CONTRIBUTION FROM THE DEPARTMENTS OF CHEMISTRY OF THE UNIVERSITY OF CALIFORNIA,
LOS ANGELES,[1] CALIFORNIA 90024 AND DAVIS, CALIFORNIA 95616

The Crystal and Molecular Structure of 1-Thia-4-telluracyclohexane 4,4-Diiodide, $C_4H_8STeI_2$

BY CAROLYN KNOBLER,[2a] J. D. McCULLOUGH,[2a,b] AND HAKON HOPE[2c]

Received August 4, 1969

1-Thia-4-telluracyclohexane 4,4-diiodide forms dark purple needles with $a = 18.817$ (12) Å, $b = 9.728$ (8) Å, and $c = 21.746$ (12) Å. The space group is Pbca with $Z = 16$ so that there are two molecules of $C_4H_8STeI_2$ in the asymmetric unit. The intensities of 4296 unique counter-measured reflections were corrected for absorption and used in the structure determination. The phase problem was solved by use of Long's program and the structure was refined by use of full-matrix least-squares procedures to a conventional R index of 5.0% for the 2766 observed reflections. Both molecules have essentially the same structure with approximate mirror symmetry and with the six-membered ring in the chair conformation. The configuration about Te approximates a trigonal bipyramid with I atoms in axial positions and two C atoms plus an unshared electron pair equatorially distributed. The observed bonded distances (in Å) range as follows: Te–I, 2.851 (2) to 2.985 (2); Te–C, 2.13 (2) to 2.18 (2); S–C, 1.79 (3) to 1.88 (3); and C–C, 1.49 (4) to 1.54 (4). Among the bond angles, the more interesting are I–Te–I, 174.9 (1)° and 178.1 (1)°; C–Te–C, 100 (1) and 100 (1)°; C–S–C, 99 (1) and 100 (1)°; and the eight C–Te–I angles, which range from 87.4 (6) to 91.8 (6)°.

Introduction

A study of the structure of 1-thia-4-telluracyclohexane 4,4-diiodide is of interest for two reasons; one, the determination of the structure of the 1,4-thiatellurane ring, and two, a study of the heavy-atom bonding system. An earlier attempt to determine the structure of the parent compound, 1,4-thiatellurane, was complicated by the presence of a type of disorder which gives the molecule a pseudo center of symmetry.[3] The project was therefore set aside. Interest in the heavy-atom bonding systems in compounds such as R_2TeI_2 and $R_2Se \cdot I_2$ lies in the varying degrees of combination, through intermolecular bonding, of the axial I–M–I "molecular" type units with the linear M···I–I "complex" type. In both types, bonding systems consisting of nearly linear chains, –I–M–I–I–M–I–, have been found, and within these chains, the M–I and I–I bonded distances vary considerably from one compound to another.[4–7] This variability in bond length is probably due to tendencies toward weaker bonding and larger coordination numbers as the atomic numbers of the atoms increase.

Preliminary Study

Crystals of 1,4-thiatellurane 4,4-diiodide were prepared as described by McCullough[3] and specimens suitable for the X-ray studies were grown by slow evaporation of solutions in ethylene chloride. The crystals are dark purple needles with a metallic luster and are elongated on the b axis of the orthorhombic unit. The cell constants, based on λ Mo Kα_1 0.70926 Å, were found to be $a = 18.817$ (12) Å, $b = 9.728$ (8) Å, and $c = 21.746$ (12) Å at 23°. The systematic extinctions 0kl with k odd, h0l with l odd, and hk0 with h odd were noted and these correspond to the space group Pbca. The density was observed by flotation to be 3.15 (3) g cm^{-3} which compares favorably with the value 3.134 (5) g cm^{-3} calculated from the X-ray data with $Z = 16$. Thus the crystallographic asymmetric unit consists of two molecules of $C_4H_8STeI_2$.

The initial intensity data consisted of multiple-film Weissenberg photographs of the levels h0l through h7l and hk0 through hk2 prepared with Cu Kα radiation. The intensities were estimated visually and corrected for absorption ($\mu = 760$ cm^{-1} for Cu Kα) and for the usual geometric factors to give a set of 3765 F_o values. These were used as input to obtain a three-dimensional Patterson summation.[8] However, interpretation of the summation was not straightforward, so attention was turned to Long's sign prediction program. In this case 222 reflections with $|E| \geq 1.80$ were used. A three-dimensional Fourier summation based on the sign set with the highest consistency index, 0.993, showed all six heavy atoms. A set of structure factors calculated on the basis of two Te and four I atoms with isotropic B values of 3.5 Å^2 at this point showed an R index of 0.32.

A difference Fourier summation from which the six heavy atom contributions were subtracted showed the two sulfur atoms, but the carbon atoms were not clearly located until another difference map was prepared which was phased on the eight heaviest atoms. The R index at this stage, based on all atoms (except hydrogen) with isotropic B values of 3.5 Å^2, was 0.20. Two cycles of

---

[1] Contribution No. 2402.

[2] (a) University of California, Los Angeles; (b) author to whom correspondence should be sent; (c) University of California, Davis.

[3] J. D. McCullough, *Inorg. Chem.*, **4**, 862 (1965).

[4] G. Y. Chao and J. D. McCullough, *Acta Crystallogr.*, **14**, 490 (1961).

[5] G. Y. Chao and J. D. McCullough, *ibid.*, **15**, 887 (1962).

[6] H. Hope and J. D. McCullough, *ibid.*, **17**, 712 (1964).

[7] H. Maddox and J. D. McCullough, *Inorg. Chem.*, **5**, 522 (1966).

[8] Fourier summations were computed by use of UCLAFOUR written by Gantzel and Hope and the least-squares refinement was carried out by use of the full-matrix program ACA No. 317 (Modified) written by Gantzel, Sparks, and Trueblood. This program minimizes $\Sigma w(\Delta|F|)^2$ and the weights, w, were assigned by the method of E. W. Hughes, *J. Amer. Chem. Soc.*, **63**, 1737 (1941). The R index was defined as $\Sigma||F_o| - |F_c||/\Sigma|F_o|$, and the esd values for the parameters were obtained from the final least-squares inverse matrix. The phase problem was solved by use of Long's program, ACA (new) No. 2; thermal ellipsoid plots were prepared by use of Johnson's ORTEP routine and hydrogen positions were calculated by use of HPSON, written by Hope. The C–H distances were taken as 1.0 Å and the H–C–H angles as 109.5°.

TABLE I

ATOMIC POSITIONAL PARAMETERS IN $C_4H_8STeI_2$

(a) Nonhydrogen Atoms

Molecule A

	x	*y*	*z*
I(1)	0.23678 (6)[a]	0.2655 (2)	0.50188 (6)
I(2)	0.54532 (6)	0.2982 (1)	0.50917 (5)
Te	0.38928 (5)	0.2945 (1)	0.50384 (5)
S	0.4029 (3)	0.1425 (5)	0.3500 (2)
C(1)	0.3972 (11)	0.0790 (17)	0.4766 (10)
C(2)	0.3632 (10)	0.0449 (17)	0.4161 (9)
C(3)	0.3600 (10)	0.3069 (19)	0.3632 (9)
C(4)	0.3893 (11)	0.3883 (19)	0.4156 (9)

Molecule B

	x	*y*	*z*
I(1)	0.09675 (8)	−0.1167 (1)	0.15693 (6)
I(2)	0.10189 (9)	0.4828 (1)	0.16556 (7)
Te	0.10051 (6)	0.1901 (1)	0.15934 (5)
S	0.1875 (3)	0.1543 (7)	0.3083 (2)
C(1)	0.2117 (8)	0.1797 (20)	0.1814 (8)
C(2)	0.2330 (10)	0.2379 (25)	0.2448 (8)
C(3)	0.1023 (11)	0.2357 (24)	0.3019 (8)
C(4)	0.0547 (10)	0.1829 (18)	0.2502 (9)

(b) Calculated Hydrogen Positions

	Molecule A			Molecule B		
	x	*y*	*z*	*x*	*y*	*z*
H(1)	0.373	0.022	0.509	0.238	0.236	0.150
H(1)′	0.448	0.054	0.475	0.227	0.083	0.179
H(2)	0.311	0.068	0.418	0.223	0.337	0.246
H(2)′	0.369	−0.055	0.408	0.286	0.221	0.250
H(3)	0.309	0.289	0.372	0.110	0.336	0.294
H(3)′	0.365	0.363	0.325	0.076	0.223	0.341
H(4)	0.361	0.475	0.418	0.010	0.237	0.250
H(4)′	0.440	0.412	0.405	0.043	0.083	0.259

[a] Numbers in parentheses here and in succeeding tables are the standard deviations in the least significant digits.

TABLE II

ANISOTROPIC THERMAL PARAMETERS[a] IN Å²

Molecule A

Atom	B_{11}	B_{22}	B_{33}	B_{12}	B_{13}	B_{23}
I(1)	2.54 (4)	6.38 (8)	4.86 (6)	0.62 (5)	−0.25 (4)	−0.29 (5)
I(2)	2.60 (4)	3.45 (5)	3.85 (6)	0.19 (3)	−0.51 (3)	−0.38 (4)
Te	2.42 (4)	2.75 (4)	2.65 (4)	0.25 (3)	−0.50 (3)	−0.38 (3)
S	4.9 (3)	3.8 (2)	3.3 (2)	−0.3 (2)	0.7 (2)	−0.7 (2)
C(1)	4.6 (8)	1.1 (5)	6.2 (9)	−0.5 (6)	−0.9 (8)	−0.6 (6)
C(2)	4.0 (8)	1.9 (6)	4.1 (8)	0.8 (6)	0.2 (6)	0.1 (5)
C(3)	3.8 (8)	3.4 (8)	3.7 (8)	−0.7 (7)	−1.0 (6)	1.1 (6)
C(4)	4.9 (9)	2.6 (7)	4.2 (8)	−0.4 (7)	−1.2 (7)	0.3 (6)

Molecule B

	B_{11}	B_{22}	B_{33}	B_{12}	B_{13}	B_{23}
I(1)	5.79 (7)	2.65 (5)	4.40 (6)	−0.19 (4)	0.25 (5)	−0.42 (4)
I(2)	6.75 (7)	2.59 (5)	4.88 (6)	−0.13 (5)	−0.64 (6)	−0.07 (4)
Te	3.15 (4)	2.56 (4)	2.52 (4)	−0.03 (4)	−0.56 (3)	−0.08 (3)
S	5.1 (2)	7.3 (3)	3.2 (2)	−2.4 (2)	−1.4 (2)	2.2 (2)
C(1)	1.6 (6)	5.4 (9)	3.4 (7)	−0.3 (6)	−0.6 (5)	−1.2 (7)
C(2)	3.4 (8)	6.9 (9)	3.0 (7)	−1.6 (8)	−0.4 (6)	0.1 (8)
C(3)	5.0 (9)	5.6 (9)	2.4 (7)	−1.9 (8)	−0.2 (6)	0.1 (7)
C(4)	4.1 (8)	3.2 (7)	3.4 (7)	1.3 (7)	1.3 (6)	0.5 (6)

[a] The anisotropic temperature factor expression has the form $\exp[-(b_{11}h^2 + b_{22}k^2 + b_{33}l^2 + b_{12}hk + b_{13}hl + b_{23}kl)]$. The relationships between the tabulated B values and the b parameters above are given by $B_{11} = 4a^2b_{11}$, $B_{12} = 2abb_{12}$, etc.

full-matrix least-squares refinement were then computed. The isotropic thermal parameters for I, Te, and S atoms were permitted to refine but the B's were held fixed at 3.5 Å² for carbon. The R index dropped only slightly, to 0.19. While there was little doubt that the R index could have been further reduced by the introduction of anisotropic thermal parameters in further refinement, an automated diffractometer had become available and we decided to measure a new data set by use of molybdenum radiation. Refinement by use of the copper data was therefore terminated.

Molybdenum Data and Refinement

The crystal selected for the intensity measurements with molybdenum radiation was an elongated (0.3 mm) fragment with a cross section approximating a right triangle with legs of 0.09 and 0.12 mm. It was mounted with the long direction (the crystallographic b axis) along the φ axis of a Picker full-circle diffractometer. The cell dimensions quoted above were obtained from five axis reflections measured at both 2θ and -2θ, and all deviations from mean values were well below 0.010 Å. The intensities of all 4296 independent reflections with 2θ less than 52° were measured with the diffractometer in automatic mode. The Mo K radiation was filtered through Zr foil and counted with a scintillation detector. The 2θ–θ scan technique (scan speed 2°/min) was used with the scan range given by $[2\theta(\alpha_1) - 0.8°]$ to $[2\theta(\alpha_2) + 0.8°]$. Background counts (20 sec) were taken at each end of the scan range. The automatic attenuator mechanism was set to keep the count rate below ~10,000 counts/sec. The intensities of two check reflections were measured about four times a day. These intensities remained constant during the first half of the run, but showed a gradual decline during the second half. The decrease amounted to a maximum of 5% at the end of the run and was ignored in processing the data.

In order approximately to correct the intensity data for absorption ($\mu = 95\ \text{cm}^{-1}$ for Mo Kα), the variations in intensity of the 0k0 reflections as a function of φ were measured. The reflections 040, 060, and 0,10,0 gave the same φ dependence within ±1% while 020 showed a somewhat larger variation. Absorption corrections were applied to all reflections by use of the mean curve for 040, 060, and 0,10,0, with the maximum correction amounting to about 30%. Lorentz and polarization corrections were applied in the usual manner.

By a procedure related to one used by previous workers,[9] each recorded number of counts, N, was assigned an estimated standard deviation, $\sigma(N) = [N + (0.01N)^2]^{1/2}$. A total of 2766 reflections for which the net intensity was greater than twice its standard deviation were recorded as observed.

With the final parameters from the refinement with Cu data as a starting point, the refinement was resumed with the Mo data. The first two cycles of least-squares refinement were carried out isotropically and R decreased to 0.11. Next, anisotropic thermal parameters for I, Te, and S atoms were allowed to refine for two cylces (R = 0.053) and finally, the thermal parameters for carbon were allowed to vary anisotropically for two cycles, during which R decreased to 0.049.

---

(9) S. W. Peterson and H. A. Levy, *Acta Crystallogr.*, **10**, 70 (1957).

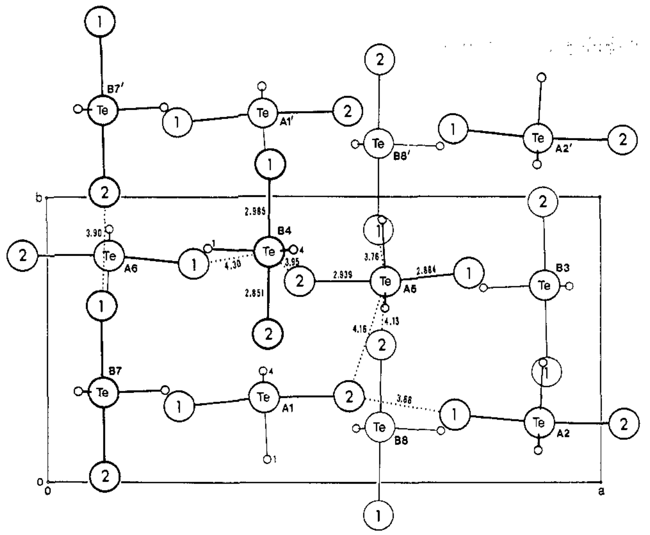

Figure 1.—Projection of a selected portion of the crystal structure of $C_4H_8STeI_2$ down the c axis. The labels A1, B8, etc., designate the crystallographically nonequivalent molecules A and B, and the eight equivalent positions of the space group Pbca: (1) x, y, z; (2) $\frac{1}{2} + x, \frac{1}{2} - y, 1 - z$; (3) $1 - x, \frac{1}{2} + y, \frac{1}{2} - z$; (4) $\frac{1}{2} - x, 1 - y, \frac{1}{2} + z$; (5) $1 - x, 1 - y, 1 - z$; (6) $\frac{1}{2} - x, \frac{1}{2} + y, z$; (7) $x, \frac{1}{2} - y, \frac{1}{2} + z$; (8) $\frac{1}{2} + x, y, \frac{1}{2} - z$. For purposes of clarity, the atoms S, C(2), C(3), and all hydrogen atoms are omitted.

At this point a three-dimensional difference Fourier summation was computed, both as a check on the refined structure and for possible location of the hydrogen atoms. The maximum fluctuations on this summation were ± 0.8 e Å^{-3} or ± 1.6 times the esd of the electron density, 0.5 e Å^{-3}. Thus, the anticipated diffraction effect of a hydrogen atom was about at the noise level, and while nine of the sixteen hydrogen atoms showed up rather clearly at reasonable positions and with maxima in the range 0.4–0.6 e Å^{-3}, information on others was less convincing. A set of hydrogen positions was computed and nine of the locations agreed reasonably well with the maxima mentioned above. Although attempts to refine the hydrogen positions with isotropic B values held constant at 6 Å^2 were unsuccessful, inclusion of the hydrogen atoms at the calculated parameters given in Table I(b) in a structure factor calculation did reduce R slightly, to 0.048.

A set of final structure factors for all measured reflections was calculated on the basis of the final positional and thermal parameters given in Tables I and II. The resulting values of F_c are listed with the respective F_o values in Table III. The value of R for these 4296 reflections, including 1530 designated as "unobserved," is 0.087.

The atomic scattering curve used for iodine was based on the I^0 values of Doyle and Turner.[10] These authors did not give a curve for tellurium so their values for Sb^0 and I^0 were averaged to give a curve for Te^0. The curve used for sulfur was that for S^0 given in Table 3.3.1A of the "International Tables for X-Ray Crystallography,"[11] that for carbon was based on the diamond values of McWeeny,[12] and the hydrogen curve was based on the bonded values of Stewart, Davidson, and Simpson.[13] The real part of the anomalous scat-

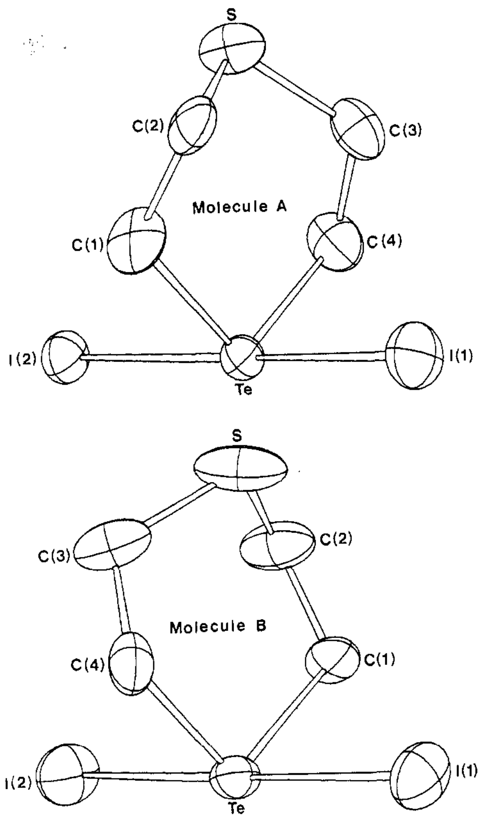

Figure 2.—ORTEP plots of the two independent molecules of $C_4H_8STeI_2$ at angles of about 45° with the respective I–Te–I axes and with the respective C–Te–C planes. The thermal ellipsoids are at the 50% probability level and the hydrogen atoms are omitted.

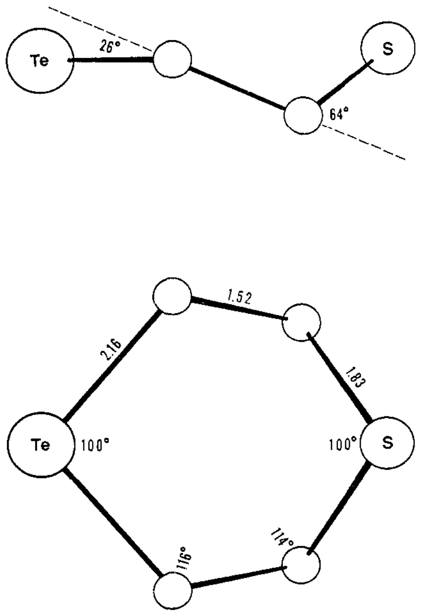

Figure 3.—Views of the structure of the 1,4-thiatellurane ring showing values for the chemically equivalent bond distances (in Å) and bond angles (in degrees), averaged over the two molecules in the asymmetric unit.

---

[10] P. A. Doyle and P. S. Turner, *Acta Crystallogr.*, **A24**, 392 (1968).

[11] "International Tables for X-Ray Crystallography," Vol. III, The Kynoch Press, Birmingham, England, 1962.

[12] R. McWeeny, *Acta Crystallogr.*, **7**, 180 (1954).

[13] R. F. Stewart, E. R. Davidson, and W. T. Simpson, *J. Chem. Phys.*, **42**, 3178 (1965).

TABLE III

OBSERVED AND CALCULATED STRUCTURE FACTORS[a]

H= 0, K= 0		
4	392	379
6	1665	2046
8	636	637
10	33*	119
12	1187	1236
14	507	506
16	94	22
18	486	475
20	384	366
22	51	-44
24	213	207
26	202	188
H= 1, K= 0		
4	441	437
6	133	134
8	545	-532
10	216	211
12	161	153
14	369	-368
16	130	134
18	84	79
20	229	-217
22	21*	13
24	35*	40
26	94	-90
H= 2, K= 0		
2	13*	-52
4	227	-218
6	271	271
8	14*	12
10	256	-250
12	171	166
14	30	17
16	196	-192
18	75	76
20	18*	3
22	111	-100
24	27*	15
26	20*	-3
H= 3, K= 0		
2	678	-701
4	770	783
6	249	242
8	637	-635
10	493	491
12	295	284
14	356	-357
16	253	249
18	247	236
20	230	-222
22	75	72
24	154	141
26	98	-96
H= 4, K= 0		
0	867	-893
2	456	441
4	768	781
6	650	-647
8	256	250
10	499	506
12	383	-383
14	61	-53
16	363	351
18	178	-178
20	99	-90
22	150	142
24	79	-84
26	105	-94
H= 5, K= 0		
2	81	-77
4	115	111
6	84	85
8	139	139
10	138	167
12	112	113
14	133	134
16	113	116
18	97	86
20	121	120
22	83	82
24	69	43
26	49	51
H= 6, K= 0		
0	1258	-1357
2	169	-158
4	46	-37
6	1005	-1071
8	339	-330
10	138	137
12	667	-708
14	274	-278
16	119	111
18	345	-346
20	212	-211
22	78	68
24	155	-152
26	122	-109
H= 7, K= 0		
2	701	703
4	531	-519
6	21*	31
8	715	723
10	169	-165
12	22*	31
14	517	524
16	32	15
18	18*	17
20	339	332
22	106	100
24	20*	-10
26	178	172
H= 8, K= 0		
0	499	488
2	247	228
4	76	75
6	394	388
8	223	229
10	33	26
12	319	319
14	195	201
16	27*	-6
18	183	182
20	112	111
22	20*	21
24	81	97
26	78	67
H= 9, K= 0		
2	348	335
4	207	-200
6	85	-83
8	337	337
10	141	-140
12	71	-75
14	271	269
16	49	-56
18	62	-45
20	152	149
22	45	-33
26	38	-18
H= 10, K= 0		
0	522	506
2	515	-508
4	588	-596
6	445	451
8	308	-308
10	435	-445
12	244	240
14	32	-32
16	307	-302
18	133	132
20	70	74
22	157	-144
24	71	55
H= 11, K= 0		
2	265	-256
4	219	210
6	65	69
8	281	-280
10	112	110
12	65	66
14	199	-203
16	51	43
18	36	32
20	131	-128
22	48	-17
24	32*	8
H= 12, K= 0		
0	33*	-48
2	267	-258
4	280	-286
6	18*	-1
8	160	-160
10	224	-230
12	28*	-12
14	78	-74
16	126	-128
18	19*	14
20	19*	-15
22	49	-51
H= 13, K= 0		
2	346	-337
4	241	233
6	53	68
8	323	-328
10	132	130
12	86	90
14	269	-272
16	54	41
18	71	63
20	171	-167
22	20*	3
H= 14, K= 0		
0	715	-707
2	239	-224
4	174	-167
6	601	-615
8	227	-231
10	88	-83
12	396	-397
14	195	-202
16	23*	-11
18	204	-202
20	138	-149
22	48	16
H= 15, K= 0		
2	25*	-32
4	17*	21
6	54	-59
8	18*	-18
10	18*	11
12	64	-66
14	22*	-11
16	21*	-8
18	48	-35
20	20*	-3
H= 16, K= 0		
0	214	-209
2	133	129
4	191	193
6	196	-194
8	68	60
10	196	195
12	123	-114
14	30*	17
16	145	149
18	67	-62
20	20*	-1
H= 17, K= 0		
2	205	200
4	213	-208
6	60	-71
8	127	134
10	165	-162
12	101	-107
14	73	77
16	88	-86
18	98	-93
H= 18, K= 0		
0	242	226
2	144	142
4	139	136
6	199	199
8	140	146
10	73	78
12	170	169
14	104	101
16	60	53
18	95	100
H= 19, K= 0		
2	53	58
4	109	-105
6	69	-65
8	22*	19
10	132	-127
12	94	-97
14	21*	-4
16	111	-111
H= 20, K= 0		
0	282	274
2	28*	27
4	23*	-5
6	242	234
8	57	58
10	30*	-28
12	157	155
14	60	67
H= 21, K= 0		
2	82	-76
4	43	44
6	21*	2
8	89	-87
10	21*	13
12	21*	-0
H= 22, K= 0		
0	76	76
2	25*	0
4	21*	-4
6	51	52
8	21*	6
10	23*	-21
H= 23, K= 0		
2	62	-56
4	54	55
6	37	26
H= 1, K= 1		
1	93	-97
2	136	-131
3	224	-212
4	151	147
5	221	-214
6	238	232
7	18*	7
8	19*	5
9	157	-152
10	235	230
11	233	-228
12	250	251
13	34	35
14	43	43
15	62	-66
16	191	190
17	165	-166
18	198	192
19	30*	25
20	68	66
21	19*	-11
22	132	127
23	92	-91
24	129	119
25	21*	9
26	50	45
27	22*	10
H= 2, K= 1		
0	35	-14
1	36	-38
2	315	302
3	11*	8
4	24	27
5	40	41
6	22	-12
7	46	42
8	243	229
9	60	-60
10	79	78
11	29	20
12	17*	14
13	69	67
14	170	170
15	67	-68
16	94	88
17	17*	3
18	17*	20
19	74	67
20	61	60
21	61	-68
22	128	124
23	22*	9
24	19*	18
25	50	43
26	20*	25
27	43	-39
H= 3, K= 1		
1	51	-48
2	118	112
3	91	-85
4	54	54
5	43	43
6	46	-44
7	59	-54
8	154	147
9	27	-26
10	59	57
11	30	33
12	17*	-15
13	55	-59
14	140	138
15	15*	9
16	39	35
17	26*	35
18	17*	14
19	28*	-17
20	70	65
21	20*	5
22	18*	8
23	19*	18
24	24*	10
25	20*	2
26	20*	22
27	22*	-2
H= 4, K= 1		
0	22	-20
1	31	28
2	85	-82
3	63	-64
4	84	-77
5	30	-25
6	11*	-11
7	78	72
8	79	-75
9	113	-115
10	30	34
11	48	-49
12	58	-56
13	14*	-5
14	14*	22
15	97	-105
16	54	58
17	21*	22
18	46	-40
19	21*	1
20	37	43
21	58	-61
22	75	70
23	19*	8
24	20*	-20
25	28*	-2
26	40	39
27	34*	-29
H= 5, K= 1		
1	16*	-14
2	207	196
3	180	173
4	154	-149
5	108	73
6	68	-62
7	69	-66
8	121	118
9	89	91
10	132	-136
11	175	174
12	84	-85
13	45	-45
14	58	57
15	21*	16
16	70	-61
17	168	164
18	106	-107
19	32	-36
20	18*	14
21	18*	-9
22	33	-40
23	119	112
24	92	-88
25	20*	-17
26	20*	-0
H= 6, K= 1		
0	804	-813
1	106	-98
2	690	-679
3	34	20
4	721	-722
5	35	-26
6	549	-551
7	109	-106
8	554	-553
9	23	14
10	497	-502
11	67	-62
12	354	-357
13	101	-101
14	301	-302
15	16*	2
16	322	-327
17	63	-63
18	127	-126
19	56	-58
20	154	-148
21	18*	-11
22	151	-154
23	25*	-32
24	53	-60
25	38	-39
26	46	-44
H= 7, K= 1		
1	32	-28
2	13*	-1
3	91	90
4	16*	-22
5	12*	10
6	13*	2
7	102	-93
8	24	24
9	66	62
10	37	-35
11	61	61
12	15*	-0
13	61	-58
14	37	31
15	17*	19
16	31	-44
17	22*	34
18	17*	3
19	27*	-33
20	38	20
21	19*	0
22	28*	-16
23	28*	23
24	24*	1
25	20*	-8
26	21*	8
H= 8, K= 1		
0	121	-115
1	24	17
2	306	-290
3	23	28
4	225	-217
5	69	-65
6	106	-101
7	54	-47
8	224	-221
9	14*	3
10	155	-152
11	81	-78
12	53	-51
13	69	-67
14	128	-132
15	41	46
16	100	-99
17	65	-61
18	17*	-3
19	71	-66
20	40	-48
21	32	31
22	77	-80
23	43	-37
24	19*	19
25	44	-40
26	20*	-10
H= 9, K= 1		
1	52	49
2	186	-177
3	33	-32
4	91	88
5	13*	4
6	14*	-15
7	72	75
8	176	-178
9	29	-14
10	32	30
11	66	-62
12	15*	-5
13	48	42
14	152	-145
15	16*	2
16	19*	-10
17	69	-67
18	17*	6
19	29*	21
20	67	-62
21	18*	9
22	32	-22
23	64	-59
24	20*	28
25	20*	4
H= 10, K= 1		
0	116	-121
1	56	47
2	90	-85
3	14*	1
4	71	-74
5	17*	-38
6	96	-93
7	29	27
8	101	-104
9	16*	-1
10	18*	4
11	25*	-26
12	51	-51
13	22*	15
14	42	-44
15	20*	11
16	32	17
17	25*	-13
18	21*	-9
19	18*	-0
20	18*	-17
21	18*	14
22	25*	24
23	24*	-6
24	19*	13
25	20*	-0
H= 11, K= 1		
1	84	84
2	57	-56
3	27	-25
4	18*	-24
5	15*	9
6	30	-10
7	146	151
8	148	-151
9	31	-22
10	40	-40
11	64	-70
12	16*	-26
13	104	110
14	158	-159
15	17*	-8
16	27*	-33
17	59	-59
18	18*	-18
19	59	62
20	117	-119
21	19*	-3
22	19*	-20
23	37	-45
24	23*	-15
H= 12, K= 1		
0	332	317
1	40	-20
2	465	463
3	21*	-13
4	451	454
5	46	29
6	257	254
7	31	17
8	401	409
9	28*	12
10	307	309
11	41	29
12	233	232
13	40	38
14	229	228
15	33	-30
16	222	229
17	18*	24
18	123	123
19	48	47
20	121	118
21	20*	-22
22	139	139
23	28*	19
H= 13, K= 1		
1	134	132
2	17*	4
3	70	65
4	61	-70
5	129	125
6	131	-136
7	82	84
8	57	-51
9	66	63
10	142	-139
11	97	98
12	180	-179
13	65	57
14	70	-69
15	52	49
16	130	-128
17	40	44
18	151	-150
19	29*	28
20	65	-72
21	20*	25
22	93	-89
23	24*	23
H= 14, K= 1		
0	109	-91
1	24*	-15
2	92	-90
3	39	-22
4	91	-87
5	53	49
6	87	-88
7	28*	1
8	64	-65
9	17*	-29
10	66	-59
11	59	56
12	99	-102
13	33	6
14	38	-34
15	39	-33
16	33	-32
17	37	44
18	81	-81
19	28*	3
20	27*	-14
21	20*	-17
22	26*	-12
H= 15, K= 1		
1	17*	-5
2	69	79
3	85	88
4	92	-86
5	29*	19
6	38	-39
7	36	-41
8	58	58
9	56	54
10	71	-69
11	70	67
12	64	-70
13	40	-32
14	51	49
15	33	19
16	51	-51
17	52	56
18	70	-66
19	31*	-31
20	26*	25
21	30*	2
H= 16, K= 1		
0	214	217
1	18*	-4
2	103	99
3	19*	16
4	95	95
5	18*	17
6	162	162
7	18*	-13
8	105	112
9	30	13
10	24*	22
11	18*	-0
12	101	100
13	19*	7
14	60	51
15	21*	24
16	20*	-2
17	19*	8
18	40	22
19	19*	-5
20	32*	25
H= 17, K= 1		
1	52	-53
2	18*	22
3	26*	27
4	18*	-21
5	19*	-25
6	33	15
7	43	-49
8	41	24
9	18*	15
10	18*	-8
11	26*	-15
12	37	31
13	35	-47
14	19*	16
15	19*	-0
16	19*	3
17	19*	1
18	36	31
19	20*	-24
H= 18, K= 1		
0	38	17
1	33	25
2	35	-39
3	19*	17
4	53	-50
5	36	-22
6	19*	25
7	29*	19
8	46	-52
9	44	37
10	58	-50
11	19*	-15
12	24*	10
13	19*	17
14	42	-37
15	36	43
16	69	-65
17	20*	-8
18	20*	7
H= 19, K= 1		
1	39	-45
2	48	-59
3	79	-82
4	78	81
5	48	-41
6	45	41
7	22*	-27
8	20*	-24
9	67	-63
10	77	83
11	59	-53
12	64	61
13	20*	-26
14	22*	6
15	23*	-34
16	63	56
H= 20, K= 1		
0	246	231
1	41	15
2	261	251
3	26*	-0
4	266	262
5	43	-8
6	206	203
7	50	27
8	193	191
9	32*	21
10	211	205
11	34*	10
12	157	153
13	40	18
14	105	115
15	21*	16
H= 21, K= 1		
1	21*	15
2	27*	-27
3	21*	-30
4	21*	24
5	29*	-11
6	21*	27
7	21*	26
8	21*	-28
9	21*	-26
10	27*	20
11	31*	-16
12	31*	35
13	45	35
H= 22, K= 1		
0	86	-91
1	21*	-15
2	24*	-18
3	21*	-0
4	22*	-26
5	21*	15
6	72	-72
7	23*	-1
8	43	-32
9	44	-7
10	31*	-4
H= 23, K= 1		
1	25*	-3
2	44	23
3	32*	-16
4	22*	5
5	21*	-4
6	21*	4
7	22*	-9
H= 0, K= 2		
0	915	-993
1	66	-65
2	776	-812
3	69	63
4	889	-945
5	191	-172
6	746	-741
7	122	-122
8	780	-791
9	25*	-51
10	545	-550
11	167	-184
12	432	-437
13	72	-107
14	458	-454
15	25*	-56
16	345	-336
17	146	-148
18	204	-202
19	22*	-49
20	277	-278
21	94	-93
22	108	-108
23	56	-63
24	93	-88
25	37	-30
26	128	-121
27	62	-63
H= 1, K= 2		
1	15*	-23
2	81	-73
3	303	-292
4	176	167
5	22	-18
6	12*	6
7	43	-43
8	35	-30
9	175	-173
10	82	81
11	90	-87
12	15*	-5
13	53	-56
14	69	60
15	54	-58
16	61	58
17	103	-99
18	17*	6
19	38	-38
20	35	38
21	19*	-15
22	42	40
23	71	-67
24	20*	2
25	36	-26
26	39	34
27	21*	-7
H= 2, K= 2		
0	151	129
1	95	88
2	16*	-17
3	39	-35
4	49	43
5	123	-115
6	83	78
7	33	32
8	28	11
9	140	-137
10	42	42
11	54	-53
12	56	56
13	50	-53
14	28	-5
15	69	-71
16	64	65
17	34	-40
18	28*	30
19	67	-59
20	17*	9
21	33	-41
22	53	46
23	19*	-22
24	37	19
25	44	-39
26	20*	7
27	25*	-13
H= 3, K= 2		
1	228	207
2	153	-145
3	167	-159
4	158	148
5	114	103
6	86	-81
7	247	238
8	119	-117
9	111	-111
10	22	15
11	53	-49
12	81	-89
13	110	110
14	51	-54
15	47	-45
16	16*	6
17	63	-56
18	86	-85
19	22*	13
20	29	-15
21	18*	-5
22	18*	1
23	43	-42
24	40	-48
25	41	-35
26	20*	2
27	20*	6
H= 4, K= 2		
0	329	-287
1	106	-98
2	126	-121
3	11*	-3
4	168	-161
5	54	51
6	123	-122
7	21	-26
8	51	-51
9	12*	8
10	77	-75
11	18*	28
12	132	-134
13	17*	-20
14	48	47
15	17*	11
16	45	-44
17	16*	-4
18	24*	-21
19	16*	-2
20	64	61
21	18*	20
22	18*	-15
23	18*	-0
24	22*	-4
25	19*	-6
26	43	54
H= 5, K= 2		
1	198	194
2	14*	-7
3	157	153
4	122	-115
5	127	124
6	72	-73
7	192	193
8	63	-63
9	107	110
10	93	-92
11	46	50
12	97	-101
13	115	116
14	103	-106
15	58	61
16	104	-107
17	21*	24
18	70	-74
19	54	48
20	76	-77
21	27*	21
22	60	-61
23	19*	10
24	51	-52
25	20*	9
26	45	-41
H= 6, K= 2		
0	427	392
1	83	-79
2	428	416
3	14*	6
4	427	415
5	76	71
6	288	285
7	49	-43
8	386	388
9	71	72
10	248	249
11	36	34
12	238	242
13	15*	1
14	257	260
15	22*	24
16	132	135
17	17*	12
18	126	128
19	36	26
20	166	166
21	29*	21
22	50	44
23	19*	-0
24	73	75
25	20*	21
26	90	80
H= 7, K= 2		
1	289	277
2	41	8
3	431	423
4	169	-159
5	319	318
6	88	-91
7	139	135
8	107	-107
9	317	319
10	201	-200
11	277	281
12	123	-122
13	93	95
14	160	-154
15	172	179
16	178	-176
17	151	149
18	104	-100
19	69	68
20	118	-117
21	66	73
22	131	-128
23	60	61
24	59	-49
25	64	58
26	80	-77
H= 8, K= 2		
0	193	-181
1	72	70
2	253	-240
3	33	-31
4	233	-227
5	13*	15
6	186	-186
7	35	38
8	241	-241
9	39	-44
10	146	-149
11	39	41
12	125	-125
13	24*	20
14	173	-172
15	33	-34
16	104	-101
17	46	50
18	94	-94
19	22*	-6
20	108	-108
21	18*	-11
22	56	-56
23	19*	13
24	44	-49
25	19*	1
H= 9, K= 2		
1	56	-48
2	34	24
3	197	192
4	52	-46
5	14*	-15
6	26	6
7	48	-46
8	54	-53
9	86	82
10	68	-65
11	51	49
12	15*	-2
13	15*	-15
14	37	-42
15	16*	-11
16	39	-35
17	56	49
18	17*	2
19	23*	-3
20	45	-45
21	18*	-35
22	32	-14
23	43	34
24	19*	1
25	27*	0
H= 10, K= 2		
0	201	186
1	29	-6
2	178	168
3	17*	24
4	187	187
5	38	39
6	147	148
7	14*	-8
8	123	125
9	42	50
10	108	103
11	15*	-2
12	93	88
13	52	56
14	19*	5
15	36	32
16	70	73
17	27*	22
18	26*	22
19	34	36
20	47	-39
21	23*	3
22	21*	27
23	20*	19
24	19*	-2
H= 11, K= 2		
1	79	-71
2	29	-6
3	100	-101
4	43	36
5	43	-53
6	19*	-4
7	64	-67
8	30	23
9	66	-71
10	53	43
11	71	-70
12	16*	3
13	73	-76
14	36	36
15	49	-41
16	45	46
17	47	-52
18	18*	11
19	46	-46
20	27*	33
21	43	-32
22	37	41
23	35	-34
24	22*	13
H= 12, K= 2		
0	127	127
1	45	43
2	136	135
3	27	16
4	139	139
5	32	16
6	117	117
7	69	63
8	103	105
9	60	60
10	93	94
11	51	48
12	55	55
13	64	62
14	47	46
15	69	66
16	56	57
17	54	53
18	18*	18
19	52	38
20	29*	13
21	60	57
22	20*	24
23	43	37
H= 13, K= 2		
1	69	-67
2	19*	-7
3	206	-206
4	46	39
5	81	-86
6	17*	-12
7	46	-41
8	57	55
9	143	-137
10	69	66
11	102	-101
12	26*	-14
13	49	-58
14	65	63
15	59	-51
16	46	42
17	59	-68
18	26*	-6
19	44	-51
20	50	55
21	31*	-7
22	44	33
H= 14, K= 2		
0	320	314
1	40	35
2	300	292
3	40	13
4	269	267
5	17*	-2
6	270	267
7	66	58
8	246	241
9	68	68
10	189	198
11	35	34
12	186	185
13	44	40
14	184	182
15	60	59
16	93	97
17	29*	33
18	95	96
19	20*	27
20	114	113
21	60	60
22	46	37
H= 15, K= 2		
1	17*	17
2	18*	18
3	17*	-1
4	18*	-10
5	25*	-25
6	36	31
7	42	44
8	33	19
9	17*	1
10	17*	-5
11	17*	-20
12	37	36
13	64	63
14	18*	16
15	20*	7
16	18*	-0
17	19*	-10
18	19*	18
19	33*	38
20	20*	9
21	20*	17
H= 16, K= 2		
0	23*	-9
1	18*	-15
2	36	-35
3	32	14
4	64	-55
5	17*	-2
6	21*	-9
7	28*	4
8	32	-26
9	28*	16
10	57	-54
11	18*	-11
12	18*	-6
13	18*	8
14	18*	-8
15	19*	14
16	49	-54
17	38	-22
18	26*	-3
19	20*	15
20	24*	-4
H= 17, K= 2		
1	24*	-32
2	31	-12
3	46	-49
4	36	35
5	27*	-17
6	46	42
7	38	-45
8	18*	-2
9	31	-25
10	18*	32
11	37	11
12	66	60
13	18*	-10
14	19*	11
15	22*	-6
16	25*	29
17	23*	6
18	49	50
19	20*	13
H= 18, K= 2		
0	146	-147
1	19*	-17
2	129	-126
3	31*	-10
4	131	-127
5	19*	14
6	118	-117
7	37	-22
8	122	-120
9	55	-54
10	87	-92
11	24*	6
12	103	-104
13	20*	-24
14	87	-88
15	25*	-37
16	72	-63
17	30*	-7
H= 19, K= 2		
1	91	-90
2	21*	3
3	52	-50
4	44	37
5	65	-67
6	34*	43
7	72	-72
8	21*	36
9	39	-47
10	71	69
11	33*	-37
12	61	66
13	55	-47
14	45	39
15	38	-43
16	70	68
H= 20, K= 2		
0	112	-102
1	42	-26
2	64	-60
3	23*	-4
4	57	-45
5	22*	8
6	99	-91
7	23*	-26
8	75	-62
9	28*	-27
10	37	-27
11	21*	6
12	58	-64
13	27*	-22
14	53	-56
H= 21, K= 2		
1	69	-73
2	21*	22
3	36	-35
4	21*	-3
5	63	-55
6	20*	6
7	61	-63
8	46	39
9	21*	-31
10	33*	18
11	33*	-44
12	21*	11
H= 22, K= 2		
0	36*	-33
1	21*	-2
2	21*	-10
3	21*	-4
4	30*	-14
5	21*	-13
6	21*	-24
7	22*	-9
8	21*	-10
9	20*	0
10	21*	4
H= 23, K= 2		
1	22*	25
2	21*	13
3	31*	21
4	21*	-9
5	33*	24
6	27*	-13
H= 1, K= 3		
1	104	97
2	123	122
3	972	1061
4	242	-235
5	183	181
6	197	-190
7	90	-84
8	101	95
9	762	769
10	152	-155
11	237	231
12	186	-232
13	24*	-117
14	28*	1
15	434	432
16	96	-114
17	170	166
18	179	-178
19	106	-99
20	20*	-13
21	200	189
22	47	-47
23	117	108
24	118	-110
25	60	-49
26	21*	-26
H= 2, K= 3		
0	375	360
1	700	706
2	137	-132
3	62	61
4	264	-261
5	575	-576
6	166	164
7	457	458
8	53	-52
9	98	94
10	254	-258
11	414	-409
12	95	95
13	252	255
14	16*	25
15	131	123
16	209	-209
17	229	-221
18	22*	-27
19	75	70
20	21*	31
21	94	101
22	112	-118
23	134	-132
24	33*	-30
25	20*	9
26	23*	-22
H= 3, K= 3		
1	157	145
2	58	-60
3	130	-121
4	59	57
5	104	97
6	12*	2
7	218	217
8	99	-99
9	146	-146
10	35	-38
11	20*	1
12	16*	1
13	154	153
14	50	-49
15	122	-124
16	43	-29
17	25*	-16
18	17*	7
19	81	82
20	20*	-37
21	70	-73
22	20*	-29
23	33*	-30
24	20*	12
25	27*	16
26	25*	-12
H= 4, K= 3		
0	277	269
1	282	270
2	73	-71
3	63	61
4	140	-129
5	221	-214
6	182	178
7	228	227
8	13*	-2
9	201	201
10	137	-134
11	217	-213
12	43	46
13	211	215
14	26*	37
15	163	159
16	122	-120
17	122	-122
18	17*	-18
19	120	121
20	20*	35
21	113	111
22	83	-82
23	64	-65
24	20*	-24
25	51	60
26	21*	14
H= 5, K= 3		
1	201	194
2	152	-147
3	910	-946
4	169	160
5	88	76
6	159	153
7	254	251
8	186	-184
9	654	-672
10	98	96
11	98	-92
12	183	174
13	190	186
14	89	-99
15	361	-366
16	51	62
17	145	-146
18	127	130
19	134	127
20	42	-45
21	181	-170
22	20*	17
23	141	-133
24	77	79
25	73	63
26	21*	7
H= 6, K= 3		
0	294	277
1	247	-232
2	472	473
3	50	-46
4	523	513
5	387	377
6	284	280
7	83	-80
8	368	367
9	15*	12
10	347	354
11	361	363
12	193	200
13	16*	19
14	155	152
15	17*	-5
16	242	240
17	270	269
18	120	124
19	44	44
20	57	56
21	22*	28
24	53	52
25	44	46
H= 7, K= 3		
1	108	106
2	100	-93
3	235	-234
4	64	63
5	27	20
6	14*	16
7	116	112
8	59	-61
9	161	-163
10	45	43
11	25*	3
12	33	34
13	96	93
14	61	-59
15	85	-84
16	17*	1
17	30*	-7
18	38	28
19	51	42
20	39	-29
21	41	-34
22	20*	-6
23	20*	3
24	37	22
25	35	20
H= 8, K= 3		
0	200	-193
1	408	-387
2	178	173
3	24*	-1
4	240	235
5	449	452
6	128	-123
7	256	-261
8	33	40
9	15*	5
10	228	232
11	382	381
12	60	-60
13	101	-103
14	17*	-24
15	23*	-25
16	153	148
17	281	272
18	19*	-1
19	18*	-15
20	52	-50
21	45	-31
22	81	79
23	161	152
24	24*	7
25	23*	21
H= 9, K= 3		
1	259	-256
2	109	107
3	446	441
4	81	-76
5	169	-163
6	32	-35
7	271	-270
8	143	139
9	329	331
10	16*	-6
11	27*	-21
12	41	-47
13	188	-183
14	99	100
15	193	196
16	18*	4
17	50	50
18	25*	-35
19	105	-99
20	53	54
21	100	94
22	26*	21
23	79	74
24	35	-31
H= 10, K= 3		
0	81	75
1	15*	-2
2	104	107
3	37	34
4	125	122
5	15*	-10
6	19*	27
7	16*	-15
8	63	63
9	29	34
10	89	84
11	16*	-19
12	32	36
13	22*	-12
14	23*	22
15	36	33
16	39	38
17	17*	-13
18	18*	-3
19	22*	-11
20	19*	2
21	18*	-0
22	26*	4
23	20*	-9
24	20*	2
H= 11, K= 3		
1	279	-276
2	132	130
3	240	231
4	63	-65
5	142	-139
6	16*	-18
7	303	-304
8	141	141
9	197	192
10	17*	-19
11	29*	-34
12	18*	-23
13	233	-233
14	123	120
15	139	131
16	36	31
17	20*	23
18	19*	-27
19	122	-122
20	81	77
21	86	80
22	30*	28
23	37	28
H= 12, K= 3		
0	146	-141
1	287	280
2	324	-313
3	18*	5
4	379	-379
5	306	-301
6	123	-121
7	215	212
8	231	-230
9	18*	2
10	303	-308
11	237	-228
12	118	-125
13	84	80
14	110	-110
15	38	39
16	218	-219
17	177	-168
18	85	-85
19	19*	7
20	56	-53
21	33*	41
22	120	-111
23	102	-97
H= 13, K= 3		
1	238	-227
2	20*	16
3	359	-348
4	66	62
5	250	-248
6	67	66
7	144	-142
8	62	65
9	283	-280
10	87	86
11	191	-199
12	100	93
13	68	-71
14	98	90
15	175	-181
16	82	80
17	108	-113
18	90	90
19	40	-31
20	71	63
21	92	-88
22	55	52
H= 14, K= 3		
0	219	219
1	91	91
2	39	44
3	19*	12
4	37	35
5	140	-136
6	182	181
7	77	78
8	87	87
9	30*	15
10	33	2
11	124	-123
12	107	108
13	51	46
14	77	77
15	19*	17
16	20*	2
17	105	-101
18	58	52
19	24*	35
20	65	66
21	20*	9
H= 15, K= 3		
1	76	74
2	76	-70
3	355	-340
4	70	60
5	37	9
6	53	54
7	102	102
8	62	-63
9	249	-249
10	49	50
11	43	-42
12	76	75
13	106	105
14	59	-55
15	148	-143
16	41	31
17	60	-57
18	46	51
19	83	73
20	26*	-24
H= 16, K= 3		
0	172	-169
1	116	-105
2	88	-86
3	24*	-18
4	79	-84
5	83	82
6	118	-123
7	101	-91
8	84	-85
9	61	-66
10	39	-35
11	66	69
12	70	-69
13	78	-71
14	46	-48
15	52	-62
16	20*	-5
17	20*	37
18	20*	-12
19	34*	-27
H= 17, K= 3		
1	83	87
2	39	-43
3	40	-22
4	35	30
5	78	85
6	19*	7
7	79	76
8	31*	-40
9	19*	-10
10	24*	15
11	70	65
12	19*	5
13	54	59
14	25*	-32
15	20*	6
16	20*	-7
17	53	40
18	20*	1
H= 18, K= 3		
0	40	-42
1	117	-120
2	64	62
3	21*	-30
4	93	94
5	100	97
6	39	-41
7	127	-123
8	48	43
9	65	-70
10	88	87
11	55	61
12	20*	-0
13	99	-100
14	25*	15
15	78	-78
16	76	79
17	45	37
H= 19, K= 3		
1	67	70
2	35*	23
3	280	275
4	50	-38
5	89	87
6	40	-38
7	49	51
8	27*	7
9	213	214
10	45	-48
11	93	89
12	57	-53
13	38	29
14	31*	-7
15	126	128
H= 20, K= 3		
0	197	-188
1	22*	-9
2	176	-170
3	23*	-11
4	168	-161
5	29*	-28
6	174	-164
7	35*	-31
8	144	-146
9	39	-21
10	114	-115
11	42	-47
12	120	-121
13	57	-41
H= 21, K= 3		
1	22*	-26
2	23*	35
3	85	82
4	28*	-33
5	21*	-8
6	21*	-14
7	53	-50
8	29*	30
9	79	69
10	21*	-18
11	21*	6
H= 22, K= 3		
0	95	83
1	76	70
2	26*	30
3	22*	0
4	30*	22
5	65	-65
6	72	66
7	49	39
8	33*	41
H= 23, K= 3		
1	31*	29
2	22*	-7
3	22*	-1
H= 0, K= 4		
0	367	363
1	518	512
2	442	444
3	46	44
4	526	530
5	353	-346
6	345	336
7	441	434
8	296	293
9	235	239
10	378	371
11	193	-190
12	289	290
13	313	311
14	95	89
15	249	246
16	236	229
17	20*	-41
18	199	193
19	152	143
20	21*	13
21	237	226
22	91	94
23	21*	3
24	113	104
25	68	59

TABLE III (*Continued*)

H= 1, K= 4		
1	368	354
2	69	-67
3	57	-51
4	51	52
5	237	224
6	74	-71
7	352	342
8	26	-33
9	47	-32
10	25	19
11	133	124
12	78	-75
13	274	271
14	18*	-28
15	26*	-15
16	18*	-4
17	66	67
18	42	-54
19	164	161
20	21*	-19
21	19*	3
22	20*	-12
23	43	37
24	22*	-24
25	93	89
26	22*	-25
H= 2, K= 4		
0	165	-148
1	122	120
2	140	-135
3	73	67
4	84	-78
5	58	-55
6	101	-94
7	113	110
8	178	-177
9	153	154
10	14*	-4
11	25	-29
12	96	-103
13	128	120
14	105	-108
15	142	143
16	28*	-17
17	17*	7
18	32	-44
19	75	78
20	22*	-64
21	91	97
22	26*	-21
23	19*	7
24	20*	-21
25	46	48
26	30*	-25
H= 3, K= 4		
1	186	172
2	26	-19
3	435	-428
4	20*	24
5	84	84
6	19*	6
7	218	213
8	13*	0
9	308	-309
10	85	86
11	14*	17
12	24*	-21
13	193	198
14	16*	-3
15	157	-154
16	69	75
17	17*	-10
18	37	-29
19	157	156
20	19*	4
21	50	-51
22	46	54
23	20*	-9
24	21*	-33
25	113	105
H= 4, K= 4		
0	187	174
1	294	-287
2	156	149
3	32	-27
4	84	79
5	340	337
6	100	98
7	211	-209
8	187	187
9	82	-82
10	16*	-7
11	249	253
12	56	57
13	86	-89
14	128	124
15	108	-111
16	17*	-10
17	159	159
18	18*	-13
19	31	-32
20	70	69
21	105	-103
22	19*	-5
23	62	64
24	22*	-23
25	21*	1
H= 5, K= 4		
1	254	-249
2	46	41
3	222	-226
4	22*	-16
5	165	-167
6	29	29
7	210	-206
8	61	63
9	164	-166
10	15*	19
11	109	-109
12	34	35
13	127	-131
14	48	44
15	86	-88
16	33	35
17	34	-41
18	37	20
19	42	-50
20	42	36
21	35	-29
22	20*	26
23	29*	-20
24	26*	10
25	20*	-13
H= 6, K= 4		
0	194	-189
1	299	-287
2	202	-196
3	58	-60
4	327	-323
5	271	273
6	177	-179
7	166	-170
8	103	-104
9	130	-138
10	270	-272
11	220	224
12	135	-135
13	115	-113
14	38	-23
15	136	-138
16	173	-180
17	119	116
18	104	-99
19	48	-48
20	19*	-12
21	98	-101
22	61	-65
23	56	57
24	71	-64
25	38	-26
H= 7, K= 4		
1	681	-680
2	61	50
3	141	-138
4	41	37
5	562	-573
6	51	50
7	586	-603
8	99	98
9	110	-107
10	37	31
11	339	-347
12	91	84
13	409	-416
14	122	123
15	69	-74
16	23*	19
17	150	-151
18	88	95
19	238	-243
20	63	68
21	50	-47
22	20*	11
23	44	-39
24	67	66
H= 8, K= 4		
0	252	248
1	51	46
2	114	112
3	23*	19
4	163	160
5	110	-106
6	192	194
7	40	32
8	108	107
9	38	36
10	131	132
11	99	-99
12	122	123
13	17*	0
14	79	78
15	47	47
16	91	92
17	79	-82
18	58	62
19	29*	8
20	63	65
21	34	37
22	37	36
23	25*	-32
24	33*	36
H= 9, K= 4		
1	128	-126
2	27	8
3	77	83
4	15*	-7
5	98	-101
6	45	49
7	143	-145
8	21*	-22
9	98	96
10	22*	-14
11	39	-40
12	59	60
13	104	-104
14	17*	-21
15	82	82
16	18*	-0
17	18*	-6
18	28*	32
19	75	-75
20	19*	-13
21	56	57
22	20*	-7
23	20*	11
24	20*	16
H= 10, K= 4		
0	184	-183
1	270	269
2	108	-100
3	36	28
4	42	-42
5	322	-333
6	108	-111
7	149	154
8	114	-115
9	16*	11
10	16*	-11
11	249	-258
12	48	-43
13	33	26
14	99	-105
15	43	52
16	18*	15
17	167	-168
18	19*	29
19	19*	-17
20	71	-65
21	31*	40
22	20*	10
23	80	-80
H= 11, K= 4		
1	207	207
2	60	-56
3	32	-27
4	29	31
5	167	167
6	18*	-16
7	209	214
8	39	-36
9	18*	-14
10	17*	25
11	104	103
12	17*	-20
13	166	175
14	24*	-36
15	19*	6
16	18*	-6
17	55	57
18	19*	-12
19	120	120
20	33	-24
21	37	23
22	20*	-6
H= 12, K= 4		
0	71	-72
1	55	51
2	26*	-21
3	17*	-19
4	30*	31
5	111	-121
6	73	-68
7	34	-26
8	48	-43
9	68	-63
10	37	45
11	135	-138
12	19*	-25
13	55	-65
14	37	-39
15	60	-61
16	35	37
17	111	-114
18	27*	-1
19	59	-61
20	20*	-19
21	54	-52
22	20*	15
H= 13, K= 4		
1	262	259
2	19*	-15
3	29*	16
4	26*	-2
5	216	213
6	26*	-25
7	260	272
8	18*	-10
9	29*	-1
10	18*	8
11	120	119
12	35	-41
13	203	215
14	27*	-17
15	19*	-13
16	19*	5
17	64	61
18	37	-37
19	144	149
20	20*	-3
21	204	-8
H= 14, K= 4		
0	132	-129
1	162	-164
2	130	-129
3	43	-51
4	148	-145
5	112	116
6	135	-138
7	141	-144
8	89	-94
9	98	-104
10	109	-111
11	56	56
12	88	-90
13	107	-104
14	47	-49
15	129	-128
16	71	-70
17	21*	7
18	66	-69
19	44	-54
20	25*	-19
H= 15, K= 4		
1	19*	-8
2	31*	41
3	36	-36
4	27*	-30
5	18*	-1
6	18*	-3
7	31*	-38
8	18*	17
9	38	-30
10	18*	-22
11	18*	1
12	18*	-8
13	44	-51
14	19*	14
15	19*	-24
16	19*	5
17	27*	-14
18	20*	-9
19	26*	-45
H= 16, K= 4		
0	52	48
1	95	-98
2	28*	25
3	36	-26
4	32	-18
5	100	117
6	55	45
7	75	-80
8	49	53
9	41	-37
10	38	-33
11	84	96
12	37	28
13	45	-41
14	55	50
15	50	-49
16	20*	-22
17	69	73
18	20*	12
H= 17, K= 4		
1	33*	-20
2	19*	5
3	160	166
4	28*	-1
5	19*	-14
6	19*	-19
7	45	-47
8	19*	2
9	111	121
10	19*	-21
11	19*	4
12	20*	-17
13	49	-57
14	20*	10
15	49	60
16	29*	-24
17	21*	1
H= 18, K= 4		
0	89	82
1	47	48
2	43	33
3	22*	22
4	55	45
5	21*	-22
6	71	77
7	39	36
8	49	42
9	46	48
10	44	34
11	20*	-11
12	37	41
13	40	41
14	24*	35
15	69	56
H= 19, K= 4		
1	78	73
2	22*	-18
3	158	159
4	36*	-16
5	89	80
6	27*	-9
7	59	59
8	35*	-35
9	123	121
10	47	-26
11	57	59
12	33*	-14
13	28*	26
14	54	-45
H= 20, K= 4		
0	22*	-1
1	80	82
2	43	21
3	22*	15
4	23*	25
5	76	-68
6	26*	10
7	68	66
8	21*	0
9	54	50
10	34*	30
11	47	-57
12	22*	10
H= 21, K= 4		
1	126	116
2	22*	-16
3	40	39
4	22*	2
5	109	103
6	22*	-3
7	111	112
8	22*	-18
9	22*	33
H= 22, K= 4		
0	22*	-3
1	27*	17
2	22*	17
3	35*	1
4	27*	24
5	22*	-7
6	22*	-11
H= 1, K= 5		
1	514	-515
2	93	-87
3	232	-231
4	88	88
5	450	-448
6	14*	-4
7	451	-448
8	47	-48
9	192	-196
10	96	94
11	258	-262
12	16*	2
13	251	-249
14	20*	-25
15	143	-143
16	59	60
17	144	-147
18	18*	10
19	112	-106
20	19*	-3
21	87	-82
22	36	36
23	63	-69
24	21*	10
25	37	-24
H= 2, K= 5		
0	173	-168
1	113	113
2	106	100
3	26	16
4	150	151
5	125	-125
6	165	-167
7	73	77
8	22*	16
9	31	-28
10	140	140
11	98	-91
12	85	-83
13	42	48
14	16*	-9
15	24*	12
16	82	79
17	28*	-37
18	39	-43
19	19*	32
20	19*	-6
21	19*	-7
22	33	29
23	20*	6
24	20*	-6
25	21*	28
H= 3, K= 5		
1	13*	-19
2	66	64
3	116	-111
4	49	-48
5	15*	-18
6	33	36
7	14*	7
8	16*	14
9	57	-57
10	35	-38
11	15*	-8
12	15*	29
13	15*	-1
14	16*	8
15	16*	-5
16	24*	-2
17	23*	26
18	18*	7
19	18*	7
20	18*	-6
21	19*	20
22	19*	1
23	35	29
24	20*	-8
25	20*	6
H= 4, K= 5		
0	116	-120
1	87	83
2	148	147
3	13*	-5
4	151	147
5	155	-156
6	83	-80
7	25	16
8	114	122
9	76	-75
10	67	66
11	120	-119
12	15*	-2
13	51	-39
14	27*	30
15	68	-67
16	51	48
17	72	-72
18	34	28
19	43	-35
20	24*	2
21	64	-65
22	34	21
23	20*	-16
24	20*	27
H= 5, K= 5		
1	312	305
2	57	53
3	39	41
4	53	-51
5	283	280
6	29	-30
7	280	279
8	70	70
9	67	75
10	78	-75
11	163	165
12	25*	-29
13	172	171
14	53	54
15	94	93
16	73	-79
17	110	114
18	18*	-10
19	97	91
20	19*	20
21	76	76
22	44	-58
23	69	73
24	21*	3
H= 6, K= 5		
0	25*	11
1	87	-84
2	211	-209
3	38	-45
4	175	-175
5	40	-39
6	18*	3
7	138	-140
8	141	-144
9	89	-97
10	113	-111
11	77	-77
12	33	-34
13	179	-183
14	63	-68
15	102	-100
16	54	-50
17	114	-112
18	19*	-27
19	129	-128
20	19*	-11
21	71	-70
22	21*	-26
23	86	-83
24	20*	-15
H= 7, K= 5		
1	36	42
2	28	20
3	23*	-18
4	31	-30
5	17*	17
6	27	19
7	45	42
8	27	31
9	23*	-21
10	15*	6
11	16*	1
12	23*	19
13	35	31
14	23*	12
15	17*	-11
16	18*	-0
17	17*	-10
18	18*	13
19	18*	4
20	28*	16
21	26*	2
22	25*	9
23	20*	-9
24	20*	2
H= 8, K= 5		
0	227	223
1	104	-104
2	15*	-11
3	41	-38
4	31	-32
5	30	31
6	164	158
7	111	-113
8	37	33
9	73	-77
10	27	-34
11	26*	-36
12	115	117
13	114	-106
14	55	43
15	80	-76
16	17*	-11
17	64	-72
18	40	37
19	76	-74
20	32*	39
21	47	-42
22	19*	1
23	59	-62
H= 9, K= 5		
1	38	-23
2	23*	-32
3	48	49
4	25*	24
5	29	-32
6	15*	1
7	43	-43
8	36	-46
9	22*	18
10	16*	18
11	16*	-26
12	16*	2
13	24*	-30
14	40	-39
15	17*	-18
16	37	29
17	46	-45
18	18*	-8
19	33	-31
20	19*	-19
21	39	-30
22	27*	23
23	44	-47
H= 10, K= 5		
0	89	-89
1	23*	-11
2	59	-59
3	18*	-9
4	92	-93
5	25*	20
6	68	-71
7	23*	-8
8	54	-50
9	29	-28
10	60	-66
11	16*	5
12	36	-43
13	17*	14
14	34	-19
15	23*	-16
16	48	-47
17	18*	9
18	30*	-20
19	26*	18
20	31*	-18
21	19*	-4
22	23*	-12
H= 11, K= 5		
1	45	43
2	34	-37
3	142	143
4	56	61
5	26*	40
6	29	-22
7	30	34
8	37	-31
9	86	89
10	38	34
11	34	24
12	31	-23
13	29	18
14	26*	4
15	31	22
16	25*	24
17	18*	-2
18	42	-11
19	27*	12
20	19*	1
21	19*	-21
H= 12, K= 5		
0	54	50
1	48	42
2	143	134
3	17*	8
4	167	170
5	17*	2
6	51	51
7	45	31
8	104	101
9	34	28
10	130	130
11	17*	19
12	29*	24
13	51	52
14	45	50
15	18*	19
16	95	87
17	53	50
18	29*	19
19	52	43
20	20*	31
21	20*	11
H= 13, K= 5		
1	295	288
2	19*	12
3	306	299
4	53	-43
5	293	286
6	18*	-6
7	238	238
8	18*	-16
9	221	224
10	42	-40
11	211	213
12	19*	-10
13	147	145
14	49	-40
15	128	131
16	20*	-27
17	132	132
18	25*	-18
19	73	77
20	20*	-25
H= 14, K= 5		
0	185	-177
1	19*	23
2	64	-61
3	18*	6
4	71	-75
5	27*	-7
6	127	-122
7	18*	19
8	74	-75
9	36	27
10	50	-55
11	18*	7
12	85	-82
13	26*	18
14	55	-58
15	19*	13
16	22*	-45
17	35	23
18	20*	-22
19	20*	4
H= 15, K= 5		
1	82	87
2	19*	4
3	61	62
4	18*	-12
5	96	92
6	18*	3
7	68	60
8	19*	24
9	51	53
10	18*	-5
11	68	65
12	19*	8
13	19*	19
14	19*	13
15	34	46
16	34	-20
17	48	38
18	20*	17
H= 16, K= 5		
0	92	96
1	23*	17
2	47	52
3	19*	6
4	58	52
5	19*	12
6	71	67
7	34	28
8	40	37
9	42	43
10	53	45
11	25*	15
12	61	52
13	30*	24
14	25*	28
15	33*	40
16	21*	21
17	23*	11
H= 17, K= 5		
1	40	-44
2	19*	-4
3	59	-58
4	20*	8
5	61	-67
6	19*	-5
7	19*	-31
8	19*	-3
9	45	-46
10	27*	-4
11	60	-66
12	20*	-4
13	40	-26
14	20*	5
15	30*	-30
16	21*	0
H= 18, K= 5		
0	21*	-27
1	20*	11
2	70	-69
3	42	24
4	86	-79
5	20*	15
6	20*	-25
7	21*	46
8	56	-59
9	62	51
10	51	-50
11	20*	31
12	32*	-34
13	54	50
14	31*	-26
H= 19, K= 5		
1	146	-142
2	22*	16
3	184	-181
4	31*	-4
5	158	-145
6	21*	12
7	128	-119
8	21*	4
9	145	-146
10	21*	4
11	115	-115
12	30*	12
H= 20, K= 5		
0	90	76
1	22*	-4
2	69	73
3	22*	17
4	59	69
5	25*	34
6	72	72
7	32*	26
8	69	74
9	22*	32
10	39	40
H= 21, K= 5		
1	22*	-5
2	22*	-6
3	21*	-8
4	22*	2
5	32*	1
6	23*	-15
7	21*	1
H= 0, K= 6		
0	229	234
1	210	-203
2	233	-228
3	106	-108
4	211	-213
5	89	86
6	221	224
7	186	-186
8	148	-147
9	216	-219
10	167	-160
11	68	64
12	144	143
13	197	-195
14	75	-72
15	253	-250
16	95	-87
17	23*	-10
18	87	82
19	100	-101
20	20*	-8
21	192	-180
22	49	-55
23	27*	-20
24	65	34
H= 1, K= 6		
1	255	-251
2	80	-98
3	16*	15
4	91	90
5	204	-196
6	27*	18
7	286	-286
8	84	-84
9	44	-33
10	107	101
11	63	-67
12	35	31
13	212	-207
14	73	-72
15	60	-63
16	77	73
17	25*	-25
18	46	37
19	149	-144
20	41	-46
21	64	-57
22	59	51
23	20*	6
24	21*	23
H= 2, K= 6		
0	237	225
1	88	-82
2	146	136
3	30	-38
4	136	133
5	14*	19
6	184	187
7	100	-99
8	146	145
9	96	-96
10	61	56
11	33	-28
12	165	165
13	85	-77
14	80	77
15	115	-108
16	45	37
17	28*	-33
18	100	93
19	29*	-44
20	30*	45
21	95	-87
22	20*	7
23	20*	-17
24	49	52
H= 3, K= 6		
1	84	-83
2	185	-182
3	278	284
4	160	163
5	24*	14
6	19*	-25
7	206	-212
8	134	-142
9	187	188
10	127	133
11	88	91
12	17*	-8
13	200	-193
14	111	-114
15	67	61
16	85	82
17	66	65
18	26*	18
19	153	-149
20	61	-68
21	20*	-9
22	42	42
23	45	43
H= 4, K= 6		
0	316	-319
1	125	126
2	15*	0
3	51	48
4	38	15
5	132	-130
6	287	-290
7	74	70
8	46	-48
9	40	43
10	43	40
11	114	-115
12	208	-207
13	31	30
14	58	-42
15	103	104
16	38	23
17	81	-69
18	132	-124
19	19*	-4
20	48	-40
21	80	79
22	28*	21
23	28*	-32
H= 5, K= 6		
1	146	149
2	16*	11
3	188	187
4	16*	18
5	149	153
6	16*	-0
7	134	136
8	43	34
9	131	139
10	19*	25
11	94	83
12	17*	-2
13	60	58
14	40	46
15	82	76
16	18*	25
17	50	47
18	19*	3
19	19*	27
20	31*	28
21	35	27
22	21*	19
23	28*	10
H= 6, K= 6		
0	54	-57
1	159	155
2	149	147
3	36	32
4	169	167
5	134	-133
6	74	-76
7	96	97
8	100	99
9	99	102
10	152	151
11	101	-101
12	87	-79
13	57	53
14	45	55
15	109	110
16	103	102
17	69	-52
18	67	-64
19	20*	10
20	20*	23
21	97	96
22	54	55
23	29*	-29
H= 7, K= 6		
1	511	504
2	178	174
3	204	196
4	159	-158
5	390	384
6	17*	22
7	507	524
8	137	131
9	157	157
10	123	-124
11	193	194
12	28*	14
13	380	377
14	77	90
15	103	110
16	57	-58
17	91	85
18	19*	-17
19	218	218
20	48	57
21	71	75
22	29*	-27
H= 8, K= 6		
0	56	-58
1	40	-33
2	108	-109
3	28*	-8
4	161	-160
5	26*	23
6	17*	-17
7	46	-5
8	81	-73
9	24*	18
10	129	-131
11	75*	20
12	17*	-17
13	18*	9
14	40	-28
15	27*	-26
16	91	-94
17	24*	9
18	19*	14
19	20*	16
20	20*	-18
21	28*	-24
22	43	-39
H= 9, K= 6		
1	128	124
2	56	56
3	120	-119
4	48	-42
5	57	57
6	17*	10
7	119	116
8	64	65
9	85	-87
10	30	-33
11	17*	2
12	36	15
13	104	100
14	60	60
15	19*	-37
16	45	-33
17	48	-50
18	26*	11
19	59	61
20	57	47
21	20*	-17
H= 10, K= 6		
0	209	205
1	109	-103
2	54	-53
3	21*	-25
4	69	-64
5	167	171
6	202	201
7	51	-42
8	28*	-35
9	38	-39
10	55	-49
11	159	157
12	140	139
13	18*	14
14	18*	1
15	43	-50
16	50	-42
17	120	116
18	78	87
19	20*	22
20	28*	17
21	37	-36
H= 11, K= 6		
1	142	-139
2	97	-96
3	25*	-17
4	78	71
5	122	-117
6	18*	8
7	154	-153
8	83	-79
9	38	-32
10	48	49
11	60	-63
12	19*	17
13	128	-124
14	70	-63
15	53	-45
16	30*	23
17	45	-32
18	19*	17
19	100	-95
20	21*	-31
H= 12, K= 6		
0	58	-55
1	44	-44
2	72	-74
3	26*	28
4	77	-80
5	104	106
6	37	-43
7	18*	19
8	73	-77
9	49	40
10	62	-52
11	119	117
12	19*	-25
13	67	62
14	37	-47
15	36	52
16	33*	-41
17	103	103
18	20*	-8
19	57	60
H= 13, K= 6		
1	231	-222
2	77	-73
3	21*	-7
4	68	62
5	146	-146
6	22*	2
7	236	-230
8	82	-76
9	29*	-13
10	57	47
11	74	-72
12	20*	7
13	198	-197
14	68	-64
15	24*	-20
16	50	36
17	20*	-16
18	20*	13
19	123	-122
H= 14, K= 6		
0	114	-103
1	74	69
2	52	49
3	46	38
4	53	53
5	46	-36
6	107	-98
7	79	80
8	24*	22
9	92	95
10	49	53
11	19*	2
12	79	-72
13	69	66
14	20*	-1
15	105	104
16	28*	38
17	32*	18
18	37	-43
H= 15, K= 6		
1	40	10
2	19*	12
3	58	57
4	19*	3
5	27*	25
6	20*	-32
7	19*	10
8	19*	11
9	42	53
10	19*	2
11	19*	31
12	40	-40
13	20*	17
14	24*	12
15	47	42
16	20*	1
H= 16, K= 6		
0	75	-63
1	68	69
2	30*	9
3	20*	13
4	43	30
5	82	-78
6	68	-65
7	64	58
8	19*	7
9	30*	27
10	34	27
11	56	-54
12	60	-57
13	22*	21
14	21*	-1
15	42	36
H= 17, K= 6		
1	21*	7
2	75	67
3	115	-107
4	71	-68
5	20*	-24
6	20*	-2
7	49	42
8	48	49
9	84	-79
10	49	-49
11	29*	-24
12	20*	-12
13	66	65
14	21*	29
H= 18, K= 6		
0	38	46
1	21*	-22
2	21*	3
3	27*	-8
4	25*	-4
5	24*	-2
6	48	-44
7	22*	-26
8	34*	17
9	21*	-32
10	21*	-14
11	21*	-23
12	49	38
H= 19, K= 6		
1	64	-60
2	41	11
3	162	-154
4	35*	-18
5	74	-68
6	22*	8
7	40	-39
8	24*	12
9	104	-110
10	21*	-18
H= 20, K= 6		
0	96	85
1	42	-45
2	22*	5
3	23*	-15
4	22*	1
5	23*	37
6	68	69
7	44	-40
H= 1, K= 7		
1	206	205
2	324	-328
3	328	331
4	294	298
5	179	181
6	112	109
7	188	190
8	266	-268
9	270	270
10	199	193
11	116	112
12	157	154
13	121	115
14	160	-164
15	182	176
16	101	93
17	72	69
18	139	133
19	41	49
20	83	-84
21	100	93
22	23*	34
H= 2, K= 7		
0	410	-407
1	150	145
2	223	222
3	16*	11
4	285	285
5	170	-167
6	335	-341
7	98	94
8	105	106
9	56	52
10	288	286
11	134	-132
12	220	-219
13	39	41
14	37	29
15	42	30
16	209	205
17	83	-82
18	83	-88
19	27*	10
20	31*	-19
21	20*	16
22	127	123
H= 3, K= 7		
1	61	58
2	134	129
3	34	-26
4	87	-84
5	56	53
6	16*	-31
7	16*	16
8	120	117
9	21*	-26
10	47	-39
11	39	29
12	33	-37
13	19*	2
14	91	89
15	30*	-29
16	34	-2
17	19*	-11
18	30*	-30
19	26*	-8
20	50	53
21	20*	-24
22	21*	1
H= 4, K= 7		
0	347	-347
1	113	112
2	38	19
3	30	10
4	76	73
5	57	-59
6	262	-260
7	105	106
8	57	-52
9	31	36
10	110	115
11	17*	-9
12	188	-191
13	68	70
14	52	-51
15	60	49
16	89	91
17	30*	13
18	81	-82
19	37	30
20	38	-43
21	46	46
22	66	63
H= 5, K= 7		
1	105	-96
2	368	368
3	220	-210
4	311	-314
5	107	-106
6	79	-82
7	83	-81
8	325	336
9	215	-208
10	175	-176
11	79	-74
12	114	-118
13	55	-53
14	221	222
15	173	-172
16	59	-66
17	38	-51
18	111	-104
19	35	-38
20	120	123
21	111	-110
22	21*	-2
H= 6, K= 7		
0	120	115
1	86	-88
2	166	-162
3	36	38
4	214	-212
5	158	157
6	117	109
7	26*	-2
8	99	-99
9	75	72
10	195	-197
11	149	146
12	62	-64
13	73	76
14	29*	-29
15	74	71
16	153	-153
17	116	116
18	45	35
19	78	80
20	20*	-1
21	45	43
H= 7, K= 7		
1	18*	14
2	92	95
3	38	-17
4	108	-109
5	24*	34
6	25*	-22
7	18*	5
8	83	86
9	18*	-11
10	69	-72
11	36	26
12	19*	-40
13	19*	-3
14	43	45
15	19*	-4
16	49	-40
17	33*	20
18	37	-43
19	20*	7
20	26*	31
21	21*	-4
H= 8, K= 7		
0	187	189
1	104	-102
2	273	-262
3	37	16
4	348	-352
5	149	149
6	149	152
7	30	-28
8	173	-168
9	42	31
10	292	-296
11	152	149
12	93	96
13	20*	18
14	62	-59
15	49	32
16	215	-214
17	104	106
18	20*	38
19	31*	34
20	20*	-17
H= 9, K= 7		
1	52	-39
2	229	-229
3	75	68
4	201	203
5	18*	-18
6	36	39
7	43	-27
8	214	-214
9	84	78
10	106	109
11	21*	1
12	60	60
13	18*	-13
14	142	-140
15	77	79
16	46	37
17	19*	19
18	59	61
19	20*	7
20	78	-85
H= 10, K= 7		
0	90	89
1	26*	17
2	59	51
3	18*	-4
4	60	60
5	29*	-16
6	60	65
7	22*	13
8	51	55
9	18*	3
10	61	47
11	18*	-6
12	59	52
13	18*	-8
14	38	35
15	19*	-1
16	25*	43
17	32*	-9
18	21*	25
19	20*	-16
H= 11, K= 7		
1	63	-71
2	185	-180
3	24*	8
4	139	142
5	77	-77
6	32	24
7	45	-44
8	191	-200
9	19*	18
10	57	58
11	53	-44
12	42	42
13	19*	-9
14	149	-153
15	32*	27
16	20*	13
17	20*	-10
18	20*	39
H= 12, K= 7		
0	234	-230
1	62	62
2	99	94
3	36	4
4	148	154
5	99	-101
6	177	-175
7	42	29
8	45	48
9	19*	-2
10	135	142
11	95	-100
12	119	-120
13	32*	-4
14	20*	1
15	21*	0
16	115	115
17	83	-81
18	38	-44
H= 13, K= 7		
1	193	-183
2	37	39
3	245	-240
4	54	-54
5	174	-176
6	35	-24
7	160	-158
8	47	37
9	179	-182
10	27*	-33
11	136	-133
12	33*	-44
13	113	-105
14	20*	20
15	101	-104
16	21*	-28
17	89	-88
H= 14, K= 7		
0	33*	-21
1	24*	41
2	121	121
3	20*	-6
4	155	158
5	38	-39
6	31*	-31
7	30*	21
8	91	90
9	20*	-13
10	121	124
11	26*	-31
12	20*	-10
13	20*	6
14	37	32
15	27*	-3
16	97	95
H= 15, K= 7		
1	21*	-22
2	129	131
3	73	-78
4	133	-132
5	33*	-25
6	45	-47
7	22*	-9
8	124	125
9	69	-70
10	81	-85
11	36	-22
12	68	-71
13	20*	-2
14	73	82
H= 16, K= 7		
0	57	58
1	46	-41
2	61	-65
3	21*	-6
4	83	-90
5	30*	26
6	31*	29
7	21*	-37
8	40	-44
9	27*	-20
10	79	-81
11	22*	16
12	20*	22
13	30*	-24
H= 17, K= 7		
1	22*	30
2	47	55
3	33*	34
4	26*	-36
5	34*	39
6	31*	5
7	21*	24
8	43	38
9	28*	26
10	21*	-20
11	37	40
H= 18, K= 7		
0	171	166
1	50	-41
2	22*	18
3	22*	-18
4	22*	-4
5	22*	25
6	139	143
7	53	-54
8	29*	37
9	22*	-31
H= 19, K= 7		
1	103	95
2	69	-68
3	132	128
4	64	71
5	102	98
6	23*	14
H= 0, K= 8		
0	48	-45
1	39	39
2	187	-188
3	31	6
4	193	-195
5	21*	20
6	46	-43
7	121	121
8	134	-140
9	58	65
10	141	-136
11	45	49
12	53	-58
13	140	138
14	67	-66
15	57	48
16	85	-84
17	37	31
18	34*	-47
19	125	123
20	22*	-34
21	63	48
H= 1, K= 8		
1	152	150
2	19*	-40
3	33	30
4	16*	17
5	132	133
6	19*	-1
7	113	111
8	34	-43
9	39	37
10	20*	5
11	110	117
12	18*	-10
13	95	91
14	27*	-27
15	39	36
16	35	7
17	55	64
18	29*	-23
19	59	50
20	25*	-2
21	36	30
H= 2, K= 8		
0	129	-127
1	17*	23
2	171	-169
3	19*	8
4	191	-192
5	31	13
6	104	-100
7	62	63
8	141	-143
9	17*	6
10	124	-123
11	46	45
12	85	-83
13	53	55
14	73	-74
15	20*	19
16	77	-71
17	23*	35
18	49	-46
19	46	40
20	49	-45
21	23*	17
H= 3, K= 8		
1	18*	21
2	61	-63
3	96	-105
4	47	47
5	25*	9
6	16*	-15
7	17*	21
8	60	-60
9	79	-78
10	23*	18
11	39	41
12	34	-23
13	36	41
14	38	-27
15	40	-39
16	19*	7
17	38	33
18	19*	-25
19	26*	33
20	23*	-7
H= 4, K= 8		
0	71	34
1	43	-38
2	127	131
3	17*	18
4	130	134
5	38	33
6	36	34
7	71	-68
8	109	108
9	17*	9
10	102	100
11	18*	8
12	44	43
13	61	-53
14	73	71
15	20*	15
16	64	63
18	54	42
19	32*	-49
20	51	48
H= 5, K= 8		
1	84	-87
2	17*	-6
3	52	-46
4	17*	-23
5	61	-62
6	39	-34
7	57	-58
8	45	-46
9	34	-34
10	49	-49
12	18*	-41
13	38	-40
14	52	-55
15	31*	-20
16	42	-45
17	19*	-6
18	29*	-34
19	20*	-9
20	52	-44
H= 6, K= 8		
0	70	-66
1	37	-41
2	55	31
3	25*	13
4	77	74
5	19*	1
6	44	-39
7	63	-60
8	24*	29
9	18*	20
10	53	45
11	18*	-10
12	19*	-8
13	66	-62
14	39	9
15	19*	13
16	19*	20
17	28*	-12
18	20*	20
19	23*	-41
H= 7, K= 8		
1	259	-252
2	18*	16
3	150	-143
4	48	-47
5	215	-215
6	27*	-16
7	222	-221
8	18*	-9
9	103	-104
10	51	-49
11	169	-166
12	19*	-26
13	168	-167
14	49	-34
15	60	-53
16	49	-51
17	101	-100
18	27*	-18
19	83	-86

TABLE III (*Continued*)

H= 8, K= 8		
0	43	44
1	37	41
2	19*	24
3	18*	-16
4	44	44
5	43	-28
6	38	27
7	19*	38
8	30*	19
9	18*	2
10	24*	19
11	18*	-5
12	19*	29
13	19*	20
14	33	-14
15	19*	-5
16	20*	-18
17	25*	4
18	20*	5
19	24*	9
H= 9, K= 8		
1	29*	-7
2	19*	1
3	33	31
4	29*	-23
5	40	-29
6	26*	-15
7	18*	-1
8	27*	4
9	27*	25
10	34	-28
11	18*	-18
12	29*	-20
13	19*	16
14	22*	-10
15	19*	18
16	20*	-32
17	76	-10
H= 10, K= 8		
0	58	49
1	19*	21
2	39	-40
3	19*	-9
4	37	-39
5	40	-25
6	27*	7
7	24*	19
8	24*	-19
9	19*	-26
10	19*	-27
11	24*	-34
12	18*	-9
13	26*	22
14	19*	-14
15	19*	-24
16	32*	-11
17	40	-32
H= 11, K= 8		
1	89	72
2	19*	17
3	19*	1
4	19*	-4
5	56	60
6	18*	1
7	71	69
8	19*	9
9	22*	7
10	23*	8
11	52	54
12	23*	-3
13	59	61
14	19*	15
15	24*	15
16	24*	21
H= 12, K= 8		
0	139	137
1	22*	-9
2	100	95
3	19*	-21
4	82	82
5	19*	-7
6	112	109
7	33	-37
8	94	94
9	57	-55
10	46	56
11	36	-38
12	79	73
13	40	-31
14	53	65
15	56	-58
H= 13, K= 8		
1	83	85
2	20*	4
3	20*	32
4	28*	17
5	94	93
6	20*	-7
7	81	76
8	20*	6
9	20*	29
10	20*	16
11	66	70
12	32*	-9
13	42	51
14	20*	23
H= 14, K= 8		
0	67	76
1	23*	-26
2	89	86
3	26*	-17
4	94	86
5	24*	-4
6	80	83
7	45	-50
8	83	75
9	34*	-34
10	49	52
11	20*	-20
12	61	59
13	57	-56
H= 15, K= 8		
1	33*	-42
2	22*	-7
3	21*	-10
4	20*	6
5	32*	-40
6	21*	19
7	27*	-38
8	20*	4
9	20*	-19
10	20*	8
11	28*	-33
12	37	26
H= 16, K= 8		
0	21*	-5
1	21*	-8
2	21*	11
3	21*	4
4	21*	9
5	21*	-1
6	20*	8
7	20*	-16
8	20*	-4
9	20*	18
10	20*	6
H= 17, K= 8		
1	21*	11
2	41	-18
3	36*	35
4	30*	19
5	21*	11
6	29*	26
7	21*	-8
H= 18, K= 8		
0	70	-71
1	39	20
2	60	-46
3	22*	9
H= 1, K= 9		
1	91	-96
2	37	21
3	108	-104
4	43	-48
5	93	-95
6	50	-48
7	38	-45
8	18*	1
9	62	-69
10	47	-50
11	100	-97
12	84	-79
13	32*	-37
14	23*	-18
15	25*	-24
16	33*	-46
17	52	-53
18	83	-83
H= 2, K= 9		
0	30*	10
1	18*	-14
2	81	-78
3	37	-33
4	117	-118
5	18*	19
6	17*	-3
7	28*	23
8	37	-32
9	19*	-21
10	134	-130
11	33	28
12	21*	9
13	42	35
14	19*	-4
15	27*	-43
16	117	-111
17	20*	16
18	22*	-15
H= 3, K= 9		
1	18*	8
2	18*	-21
3	18*	-2
4	17*	7
5	17*	-4
6	17*	-9
7	17*	-5
8	26*	-32
9	17*	-1
10	29*	-23
11	26*	17
12	33	-7
13	18*	18
14	19*	-19
15	19*	-0
16	20*	-24
17	20*	8
18	38	1
H= 4, K= 9		
0	111	123
1	19*	-27
2	28*	33
3	17*	-20
4	17*	23
5	33	23
6	97	92
7	26*	-25
8	61	62
9	18*	-29
10	18*	-14
11	18*	-5
12	62	56
13	19*	-0
14	48	48
15	23*	-34
16	20*	-21
17	39	-12
18	20*	13
H= 5, K= 9		
1	76	74
2	29*	-33
3	80	72
4	18*	15
5	84	83
6	23*	24
7	20*	29
8	55	-53
9	52	53
10	18*	5
11	97	99
12	44	43
13	28*	28
14	48	-48
15	25*	27
16	20*	8
17	67	62
18	52	48
H= 6, K= 9		
0	120	116
1	19*	9
2	157	160
3	23*	-5
4	174	176
5	18*	-19
6	104	106
7	60	-42
8	118	120
9	43	-41
10	142	138
11	37	-44
12	72	74
13	51	-46
14	54	51
15	29*	-30
16	102	103
17	20*	-25
H= 7, K= 9		
1	39	-36
2	26*	-17
3	18*	-1
4	32	21
5	26*	-7
6	26*	1
7	36	-33
8	18*	-2
9	19*	-5
10	38	33
11	26*	-4
12	31*	9
13	39	-38
14	19*	-7
15	20*	-12
16	27*	18
17	20*	9
H= 8, K= 9		
0	83	84
1	30*	18
2	171	170
3	19*	2
4	208	207
5	34	-34
6	70	63
7	19*	-27
8	105	103
9	19*	10
10	177	179
11	37	-39
12	36	51
13	44	-44
14	46	40
15	44	5
16	124	124
H= 9, K= 9		
1	39	-24
2	28*	36
3	19*	6
4	31*	-14
5	30*	-27
6	20*	-2
7	19*	-0
8	52	49
9	19*	-1
10	19*	2
11	40	-43
12	19*	-12
13	23*	-9
14	45	44
15	27*	-6
H= 10, K= 9		
0	58	-63
1	20*	7
2	41	-44
3	19*	2
4	37	-46
5	32*	-21
6	54	-55
7	19*	10
8	48	-52
9	29*	26
10	19*	-30
11	31*	-10
12	44	-49
13	20*	2
14	33*	-32
15	31*	17
H= 11, K= 9		
1	21*	18
2	51	43
3	31*	-20
4	20*	-7
5	21*	-5
6	22*	24
7	24*	13
8	54	61
9	30*	-11
10	20*	14
11	20*	-17
12	20*	21
13	28*	8
14	73	71
H= 12, K= 9		
0	21*	-14
1	21*	3
2	80	-79
3	21*	-3
4	114	-112
5	21*	10
6	20*	-4
7	20*	23
8	44	-38
9	20*	-5
10	109	-112
11	25*	16
12	20*	-13
13	21*	30
H= 13, K= 9		
1	110	108
2	21*	-6
3	81	76
4	21*	22
5	90	86
6	20*	21
7	88	90
8	23*	19
9	55	62
10	21*	29
11	65	60
H= 14, K= 9		
0	22*	-14
1	21*	-17
2	67	-69
3	21*	1
4	88	-85
5	24*	16
6	21*	-4
7	21*	-4
8	50	-49
9	20*	-22
10	72	-63
H= 15, K= 9		
1	21*	7
2	38	-27
3	61	9
4	33*	27
5	21*	17
6	39	23
7	37	4
H= 16, K= 9		
0	22*	-1
1	22*	-9
2	22*	37
3	28*	2
4	40	47
H= 0, K= 10		
0	330	331
1	202	208
2	92	88
3	27*	13
4	52	47
5	224	-217
6	302	296
7	149	144
8	119	115
9	40	34
10	33*	-5
11	196	-194
12	210	206
13	86	80
14	99	94
15	43	31
16	22*	-14
H= 1, K= 10		
1	29*	23
2	110	-111
3	205	-206
4	95	93
5	19*	-4
6	29*	27
7	47	43
8	95	-91
9	156	-152
10	49	58
11	37	-28
12	48	40
13	39	41
14	62	-63
15	88	-86
16	21*	12
H= 2, K= 10		
0	172	173
1	67	64
2	85	80
3	19*	1
4	78	75
5	60	-58
6	143	140
7	37	32
8	81	75
9	20*	16
10	38	45
11	63	-60
12	102	98
13	21*	21
14	57	50
15	28*	12
16	21*	21
H= 3, K= 10		
1	130	123
2	165	-165
3	241	-227
4	140	141
5	84	75
6	57	59
7	150	147
8	142	-146
9	163	-169
10	92	84
11	28*	16
12	86	82
13	124	120
14	104	-101
15	101	-97
H= 4, K= 10		
0	213	-205
1	161	-152
2	20*	-15
3	26*	-18
4	20*	10
5	156	154
6	182	-184
7	109	-115
8	46	-51
9	32*	-38
10	20*	26
11	139	132
12	136	-131
13	60	-64
14	57	-59
15	43	-42
H= 5, K= 10		
1	20*	-7
2	20*	7
3	21*	-9
4	32*	29
5	20*	-2
6	45	36
7	21*	-8
8	37	25
9	20*	-12
10	41	39
11	20*	-4
12	52	48
13	34*	-11
14	37	45
15	36	-10
H= 6, K= 10		
0	178	-170
1	146	-139
2	20*	12
3	31*	-20
4	31*	34
5	141	139
6	140	-141
7	102	-99
8	22*	-10
9	47	-35
10	46	37
11	117	119
12	101	-108
13	61	-58
14	46	-29
H= 7, K= 10		
1	49	-30
2	150	146
3	261	259
4	88	-91
5	20*	-4
6	28*	-18
7	65	-64
8	168	167
9	199	195
10	27*	-20
11	37	24
12	37	-23
13	69	-61
14	140	138
H= 8, K= 10		
0	22*	42
1	37	39
2	21*	-15
3	36	11
4	21*	-24
5	59	-53
6	42	45
7	29*	32
8	20*	-3
9	20*	7
10	20*	-13
11	42	-43
12	25*	22
13	20*	8
H= 9, K= 10		
1	74	-68
2	87	92
3	89	86
4	62	-71
5	42	-53
6	20*	-9
7	79	-78
8	95	96
9	60	61
10	38	-17
11	24*	-23
12	20*	-14
H= 10, K= 10		
0	117	116
1	127	129
2	39	-32
3	50	27
4	71	-65
5	130	-130
6	110	101
7	104	102
8	20*	-8
9	23*	35
10	43	-58
11	108	-104
H= 11, K= 10		
1	53	34
2	69	-63
3	98	-96
4	49	50
5	46	28
6	71*	11
7	25*	43
8	54	-67
9	74	-71
10	21*	16
H= 12, K= 10		
0	53	-59
1	35*	31
2	108	-104
3	22*	9
4	103	-105
5	37	-26
6	68	-54
7	48	40
8	77	-82
H= 13, K= 10		
1	37*	34
2	88	-97
3	127	-124
4	66	74
5	22*	15
6	27*	19
H= 14, K= 10		
0	156	-149
1	78	-69
2	77	-72
H= 1, K= 11		
1	19*	-6
2	19*	-18
3	20*	-14
4	55	57
5	19*	0
6	20*	19
7	19*	2
8	41	22
9	20*	-18
10	82	80
11	25*	-15
12	29*	27
H= 2, K= 11		
0	21*	6
1	31*	-34
2	69	68
3	19*	-20
4	63	55
5	37	31
6	19*	-6
7	19*	-5
8	74	70
9	47	-31
10	53	59
11	20*	32
12	20*	1
H= 3, K= 11		
1	20*	-5
2	19*	27
3	24*	-4
5	19*	-17
6	19*	8
7	19*	-12
8	19*	21
9	20*	-2
10	19*	-9
11	20*	-2
12	22*	11
H= 4, K= 11		
0	87	-61
1	20*	-19
2	24*	-20
3	19*	0
4	30*	-31
5	28*	15
6	50	-53
7	19*	-3
8	19*	-3
9	19*	-23
10	19*	-19
11	28*	17
H= 5, K= 11		
1	20*	-19
2	20*	27
3	19*	-7
4	33	-35
5	20*	-15
6	28*	2
7	27*	-27
8	22*	9
9	22*	3
10	50	-49
11	20*	1
H= 6, K= 11		
0	81	-77
1	35*	16
2	135	-133
3	20*	17
4	125	-120
5	20*	-19
6	55	-62
7	19*	7
8	108	-110
9	20*	12
10	92	-98
H= 7, K= 11		
1	21*	11
2	27*	-12
3	34*	28
4	20*	-5
5	26*	21
6	19*	7
7	30*	20
8	20*	-14
9	20*	21
H= 8, K= 11		
0	69	-62
1	29*	19
2	114	-111
3	27*	7
4	104	-99
5	39	-36
6	55	-50
7	20*	15
8	103	-99
H= 9, K= 11		
1	21*	16
2	41	-30
3	20*	-11
4	20*	24
5	20*	12
6	27*	-1
7	26*	17
H= 10, K= 11		
0	22*	18
1	21*	-1
2	27*	41
3	21*	-7
4	55	46
5	31*	-2
H= 0, K= 12		
0	161	-151
1	55	47
2	81	-82
3	23*	12
4	34*	-46
5	44	-44
6	125	-123
H= 1, K= 12		
1	25*	14
2	22*	21
3	27*	1
4	26*	-21
5	24*	20
6	20*	-4
H= 2, K= 12		
0	70	-70
1	20*	9
2	50	-45
3	28*	4
4	28*	-36
5	35	-20
6	64	-63
H= 3, K= 12		
1	20*	-3
2	37	37
3	30*	-35
4	40	-33
5	19*	8
H= 4, K= 12		
0	82	85
1	40	-35
2	39	27
3	20*	-10
4	19*	8
5	38	24
H= 5, K= 12		
1	40	42
2	20*	1
3	29*	33

[a] The data are separated into groups having common values of *h* and *k*. The three columns in each group list values of *l*, F_o, and F_c in that order. Reflections designated as "unobserved" are indicated by an asterisk.

TABLE IV

BOND DISTANCES IN $C_4H_8STeI_2$ IN Å

Bond	Molecule A	Molecule B	Average
Te–I(1)	2.884 (2)	2.985 (2)	*a*
Te–I(2)	2.939 (2)	2.851 (2)	
Te–C(1)	2.18 (2)	2.15 (2)	2.16
Te–C(4)	2.13 (2)	2.16 (2)	
S–C(2)	1.88 (3)	1.82 (3)	1.83
S–C(3)	1.82 (3)	1.79 (3)	
C(1)–C(2)	1.50 (4)	1.54 (4)	1.52
C(3)–C(4)	1.49 (4)	1.53 (4)	

[a] Although the individual Te–I bond distances have esd values of 0.002 Å, an average of the four observed values has little significance because of the influence of secondary bonding. See text.

TABLE V

BOND ANGLES IN $C_4H_8STeI_2$ (DEG)

Atoms	Molecule A	Molecule B	Average
I(1)–Te–I(2)	174.9 (1)	178.1 (1)	*a*
I(1)–Te–C(1)	88.3 (6)	91.6 (6)	*a*
I(1)–Te–C(4)	91.6 (6)	89.6 (6)	*a*
I(2)–Te–C(1)	87.4 (6)	88.9 (6)	*a*
I(2)–Te–C(4)	91.8 (6)	88.5 (6)	*a*
C(1)–Te–C(4)	100 (1)	100 (1)	100
C(2)–S–C(3)	99 (1)	100 (1)	100
Te–C(1)–C(2)	115 (1)	116 (1)	116
Te–C(4)–C(3)	117 (1)	115 (1)	
S–C(2)–C(1)	113 (2)	113 (2)	114
S–C(3)–C(4)	115 (2)	116 (2)	

[a] Due to the influence of secondary bonding, the averages of these angles are of little significance.

tering correction was applied to the curves for I, Te, and S by use of the $\Delta f'$ values of Templeton and Dauben for Mo Kα radiation given in Table 3.3.2C of ref 11.

TABLE VI

DIHEDRAL OR TORSION ANGLES IN 1,4-THIATELLURANE RING (ESD ~2°)

	Angle, deg		
Atoms	Molecule A	Molecule B	Average
Te–C(1)–C(2)–S	60	58	58
Te–C(4)–C(3)–S	58	56	
C(1)–Te–C(4)–C(3)	29	26	29
C(4)–Te–C(1)–C(2)	31	28	
C(2)–S–C(3)–C(4)	75	77	77
C(3)–S–C(2)–C(1)	77	77	

TABLE VII

ATOM DISPLACEMENTS FROM LEAST-SQUARES PLANES THROUGH FOUR CARBON ATOMS (Å)

	C(1)	C(2)	C(3)	C(4)	Te	S
Molecule A	−0.02	0.02	−0.02	0.02	0.63	−1.08
Molecule B	0.01	−0.01	0.01	−0.01	−0.57	1.05

Discussion of the Structure

Some of the more interesting features of the crystal structure of 1,4-thiatellurane 4,4-diiodide are shown in Figure 1 and ORTEP views of the two independent molecules are shown in Figure 2. Views of the 1,4-thiatellurane ring with averaged values of bond distances and angles are given in Figure 3, while the individual observed values of the bond distances, bond angles and torsion angles are given in Tables IV, V, and VI.

The 1,4-thiatellurane ring has the expected chair conformation, but with pronounced deviations from the geometry of the cyclohexane ring. These deviations are apparent in Figure 3 and the numerical details are given in Tables IV–VII. In each molecule, the four carbon atoms are coplanar within the standard deviations of the positional parameters. Individual atom displacements from the least-squares planes through the carbon atoms are given in Table VII. The planes of the C(1)–Te–C(4) systems make dihedral angles of 27 (1)° in molecule A and 25 (1)° in molecule B with the respective least-squares planes through the carbon atoms. In contrast, the dihedral angles that these least-squares planes make with the C(2)–S–C(3) systems are 64 (2)° in molecule A and 63 (2)° in molecule B. This geometry has the effect of bringing the sulfur atoms close to the planes of the C–Te–C systems. These distances are 0.063 (7) Å in molecule A and 0.122 (7) Å in molecule B. In each case, the S atom is on the opposite side of the C–Te–C plane from the locations of C(2) and C(3).

The molecular structure of 1,4-thiatellurane diiodide is very much like that of 1,4-thiaselenane dibromide,[14] except for displacement of the iodine atoms caused by intermolecular interactions. The molecules approximate mirror symmetry through the I, Te, and S atoms and the configuration about tellurium approximates a trigonal bipyramid with C(1), C(4), and an unshared pair of electrons in equatorial positions and the iodine atoms in axial positions. This type of geometry about tellurium has been observed previously in diphenyltellurium dibromide,[15] dimethyltellurium dichloride,[16] and *p,p*-dichlorodiphenyltellurium diiodide,[5] as well as in numerous selenium compounds of the general type R_2SeX_2.[14]

The main features of the intermolecular bonding are shown in Figure 1. Two sets of loosely bonded linear polymers are formed and there are significant "cross links" between the sets. In each set, systems of the type $\cdots I(1)–Te–I(2)\cdots I(1)–Te–I(2)\cdots$ are found. In the A molecules these systems are lined up along the crystallographic *a* axis while in the B molecules they are lined up along *b*. The intermolecular $I(1)\cdots I(2)$ separations in the chains are 3.66 Å in the A set and 3.90 Å in the B set whereas the van der Waals radius of 2.15 Å[17] for iodine would suggest a normal, nonbonded contact of 4.30 Å. The cross linking between chains consists of secondary bonding of the tellurium atoms in one chain with iodine atoms in another. These secondary bonds increase the equatorial ligancy about tellurium to five in molecule A and to four in molecule B. Thus, the configuration about each tellurium atom approximates a pentagonal bipyramid, but for Te(B), one equatorial iodine atom is absent. The bonding arrangements about the tellurium atoms are shown in Figure 4. Each iodine atom forms a strong bond with the tellurium atom in its own molecule and a secondary bond with an iodine atom in a neighboring molecule in the same chain, to give a nearly linear group. In each case, the central iodine atom makes a secondary bond with a tellurium atom of the opposite set, *i.e.*, I(A) with Te(B) and I(B) with Te(A), so that the $Te–I\cdots Te$ bond angle is in the range 103 to 125°. The result is a nearly planar group of two iodine and two tellurium atoms arranged thus

$$\begin{array}{ccc} & \text{Te} & \\ & \vdots & \\ \text{Te}\text{———} & \text{I} & \cdots\cdots\cdots\cdots\text{I} \end{array}$$

In one case, I(2) of set A, an additional tellurium atom forms a secondary bond with the central iodine atom so that the second $Te—I\cdots Te$ angle is 108° and the $Te\cdots I\cdots Te$ angle is 97°. Further details of the coordination about the tellurium and iodine atoms are given in Table VIII.

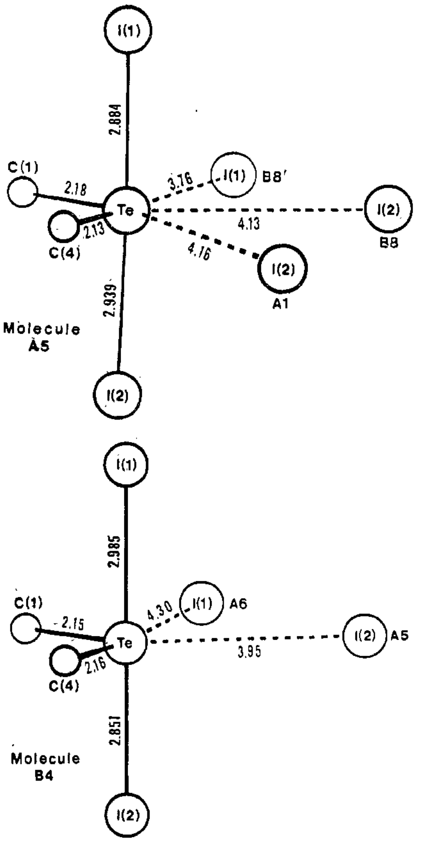

Figure 4.—Views showing the bonding configuration about Te(A5) and Te(B4). Primary (intramolecular) bonds are shown by full lines, secondary (intermolecular) bonds by dotted lines. The bond angles about these tellurium atoms are given in Table VIII and the atom numbering is the same as used in that table and in Figure 1.

An examination of the data in Table VIII shows that there is excellent correlation between the strength of the bond (as indicated by bond distance) that an iodine atom forms with the Te atom in its own molecule and the strengths of the secondary bonds which it forms. Thus, I(1) of molecule B forms the longest primary bond with Te, 2.985 Å, but it also forms the shortest intermolecular bond with Te at 3.76 Å. On the other hand,

---

[14] L. Battelle, C. Knobler, and J. D. McCullough, *Inorg. Chem.*, **6**, 958 (1967). See also the references therein.

[15] G. D. Christofferson and J. D. McCullough, *Acta Crystallogr.*, **11**, 249 (1958).

[16] G. D. Christofferson, R. A. Sparks, and J. D. McCullough, *ibid.*, **11**, 782 (1958).

[17] L. Pauling, "Nature of the Chemical Bond," 3rd ed, Cornell University Press, Ithaca, N. Y., 1960, p 260.

TABLE VIII

COORDINATION ABOUT TELLURIUM AND IODINE ATOMS IN $C_4H_8STeI_2$

Angle, deg[b]	Bonded atom	Dist, Å
	About Te(A5)[a]	
	I(1) (A5) ax[c]	2.884
174.9		
	I(2) (A5) ax	2.939
87.4[d]		
	C(1) (A5) eq	2.18
100		
	C(4) (A5) eq	2.13
61.9		
	I(2) (A1) eq	4.16
63.0		
	I(2) (B8) eq	4.13
59.0		
	I(1) (B8') eq	3.76
78.1		
	C(1) (A5)[e] eq	2.18
	About Te(B4)	
	I(1) (B4) ax	2.985
178.1		
	I(2) (B4) ax	2.851
91.6[f]		
	C(1) (B4) eq	2.15
100		
	C(4) (B4) eq	2.16
138.9		
	I(2) (A5) eq	3.95
52.5		
	I(1) (A6) eq	4.30
66.5		
	C(1) (B4) eq	2.15

Angle, deg[b]	Bonded atom	Dist, Å
	About I(1) (A6)	
	Te (A6) ax	2.884
174.9		
	I(2) (A5) ax	3.66
58.9		
	Te (B4)	4.30
124.9		
	Te (A6) ax	2.884
	About I(2) (A5)[g]	
	Te (A5) ax	2.939
167.9		
	I(1) (A6) ax	3.66
68.6		
	Te (B4)	3.95
102.9		
	Te (A5) ax	2.939
	About I(1) (B8')	
	Te (B8') ax	2.985
175.3		
	I(2) (B8) ax	3.90
65.3		
	Te (A5)	3.76
118.3		
	Te (B8') ax	2.985
	About I(2) (B8)	
	Te (B8) ax	2.851
174.2		
	I(1) (B8') ax	3.90
55.7		
	Te (A5)	4.13
118.9		
	Te (B8) ax	2.851

[a] The atom and molecule numbering is keyed to Figure 1. [b] The angles are those formed at the central atom by the bonds to the two bracketed atoms. [c] The atoms are designated ax for axial and eq for equatorial where this designation is useful. [d] The ten axial–equatorial angles at Te(A) range from 72.3 to 112.8°. [e] One atom is repeated in each coordination group to facilitate the designation of angles. [f] The eight axial–equatorial angles at Te(B) range from 77.3 to 104.1°. [g] An additional tellurium atom, Te-(A1), at a distance of 4.16 Å from the central atom, is located as indicated in the text.

I(2) of molecule B forms the shortest primary bond with Te, 2.851 Å, and its only intermolecular bond with Te has a length of 4.13 Å.

The thermal ellipsoids of the iodine atoms show an interesting correlation with the observed structure. In molecule A, the I–Te–I axis is lined up with the crystallographic *a* axis and the major vibrations of the iodine atoms are perpendicular to *a* and hence to the direction of the Te–I bonds. In molecule B, where the alignment is along *b*, the major vibrations of the iodine atoms are perpendicular to *b* and (again) to the direction of the Te–I bonds. This effect is smaller in I(2)A than in the other three iodine atoms, and inspection of the structure shows that this atom is more restricted in its vibrations by the larger number of secondary bonds and by their directions.

Acknowledgment.—The authors are pleased to acknowledge the financial support of this research by the National Science Foundation through Grant GP-6356 with the University of California at Los Angeles and Grant GP6635 with the University of California at Davis.