4) Å,[10] and in *trans*-dibenzenethiosulfonatobis(tetramethylthiourea)tellurium(II) to be 2.724(6) Å.[10] The differences between these values and those of the present work are significant, and presumably must be due to packing forces within the crystals. It may be noted that in the latter of these two structures, the deviation in the S–Te–S angle from 90° is approximately ten degrees.

The lengthening of the Te–S_1(thiourea) bond relative to the average value quoted earlier, may be explained by a combination of hydrogen-bonding and steric interaction effects. For example, the thiourea sulfur atom lies only 3.44 Å distant from one of the methyl groups (C_{Me4}) on the tetramethylthiourea ligand in the chloride salt (3.45 Å in the bromide). Commonly accepted values of the van der Waals radii are 2.0 Å for a methyl group [11] and 1.7 Å for sulfur,[12] and the resultant sum of 3.7 Å for a van der Waals contact of this type indicates a slight interaction between the thiourea sulfur and the methyl group. A glance at Fig. 1 confirms that the interaction might well be expected to increase the bond length of the Te–S(thiourea) bond.

Hydrogen bonds of the type N–H· · ·Cl^- are normally found to be in the range 3.2–3.4 Å.[13] In the present work, both of the $-NH_2$ groups of thiourea are found to engage in hydrogen bonding. For example, the distance from the chloride ion whose position is given in Table 3 to N_2 at (x_2, y_2-1, z_2) is 3.24 Å (where (x_2, y_2, z_2) are the coordinates given for N_2 in Table 3), to N_1 at (x_1, y_1, z_1) is 3.19 Å, and to N_1 at ($-x_1$, $-y_1$, $1-z_1$) is 3.21 Å. Corresponding distances in the bromide salt are 3.38 Å, 3.34 Å, and 3.37 Å. The halide ions lie quite near the planes of the thiourea group. As an example, the chloride ion in the first of these structures lies 0.51 Å from the plane through the S_1 thiourea group.

The other bond lengths and angles reported in Tables 7 and 8 are normal values for these bond types. The rather large variation in the bond lengths of the nitrogen – methyl carbon bonds is not significant.

The shape of the complex ion may be indicated by the angles between the primary TeS_4 plane and the Te – S – C plane for each ligand. In the chloride salt, the thiourea ligand makes an angle of 70°, while the tetramethylthiourea ligand makes an angle of 101°. The corresponding values for the bromide salt are 70° and 100°. The planarity of the SCN_2 moieties is quite good in all cases, with the maximum deviation from a least squares plane through these atoms (with the coordinates of sulfur weighted three times as heavily as those of the lighter atoms) being 0.02 Å. The two $-N(CH_3)_2$ groups of tetramethylthiourea are staggered with respect to one another, the angle between the two C – N – C planes being 52.0° in the chloride salt and 51.5° in the bromide salt.

With regard to the lack of success in synthesizing salts of the $[Te(tmtu)_4]^{2+}$ cation, the present work finds distances of 3.3 – 3.8 Å between methyl carbon atoms of the tetramethylthiourea ligand and nitrogen atoms of the thiourea ligand. This would indicate that an attempt to substitute tetramethylthiourea for thiourea would incur rather severe steric difficulties, and might thus be precluded on these grounds.

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