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The Crystal and Molecular Structure of Dibenzoselenophene, $C_{12}H_8Se$

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Dibenzoselenophene forms colorless, orthorhombic crystals with cell dimensions $a = 19.851$ (20), $b = 21.244$ (10) and $c = 8.895$ (10) Å. The space group is *Pbca*; there are 16 molecules in the unit cell, and two molecules in the asymmetric unit. The intensities of 4063 reflections were measured on a Picker automated diffractometer and were corrected for absorption and secondary extinction. The structure was solved by use of three-dimensional Patterson and difference Fourier syntheses and refined by full-matrix least-squares procedures to a final R index of 0·035 for 3002 observed reflections. The individual five- and six-membered rings are planar, but the six-membered rings show significant dihedral angles (0·5 to 1·2°) with the respective five-membered rings. The independently observed values for chemically equivalent bond lengths and angles are in good agreement, with the following average values after correction for thermal motion: Se–C, 1·899 (5) Å; C–C (in the six-membered rings), 1·371 (7) to 1·398 (7) Å; C–C (between the six-membered rings), 1·453 (7) Å; C–Se–C, 86·7 (2)° and C–C–C (in the six-membered rings) 118·1 (5) to 121·6 (5)°.

Introduction

Studies of the donor properties of a wide variety of organoselenium compounds toward molecular iodine in carbon tetrachloride solution have shown dibenzoselenophene to be the weakest donor of some twenty such compounds investigated (McCullough & Mulvey, 1960; McCullough & Brunner, 1967). This is probably due to the fact that the selenium atom, which is the usual seat of donor properties in organoselenium compounds (Chao & McCullough, 1961; Hope & McCullough, 1964; Maddox & McCullough, 1966), is involved in an aromatic ring system. Actually, the donor strength of dibenzoselenophene toward I_2 is scarcely greater than that of aromatic hydrocarbons with approximately the same number of atoms, as shown in Table 1. Since there appears to have been no detailed structural study of a compound with selenium in a similar aromatic environment, the present investigation of dibenzoselenophene was undertaken.

Table 1. *Formation constants, K_c, for complexes of* I_2 *with various donors, D, in carbon tetrachloride at* 25°

$K_c = [DI_2]/[D]\,[I_2]$

Donor	K_c (liter mole^{-1})	References
Tetrahydroselenophene	2.2×10^3	1
Dimethylselenide	4.8×10^2	2
Diphenylselenide	2.8×10^1	3
Dibenzoselenophene	1.9×10^0	4
Diphenyl	3.1×10^{-1}	5
Naphthalene	2.5×10^{-1}	6
Phenanthrene	1.4×10^{-1}	6

Table 1 (*cont.*)

References: (1) McCullough & Brunner (1967);
(2) Tideswell & McCullough (1957);
(3) McCullough (1942);
(4) McCullough & Mulvey (1960);
(5) de Maine (1957);
(6) Keefer & Andrews (1952).

Experimental

The dibenzoselenophene used in this study was prepared by the method of McCullough, Campbell & Gould (1950), and crystals were grown by the slow evaporation of a solution in ethanol. The colorless crystals belong to the orthorhombic system with elongation along **c** and principal faces of the form $\{hk0\}$. A preliminary photographic investigation showed a somewhat rapid decline of intensity with increasing θ. This indicated that the measurement of intensity data on the diffractometer would require either long counting times or a large crystal in order to obtain reasonably low relative counting errors for the high angle reflections. It was also noted that the crystals could not be exposed to X-rays for more than about a week without suffering measurable radiation damage. For these reasons, the decision was made to use a fairly large crystal for the intensity measurements. An apparently flawless crystal was ground to a sphere 0·46 mm in diameter, coated with a water-based glue, and mounted on a Picker full-circle diffractometer without prior orientation. Crystal setting parameters and cell dimensions were obtained by a least-squares fit to 12 sets of measured diffractometer angles. The cell dimensions so obtained were: $a = 19.851(20)$, $b = 21.244(10)$ and $c = 8.895(10)$ Å at

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* Contribution No. 2401.

23 °C, based on $\lambda(\text{Cu } K\beta) = 1{\cdot}39217$ and $\lambda(\text{Cu } K\alpha_1) = 1{\cdot}54051$ Å.

The intensity symmetry and systematic absences ($0kl$, absent if $k=2n+1$; $h0l$, absent if $l=2n+1$ and $hk0$, absent if $h=2n+1$) uniquely determine the space group to be *Pbca*. The density observed by flotation in aqueous zinc chloride solution is 1·62(2) g.cm^{-3}, which compares favorably with the value 1·637(3) g.cm^{-3} calculated for $Z=16$. Thus, there are two molecules of $C_{12}H_8Se$ in the crystallographic asymmetric unit.

The intensities of 4063 reflections accessible below $2\theta = 161°$ were measured with the diffractometer in automatic mode. Nickel filtered Cu $K\alpha$ radiation was used in conjunction with a scintillation counter and pulse-height analyzer. The θ–2θ scan technique was employed with a scan speed of 2° min^{-1}, and backgrounds were measured for 20 sec at each end of the scan range. Attenuators were automatically inserted when the count rate exceeded 10,000 c.p.s. Measurements of two reference reflections were repeated at 8 hr intervals. No systematic drift was in evidence. The difference between the highest and lowest net check intensities was 4%, with most variations within ±1%. However, we believe that the intensities of a few reflections were incorrectly measured, owing to an intermittent malfunctioning of the shutter system. Most of these errors were obvious and were discovered in time for correction, but seven were unnoticed and were processed part way into the refinement. It was then noted that their F_o values were much too low and they were removed from subsequent calculations. These reflections are noted later. Lorentz, polarization and absorption corrections ($\mu r = 1{\cdot}37$) were applied. Each recorded number of counts, N, was assigned an estimated standard deviation by use of the expression

$$S(N) = N^{1/2} + 0{\cdot}01N.$$

Altogether, 3009 reflections for which the net intensity exceeded three standard deviations were recorded as 'observed'.

Determination and refinement of the structure

The structure determination and refinement proceeded by the following steps:

(1) A three-dimensional Patterson synthesis was readily interpreted to give the positions of the two Se atoms in the asymmetric unit.

(2) A three-dimensional difference Fourier synthesis phased on the Se atoms, but with the Se contributions otherwise subtracted, clearly showed the positions of all 24 carbon atoms.

(3) Two cycles of full-matrix least-squares refinement with isotropic thermal parameters for all 26 non-hydrogen atoms reduced the usual R index ($R = \sum||F_o| - |F_c||/\sum|F_o|$) from 0·24 to 0·14.

(4) In two more cycles of least-squares refinement the thermal parameters for Se were allowed to go anisotropic, with a resulting decrease in R to 0·089.

(5) In the next two cycles of least-squares refinement, anisotropic thermal parameters were allowed to refine for all 26 non-hydrogen atoms. This caused a reduction in R to 0·062.

At this stage it was noted that the F_o values for seven reflections (2,14,1, 713, 8,15,1, 10,0,2, 14,1,1, 14,5,1, and 14,6,0) were much lower than their respective values of F_c. As stated earlier, it was assumed that these reflections were affected by malfunctioning of the shutter. They were therefore removed from all subsequent calculations.

(6) A difference Fourier synthesis with the contributions of Se and C subtracted showed maxima which could be reasonably interpreted as being due to hydrogen atoms. However, to support these conclusions, hydrogen atom positions were also computed by use of the program *HPOSN*.

(7) Three more cycles of least-squares refinement were computed in which hydrogen atoms were included with isotropic thermal parameters held constant at 5 Å^2. All positional parameters as well as the anisotropic parameters for Se and C were allowed to refine. The resulting value of R was 0·041.

(8) A comparison of F_o and F_c values at this stage suggested that many of the stronger, low order reflections might be suffering from the effects of secondary extinction. The intensities of all observed reflections were therefore processed and corrected by use of the program *SECEXT* and R was thus reduced to 0·036.

(9) After correction of the intensity data for the effects of secondary extinction, two final cycles of least-squares refinement were computed. In these cycles, all positional and thermal parameters (anisotropic for Se and C, isotropic for H) were allowed to vary. Including the overall scale factor, 299 variables were thus refined. The final R index for the 3002 observed reflections was 0·035 and the final shifts averaged less than 15% of the corresponding estimated standard deviations. The largest final shift for a non-hydrogen atom was $0{\cdot}4\,\sigma$ for a positional parameter and $0{\cdot}5\,\sigma$ for a thermal parameter, while for hydrogen, the maximum final shift was $0{\cdot}8\,\sigma$ for a positional parameter and $0{\cdot}9\,\sigma$ for a thermal parameter.

(10) A final three-dimensional difference Fourier synthesis was computed with all atoms subtracted at the positions indicated in Table 2 and with the thermal parameters given in Table 3. The maximum fluctuations of the electron density in this summation, ±0·25 e.Å^{-3} were about half the electron density shown by the hydrogen atoms as observed earlier, and about three times the e.s.d. of the electron density, 0·08 e.Å^{-3}.

(11) 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 2 and 3. The resulting values of F_c are listed with the respective F_o values in Table 4. The value of R for these 4056 reflections, including 1054 designated as 'unobserved', is 0·051.

Table 2. *Final atomic positional parameters with their standard deviations in parentheses*

Molecule *A*

	x	*y*	*z*
Se	0·20602 (3)	0·01622 (2)	0·02930 (6)
C(1)	0·2217 (2)	0·0358 (2)	0·4689 (5)
C(2)	0·1543 (2)	0·0286 (2)	0·5095 (5)
C(3)	0·1083 (2)	0·0714 (3)	0·4563 (6)
C(4)	0·1280 (3)	0·1200 (2)	0·3659 (6)
C(5)	0·1940 (2)	0·1273 (2)	0·3236 (5)
C(6)	0·2423 (2)	0·0844 (2)	0·3742 (4)
C(7)	0·3136 (2)	0·0840 (2)	0·3402 (4)
C(8)	0·3492 (2)	0·1255 (2)	0·2477 (5)
C(9)	0·4173 (3)	0·1185 (2)	0·2304 (6)
C(10)	0·4522 (2)	0·0705 (2)	0·3011 (6)
C(11)	0·4188 (2)	0·0287 (2)	0·3917 (5)
C(12)	0·3495 (2)	0·0355 (2)	0·4097 (5)
H(2)*	0·143 (2)	−0·004 (2)	0·572 (5)
H(3)	0·068 (2)	0·069 (2)	0·485 (5)
H(4)	0·099 (2)	0·149 (2)	0·342 (5)
H(5)	0·211 (2)	0·165 (2)	0·262 (5)
H(8)	0·322 (2)	0·158 (2)	0·206 (5)
H(9)	0·443 (2)	0·145 (2)	0·158 (5)
H(10)	0·503 (2)	0·064 (2)	0·299 (5)
H(11)	0·446 (2)	−0·001 (2)	0·434 (4)

Molecule *B*

	x	*y*	*z*
Se	0·45254 (3)	0·09762 (2)	0·78198 (6)
C(1)	0·5087 (2)	0·1479 (2)	0·6581 (5)
C(2)	0·5783 (2)	0·1421 (2)	0·6421 (6)
C(3)	0·6111 (2)	0·1811 (3)	0·5466 (6)
C(4)	0·5768 (3)	0·2257 (2)	0·4643 (6)
C(5)	0·5077 (3)	0·2316 (2)	0·4815 (5)
C(6)	0·4721 (2)	0·1922 (2)	0·5786 (5)
C(7)	0·4001 (2)	0·1913 (2)	0·6052 (5)
C(8)	0·3516 (2)	0·2289 (2)	0·5396 (6)
C(9)	0·2843 (3)	0·2215 (2)	0·5756 (7)
C(10)	0·2656 (2)	0·1766 (2)	0·6769 (6)
C(11)	0·3123 (3)	0·1384 (2)	0·7447 (6)
C(12)	0·3798 (2)	0·1458 (2)	0·7081 (5)
H(2)	0·595 (2)	0·117 (2)	0·696 (5)
H(3)	0·658 (2)	0·176 (2)	0·541 (6)
H(4)	0·601 (2)	0·252 (2)	0·384 (5)
H(5)	0·485 (2)	0·257 (2)	0·427 (5)
H(8)	0·362 (2)	0·256 (2)	0·469 (5)
H(9)	0·250 (2)	0·247 (2)	0·520 (5)
H(10)	0·224 (2)	0·173 (2)	0·701 (5)
H(11)	0·302 (2)	0·115 (2)	0·816 (4)

* Hydrogen atoms are assigned the same numbers as the carbon atoms to which they are bonded.

The atomic scattering curve used for selenium was that given in Table 3.3.1A of *International Tables for X-ray Crystallography* (1962) corrected for dispersion for Cu *Kα* radiation by use of the $\Delta f'$ values in Table 3.3.2B. The factors used for carbon were the graphite values of McWeeny (1954) and those for hydrogen were the bonded values of Stewart, Davidson & Simpson (1965).

(12) Analysis of possible rigid-body motion of each of the two molecules of dibenzoselenophene was carried out by use of the program (ACA No. 1) written by Schomaker & Trueblood (1968) which is based on the

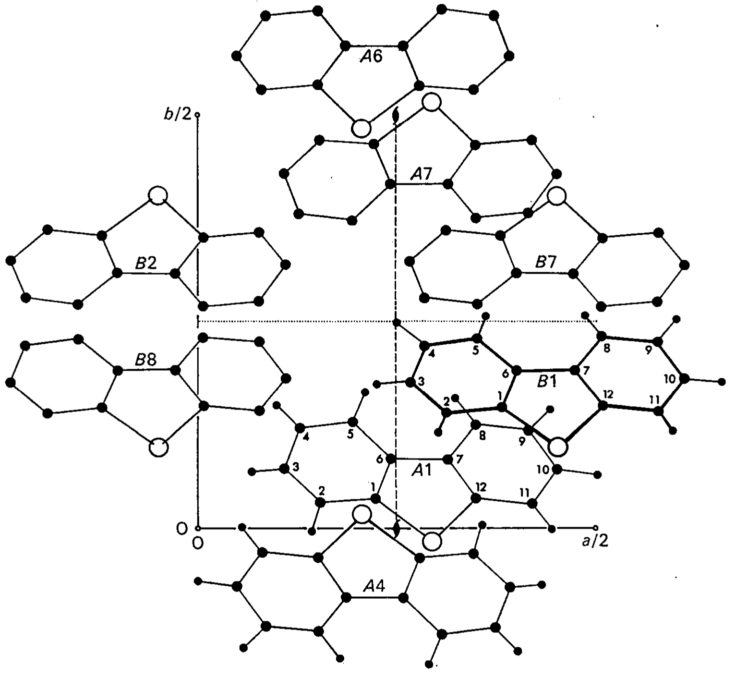

Fig. 1. Projection of a selected portion of the structure of dibenzoselenophene down the *c* axis. The labels *A*1, *B*1, *etc.* designate the crystallographically nonequivalent molecules *A* and *B* and the eight equivalent positions of the space group. The position numbering is indicated in Table 12. Hydrogen atoms are shown only in molecules *A*1, *B*1 and *A*4.

treatment presented in their paper on the rigid-body motions of molecules in crystals. The more significant results of the application of this program to dibenzoselenophene are presented in Table 5 and the bond lengths and angles, corrected for the effects of the implied librational motion, are listed with the uncorrected values in Tables 6 and 7.

The various Fourier summations were computed by use of *UCLAFOUR* written by Gantzel & Hope, and the least-squares refinement was carried out by use of the full-matrix program (ACA No.317, modified) written by Gantzel, Sparks & Trueblood. This program minimized $\sum w(\Delta|F|)^2$ and provides for anisotropic thermal parameters of 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 weighting scheme was that of Hughes (1941). Hydrogen positions were checked by use of *HPOSN*, written by H. Hope. This routine calculates H atom positions by use of the known molecular geometry around the carbon atom to which the hydrogen atom is assumed to be bonded. Correction of the observed intensities for the effects of secondary extinction were calculated by use of the

Table 3. *Final thermal parameters (in* Å^2)* *with their standard deviations in parentheses*

Molecule A

	B_{11}	B_{22}	B_{33}	B_{12}	B_{13}	B_{23}
Se	5·73 (2)	4·42 (2)	5·02 (2)	−0·08 (2)	0·06 (2)	−1·23 (2)
C(1)	5·0 (2)	4·5 (2)	3·7 (2)	−0·2 (2)	−0·1 (2)	−0·5 (2)
C(2)	5·4 (2)	6·5 (2)	4·4 (2)	−0·4 (2)	0·7 (2)	−0·3 (2)
C(3)	4·6 (2)	9·3 (3)	5·4 (2)	0·6 (2)	0·1 (2)	−1·5 (2)
C(4)	6·3 (2)	6·4 (2)	5·8 (2)	1·8 (2)	−0·9 (2)	−1·4 (2)
C(5)	6·2 (2)	4·4 (2)	4·8 (2)	0·7 (2)	−0·3 (2)	−0·6 (2)
C(6)	4·9 (2)	3·7 (1)	3·4 (1)	0·2 (1)	−0·2 (1)	−0·4 (1)
C(7)	5·5 (2)	3·2 (1)	3·3 (1)	0·0 (1)	−0·1 (2)	−0·3 (1)
C(8)	6·5 (2)	4·2 (2)	4·7 (2)	−0·4 (2)	0·2 (2)	0·5 (2)
C(9)	7·0 (2)	5·5 (2)	5·2 (2)	−1·8 (2)	1·2 (2)	−0·1 (2)
C(10)	5·0 (2)	6·3 (2)	5·8 (2)	−0·8 (2)	0·7 (2)	−1·0 (2)
C(11)	4·9 (2)	5·0 (2)	5·0 (2)	0·0 (2)	−0·4 (2)	−0·5 (2)
C(12)	5·0 (2)	3·7 (1)	3·7 (2)	−0·5 (1)	0·0 (2)	−0·3 (1)

	B
H(2)	6·5 (1·1)
H(3)	9·6 (1·4)
H(4)	7·0 (1·1)
H(5)	5·3 (1·0)
H(8)	6·6 (1·1)
H(9)	6·8 (1·1)
H(10)	7·0 (1·1)
H(11)	5·9 (1·0)

Molecule B

	B_{11}	B_{22}	B_{33}	B_{12}	B_{13}	B_{23}
Se	5·86 (2)	5·30 (2)	4·95 (2)	−0·73 (2)	−0·03 (2)	1·12 (2)
C(1)	4·8 (2)	3·9 (2)	4·0 (2)	−0·5 (2)	0·1 (2)	−0·3 (1)
C(2)	5·3 (2)	5·0 (2)	5·5 (2)	−0·2 (2)	−0·3 (2)	−0·1 (2)
C(3)	5·1 (2)	6·3 (2)	6·5 (2)	−0·9 (2)	0·6 (2)	−0·3 (2)
C(4)	6·9 (2)	5·3 (2)	6·2 (2)	−1·2 (2)	1·7 (2)	0·3 (2)
C(5)	7·0 (2)	4·0 (2)	4·8 (2)	0·0 (2)	0·5 (2)	0·4 (2)
C(6)	5·2 (2)	3·3 (1)	3·9 (2)	−0·4 (1)	0·2 (2)	−0·5 (1)
C(7)	4·9 (2)	3·6 (1)	4·4 (2)	0·0 (1)	0·0 (2)	−1·0 (1)
C(8)	6·6 (2)	4·0 (2)	5·9 (2)	0·6 (2)	−0·4 (2)	−1·0 (2)
C(9)	5·8 (2)	5·6 (2)	8·4 (3)	1·3 (2)	−1·0 (2)	−2·3 (2)
C(10)	4·5 (2)	7·9 (2)	7·9 (3)	−0·1 (2)	0·3 (2)	−3·6 (2)
C(11)	6·1 (2)	6·2 (2)	5·4 (2)	−1·5 (2)	0·8 (2)	−1·1 (2)
C(12)	4·8 (2)	4·6 (2)	4·4 (2)	−0·3 (2)	0·2 (2)	−1·2 (2)

	B
H(2)	5·1 (1·0)
H(3)	7·9 (1·2)
H(4)	7·6 (1·1)
H(5)	4·6 (0·9)
H(8)	5·7 (1·0)
H(9)	8·1 (1·1)
H(10)	7·5 (1·2)
H(11)	6·0 (1·0)

* The anisotropic B_{ii} and B_{ij} values in the Table are related to the b_{ii} and b_{ij} values in the anisotropic temperature factor expression as follows: $B_{11}=4a^2b_{11}$, $B_{22}=4b^2b_{22}$, $B_{12}=2abb_{12}$, *etc.*

Table 4. *Observed and calculated structure factors for dibenzoselenophene*

The data are separated into groups having common *k* and *l* values. The three columns of each group list values of *h*, $10F_o$ and $10F_c$ in that order. The asterisks indicate reflections designated as unobserved.

K= 23, L= 3		
1	46*	-36
2	79	70
3	138	139
4	27*	15
5	195	-201
6	85	96
7	163	185
8	28*	31
9	27*	-21
10	25*	45
11	25*	29
K= 24, L= 3		
0	249	-252
1	141	-141
2	48*	-80
3	168	173
4	128	-137
5	79	45
6	26*	21
7	43*	34
8	130	147
9	41	85
K= 25, L= 3		
1	89	-99
2	69	-84
3	88	92
4	183	-196
5	158	-169
6	23*	-28
K= 26, L= 3		
0	41*	-50
1	103	-125
2	79	92
K= 0, L= 4		
0	2300	2324
1	1327	-1361
2	181	-161
3	193	-170
4	508	542
5	1371	-1378
6	313	320
7	1810	-1820
8	1102	-1114
9	342	346
10	67*	-60
11	479	-482
12	1046	-1083
13	679	701
14	210	217
15	86	78
16	154	-157
17	111	122
18	171	194
19	285	284
20	313	292
21	99	-108
22	29*	-30
23	100	14
K= 1, L= 4		
1	486	510
2	511	511
3	267	282
4	402	428
5	48*	-37
6	206	207
7	174	-157
8	542	535
9	443	-436
10	53*	-57
11	479	-490
12	271	-270
13	384	-387
14	251	-263
15	236	-241
16	132	-123
17	34*	-7
18	33*	0
19	151	171
20	93	-78
21	63	53
22	57*	10
23	55	32
K= 2, L= 4		
0	1253	1280
1	674	-702
2	667	-666
3	635	616
4	640	622
5	351	-354
6	79	-52
7	509	-528
8	641	-654
9	374	382
10	392	402
11	496	-513
12	820	-826
13	448	459
14	165	169
15	214	204
16	206	-214
17	64*	65
18	91	93
19	125	119
20	173	164
21	75	-90
22	74	-69
23	92	63
K= 3, L= 4		
1	877	883
2	606	591
3	1127	1121
4	1471	1456
5	106	-94
6	580	592
7	395	-369
8	559	571
9	713	-717
10	106	101
11	485	-495
12	192	-191
13	355	-360
14	178	-173
15	177	-166
16	375	-363
17	288	296
18	34*	17
19	103	108
20	125	-115
21	163	158
22	28*	37
23	79	88
K= 4, L= 4		
0	515	505
1	655	-660
2	1304	-1313
3	1006	1022
4	540	440
5	627	624
6	313	305
7	571	565
8	256	246
9	551	572
10	941	964
11	538	-540
12	76	-83
13	147	131
14	477	474
15	411	-417
16	39*	-24
17	112	-104
18	149	-136
19	32*	-35
20	30*	2
21	116	-96
22	171	-157
23	150	156
K= 5, L= 4		
1	313	280
2	1163	-1108
3	36*	35
4	639	650
5	61	-86
6	375	-368
7	42*	75
8	398	426
9	87	82
10	80	46
11	89	-73
12	71*	-51
13	47*	-43
14	70*	-5
15	171	-111
16	364	-367
17	153	165
18	33*	28
19	70	-64
20	88	-79
21	60	55
22	28*	24
23	24*	28
K= 6, L= 4		
0	231	-231
1	40*	-16
2	2251	-2028
3	950	980
4	106	84
5	557	582
6	258	262
7	349	334
8	82	70
9	605	629
10	781	806
11	519	-538
12	129	-125
13	40*	-39
14	209	215
15	482	-488
16	37*	6
17	184	-178
18	157	-144
19	29*	-12
20	44*	-29
21	130	-123
22	182	-172
K= 7, L= 4		
1	678	-698
2	1653	-1636
3	111	95
4	60	-31
5	545	-557
6	929	-960
7	566	580
8	115	94
9	491	483
10	259	-272
11	544	553
12	276	278
13	216	213
14	270	256
15	108	-111
16	33*	16
17	58*	36
18	331	325
19	191	-197
20	27*	-10
21	104	-117
22	26*	-29
K= 8, L= 4		
0	1089	1070
1	958	-969
2	531	-540
3	438	413
4	258	258
5	139	-139
6	87	99
7	82	-110
8	275	-283
9	319	352
10	215	202
11	278	-286
12	120	-122
13	368	371
14	139	133
15	81	-55
16	59*	-77
17	48*	26
18	59*	-54
19	63	19
20	118	112
21	113	-113
22	48*	-48
K= 9, L= 4		
1	1406	-1410
2	277	-310
3	189	192
4	101	93
5	471	-460
6	1085	-1159
7	453	454
8	34*	29
9	40*	10
10	242	-249
11	129	121
12	324	334
13	427	431
14	291	278
15	114	-103
16	55*	-27
17	123	116
18	305	291
19	144	-155
20	56*	-55
21	32*	-40
22	22*	20
K= 10, L= 4		
0	647	676
1	882	-874
2	575	581
3	256	-244
4	301	308
5	641	-638
6	94	-100
7	609	-607
8	633	-620
9	35*	-27
10	268	-256
11	280	-291
12	343	-346
13	368	379
14	81	111
15	175	177
16	34*	-28
17	205	213
18	60*	60
19	122	119
20	133	128
21	26*	-22
K= 11, L= 4		
1	174	163
2	316	-327
3	736	750
4	700	724
5	339	-337
6	493	-498
7	273	276
8	551	542
9	252	-269
10	209	-205
11	195	-214
12	42*	-54
13	47*	34
14	36*	-37
15	164	-180
16	268	-261
17	220	230
18	174	156
19	76	-38
20	37*	-64
21	40*	41
K= 12, L= 4		
0	333	346
1	292	-287
2	376	381
3	89	71
4	77	92
5	197	-202
6	34*	-46
7	337	-337
8	196	-210
9	71*	76
10	111	-90
11	91	-75
12	343	-355
13	186	190
14	34*	-3
15	66*	-30
16	40*	-39
17	92	78
18	73	41
19	98	82
20	43*	45
K= 13, L= 4		
1	440	447
2	342	-352
3	587	609
4	991	1034
5	401	-413
6	47*	-53
7	173	188
8	581	575
9	500	-489
10	36*	-1
11	150	-141
12	191	-197
13	170	-187
14	61*	-42
15	119	-116
16	403	-405
17	181	197
18	27*	27
19	128	-25
20	79	-77
K= 14, L= 4		
0	265	-267
1	302	-305
2	154	-134
3	434	433
4	255	-267
5	211	209
6	37*	82
7	146	164
8	168	166
9	186	190
10	180	177
11	72*	-70
12	72	60
13	39*	-23
14	56*	-58
15	262	-281
16	30*	-19
17	79	-72
18	30*	-66
19	24*	-16
K= 15, L= 4		
1	231	-230
2	233	-229
3	169	170
4	631	648
5	247	-252
6	236	-242
7	255	264
8	366	360
9	289	-294
10	48*	38
11	34*	-27
12	34*	-18
13	72	65
14	129	145
15	167	-174
16	261	-264
17	76	91
18	76	81
19	69	-86
K= 16, L= 4		
0	442	-433
1	35*	-9
2	231	-213
3	256	260
4	191	-193
5	271	273
6	58*	55
7	143	153
8	214	213
9	84	90
10	128	130
11	80	-99
12	334	333
13	50*	-30
14	67	77
15	105	-116
16	40*	37
17	81	-85
18	28*	-60
K= 17, L= 4		
1	285	-271
2	272	-270
3	196	207
4	51*	26
5	433	-425
6	513	-496
7	481	474
8	144	147
9	52*	16
10	109	-113
11	227	239
12	46*	-57
13	130	134
14	207	206
15	130	-151
16	32*	0
17	90	74
K= 18, L= 4		
0	35*	9
1	63*	-48
2	176	187
3	50*	-63
4	68*	-58
5	41*	-2
6	147	-161
7	35*	49
8	90	88
9	32*	-13
10	67	-49
11	70	84
12	270	271
13	104	129
14	23*	-13
15	26*	-7
16	25*	27
K= 19, L= 4		
1	228	-227
2	177	-165
3	48*	55
4	32*	-34
5	341	-327
6	482	-476
7	389	391
8	64*	83
9	48*	-34
10	88	-102
11	47*	67
12	34*	-32
13	139	146
14	193	169
15	27*	-18
K= 20, L= 4		
0	94	-112
1	31*	46
2	228	208
3	232	-241
4	36*	2
5	254	-268
6	117	-119
7	77	-70
8	42*	-60
9	139	-140
10	248	-235
11	26*	43
12	37*	-59
13	26*	-24
14	122	-128
K= 21, L= 4		
1	44	48
2	70	-34
3	281	270
4	177	180
5	251	-237
6	106	-109
7	96	109
8	65	73
9	204	-215
10	59	-70
11	27*	-36
12	24*	-21
13	22*	40
K= 22, L= 4		
0	57*	-48
1	28*	-4
2	298	288
3	97	-106
4	44*	-47
5	49*	-34
6	43*	25
7	55	-60
8	34*	33
9	34*	-43
10	154	-147
11	26*	42
K= 23, L= 4		
1	87	95
2	26*	45
3	143	134
4	146	143
5	141	-146
6	46*	39
7	104	110
8	133	139
9	176	-189
K= 24, L= 4		
0	211	-224
1	93	110
2	154	178
3	57	54
4	75	-86
5	129	143
6	23*	-30
7	101	100
K= 25, L= 4		
1	27*	-17
2	62	71
3	89	94
4	96	103
K= 1, L= 5		
1	809	-802
2	805	-816
3	676	-712
4	297	295
5	627	626
6	1509	-1525
7	148	-158
8	463	456
9	870	884
10	259	-263
11	309	314
12	158	-155
13	70*	-79
14	435	436
15	304	304
16	102	-115
17	70*	-62
18	256	244
19	48*	-40
20	75*	-96
21	114	-120
22	29*	31
K= 2, L= 5		
0	470	464
1	389	-400
2	195	206
3	778	-775
4	106	107
5	955	-949
6	100	94
7	538	-559
8	350	-341
9	204	-220
10	432	-447
11	35*	31
12	406	-412
13	170	180
14	416	-415
15	142	146
16	157	164
17	210	212
18	33*	13
19	139	144
20	65	56
21	36	-30
22	128	73
K= 3, L= 5		
1	316	322
2	468	-465
3	37*	-47
4	944	958
5	656	674
6	626	-446
7	819	-815
8	818	816
9	71*	57
10	321	-324
11	79	-70
12	63*	-44
13	400	-403
14	227	217
15	143	133
16	171	-169
17	180	-182
18	194	200
19	156	152
20	100	-83
21	27*	9
22	25*	21
K= 4, L= 5		
0	79	70
1	483	-493
2	589	598
3	40*	-2
4	308	303
5	476	-447
6	128	-105
7	256	-288
8	190	-170
9	47*	-47
10	490	-486
11	35*	38
12	193	201
13	436	333
14	169	-149
15	137	144
16	149	154
17	53*	18
18	31*	-11
19	103	100
20	42*	25
21	34*	-16
22	111	116
K= 5, L= 5		
1	722	743
2	176	-161
3	269	270
4	1064	1098
5	565	590
6	323	-304
7	757	-753
8	674	693
9	353	-356
10	201	-192
11	413	-418
12	34*	1
13	387	-390
14	75*	-61
15	172	184
16	529	-537
17	43*	-28
18	58*	82
19	193	205
20	102	-92
21	79	86
22	64	73
K= 6, L= 5		
0	671	-638
1	431	-432
2	508	495
3	489	505
4	327	-328
5	341	349
6	80	80
7	237	224
8	313	323
9	469	470
10	225	-222
11	413	-411
12	443	441
13	82	-68
14	36*	-14
15	291	-292
16	74*	-95
17	164	-165
18	45*	-43
19	35*	32
20	80	-63
21	60	-43
22	21*	-12
K= 7, L= 5		
1	294	300
2	180	166
3	164	-168
4	664	678
5	267	278
6	392	-393
7	264	-285
8	619	638
9	199	195
10	88	-93
11	244	-251
12	119	-107
13	280	-286
14	48*	50
15	46*	49
16	263	-257
17	93	-72
18	30*	-6
19	109	110
20	95	-95
21	39*	-49
K= 8, L= 5		
0	1310	-1321
1	59*	29
2	276	252
3	716	746
4	603	-614
5	681	711
6	34*	-42
7	193	193
8	399	398
9	542	586
10	71*	67
11	210	-220
12	460	462
13	37*	-18
14	67*	-42
15	352	-352
16	72	71
17	208	-205
18	39*	-28
19	33*	14
20	144	-142
21	78	-68
K= 9, L= 5		
1	419	-429
2	363	-371
3	481	-502
4	178	188
5	120	131
6	648	-632
7	230	233
8	166	172
9	483	480
10	132	-122
11	350	366
12	47*	61
13	182	176
14	213	207
15	124	119
16	48*	-41
17	153	-164
18	155	160
19	32*	-43
20	45*	-64
21	83	-102
K= 10, L= 5		
0	819	-843
1	476	-499
2	176	182
3	192	156
4	406	-405
5	154	-151
6	58*	47
7	92	-99
8	343	336
9	370	375
10	164	-188
11	244	-196
12	218	212
13	237	250
14	152	-148
15	144	-147
16	69*	74
17	31*	-34
18	37*	47
19	37*	18
20	61	-64
K= 11, L= 5		
1	582	-597
2	235	-234
3	620	-664
4	72*	63
5	139	143
6	565	-562
7	90	-55
8	189	-205
9	276	279
10	54	-61
11	221	210
12	36*	-29
13	252	267
14	313	317
15	59*	72
16	37*	14
17	64	-75
18	209	211
19	28*	-58
20	22*	15
K= 12, L= 5		
0	133	-137
1	732	-749
2	1023	1012
3	443	-437
4	90	-98
5	559	-563
6	113	-118
7	407	-418
8	132	143
9	94	111
10	383	-368
11	292	-278
12	233	244
13	356	342
14	224	-214
15	149	161
16	91	102
17	123	133
18	89	94
19	134	141
K= 13, L= 5		
1	567	548
2	516	-535
3	47*	-8
4	193	198
5	37*	9
6	142	-146
7	44*	-32
8	83	84
9	46*	-57
10	37*	-3
11	63*	-52
12	36*	-62
13	35*	61
14	74	76
15	35*	-37
16	99	-117
17	29*	-7
18	28*	46
19	38*	29
K= 14, L= 5		
0	122	-127
1	404	-404
2	418	403
3	130	140
4	163	-170
5	432	-428
6	129	-126
7	349	-351
8	37*	40
9	149	145
10	569	-564
11	200	-187
12	162	166
13	250	259
14	202	-203
15	37*	36
16	31*	-12
17	27*	29
18	36*	42
K= 15, L= 5		
1	357	364
2	124	128
3	229	230
4	195	198
5	104	-92
6	131	142
7	87	-84
8	133	148
9	399	-415
10	61*	-4
11	335	-345
12	184	-187
13	33*	-65
14	47*	-50
15	29*	-42
16	28*	-56
17	39*	49
K= 16, L= 5		
0	338	-330
1	211	-209
2	235	239
3	474	476
4	37*	-54
5	57*	31
6	36*	-12
7	81	106
8	132	124
9	164	160
10	246	-233
11	192	-192
12	218	218
13	35*	0
14	185	-198
15	139	-146
16	39*	54
17	24*	-27
K= 17, L= 5		
1	164	181
2	244	261
3	194	195
4	165	162
5	95	-88
6	187	186
7	84	102
8	51*	41
9	154	-158
10	32*	17
11	125	-124
12	30*	53
13	29*	85
14	44*	-70
15	94	-89
16	23*	-43
K= 18, L= 5		
0	493	-476
1	96	-104
2	100	108
3	305	306
4	174	-184
5	212	214
6	88	91
7	206	212
8	282	271
9	242	235
10	56*	-37
11	190	-202
12	212	211
13	27*	-32
14	28*	-43
15	130	-150
K= 19, L= 5		
1	175	-173
2	33*	-3
3	46*	-57
4	78	-76
5	168	-197
6	56*	58
7	215	208
8	31*	-26
9	41*	64
10	28*	-20
11	134	143
12	28*	71
13	69	77
14	23*	-25
K= 20, L= 5		
0	422	-429
1	130	-128
2	178	173
3	151	163
4	127	-130
5	45*	56
6	51*	-34
7	30*	-15
8	202	197
9	158	172
10	96	-101
11	64	-71
12	195	191
K= 21, L= 5		
1	186	-195
2	116	-139
3	47*	-57
4	179	-179
5	127	-133
6	63	-75
7	194	201
8	158	-168
9	27*	50
10	24*	-2
11	118	131
K= 22, L= 5		
0	157	-167
1	103	-97
2	208	206
3	59*	-67
4	75	-113
5	205	-207
6	36*	-48
7	162	-178
8	39*	58
9	23*	21
K= 23, L= 5		
1	48*	-7
2	33*	34
3	117	129
4	76	-78
5	159	-170
6	31*	21
7	37*	48
K= 24, L= 5		
0	28*	-8
1	47	-26
2	141	141
3	22*	8
K= 0, L= 6		
0	155	143
1	852	-838
2	695	-697
3	1115	1123
4	362	346
5	674	677
6	210	212
7	401	401
8	39*	25
9	605	627
10	538	544
11	294	-287
12	37*	-4
13	61*	42
14	217	220
15	570	-576
16	104	120
17	432	-431
18	43*	-39
19	28*	4
20	92	10
21	85	-56
K= 1, L= 6		
1	547	-558
2	575	-495
3	575	-569
4	194	-170
5	128	-120
6	314	-306
7	317	313
8	115	-104
9	341	330
10	87	-53
11	216	217
12	63*	-73
13	60*	59
14	36*	-41
15	35*	-22
16	90	-101
17	64*	-45
18	63*	69
19	72	-64
20	53*	-16
21	77	-87
K= 2, L= 6		
0	335	331
1	632	-633
2	563	-572
3	744	741
4	159	147
5	218	209
6	102	92
7	70*	63
8	206	-211
9	558	569
10	352	348
11	419	-418
12	271	-276
13	148	138
14	56*	50
15	206	-205
16	61*	-86
17	93	-89
18	36*	-22
19	78	85
20	26*	16
21	119	-111
K= 3, L= 6		
1	718	-734
2	474	-459
3	351	-353
4	64*	-57
5	343	-342
6	241	-253
7	370	361
8	128	-120
9	540	545
10	54*	10
11	664	665
12	219	221
13	339	327
14	128	115
15	41*	16
16	38*	-21
17	32*	-24
18	116	104
19	144	-151
20	26*	-1
21	116	-121
K= 4, L= 6		
0	430	461
1	813	-801
2	140	-138
3	47*	-58
4	91	106
5	657	-657
6	43*	26
7	845	-860
8	217	-226
9	276	272
10	52*	-23
11	283	-280
12	237	-225
13	517	516
14	55*	96
15	35*	16
16	55*	-69
17	178	189
18	33*	32
19	176	170
20	80	75
21	122	-128
K= 5, L= 6		
1	135	-137
2	158	-102
3	103	123
4	148	143
5	366	-361
6	186	-186
7	219	210
8	123	119
9	103	-104
10	160	-165
11	82	58
12	168	166
13	190	197
14	35*	2
15	93	-87
16	33*	-18
17	54*	17
18	132	132
19	51*	-46
20	51*	-51
K= 6, L= 6		
0	432	421
1	695	-699
2	53*	2
3	242	-231
4	271	266
5	660	-666
6	142	-131
7	709	-700
8	169	-160
9	191	165
10	98	-87
11	361	-372
12	238	-233
13	488	494
14	102	112
15	117	110
16	54*	-32
17	179	191
18	85	87
19	125	107
20	60	70
K= 7, L= 6		
1	668	648
2	163	-160
3	700	708
4	488	458
5	336	-326
6	43*	-37
7	42*	-13
8	193	178
9	480	-475
10	71*	-54
11	449	-455
12	91	-98
13	98	-99
14	63*	-67
15	171	-163
16	185	-173
17	242	247
18	94	105
19	26*	-5
20	29*	-51
K= 8, L= 6		
0	270	272
1	659	-648
2	108	89
3	103	80
4	151	153
5	118	109
6	68*	63
7	136	138
8	45*	3
9	325	331
10	154	173
11	418	-415
12	132	-130
13	140	144
14	38*	22
15	163	-158
16	64*	-47
17	39*	21
18	31*	-25
19	31*	17
20	22*	27
K= 9, L= 6		
1	316	318
2	402	-414
3	472	483
4	750	764
5	370	-365
6	126	-124
7	76	51
8	288	282
9	378	-374
10	79	76
11	309	-315
12	36*	-28
13	42*	-30
14	37*	-26
15	237	-239
16	245	-249
17	135	149
18	27*	-11
19	35*	-34
K= 10, L= 6		
0	364	-363
1	151	-136
2	499	-495
3	841	865
4	148	-137
5	386	396
6	101	95
7	271	263
8	46*	-19
9	334	334
10	115	106
11	240	-233
K= 14, L= 6		
6	41*	19
7	165	-153
8	35*	11
9	39*	-2
10	45*	-45
11	69*	-79
12	76	87
13	145	140
14	35*	-1
15	91	83
16	32*	27
K= 15, L= 6		
1	167	-179
2	91	-91
3	179	156
4	41*	38
5	420	-422
6	297	-297
7	366	374
8	105	106
9	135	-133
10	109	-117
11	49*	44
12	54*	65
13	51*	17
14	59*	61
15	71	-71
16	22*	-29
K= 10, L= 6		
12	98*	96
13	48*	-21
14	33*	19
15	259	-267
16	29*	25
17	155	-130
18	71	-53
19	22*	-13
K= 11, L= 6		
1	362	-357
2	501	-496
3	344	353
4	325	330
5	325	-340
6	256	-257
7	384	378
8	156	156
9	96	-96
10	45*	-47
11	186	193
12	34*	28
13	269	283
14	69*	44
15	133	-136
16	97	-102
17	59*	43
18	106	115
K= 12, L= 6		
0	44*	31
1	261	-243
2	147	-152
3	621	636
4	115	-127
5	54*	26
6	116	97
7	108	109
8	92	98
9	185	184
10	67*	62
11	105	-112
12	178	180
13	64*	42
14	47*	38
15	94	-92
16	28*	-16
17	88	-65
18	31*	-38
K= 13, L= 6		
1	511	-521
2	100	-96
3	79*	97
4	63*	-74
5	465	-470
6	331	-324
7	471	455
8	54*	10
9	71*	71
10	74	-77
11	275	290
12	82	84
13	286	303
14	120	121
15	66	-71
16	89	-16
17	59	74
K= 14, L= 6		
0	70*	41
1	330	-319
2	284	295
3	131	-136
4	85	-76
5	314	-313
K= 16, L= 6		
0	72*	-74
1	39*	12
2	159	132
3	116	-90
4	35*	-5
5	264	-261
6	91	-102
7	269	-271
8	61*	-73
9	95	-106
10	204	-204
11	29*	-78
12	57*	-60
13	148	160
14	45*	-36
15	69	77
K= 17, L= 6		
1	164	156
2	112	-123
3	446	448
4	125	123
5	311	-292
6	85	-80
7	154	158
8	87	82
9	309	-308
10	38*	-44
11	67	-56
12	92	-109
13	64	-75
14	22*	19
K= 18, L= 6		
0	54*	-47
1	50*	37
2	261	272
3	32*	-0
4	51*	-60
5	81	69
6	36*	-36
7	53*	37
8	65	78
9	28*	-6
10	139	-133
11	27*	-36
12	25*	25
13	26*	-14
K= 19, L= 6		
1	63*	61
2	49*	43
3	286	285
4	245	240
5	242	-234
6	37*	31
7	131	138
8	132	155
9	214	-217
10	67	42
11	40*	-49
K= 20, L= 6		
0	206	-203
1	157	166
2	95	101
3	109	94
4	92	-97
5	197	192
6	28*	0
7	145	148
8	114	128
9	25*	13
10	58	-62
K= 21, L= 6		
1	129	-135
2	34*	62
3	134	168
4	44*	28
5	194	-195
6	113	-33
7	206	200
8	72	85
K= 22, L= 6		
0	167	-168
1	66	77
2	29*	42
3	30*	9
4	51*	-55
5	48*	62
6	27*	-30
K= 1, L= 7		
1	519	522
2	445	-435
3	351	338
4	664	651
5	239	228
6	435	-429
7	502	-489
8	581	568
9	270	-250
10	151	-147
11	126	-112
12	48*	45
13	225	-234
14	79	78
15	68	45
16	304	-300
17	34*	4
18	153	163
19	92	89
K= 2, L= 7		
0	218	-216
1	213	192
2	90	61
3	397	391
4	150	-140
5	496	485
6	37*	-35
7	366	343
8	348	343
9	193	193
10	216	-216
11	204	-185
12	228	218
13	165	-153
14	97	93
15	296	-287
16	31*	-3
17	149	-141
18	28*	-3
19	85	-100
K= 3, L= 7		
1	179	-178
2	431	-427
3	253	-261
4	471	467
5	106	92
6	532	-521
7	37*	-41
8	514	506
9	283	269
10	205	-203
11	36*	9
12	156	-160
13	162	-177
14	136	130
15	69	49
16	175	-176
17	41*	-31
18	139	145
19	51	-45
K= 4, L= 7		
0	372	-363
1	177	176
2	203	193
3	345	340
4	193	-183
5	425	417
6	43*	-47
7	C32*	304
8	139	131
9	217	234
10	115	-101
11	71*	-46
12	311	309
13	53*	6
14	33*	-8
15	132	-117
16	30*	-9
17	42*	-40
18	70	-81
19	27*	-32
K= 5, L= 7		
1	719	-714
2	317	-314
3	397	-393
4	453	440
5	192	30
6	692	-672
7	707	178
8	274	262
9	499	489
10	143	-134
11	307	307
12	67*	80
13	186	187
14	176	171
15	123	127
16	140	-149
17	49*	-17
18	83	70
19	92	-87
K= 6, L= 7		
0	458	-452
1	298	-297
2	112	101
3	197	-176
4	218	-228
5	339	-329
6	114	104
7	317	-325
8	38*	18
9	38*	-41
10	237	-240
11	90	-88
12	181	187
13	166	164
14	133	-125
15	63*	57
16	64	71
17	77	96
18	26*	-43
19	75	89
K= 7, L= 7		
1	135	-127
2	347	-337
3	46*	-4
4	325	315
5	79	68
6	543	-543
7	75*	-73
8	263	255
9	123	120
10	130	-125
11	195	122
12	34*	3
13	172	169
14	178	173
15	48*	37
16	77	-66
17	52*	-62
18	141	142
K= 8, L= 7		
0	115	-107
1	440	-441
2	609	595
3	231	-275
4	273	-213
5	510	-524
6	63*	4
7	386	-391
8	109	108
9	72*	-55
10	247	-230
11	35*	-35
12	239	238
13	214	206
14	130	-117
15	190	201
16	59*	48
17	66	41
18	27*	40
K= 9, L= 7		
1	427	419
2	290	-282
3	250	249
4	240	225
5	37*	-7
6	328	-328
7	154	-149
8	146	132
9	275	-268
10	43*	-10
11	211	-204
12	33*	-45
13	118	-125
14	87	87
15	38*	-39
16	169	-171
17	25*	39
18	63	95
K= 10, L= 7		
0	227	-222
1	244	-245
2	559	570
3	197	189
4	403	-410
5	83	-78
6	69*	44
7	64*	-72
8	99	99
9	91	89
10	389	-390
11	141	-134
12	186	181
13	49*	34
14	129	-129
15	68	-8
16	56	-42
17	23*	-14
K= 11, L= 7		
1	311	310
2	209	225
3	47*	23
4	271	261
5	36*	-11
6	134	-129
7	98	-93
8	158	159
9	284	-289
10	33*	-50
11	278	-287
12	79	-60
13	173	-185
14	58*	75
15	28*	-33
16	49*	-74
17	34*	46
K= 12, L= 7		
0	326	-306
1	127	122
2	355	348
3	437	442
4	201	-194
5	323	316
6	77	-85
7	156	142
8	137	117
9	177	171
10	216	-220
11	128	-129
12	233	232
13	70	-73
14	112	-117
15	154	-153
16	27*	64
K= 13, L= 7		
1	41*	52
2	35*	-28
3	64*	56
4	84	53
5	43*	30
6	116	126
7	234	249
8	143	139
9	37*	21
10	55*	-52
11	93	104
12	90	-108
13	48*	25
14	45*	20
15	26*	-31
K= 14, L= 7		
0	397	-382
1	35*	-42
2	163	157
3	221	211
4	189	-183
5	234	241
6	66*	-56
7	189	205
8	251	254
9	185	186
10	132	-135
11	90	-94
12	279	219
13	34*	24
14	118	-135
K= 15, L= 7		
1	365	-369
2	37*	58
3	193	-219
4	51*	53
5	130	-122
6	33*	-13
7	187	185
8	30*	-8
9	127	128
10	28*	16
11	181	169
12	33*	-40
13	194	197
14	77	81
K= 16, L= 7		
0	443	-452
1	133	-125
2	281	277
3	190	-202
4	69	-42
5	145	-140
6	30*	-36
7	74	-69
8	214	219
9	45*	36
10	148	-149
11	41*	-63
12	247	240
13	86	99
K= 17, L= 7		
1	120	-124
2	84	-79
3	32*	-40
4	46*	-17
5	154	-155
6	120	-123
7	144	153
8	73	-84
9	27*	29
10	26*	22
11	49*	36
K= 18, L= 7		
0	235	-233
1	56*	-48
2	172	147
3	95	-97
4	122	-109
5	264	-261
6	73	-73
7	197	-203
8	91	93
9	25*	-41
10	220	-220
K= 19, L= 7		
1	98	107
2	48*	26
3	167	163
4	86	-101
5	107	-98
6	26*	24
7	26*	56
8	46*	-53
K= 20, L= 7		
0	88	-77
1	29*	-41
2	225	222
3	78	79
4	66	-43
5	45*	-55
6	27*	-21
K= 21, L= 7		
1	110	118
2	113	125
3	152	151
K= 0, L= 8		
0	78	121
1	467	-449
2	110	-109
3	59*	-36
4	69*	-61
5	503	-487
6	37*	-33
7	580	-585
8	42*	22
9	35*	19
10	42*	-8
11	38*	10
12	159	164
13	447	438
14	72	79
15	28*	15
16	27*	-1
17	147	144
K= 1, L= 8		
1	227	218
2	50*	2
3	194	189
4	37*	-39
5	36*	-11
6	94	-81
7	79	-27
8	49*	-50
9	238	-229
10	106	-121
11	229	-224
12	33*	49
13	43*	-38
14	35*	-23
15	28*	-14
16	27*	3
17	42*	58
K= 2, L= 8		
0	163	173
1	524	-520
2	101	-99
3	66*	58
4	51*	74
5	206	-193
6	37*	-20
7	281	-277
8	35*	-10
9	180	174
10	56*	-58
11	263	-264
12	38*	-16
13	228	223
14	39*	34
15	62	-57
16	27*	-15
17	66	69
K= 3, L= 8		
1	582	575
2	37*	-2
3	509	510
4	37*	2
5	117	-101
6	36*	-16
7	128	-107
8	50*	25
9	292	-274
10	35*	-39
11	289	-286
12	60*	63
13	87	-74
14	40*	41
15	82	-87
16	31*	45
17	75	73
K= 4, L= 8		
0	45*	0
1	536	-533
2	81	61
3	388	384
4	63*	56
5	352	355
6	56*	29
7	118	106
8	52*	-30
9	378	383
10	75	69
11	270	-261
12	44*	-52
13	43*	18
14	41*	-22
15	269	-265
16	26*	2
17	171	-176
K= 5, L= 8		
1	40*	-21
2	99	-100
3	41*	36
4	240	250
5	302	-306
6	87	-86
7	137	139
8	35*	-19
9	106	-98
10	34*	3
11	128	-134
12	43*	-29
13	30*	5
14	28*	-9
15	135	-145
16	52*	-45
17	35*	18
K= 6, L= 8		
0	68*	-50
1	257	-253
2	59*	37
3	655	652
4	93	-118

Table 4 (*cont.*)

K= 0, L= 0		
2	343	-345
4	730	718
6	630	-623
8	1614	-1660
10	323	290
12	1662	-1685
14	358	354
16	197	-200
18	101	102
20	561	557
22	38*	-16
24	190	168
K= 1, L= 0		
2	1414	1422
4	504	463
6	1287	1288
8	1240	1225
10	244	216
12	444	-441
14	289	-292
16	500	-495
18	296	-249
20	196	-185
22	54*	44
24	47	68
K= 2, L= 0		
0	2319	2471
2	2098	-2124
4	748	730
6	48	46
8	1832	-1831
10	202	228
12	1287	-1298
14	405	420
16	193	-200
18	63*	-37
20	358	355
22	124	-114
24	161	166
K= 3, L= 0		
2	946	943
4	3130	3200
6	1441	1464
8	1821	1813
10	819	-739
12	396	-375
14	611	-616
16	663	-644
18	179	-163
20	234	-212
22	28*	40
24	112	126
K= 4, L= 0		
0	866	-855
2	2879	-2856
4	769	770
6	591	591
8	194	190
10	1530	1586
12	116	-114
14	1137	1133
16	557	-581
18	214	-206
20	38*	13
22	352	-330
24	36*	42
K= 5, L= 0		
2	387	-389
4	1071	1116
6	571	-576
8	1036	1302
10	382	-337
12	114	-111
14	106	89
16	80*	-53
18	86	74
20	139	-139
22	39*	-12
24	45*	60
K= 6, L= 0		
0	84	80
2	2674	-2741
4	316	-300
6	325	310
8	368	340
10	1982	1996
12	31*	-31
16	246	-260
18	250	-244
20	119	-126
22	346	-313
24	24*	13
K= 7, L= 0		
2	1586	-1615
4	360	327
6	2288	-2307
8	193	-185
10	288	-303
12	355	365
14	905	901
16	137	138
18	609	586
20	144	-174
22	27*	-12
24	70	-93
K= 8, L= 0		
0	2069	2048
2	792	-800
4	24*	25
6	569	531
8	956	-960
10	522	521
12	476	-506
14	763	767
16	135	127
18	154	-152
20	179	124
22	79	-79
24	126	135
K= 9, L= 0		
2	1166	-1167
4	26*	24
6	2830	-2796
8	131	137
10	503	-509
12	59*	-50
14	576	562
16	113	-104
18	448	427
20	35*	-48
22	37*	10
K= 10, L= 0		
0	1665	1694
2	364	371
4	844	851
6	555	-534
8	1111	-1144
10	452	-458
12	1028	-1040
14	343	-318
16	109	-109
18	88	96
20	264	270
22	55*	47
K= 11, L= 0		
2	104	-125
4	2029	2035
6	670	-655
8	783	797
10	390	-386
12	237	-234
14	421	406
16	393	-389
18	156	155
20	99	-100
22	29*	75
K= 12, L= 0		
0	517	540
2	126	137
4	917	888
6	186	-165
8	247	-261
10	138	-109
12	500	-507
14	305	-293
16	143	154
18	86	102
20	153	147
22	27*	9
K= 13, L= 0		
2	60	-50
4	2020	2037
6	74	41
8	1033	1055
10	306	-306
12	270	-259
14	34*	-16
16	488	-476
18	112	128
20	246	-237
22	25*	59
K= 14, L= 0		
0	392	-392
2	477	-478
4	58*	33
6	242	232
8	155	161
10	618	620
12	162	149
14	82	88
16	87	101
18	112	-114
20	89	-71
K= 15, L= 0		
2	330	-337
4	556	580
6	667	-654
8	644	641
10	98	-87
12	68*	20
14	109	-112
16	415	-393
18	145	149
20	114	-123
K= 16, L= 0		
0	799	-799
2	337	-323
4	442	-427
6	68*	66
8	385	377
10	464	466
12	240	217
14	81	-83
16	30*	-4
18	91	-100
20	68	-85
K= 17, L= 0		
2	670	-625
4	324	319
6	978	-974
8	230	227
10	194	-195
12	198	205
14	424	438
16	85	-83
18	267	255
K= 18, L= 0		
0	598	-591
2	202	196
4	85	-78
6	72	-71
8	47*	40
10	167	-172
12	51*	35
14	88	111
16	63	54
18	86	106
K= 19, L= 0		
2	643	-626
4	108	99
6	672	-664
8	72	63
10	194	-191
12	191	-198
14	373	383
16	33*	-16
K= 20, L= 0		
0	187	-190
2	713	710
4	151	150
6	122	-111
8	44*	-60
10	332	-319
12	114	-114
14	201	-213
16	57	62
K= 21, L= 0		
2	190	-186
4	557	553
6	183	-179
8	146	140
10	29*	-33
12	77	-78
14	63	18
K= 22, L= 0		
0	171	170
2	271	265
4	31*	20
6	34*	12
8	60	48
10	221	-215
12	42*	56
14	130	-134
K= 23, L= 0		
2	32*	7
4	309	292
6	32*	2
8	248	261
10	85	89
12	47*	-58
K= 24, L= 0		
0	413	-419
2	140	-160
4	106	-114
6	33*	36
8	83	120
10	120	-134
K= 25, L= 0		
2	108	-117
4	138	127
6	27*	-37
8	177	137
K= 26, L= 0		
0	140	-109
2	77	101
4	113	-129
6	45*	41
K= 1, L= 1		
1	936	951
2	766	-751
3	1179	-1181
4	352	-361
5	1779	1771
6	1685	-1688
7	1470	-1482
8	191	-214
9	785	792
10	841	-797
11	394	348
12	91	111
13	231	-236
15	676	667
16	526	515
17	597	-594
18	265	237
19	200	193
20	60*	41
21	127	-132
22	50*	-42
23	32*	-12
24	57*	-42
25	81	72
K= 2, L= 1		
0	1647	1592
1	1037	1044
2	2255	2239
3	363	-358
4	1139	1148
5	559	-534
6	512	-498
7	544	-538
8	551	-575
9	438	410
10	753	-794
11	125	-77
12	799	-786
13	248	260
14	439	-417
15	49*	-29
16	34*	55
17	50*	17
18	323	338
19	38*	7
20	171	150
21	57*	-45
22	182	163
23	26*	30
24	68	61
25	66	-67
K= 3, L= 1		
1	620	-626
2	1036	1000
3	1262	-1293
4	243	234
5	1678	1694
6	292	303
7	1551	-1562
8	292	291
9	116	137
10	243	225
11	160	-157
12	68	-65
13	506	-504
14	256	-258
15	721	713
16	335	-346
17	476	-479
18	34*	34
19	230	230
20	137	-135
21	31*	-47
22	54*	44
23	25*	33
24	76*	2
25	81	74
K= 4, L= 1		
0	1619	-1570
1	154	120
2	1271	1315
3	992	987
4	195	147
5	536	-514
6	140	143
7	675	-655
8	823	-809
9	236	226
10	802	-807
11	614	-586
12	524	-525
13	402	398
14	189	-165
15	116	-89
16	57*	-23
17	61*	63
18	127	135
19	152	143
20	137	131
21	45*	-18
22	113	49
23	55	45
24	68	66
K= 5, L= 1		
1	2506	2424
2	557	564
3	1150	-1164
4	1569	1608
5	1019	1098
6	916	920
7	1471	-1485
8	1139	1147
9	951	939
10	156	157
11	260	-268
12	330	-335
13	419	-418
15	323	317
16	603	-600
17	386	-384
18	191	-167
19	269	284
20	109	-91
21	58*	-50
22	29*	45
23	61*	-35
24	63	71
K= 6, L= 1		
0	944	-943
1	104	62
2	1145	-1117
3	997	995
4	600	-597
5	176	165
6	184	182
7	70	-73
8	682	699
9	769	762
10	369	376
11	759	-749
12	366	370
13	364	356
14	78	74
15	105	95
16	146	-152
17	236	-237
18	158	-169
19	35*	34
20	129	-112
21	104	-101
22	114	-73
23	108	114
24	47*	-65
K= 7, L= 1		
1	41*	4
2	207	211
3	544	-558
4	1467	1460
5	696	721
6	197	193
7	1040	-1055
8	442	440
9	637	599
10	59*	37
11	88	-74
12	334	-323
13	307	-300
14	324	329
15	316	321
16	135	-127
17	189	-193
18	135	-121
19	176	187
20	49*	-28
21	64	-76
22	26*	6
23	38*	-17
24	23*	27
K= 8, L= 1		
0	1090	-1095
1	1059	-1097
2	1082	-1085
3	1271	1264
4	403	-431
5	25*	14
6	201	193
7	80	-88
8	1000	1026
9	674	672
10	912	920
11	869	-876
12	841	839
13	343	328
14	143	123
15	112	-85
16	283	268
17	102	-97
18	161	-173
19	84	79
20	257	-254
21	169	-161
22	132	-123
23	98	108
24	75	-70
K= 9, L= 1		
1	182	172
2	764	-760
3	742	-742
4	620	-639
5	1008	976
6	1220	-1216
7	787	-796
8	543	-538
9	557	575
10	142	-125
11	37*	88
12	32*	187
13	95	85
14	545	552
15	290	293
16	216	222
17	315	-320
18	207	204
19	145	150
20	29*	-25
21	90	-103
22	28*	-33
23	28*	-1
K= 10, L= 1		
0	730	-723
1	770	-796
2	161	-55
3	633	651
4	197	154
5	934	-853
6	82	73
7	282	-284
8	53*	-19
9	765	780
10	31*	14
11	700	-705
12	139	124
13	222	209
14	131	-126
15	41*	-45
16	169	176
17	117	-108
18	82	86
19	114	98
20	38*	-25
21	143	-140
22	27*	1
23	77	81
K= 11, L= 1		
1	251	-251
2	542	-601
3	686	-660
4	1315	-1290
5	471	466
6	930	-938
7	473	-460
8	514	-513
9	439	442
10	213	-208
11	34*	35
12	343	362
13	338	-346
14	34*	37
15	33*	24
16	274	265
17	86	-113
18	279	271
19	64	59
20	87	63
21	96	-53
22	56	-44
K= 12, L= 1		
0	552	569
1	1047	-1071
2	1011	1005
3	835	827
4	411	403
5	62*	-75
6	308	-290
7	373	-384
8	465	-483
9	546	548
10	810	-828
11	710	-714
12	410	-412
13	676	689
14	395	-389
15	60*	54
16	65*	-49
17	142	157
18	142	200
19	161	162
20	179	187
21	166	-164
22	119	126
K= 13, L= 1		
1	293	279
2	74	-70
3	252	-245
4	237	218
5	623	593
6	308	275
7	244	-238
8	147	146
9	59*	68
10	50*	-53
11	82	-79
12	103	87
13	87	91
14	123	-120
15	288	300
16	95	-107
17	31*	-20
18	65	61
19	57	65
20	25*	4
21	26*	-30
22	24*	48
K= 14, L= 1		
0	573	562
1	839	-836
3	364	335
4	75	33
5	439	-420
6	53*	44
7	433	-433
8	181	-179
9	488	489
10	562	-557
11	742	-729
12	329	-307
13	368	366
14	91	-69
15	141	-157
16	32*	-29
17	30*	4
18	82	86
19	90	77
20	125	91
21	86	-98
K= 15, L= 1		
1	32*	33
2	308	315
3	195	203
4	860	842
5	91	75
6	652	652
7	239	-214
9	76	-65
10	83	88
11	170	-170
12	321	-332
13	140	-138
14	198	-205
15	137	-135
16	272	-275
17	28*	15
18	142	-141
19	32*	26
20	28*	-21
K= 16, L= 1		
0	343	-330
1	706	-706
2	148	131
3	701	688
4	254	-250
5	81	49
6	115	115
7	199	-196
8	274	277
9	434	431
10	196	197
11	407	-408
12	196	198
13	395	401
14	61*	31
15	263	-282
16	29*	-27
17	27*	5
18	65	-61
19	77	77
20	98	-114
K= 17, L= 1		
1	36*	-9
2	133	144
5	49*	-9
6	193	183
7	95	104
8	176	186
9	33*	-2
10	149	152
11	143	-137
12	76	-60
13	84	73
14	125	-122
15	79	-102
16	172	-177
17	68	61
18	118	-117
19	24*	31
K= 18, L= 1		
0	897	-888
1	583	-583
2	448	-437
3	515	511
4	200	-196
5	34*	-20
6	33*	24
7	87	-64
8	367	357
9	369	368
10	238	233
11	353	-340
12	363	354
13	248	235
14	50*	27
15	172	-182
16	48*	-45
17	27*	4
18	43*	-60
K= 19, L= 1		
1	332	-317
2	217	-217
3	34*	65
4	280	-281
5	125	-119
6	181	-174
7	156	161
8	155	-151
9	32*	-30
10	66*	66
11	36*	-29
12	144	142
13	88	82
14	116	119
15	91	-74
16	69	78
17	60	72
K= 20, L= 1		
0	289	-283
1	611	-613
2	215	-207
3	351	340
4	55*	-29
5	64*	-55
6	33*	33
7	128	-133
8	84	77
9	193	195
10	49*	-47
11	217	-210
12	152	151
13	170	167
14	56	52
15	105	-125
16	89	48
K= 21, L= 1		
1	72	68
2	291	-285
3	149	144
4	367	-369
5	216	-213
6	236	-234
7	286	290
8	205	-198
9	29*	-7
10	51*	-44
11	84	87
12	61	52
13	53*	55
14	105	113
15	57	-82
K= 22, L= 1		
0	501	525
1	439	-443
2	263	262
3	258	249
4	40*	-34
5	112	-104
6	34*	-25
7	145	-140
8	86	-93
9	144	143
10	157	-153
11	96	-94
12	28*	-37
13	155	181
14	37*	-56
K= 23, L= 1		
1	129	-133
2	69	65
3	81	77
4	48*	-32
5	237	-230
6	71	-77
7	152	153
8	26*	0
9	149	-161
10	134	-29
11	30*	-1
12	24*	20
13	191	49
K= 24, L= 1		
0	198	199
1	248	-254
2	185	182
3	27*	-13
4	41*	11
5	42*	-44
6	57	-65
7	29*	-44
8	96	-94
9	98	70
10	148	-161
11	107	-107
K= 25, L= 1		
1	54*	-37
2	144	161
3	180	186
4	56*	67
5	157	-153
6	135	149
7	184	197
8	48*	74
9	140	-167
K= 26, L= 1		
0	195	-224
1	81	-82
2	59	64
3	68	68
4	24*	-6
5	23*	24
6	22*	-14
K= 0, L= 2		
0	527	519
1	535	504
2	2878	-2937
3	1537	1579
4	78	-103
5	472	458
6	442	433
7	437	429
8	840	817
9	407	417
11	602	-565
12	58*	-17
13	74	70
14	1032	1023
15	469	-466
16	467	-488
17	57*	52
18	194	-189
19	54*	-46
20	31*	-28
21	94	-54
22	438	-426
23	72	87
24	25*	3
K= 1, L= 2		
1	873	863
2	1768	-1744
3	765	-773
4	1152	-1138
5	238	-240
6	867	-867
7	143	138
8	136	-144
9	975	919
10	28*	9
11	170	157
12	134	124
13	170	160
14	399	400
15	107	-106
16	370	367
17	34*	-4
18	105	85
19	98	-97
20	33*	17
21	61*	-53
22	39*	-43
23	67	-67
24	26*	-16
K= 2, L= 2		
0	843	829
1	1003	971
2	3089	-3176
3	969	977
4	306	285
5	631	605
6	118	128
7	173	-172
8	447	-458
9	447	460
10	1213	1229
11	491	-454
12	591	-598
13	252	251
14	625	626
15	83	-86
16	200	-215
17	105	-101
18	107	-105
19	32*	-24
20	94	94
21	107	-97
22	245	-231
23	70	75
24	74	58
K= 3, L= 2		
1	757	-741
2	2616	-2577
3	95	-100
4	634	-647
5	595	-611
6	1920	-1945
7	448	441
8	653	-654
9	765	725
10	438	-433
11	430	440
12	403	404
13	305	300
14	717	713
15	109	92
16	430	425
17	120	117
18	500	493
19	170	-183
20	32*	19
21	99	-97
22	37*	-41
23	48*	-59
24	78	-68
K= 4, L= 2		
0	6647	6620
1	1769	-1718
2	595	-586
3	53	-24
4	806	808
5	705	-687
6	251	259
7	677	-635
8	1471	-1470
9	230	236
10	170	159
11	453	-443
12	1127	-1134
13	398	396
14	474	490
15	114	109
16	122	-118
17	36*	2
18	50*	24
19	96	94
20	376	363
21	84	-95
22	50*	-20
23	29*	15
24	123	135
K= 5, L= 2		
1	1802	-1739
2	218	-209
3	257	238
4	108	119
5	45*	-43
6	1465	-1402
7	123	110
8	521	508
9	99	-97
10	259	-249
11	265	-248
12	129	-126
13	57*	-24
14	201	178
15	194	-191
16	199	-189
17	83	78
18	229	218
19	35*	43
20	103	-110
21	29*	-14
22	27*	17
23	28*	-5
24	28*	-18
K= 6, L= 2		
0	2312	2236
1	1331	-1277
2	294	168
3	399	378
4	917	911
5	803	-775
6	137	-126
7	451	-451
8	1591	-1574
9	157	-124
10	273	-274
11	368	-355
12	1270	-1294
13	216	209
14	49*	-21
15	367	366
16	188	-184
17	167	162
18	47*	80
19	156	156
20	335	333
21	28*	-48
22	25*	11
23	28*	1
24	148	140
K= 7, L= 2		
1	620	594
2	167	155
3	1038	1010
4	2605	2569
5	49*	-45
6	335	338
7	124	-95
8	1400	1394
9	213	-216
10	430	-405
11	229	-226
12	256	-261
13	259	-265
14	145	-144
15	284	-283
16	533	-517
17	237	246
18	38*	29
19	72	56
20	202	-189
21	98	91
22	35*	48
23	65	71
24	90	101
K= 8, L= 2		
0	38*	77
1	240	-236
2	975	-951
3	596	569
4	1014	1008
5	251	238
6	194	231
7	28*	-10
8	264	-254
9	241	237
10	381	414
11	31*	-134
12	350	-363
13	183	181
14	408	417
15	34*	-26
16	97	-89
17	68*	56
18	88	-81
19	52*	26
20	89	71
21	79	-83
22	63	-65
23	127	65
K= 9, L= 2		
1	140	145
2	219	-204
3	401	413
4	1914	1917
5	153	81
6	217	-207
7	116	121
8	1071	1045
9	487	-466
10	182	-176
11	44*	-55
12	204	-199
13	183	-177
14	113	-106
15	110	139
16	598	-593
17	169	170
18	40*	53
19	41*	-34
20	193	-177
21	57	52
22	48*	75
23	98	99
K= 10, L= 2		
0	377	-374
1	259	-258
2	1353	-1360
3	245	277
4	167	-178
5	162	193
6	294	283
7	168	176
8	395	382
9	333	326
10	1164	1185
11	233	-235
12	177	108
13	114	-106
14	273	267
15	470	-483
16	46*	-34
17	92	-74
18	185	-194
19	29*	-12
20	116	-109
21	50*	-35
22	194	-188
23	39*	28
K= 11, L= 2		
1	342	-340
2	784	-786
3	60	60
4	628	632
5	184	-188
6	1211	-1194
7	333	332
8	425	404
9	64*	27
10	102	-111
11	90	91
12	218	224
13	97	-74
14	307	304
15	146	-150
16	284	-281
17	59*	43
18	306	307
19	98	-107
20	124	-126
21	28*	-5
22	26*	3
K= 12, L= 2		
0	121	-116
1	185	-183
2	555	-573
3	134	137
4	361	-345
5	321	299
6	135	133
7	56*	39
8	123	98
9	194	191
10	592	578
11	60*	-70
12	142	120
13	184	201
14	210	206
15	182	-203
16	81	75
17	73	-63
18	101	-100
19	27*	-5
20	25*	-13
21	29*	-11
22	32*	-116
K= 13, L= 2		
1	714	-697
2	904	-908
3	185	174
4	148	134
5	389	-373
6	1693	-1635
7	463	452
8	158	150
9	98	99
10	380	-376
11	106	95
12	134	137
13	173	165
14	531	519
15	166	-177
16	45*	2
17	143	136
18	348	340
19	85	-88
20	41*	-83
21	36*	-12
K= 14, L= 2		
0	231	233
1	274	-259
2	373	368
3	152	-149
4	265	251
5	40*	-11
6	331	-317
7	164	-161
8	380	-380
9	34*	-20
10	285	-273
11	53*	-32
12	156	-173
13	284	293
14	33*	-18
15	32*	19
16	31*	9
17	109	114
18	57	59
19	25*	14
20	83	77
21	21*	-5
K= 15, L= 2		
1	182	-175
2	526	-531
3	333	328
4	564	548
5	212	-205
6	888	-882
7	283	281
8	282	285
9	86	-88
10	249	-246
11	57*	-50
12	173	-189
13	210	227
14	357	357
15	42*	-37
16	151	-153
17	111	120
18	203	200
19	38*	2
20	24*	-34
K= 16, L= 2		
0	233	223
1	203	-196
2	711	703
3	181	-179
4	255	251
5	344	-339
6	177	-164
7	129	-127
8	172	-175
9	86	-80
10	304	-291
11	59*	45
12	327	-326
13	74	-83
14	308	-313
15	30*	-17
16	79	91
17	45*	48
18	90	101
19	96*	66
K= 17, L= 2		
1	326	319
2	176	-176
3	360	324
4	1050	1038
5	330	-331
6	74	-62
7	111	111
8	522	510
9	209	-212
10	90	-101
11	45*	-52
12	158	-155
13	48*	-31
14	30*	27
15	137	-147
16	269	-269
17	48*	51
18	100	113
19	22*	-29
K= 18, L= 2		
0	108	-105
1	231	-226
2	138	139
3	174	161
4	86*	-66
5	33*	-13
6	90	95
7	73	24
8	65*	66
9	80	81
10	37*	-15
11	120	127
12	46*	57
13	30*	-18
14	88	-80
15	101	-100
16	30*	64
17	72	-87
18	25*	-10
K= 19, L= 2		
1	57*	-56
2	143	-102
3	79	-35
4	473	452
5	145	-138
6	91	-94
7	168	169
8	435	426
9	214	-223
10	31*	-8
11	97	-98
12	102	-101
13	35*	-18
14	75	-75
15	44*	-51
16	272	-271
17	76*	37
K= 20, L= 2		
0	657	-650
1	34*	-27
2	171	-127
3	57*	42
4	183	-173
5	175	180
6	45*	42
7	138	139
8	218	211
9	66	45
10	50*	41
11	36*	-52
12	257	256
13	69	-68
14	58*	-65
15	26*	26
16	87	-18
K= 21, L= 2		
1	61*	-31
2	183	-146
3	103	98
4	217	205
5	143	-147
6	298	-292
7	235	229
8	158	147
9	61	-77
10	28*	-46
11	126	141
12	48*	50
13	34*	54
14	162	175
15	23*	-14
K= 22, L= 2		
0	338	-319
1	61*	67
2	111	126
3	75	-68
4	153	-147
5	43*	39
6	40*	-27
7	57*	56
8	209	207
9	26*	-15
10	40*	-47
11	28*	13
12	210	219
13	25*	3
K= 23, L= 2		
1	32*	0
2	200	-193
3	29*	-3
4	64	-61
5	135	-132
6	321	-327
7	139	134
8	26*	27
9	44*	-1
10	42*	-55
11	77	96
12	23*	-25
K= 24, L= 2		
0	237	-240
1	170	191
2	238	234
3	113	-120
4	30*	-35
5	79	-85
6	85	-101
7	28*	-16
8	42*	44
9	33*	-16
10	176	-186
K= 25, L= 2		
1	54*	-88
2	111	-104
3	28*	24
4	75	70
5	82	-80
6	113	-128
7	24*	15
8	22*	-33
K= 26, L= 2		
0	52	70
1	36*	46
2	239	236
3	122	-136
4	26*	2
5	53	-59
K= 1, L= 3		
1	458	468
2	251	238
3	482	-488
4	1500	1567
5	1284	1306
6	122	106
8	1274	1284
9	121	114
10	397	-363
11	503	-513
12	265	-274
13	677	-667
14	203	-196
15	404	414
16	469	-457
17	325	-318
18	33*	22
19	278	277
20	176	-163
21	49*	12
22	35*	37
23	27*	35
24	53	51
K= 2, L= 3		
0	1387	-1409
1	908	-875
2	309	-338
3	1305	1299
4	574	-584
5	883	870
6	289	281
7	665	658
8	568	592
9	356	347
10	667	674
11	403	-391
12	778	730
13	112	-104
14	317	306
15	54*	-14
16	201	-221
17	270	-273
18	168	-169
19	32*	-3
20	166	-156
21	44*	-4
22	134	-112
23	55	60
24	88	-64
K= 3, L= 3		
1	230	-209
2	103	-111
3	498	-532
4	788	774
5	1145	1167
6	1127	-1134
7	861	-884
8	679	637
9	941	918
10	309	-308
11	162	158
12	168	-142
13	133	-128
14	611	617
15	394	393
16	48*	25
17	244	-244
18	93	84
19	103	95
20	96	-117
21	92	-95
22	26*	2
23	34*	-22
24	23*	-4
K= 4, L= 3		
0	2626	-2553
1	68	-76
2	338	-333
3	943	926
4	186	-192
5	253	254
6	379	330
7	381	-350
8	243	257
9	501	509
10	218	221
11	191	-182
12	512	507
13	102	92
14	217	186
15	211	-202
16	233	227
17	277	-278
18	76	-79
19	48*	74
20	164	-169
21	52*	-46
22	31*	-9
23	79	71
24	22*	-19
K= 5, L= 3		
1	276	-277
2	848	-837
3	1074	-1086
4	346	-340
5	932	924
6	2142	-2179
7	413	-424
8	165	-174
9	873	897
10	407	-401
11	617	611
12	33*	16
13	99	-89
14	583	579
15	463	457
16	134	121
17	349	-352
18	402	383
19	106	103
20	29*	-24
21	181	-195
22	25*	8
23	51*	-54
K= 6, L= 3		
0	233	209
1	540	-565
2	725	739
3	404	-353
4	201	183
5	1270	-1180
6	65	-3
7	454	-469
8	46*	19
9	523	502
10	410	-437
11	223	-235
12	405	-407
13	249	251
14	516	-509
15	61*	-65
16	135	137
17	45*	52
18	175	176
19	113	103
20	29*	28
21	77	-82
22	99	87
23	54*	26
K= 7, L= 3		
1	288	-270
2	176	86
3	1187	-1169
4	235	210
5	809	824
6	666	-679
7	833	-824
8	136	-128
9	303	327
10	87	-93
11	57*	38
12	103	95
13	439	-439
14	320	308
15	244	240
16	69	-66
17	212	-226
18	265	268
19	133	138
20	29*	-21
21	34*	-32
22	52*	23
23	72	-28
K= 8, L= 3		
0	85	134
1	771	-829
2	1537	1515
3	107	-64
4	359	336
5	510	-540
6	318	-293
7	511	-542
8	300	-289
9	222	227
10	857	-859
11	541	-536
12	166	-159
13	657	665
14	499	-493
15	142	154
16	181	195
17	222	230
18	172	175
19	208	192
20	110	113
21	82	-83
22	148	124
23	88	81
K= 9, L= 3		
1	1419	1393
2	411	-372
3	180	-175
4	1109	1109
5	697	699
6	315	296
7	715	-704
8	640	661
9	68	66
10	121	-110
11	346	-353
12	70*	-61
13	177	-174
14	178	-192
15	194	204
16	433	-450
17	68*	-72
18	45*	-10
19	157	170
20	90	-88
21	72	70
22	27*	59
K= 10, L= 3		
0	475	-464
1	436	-457
2	194	214
3	327	357
4	28*	-19
5	40*	-53
6	38*	-38
7	286	-297
8	176	188
9	609	602
10	499	-493
11	697	-696
12	211	189
13	387	379
14	181	-172
15	163	-160
16	55*	-46
17	101	-107
18	30*	22
19	99	79
20	26*	8
21	79	-80
22	66	56
K= 11, L= 3		
1	516	508
2	209	219
3	207	204
4	845	864
5	163	175
6	350	347
7	421	-426
8	589	589
9	38*	-58
10	65*	54
11	389	-391
12	351	-355
13	200	-187
14	177	-171
15	33*	1
16	315	-301
17	37*	-42
18	112	-110
19	140	154
20	51	-37
21	29*	-26
22	57	-1
K= 12, L= 3		
0	992	-999
1	737	-735
2	76	57
3	884	903
4	480	-483
5	308	309
6	65	57
7	294	279
8	657	655
9	638	639
10	314	319
11	526	-528
12	505	505
13	99	84
14	207	-225
15	348	-357
16	70	56
17	130	-141
18	57*	-65
19	26*	24
20	171	-172
21	115	-117
K= 13, L= 3		
1	202	-185
2	100	-100
3	158	-155
4	255	251
5	167	155
6	192	-178
7	74	-57
8	88	90
9	173	180
10	97	88
11	59*	-54
12	166	181
13	256	270
14	88	94
15	81	-62
16	57*	-48
17	133	-146
18	59	68
19	29*	13
20	60*	-76
21	23*	-29
K= 14, L= 3		
0	1342	-1326
1	677	-626
2	227	-226
3	685	692
4	383	-390
5	91	-82
6	223	224
7	33*	47
8	399	396
9	573	570
10	60*	44
11	368	-367
12	366	350
13	148	135
14	54*	56
15	189	-191
16	106	104
17	139	-131
18	31*	30
19	94	9
20	31*	-131
K= 15, L= 3		
1	576	-572
2	523	-508
3	418	-412
4	539	-526
5	59*	44
6	438	-436
7	171	141
8	294	-294
9	227	224
10	88	-100
11	158	160
12	121	129
13	154	151
14	119	120
15	45*	-4
16	146	157
17	27*	-58
18	189	195
19	85	-91
K= 16, L= 3		
0	255	-260
1	763	-756
2	584	567
3	368	370
4	42*	-40
5	213	-197
6	71	-65
7	328	-336
8	45*	35
9	323	311
10	341	-353
11	300	-297
12	144	153
13	384	386
14	82	-75
15	29*	39
16	27*	0
17	78	69
18	77	87
19	119	125
K= 17, L= 3		
1	218	209
2	452	-447
3	127	-122
4	242	-234
5	69*	-63
6	184	-178
7	203	208
8	207	-205
9	58*	55
10	37*	20
11	176	184
12	66*	68
13	137	135
14	72	82
15	94	107
16	32*	-38
17	55*	44
18	77	84
K= 18, L= 3		
0	321	321
1	602	-590
2	550	538
3	99	98
4	123	-119
5	442	-433
6	71	-68
7	368	-370
8	59*	-54
9	152	157
10	491	-483
11	312	-289
12	61*	-44
13	253	260
14	150	-161
15	25*	-6
16	32*	-27
17	26*	51
K= 19, L= 3		
1	108	102
2	135	122
3	194	169
4	182	178
5	227	-225
6	168	169
7	32*	-30
8	92	112
9	274	-278
10	79	77
11	93	-94
12	70	-74
13	26*	-15
14	71	-49
15	122	-117
16	50*	-67
K= 20, L= 3		
0	62*	-49
1	244	-232
2	139	179
3	203	186
4	44*	-5
5	57*	-67
6	31*	-4
7	138	-124
8	38*	31
9	113	107
10	271	-271
11	188	-189
12	78	81
13	169	191
14	67	-63
15	109	-123
K= 21, L= 3		
1	57*	49
2	215	217
3	275	279
4	135	124
5	127	-132
6	230	218
7	117	115
8	78	79
9	204	-220
10	38*	20
11	133	-138
12	60	-86
13	44*	4
14	141	-151
K= 22, L= 3		
0	230	-207
1	83	-74
2	56*	57
3	227	215
4	80	-84
5	112	118
6	28*	-11
7	97	104
8	195	205
9	130	127
10	46*	-9
11	137	-152
12	182	197
13	48*	54

Table 4 (*cont.*)

5	351	155
6	56*	41
7	146	146
8	121	-138
9	390	404
10	59*	57
11	201	-191
12	31*	-2
13	39*	37
14	31*	28
15	180	-172
16	35*	-41
17	94	-97
K= 7, L= 8		
1	394	-380
2	39*	-53
3	90	-88
4	174	179
5	243	-258
6	75*	-82
7	328	311
8	34*	-36
9	179	180
10	37*	3
11	260	256
12	30*	26
13	269	287
14	28*	-2
15	54	-44
16	27*	-56
K= 8, L= 8		
0	36*	44
1	335	-323
2	73*	54
3	105	96
4	100	-95
5	131	-121
6	87	60
7	133	-128
8	69*	71
9	151	158
10	56*	-15
11	196	-210
12	55*	43
13	127	107
14	27*	8
15	35*	-27
16	22*	-13
K= 9, L= 8		
1	222	-215
2	74*	-89
3	42*	8
4	35*	-13
5	203	-194
6	69*	54
7	302	306
8	49*	59
9	32*	34
10	42*	-43
11	205	218
12	29*	4
13	213	224
14	40*	43
15	42*	-55
K= 10, L= 8		
0	104	-94
1	299	-287
2	35*	-22
3	98	-100
4	47*	-41
5	401	-398
6	52*	-67
7	271	-254
8	91	107
9	36*	2
10	50*	-48
11	108	-119
12	40*	31
13	238	235
14	27*	-25
15	89	92
K= 11, L= 8		
1	34*	-12
2	73	-51
3	217	203
4	33*	33
5	229	-225
6	90	-88
7	138	140
8	34*	-57
9	248	-251
10	58*	-66
11	98	-104
12	28*	-14
13	26*	21
14	24*	58
K= 12, L= 8		
0	83	-78
1	172	-167
2	117	95
3	37*	-25
4	117	131
5	244	-252
6	32*	-39
7	97	-95
8	37*	5
9	29*	6
10	96	-88
11	94	-117
12	40*	19
13	112	119
K= 13, L= 8		
1	180	162
2	67	-56
3	366	373
4	144	171
5	297	-302
6	81	-91
7	90	82
8	28*	7
9	261	-259
10	28*	-8
11	183	-160
12	24*	1
13	22*	-29
K= 14, L= 8		
0	73	-81
1	71	64
2	99	80
3	207	202
4	44*	53
5	83	68
6	23*	-19
7	110	111
8	29*	11
9	65	79
10	109	-107
11	70	-64
12	24*	39
K= 15, L= 8		
1	29*	23
2	40*	-56
3	351	370
4	133	118
5	248	-263
6	52*	58
7	211	218
8	73	84
9	141	-142
10	24*	9
11	21*	1
K= 16, L= 8		
0	125	-120
1	78	88
2	68	50
3	278	296
4	119	-140
5	118	121
6	27*	22
7	132	135
8	64	79
9	55	65
K= 17, L= 8		
1	235	-235
2	61	84
3	90	96
4	26*	-26
5	218	-218
6	25*	-5
7	214	197
8	21*	3
K= 18, L= 8		
0	217	-221
1	36*	-18
2	83	94
3	33*	-63
4	62	-67
5	23*	-14
6	56	63
K= 19, L= 8		
1	165	-171
2	21*	6
K= 1, L= 9		
1	313	-293
2	166	-167
3	147	-154
4	388	382
5	138	-136
6	267	-262
7	122	96
8	283	277
9	185	190
10	145	-138
11	172	171
12	30*	4
13	85	71
14	81	75
15	35*	25
K= 2, L= 9		
0	274	-269
1	133	-112
2	64*	42
3	178	-178
4	60*	-54
5	292	-275
6	79	70
7	329	-324
8	37*	-37
9	34*	-6
10	49*	43
11	31*	13
12	97	105
13	113	106
14	25*	10
15	117	118
K= 3, L= 9		
1	130	127
2	328	-331
3	160	154
4	201	195
5	52*	-27
6	360	-355
7	33*	-21
8	210	200
9	77	-61
10	149	-160
11	47*	-35
12	30*	-1
13	45*	45
14	73	62
15	21*	-7
K= 4, L= 9		
0	135	-135
1	111	-102
2	222	219
3	233	-214
4	97	-92
5	156	-162
6	58*	64
7	149	-143
8	66	71
9	35*	39
10	116	-120
11	94	-111
12	63	63
13	50*	48
14	35*	-33
K= 5, L= 9		
1	327	326
2	219	-204
3	232	230
4	226	223
5	61*	-38
6	306	-300
7	137	-137
8	146	143
9	232	-211
10	23*	-1
11	118	-110
12	40*	42
13	82	-80
14	87	102
K= 6, L= 9		
0	139	-148
1	93	78
2	214	198
3	202	206
4	228	-235
5	104	101
6	32*	29
7	96	81
8	91	94
9	30*	-31
10	302	-317
11	92	-104
12	67	65
13	38*	-26
14	45	-55
K= 7, L= 9		
1	103	91
2	33*	-26
3	33*	16
4	268	272
5	32*	10
6	204	-211
7	59*	-52
8	144	148
9	146	-150
10	44*	-51
11	105	-103
12	74	-81
13	70	-85
K= 8, L= 9		
0	51*	-17
1	150	156
2	259	279
3	312	321
4	80	-67
5	176	159
6	31*	15
7	244	254
8	65	59
9	79	87
10	152	-153
11	29*	-12
12	177	181
13	51	-57
K= 9, L= 9		
1	227	-227
2	33*	-37
3	46*	-7
4	192	186
5	36*	-8
6	38*	-31
7	173	163
8	145	145
9	111	113
10	44*	-45
11	117	124
12	46*	-60
K= 10, L= 9		
0	280	-272
1	41*	-4
2	101	61
3	89	61
4	124	-131
5	29*	6
6	56*	32
7	60	65
8	118	123
9	28*	35
10	110	-126
11	24*	-21
12	176	177
K= 11, L= 9		
1	235	-235
2	29*	6
3	59	-5
4	80	81
5	142	-152
6	63	-50
7	168	170
8	99	110
9	80	85
10	32*	4
11	149	145
K= 12, L= 9		
0	334	-345
1	29*	-34
2	121	110
3	113	-91
4	180	-192
5	212	-212
6	49*	-3
7	165	-168
8	179	185
9	36*	-64
10	52	-72
K= 13, L= 9		
1	27*	-35
2	74	-71
3	95	90
4	83	-98
5	120	-135
6	122	-126
7	66	82
8	24*	-51
9	56	-47
K= 14, L= 9		
0	178	-185
1	27*	-25
2	243	240
3	112	-128
4	157	-164
5	95	-75
6	24*	21
7	99	-107
8	86	95
K= 15, L= 9		
1	135	136
2	35*	44
3	45	80
4	24*	-56
5	83	-79
6	24*	-41
K= 16, L= 9		
0	97	-87
1	67	65
2	231	234
3	21*	19
K= 0, L= 10		
0	31*	-13
1	173	-166
2	202	185
3	257	245
4	45*	-26
5	299	307
6	56	-57
7	29*	-2
8	28*	3
9	265	273
10	155	-150
11	145	-151
K= 1, L= 10		
1	158	-156
2	99	89
3	156	-157
4	161	168
5	111	-122
6	30*	14
7	69	52
8	41*	-27
9	59	62
10	43*	51
11	58	59
K= 2, L= 10		
0	40*	6
1	178	-171
2	108	91
3	200	194
4	70	-69
5	82	85
6	30*	25
7	74	-86
8	28*	-2
9	133	129
10	126	-131
11	128	-134
K= 3, L= 10		
1	162	-139
2	60*	59
3	91	-93
4	137	140
5	56*	-58
6	55*	52
7	122	114
8	44*	51
9	151	158
10	55	65
11	103	113
K= 4, L= 10		
0	65*	-22
1	223	-216
2	34*	-1
3	31*	-4
4	111	-92
5	156	-155
6	75	81
7	134	-141
8	80	71
9	30*	-11
10	24*	25
11	42*	-39
K= 5, L= 10		
1	70	-80
2	31*	-19
3	30*	32
4	33*	-26
5	29*	-19
6	29*	10
7	93	96
8	26*	-16
9	25*	-21
10	25*	-40
K= 6, L= 10		
0	99	-72
1	232	-231
2	30*	-50
3	30*	8
4	124	-132
5	186	-186
6	28*	-5
7	123	-117
8	67	55
9	24*	3
10	22*	3
K= 7, L= 10		
1	103	97
2	36*	52
3	189	190
4	110	-90
5	92	-94
6	73	-83
7	26*	20
8	64	-69
9	144	-135
K= 8, L= 10		
0	75	-88
1	185	-187
2	91	81
3	101	97
4	30*	1
5	50	-54
6	26*	-34
7	25*	-36
8	23*	15
9	22*	47
K= 9, L= 10		
1	89	98
2	27*	-10
3	201	202
4	47*	-37
5	156	-152
6	25*	5
7	59	78
8	28*	-31
K= 10, L= 10		
0	26*	9
1	26*	-13
2	170	170
3	188	175
4	32*	34
5	144	140
6	39*	-33
7	95	106
K= 11, L= 10		
1	104	-98
2	51*	40
3	99	92
4	37*	36
5	158	-159

Table 5. *Some results of the rigid-body analysis of dibenzoselenophene*

(*a*) Libration tensors, **L**(°)² (× 10)

Molecule *A*

$$\begin{pmatrix} 238\ (28) & 4\ (8) & 9\ (11) \\ & 83\ (7) & 31\ (7) \\ & & 135\ (8) \end{pmatrix}$$

Molecule *B*

$$\begin{pmatrix} 251\ (32) & 18\ (10) & 2\ (11) \\ & 123\ (8) & 38\ (8) \\ & & 115\ (9) \end{pmatrix}$$

(*b*) Principal axes of **L**

	Molecule *A*				Molecule *B*			
	r.m.s. amplitude (°)	Direction cosines (× 10³)			r.m.s. amplitude (°)	Direction cosines (× 10³)		
L(1)	4·9	994	044	097	5·0	986	157	060
L(2)	3·8	−106	420	902	3·9	−156	720	677
L(3)	2·6	002	−906	422	2·8	063	−676	734

(*c*) Principal axes of reduced **T**

	Molecule *A*				Molecule *B*			
	r.m.s. amplitude (Å)	Direction cosines (× 10³)			r.m.s. amplitude (Å)	Direction cosines (× 10³)		
T(1)	0·25	−999	045	020	0·25	−995	092	−032
T(2)	0·21	013	668	−745	0·22	075	526	−847
T(3)	0·19	−046	743	668	0·19	−061	845	531

(*d*) Displacement of librational axes from intersecting

Molecule *A*		Molecule *B*	
$_2\varrho_1$–$_3\varrho_1$	−0·41 Å	$_2\varrho_1$–$_3\varrho_1$	−1·03 Å
$_3\varrho_2$–$_1\varrho_2$	0·26	$_3\varrho_2$–$_1\varrho_2$	0·45
$_1\varrho_3$–$_2\varrho_3$	0·61	$_1\varrho_3$–$_2\varrho_3$	0·76

routine *SECEXT*, written by A. T. Christensen. This program is based on Zachariasen's (1963) equation and employs a least-squares successive approximation procedure.

Discussion

Views of the crystal structure of dibenzoselenophene along the crystallographic *c* and *a* axes are shown in Figs. 1 and 2 respectively and the averaged dimensions of the dibenzoselenophene molecule are shown in Fig. 3. The individual bond distances and bond angles are given in Tables 6 and 7 and are grouped so that all values for a chemically equivalent bond or angle appear together. As an aid in this comparison, Tables 6 and 7 are keyed to Fig. 3 by use of the lower-case letters *a* through *l*. Table 6 shows both the uncorrected bond distances and the values resulting from corrections for librational motion. The corrections applied to the C–C bond distances averaged 0·6σ (with a maximum correction equal to σ), but the corrections applied to the Se–C distances were about 1·7 σ. Corrections to the bond angles were in all cases less than 0·5 σ, so these corrections were omitted from Table 7.

The magnitudes and orientations of the thermal ellipsoids of the selenium and carbon atoms are shown in the *ORTEP* plots in Fig. 4 (Johnson, 1965). These plots show notable similarities in the thermal ellipsoids for corresponding atoms in the two molecules.

The individual five- and six-membered rings in the two independent molecules are closely planar. However,

Table 6. *Observed bond lengths in dibenzoselenophene* (*in* Å)*

		Molecule *A*		Molecule *B*		Average§	
	Bond†	Uncorrected	Corrected ‡	Uncorrected	Corrected	Uncorrected	Corrected
a	Se—C(1)	1·889	1·897	1·897	1·906		
a'	Se—C(12)	1·885	1·894	1·889	1·897	1·890	1·899
b	C(1)—C(2)	1·395	1·397	1·395	1·398		
b'	C(11)-C(12)	1·393	1·395	1·387	1·390	1·393	1·395
c	C(2)—C(3)	1·372	1·376	1·353	1·358		
c'	C(10)-C(11)	1·371	1·375	1·371	1·375	1·367	1·371
d	C(3)—C(4)	1·367	1·371	1·378	1·381		
d'	C(9)—C(10)	1·385	1·387	1·364	1·368	1·374	1·377
e	C(4)—C(5)	1·372	1·374	1·386	1·388		
e'	C(8)—C(9)	1·370	1·372	1·382	1·384	1·378	1·380
f	C(5)—C(6)	1·397	1·400	1·394	1·397		
f'	C(7)—C(8)	1·396	1·399	1·382	1·385	1·392	1·395
g	C(1)—C(6)	1·394	1·401	1·383	1·390		
g'	C(7)—C(12)	1·397	1·403	1·389	1·396	1·391	1·398
h	C(6)—C(7)	1·447	1·451	1·449	1·454	1·448	1·453
i	C(2)—H(2)	0·91		0·78			
i'	C(11)-H(11)	0·91		0·83		0·86	
j	C(3)—H(3)	0·84		0·94			
j'	C(10)-H(10)	1·01		0·86		0·91	
k	C(4)—H(4)	0·87		1·03			
k'	C(9)—H(9)	1·00		1·01		0·98	
l	C(5)—H(5)	1·02		0·85			
l'	C(8)—H(8)	0·95		0·88		0·93	

* Estimated standard deviations, average: Se–C, 0·005; C–C, 0·007; C–H, 0·07 Å.
† Letters are keyed to Fig. 3.
‡ Corrected for librational motion.
§ Averages of values for chemically equivalent bonds.

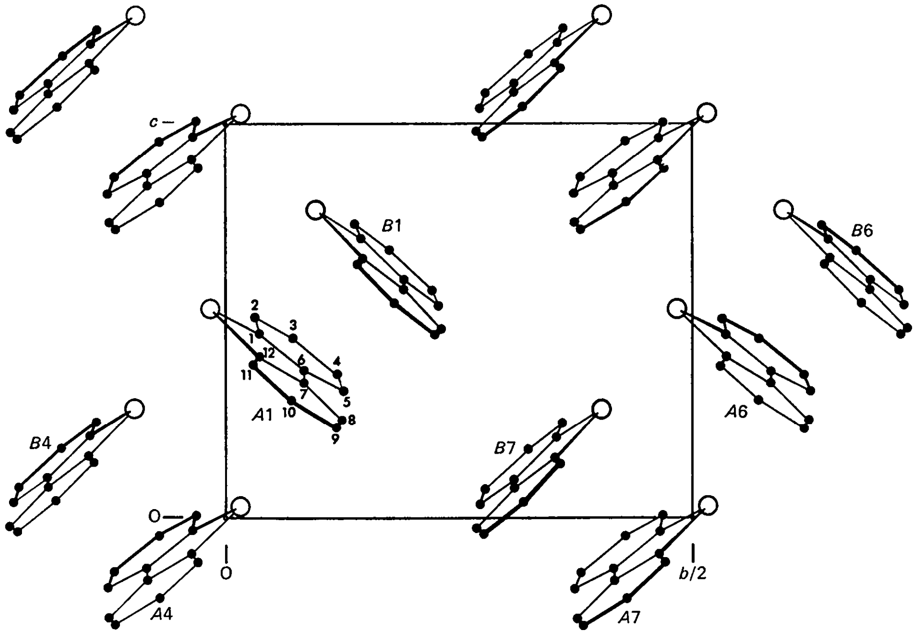

Fig. 2. Projection of a selected portion of the structure of dibenzoselenophene down **a**. The loose association of molecules *A* and *B* into pairs is indicated. Hydrogen atoms are omitted.

Table 7. *Observed bond angles in dibenzoselenophene* (*in degrees*)*

	Angle†	Molecule *A*	Molecule *B*	Average‡
a–a′	C(1)—Se——C(12)	86·7	86·6	86·7
a–g	Se——C(1)—C(6)	112·4	111·8	
a′–g′	Se——C(12)-C(7)	112·5	112·6	112·3
g–h	C(1)—C(6)—C(7)	114·2	115·1	
g′–h	C(12)-C(7)—C(6)	114·2	113·8	114·3
b–c	C(1)—C(2)—C(3)	118·4	118·8	
b′–c′	C(12)-C(11)-C(10)	118·5	119·0	118·7
c–d	C(2)—C(3)—C(4)	121·0	121·4	
c′–d′	C(11)-C(10)-C(9)	120·2	121·1	120·9
d–e	C(3)—C(4)—C(5)	121·3	119·7	
d′–e′	C(10)-C(9)—C(8)	121·6	119·6	120·6
e–f	C(4)—C(5)—C(6)	119·6	120·7	
e′–f′	C(9)—C(8)—C(7)	119·8	121·0	120·3
f–g	C(5)—C(6)—C(1)	118·4	117·3	
f′–g′	C(8)—C(7)—C(12)	117·9	118·6	118·1
g–b	C(6)—C(1)—C(2)	121·4	122·0	
g′–b′	C(7)—C(12)-C(11)	122·0	120·9	121·6
a–b	Se——C(1)—C(2)	126·2	126·2	
a′–b′	Se——C(12)-C(11)	125·5	126·5	126·1
f–h	C(5)—C(6)—C(7)	127·4	127·6	
f′–h	C(6)—C(7)—C(8)	127·9	127·6	127·6
b–i	C(1)—C(2)—H(2)	119	115	
b′–i′	C(12)-C(11)-H(11)	127	120	120
i–c	H(2)—C(2)—C(3)	123	126	
i′–c′	H(11)-C(11)-C(10)	114	121	121
c–j	C(2)—C(3)—H(3)	119	117	
c′–j′	C(11)-C(10)-H(10)	114	120	118
j–d	H(3)—C(3)—C(4)	120	122	
j′–d′	H(10)-C(10)-C(9)	125	119	122
d–k	C(3)—C(4)—H(4)	120	122	
d′–k′	C(10)-C(9)—H(9)	117	121	120
k–e	H(4)—C(4)—C(5)	118	119	
k′–e′	H(9)—C(9)—C(8)	121	119	119
e–l	C(4)—C(5)—H(5)	123	121	
e′–l′	C(9)—C(8)—H(8)	126	118	122
l–f	H(5)—C(5)—C(6)	117	118	
l′–f′	H(8)—C(8)—C(7)	114	121	118

* Estimated standard deviations, average: C–Se–C, 0·2°; Se–C–C, 0·4°; C–C–C, 0·5°; C–C–H, 3°.
† Letters are keyed to Fig. 3.
‡ Averages of values for chemically equivalent angles.

Table 8. *Plane data*

(*a*) List of least-squares planes

Plane No.	Direction cosines (×10⁴) with respect to: a	b	c	Atoms involved	r.m.s. deviations of atoms from plane, (Å×10³)
1	1668	5905	7896	Molecule *A*, selenophene ring	5
2	1594	5748	8026	Molecule *A*, C(1) through C(6)	6
3	1596	5948	7878	Molecule *A*, C(7) through C(12)	4
4	1649	5872	7925	Molecule *A*, Se and all C atoms	15
5	1179	6526	7485	Molecule *B*, selenophene ring	3
6	1350	6584	7405	Molecule *B*, C(1) through C(6)	4
7	1001	6629	7420	Molecule *B*, C(7) through C(12)	1
8	1164	6600	7422	Molecule *B*, Se and all C atoms	17

(*b*) Interplanar angles*

Planes	Angle (°)	Planes	Angle (°)
1 and 2	1·2	5 and 6	1·2
1 and 3	0·5	5 and 7	1·1
2 and 3	1·4	6 and 7	2·0
4 and 8	5·7		

* e.s.d. ~0·1°.

each molecule, as a whole, appears to be slightly but significantly bowed. The details of this analysis in terms of least-squares planes are given in Tables 8 and 9. The extent of the molecular bowing is indicated by the dihedral angles which the least-squares planes of the six-membered rings make with the least-squares planes through the respective selenophene rings. These angles range from 0·5 to 1·2°, each with an e.s.d. of 0·1°.

The observed Se–C bond distance of 1·899(5) Å (corrected for libration) is significantly shorter than the weighted average Se–C bond distance of 1·98(2) Å found in the eight non-aromatic compounds listed in Table 10. In contrast, the weighted average Se–C (aromatic) distance found in the six aromatic organoselenium compounds in Table 10 is 1·92(2) Å, so the Se–C distance observed in dibenzoselenophene does not appear to be significantly less than the values found in other aromatic compounds. It should be noted, however, that the previous values are somewhat less precise and have not been corrected for libration.

The averaged C–C bond distances for chemically equivalent bonds in the six-membered rings vary from 1·371 to 1·398 Å, a range of some 4 σ. In this connec-

Table 9. *Deviations of atoms from least-squares planes* (Å × 10^3)*

	Molecule *A*					Molecule *B*		
Plane No.:	1	2	3	4	5	6	7	8
Se	4†	34	3	13†	−3†	−38	−48	−4†
C(1)	−7†	9†		0†	1†	0†		13†
C(2)	−35	−2†		−24†	−23	−1†		−13†
C(3)	−24	−5†		−16†	−41	4†		−21†
C(4)	16	6†		18†	−51	−6†		−18†
C(5)	28	1†		26†	−16	5†		19†
C(6)	6†	−8†	23	6†	1†	−2†	−19	25†
C(7)	−1†	−30	7†	−5†	−4†	−33	0†	21†
C(8)	−13		−5†	−23†	−33		0†	3†
C(9)	3		1†	−10†	−53		0†	−18†
C(10)	13		1†	4†	−45		−1†	−22†
C(11)	15		2†	12†	−14		1†	−3†
C(12)	−3†		−5†	−2†	4†		−1†	17†
H(2)		10				52		
H(3)		40				23		
H(4)		97				−98		
H(5)		66				−65		
H(8)			27				−61	
H(9)			−86				−73	
H(10)			68				34	
H(11)			6				118	

* A negative deviation from a plane indicates that the atom with the coordinates given in Table 1 lies on that side of the plane toward the origin.

† Indicates atoms used to define the respective least-squares planes.

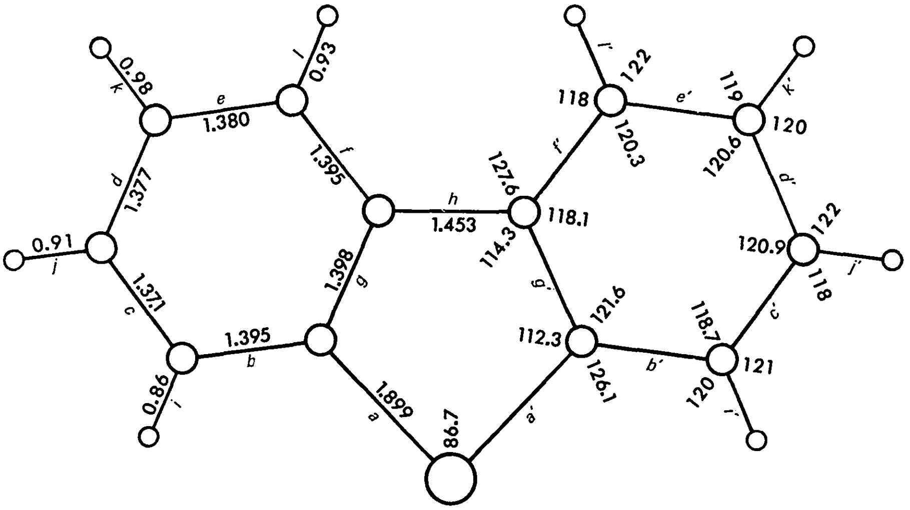

Fig. 3. The structure of the dibenzoselenophene molecule, showing averaged values for chemically equivalent bond distances (in Å) and bond angles (in degrees). The various bonds are designated by lower case letters (*a* through *l*) to aid in comparison with Tables 6 and 7.

Table 10. *Selenium–carbon bond distances in various organo-selenium compounds*

(*a*) Non-aromatic compounds

Compound	Distance	Reference
1,4-Diselenane	1·99 (4) Å 2·04 (6)	1
1,4-Diselenane.$2I_2$	1·95 (2) 1·98 (2)	2
1,4-Selenoxane.I_2	1·93 (3) 1·98 (3)	3
1,4-Selenoxane.ICl	1·93 (4) 2·02 (4)	4
1,4-Selenothiane-4,4-dibromide	2·01 (3) 2·02 (3)	5
Dimethyl selenide	1·977 (12)	6
Tetrahydroselenophene.I_2	1·960 (25)	7
Trimethylselenonium iodide	1·95 (2)	8

(*b*) Aromatic compounds

Compound	Distance	Reference
Diphenylselenium dibromide	1·91 (3) Å	9
Di-*p*-tolylselenium dichloride	1·93 (3)	10
Di-*p*-tolylselenium dibromide	1·95 (3)	10
Di-*p*-tolylselenium	1·93 (3)	11
Diphenyl diselenide	1·93 (5)	12
Benzeneseleninic acid	1·90 (2)	13

References: (1) Marsh & McCullough (1951);
(2) Chao & McCullough (1961);
(3) Maddox & McCullough (1966);
(4) Knobler & McCullough (1968);
(5) Battelle, Knobler & McCullough (1967);
(6) Goldish, Hedberg, Marsh & Schomaker (1955);
(7) Hope & McCullough (1964);
(8) Hope (1966);
(9) McCullough & Hamburger (1941);
(10) McCullough & Marsh (1950);
(11) Blackmore & Abrahams (1955);
(12) Marsh (1952);
(13) Bryden & McCullough (1954).

tion, it should be noted that the average value (1·371 Å) for bond *c* could be questioned, since one of the four values included in the average differs by almost 3σ from the average of the remaining three. If the doubtful value (1·358 Å) is omitted, the average distance for bond *c* becomes 1·375 Å. Even so, this is still the shortest C–C bond in the molecule and some 3σ shorter than bonds *b*, *f* and *g*, which have lengths of 1·395, 1·395 and 1·398 Å respectively.

The rigid-body analysis of each molecule was reasonably satisfactory. The root-mean-square ΔU_{ij} values are 0·0029 and 0·0033 Å^2 for molecules *A* and *B* respectively and are not greatly above the average e.s.d. of the input B_{ij}, which converts to 0·0025 Å^2 when placed on the scale of *U*. The principal libration axes listed in Table 5 correlate fairly well with a set of mutually perpendicular axes related to the molecular geometry. Thus, in each molecule, **L**(1) is approximately parallel to the long axis of the molecule (17° deviation in *A* and 15° in *B*), **L**(2) is approximately normal to the least-squares plane through the molecule (20° deviation in *A* and 17° in *B*) and **L**(3) is nearly parallel (11° deviation in *A* and 8° in *B*) to an axis normal to bond *h* and passing through the selenium atom.

There are few precisely determined related structures with which to compare the results of the present study. An approximate structure of selenophene has been obtained by Brown, Burden & Godfrey (1968) on the basis of microwave spectra and the assumption that some distances are the same as those in thiophene. Thus Se–C was reported as 1·863 Å and C–Se–C as 87·72° with no error estimates given. X-ray diffraction studies of dibenzothiophene sulfone (Kronfeld & Sass, 1968) and fluorene (Burns & Iball, 1955) yielded C–C

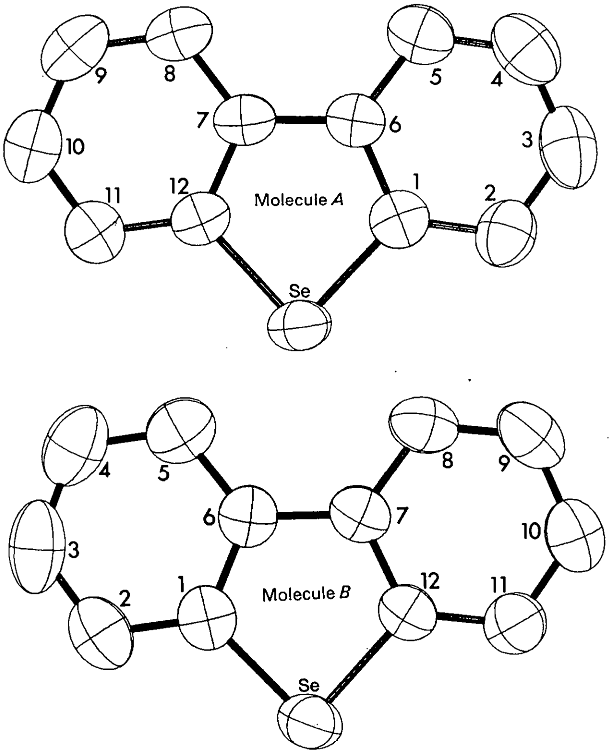

Fig. 4. *ORTEP* plots of the two independent molecules of dibenzoselenophene normal to their respective least-squares planes. The thermal ellipsoids are at the 50% probability level. Molecule *A* is viewed from the side toward the origin while molecule *B* is viewed from the opposite side. This causes a different atom numbering order in the two plots.

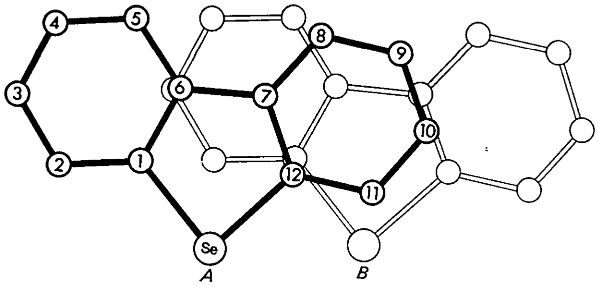

Fig. 5. Projection of a dimer pair of dibenzoselenophene molecules normal to their mean plane. The numbering system shown for molecule *A* applies also to molecule *B* without inversion.

distances and C–C–C angles comparable with the corresponding values found in dibenzoselenophene.

An interesting feature of the packing in dibenzoselenophene is the formation of loosely associated dimers, each consisting of one *A* and one *B* molecule. This pairing of *A* and *B* molecules is best illustrated in Fig. 2 and in the projection of a dimer pair normal to the mean plane, shown in Fig. 5. The dihedral angle between the least-squares planes through the individual molecules of the dimer pair is 5·7°, and the closest intermolecular contact is 3·36 Å, between C(6) of molecule *A* and C(3) of molecule *B*. Other intermolecular contacts within the dimer (*A*1–*B*1) are given in Table 12 and the distances of various atoms in one molecule from the least-squares plane of the other molecule are given in Table 11. Although the intermolecular carbon–carbon separations within a dimer pair are not notably short, some of the distances are short enough to suggest intermolecular attractions above the level of van der Waals forces.

In other respects the packing appears to be normal, but it is interesting to note that H(2) of molecule *A*4($0\bar{1}\bar{1}$) makes approximately equidistant contacts of 3·06, 3·03, 3·06, 3·12, 3·14, and 3·09 Å respectively with C(7), C(8), C(9), C(10), C(11) and C(12) which make up one of the six-membered rings of molecule *A*1(000). These contacts are repeated down the twofold screw axis parallel to **c** by which sets of neighboring *A* molecules are related.

Table 11. *Atom-plane distances within associated (dimer) pairs of molecules*

(*a*) Distances of atoms in molecule *A* from least-squares plane of molecule *B*.
(*b*) Distances of atoms in molecule *B* from least-squares plane of molecule *A*.

	a	*b*
Se	3·73 Å	3·63 Å
C(1)	3·58	3·47
C(2)	3·52	3·46
C(3)	3·37	3·32
C(4)	3·27	3·19
C(5)	3·33	3·21
C(6)	3·48	3·37
C(7)	3·54	3·43
C(8)	3·47	3·38
C(9)	3·50	3·43
C(10)	3·64	3·56
C(11)	3·71	3·63
C(12)	3·67	3·57

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Table 12. *Shorter intermolecular distances*

First atom	Molecule and position *	Second atom	Molecule and position*	Lattice translation	Distance
Se	*A*1	C(6)	*A*4	$0\bar{1}0$	3·47 Å
Se	*A*1	C(5)	*A*4	$0\bar{1}0$	3·53
Se	*B*8	H(3)	*A*1	100	3·16
C(5)	*A*1	C(4)	*B*1	000	3·50
C(6)		C(3)			3·36
C(7)		C(5)			3·63
C(7)		C(4)			3·64
C(8)		C(6)			3·62
C(8)		C(5)			3·40
C(9)		C(7)			3·64
C(8)		C(5)	*B*7		3·61
C(5)	*B*7	H(8)	*A*1		2·88
C(4)		H(8)			2·91
C(3)	*A*8	H(10)			3·09
C(4)		H(10)			3·12
C(7)	*A*1	H(2)	*A*4	$0\bar{1}\bar{1}$	3·06
C(8)		H(2)			3·03
C(9)		H(2)			3·06
C(10)		H(2)			3·12
C(11)		H(2)			3·14
C(12)		H(2)			3·09
H(11)	*A*1	H(11)	*A*5	$0\bar{1}0$	2·45

* Positions:

(1)	x	y	z	(5)	$1-x$	$1-y$	$1-z$
(2)	$\frac{1}{2}+x$	$\frac{1}{2}-y$	$1-z$	(6)	$\frac{1}{2}-x$	$\frac{1}{2}+y$	z
(3)	$1-x$	$\frac{1}{2}+y$	$\frac{1}{2}-z$	(7)	x	$\frac{1}{2}-y$	$\frac{1}{2}+z$
(4)	$\frac{1}{2}-x$	$1-y$	$\frac{1}{2}+z$	(8)	$\frac{1}{2}+x$	y	$\frac{1}{2}-z$

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The Crystal Structure of Fairfieldite*

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The mineral fairfieldite is triclinic, space group $P\bar{1}$; the cell dimensions, as determined from crystals from Foote Mine, North Carolina, are: $a=5{\cdot}79$, $b=6{\cdot}57$, $c=5{\cdot}51$ Å, $\alpha=102°16'$, $\beta=108°40'$, $\gamma=90°18'$. The cell content is $Ca_2Mn(PO_4)_2.2H_2O$. The crystal structure was solved from a three-dimensional Patterson function and refined first by successive Fourier syntheses and then by least-squares to an R value 0·075. The coordination around the Mn and P ions is octahedral and tetrahedral respectively: the average Mn–O and P–O distances are 2·20 and 1·55 Å. The Ca atom has the coordination number 7+1 with seven Ca–O bonds in the range 2·34 to 2·50 Å and one bond 2·72 Å long. The structure consists of infinite chains of Mn octahedra and P tetrahedra running along the c axes. Calcium ions occupy the vacant spaces between the chains connecting them in a three-dimensional network. The crystal structure of the fairfieldite mineral group is closely related to that of the kröhnkite mineral group. In both structures there is the same chain motif with a strictly similar connection of tetrahedra and octahedra inside the chain. Differences occur in the reciprocal array of the chains, which are shifted in the **c** direction by different amounts in the two mineral groups.

Introduction

The phosphate and arsenate minerals with the general formula $A_2B(XO_4)_2.2H_2O$, where A is Ca, B is Co, Fe, Mg, Mn, and X is As or P, may crystallize in the monoclinic or in the triclinic system. The monoclinic group comprises two minerals, brandtite and roselite, which are isostructural with the sulphate kröhnkite, $CuNa_2(SO_4)_2\ 2H_2O$. Members of the triclinic class are fairfieldite, neomesselite, collinsite and β-roselite.

The atomic arrangement in the monoclinic family was determined by Dahlman (1952) for kröhnkite and brandtite. Leone & Sgarlata (1954) redetermined the crystal structure of kröhnkite which was later refined by Rao (1961). In the present study the crystal structure of fairfieldite, which is a representative member of the triclinic group, was undertaken in an attempt to contribute to a better crystallochemical knowledge of phosphate minerals and to study its relationship with other compounds having a similar formula but belonging to the monoclinic system.

The mineral occurs as an accessory constituent in pegmatitic rocks, where it was first found by Brush

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