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# The Crystal and Molecular Structure of 3,4-Trimethylene-6a-selenaselenophthene

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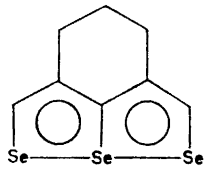
3,4-Trimethylene-6a-selenaselenophthene crystallizes in the orthorhombic space group $Pn2_1a$, with unit cell dimensions: $a = 11.437(3)$ Å, $b = 4.860(5)$ Å, and $c = 16.589(4)$ Å. There are four molecules per unit cell.

The structure has been solved by three-dimensional Patterson synthesis, and refined by full-matrix least squares. The refinement comprises 1004 *h0l*–*h4l* reflections, including 101 unobserved.

The atoms of the 6a-selenaselenophthene system and the methylene-carbons C(6) and C(8), bonded to C(3) and C(4), respectively, lie almost in the same plane. The Se-Se bond lengths are Se(1) – Se(6a) = 2.568(3) Å and Se(6a) – Se(6) = 2.554(3) Å, with the angle Se(1) – Se(6a) – Se(6) = 175.2(2)°. The other bond lengths in the selenaselenophthene system are: Se(1) – C(2) = 1.777(23) Å, Se(6a) – C(3a) = 1.906(20) Å, Se(6) – C(5) = 1.817(22) Å, C(2) – C(3) = 1.379(24) Å, C(3) – C(3a) = 1.435(23) Å, C(3a) – C(4) = 1.418(22) Å, and C(4) – C(5) = 1.400(23) Å.

In the crystals, Se(1) of the reference molecule approaches Se(6a) of a screw axis-related molecule at a distance of 3.57 Å.

The present structure investigation of 3,4-trimethylene-6a-selenaselenophthene (I) has been carried out in order to obtain further experimental evidence for the bonding in 6a-selenaselenophthenes.




(I)

## STRUCTURE DETERMINATION

Crystals of 3,4-trimethylene-6a-selenaselenophthene (I) were generously supplied by Reid.[1] The crystals are very dark purple and belong to the orthorhombic space group $Pn2_1a$.

The structure study is based on photographic data, taken with Weissenberg camera and Cu$K\alpha$ radiation. The data comprise 1004 *h0l–h4l* reflections, including 101 unobserved.

Approximate selenium positions were found from a three-dimensional Patterson map, and the carbon atoms revealed themselves during a subsequent Fourier synthesis.

The structure was refined by a full-matrix least squares procedure (*cf.* Ref. 2). The constants $a_1$ and $a_2$ in the weighting scheme were in the present case set equal to 1.0. Unobserved reflections with $K|F_c|$ greater than $F_o^{\text{threshold}}$ were included in the refinement with $F_o = F_o^{\text{threshold}}$. Anisotropic temperature factors were applied to selenium and carbon, and isotropic to hydrogen. Four low order reflections, supposed to be affected by secondary extinction, were excluded from the least squares refinement. The final $R$ factor is 0.076 when unobserved reflections are included, and 0.075 when they are omitted. For further details with respect to the structure determination, see Experimental.

## DISCUSSION

*Molecular shape and dimensions.* Bond lengths and angles in the 3,4-trimethylene-6a-selenaselenophthene molecule, together with their standard deviations, are listed in Tables 1 and 2, and shown in Fig. 1, a and b.

The molecule is presented in Fig. 1, a and b, in a projection on to the least squares plane of the atoms of the 6a-selenaselenophthene system and the methylene carbons C(6) and C(8). The equation for this plane, with weights equal to four for selenium, and one for carbon, is,

$$-0.63748\,X + 0.76127\,Y - 0.11871\,Z = -0.78216$$

with $X$, $Y$, and $Z$ in Å units. Deviations from the plane for the selenium and the carbon atoms are given in Fig. 1a. It is seen that the methylene carbons C(6) and C(8) and the atoms of the 6a-selenaselenophthene system lie almost in the same plane.

*Table 1.* Bond lengths ($l$) and standard deviations in bond lengths $\sigma(l)$ in 3,4-trimethylene-6a-selenaselenophthene. Bond lengths ($l'$) include corrections for rigid-body libration.

| Bond | $l'$ (Å) | $l$ (Å) | $\sigma(l)$ (Å) |
|---|---|---|---|
| Se(1) – Se(6a) | 2.568 | 2.563 | 0.003 |
| Se(6a) – Se(6) | 2.554 | 2.548 | 0.003 |
| Se(1) – C(2) | 1.777 | 1.771 | 0.023 |
| Se(6a) – C(3a) | 1.906 | 1.899 | 0.020 |
| Se(6) – C(5) | 1.817 | 1.811 | 0.022 |
| C(2) – C(3) | 1.379 | 1.375 | 0.024 |
| C(3) – C(3a) | 1.435 | 1.432 | 0.023 |
| C(3a) – C(4) | 1.418 | 1.414 | 0.022 |
| C(4) – C(5) | 1.400 | 1.397 | 0.023 |
| C(3) – C(6) | 1.499 | 1.494 | 0.028 |
| C(6) – C(7) | 1.507 | 1.503 | 0.024 |
| C(7) – C(8) | 1.564 | 1.561 | 0.024 |
| C(8) – C(4) | 1.549 | 1.544 | 0.030 |

*Table 2.* Bond angles ∠(ijk) in 3,4-trimethylene-6a-selenaselenophthene. The standard deviations given in parentheses refer to the last digits of the respective values.

| i | j | k | ∠(ijk)° |
|---|---|---|---|
| Se(6a) | Se(1) | C(2) | 87.7(6) |
| Se(1) | Se(6a) | C(3a) | 87.5(5) |
| Se(1) | Se(6a) | Se(6) | 175.2(2) |
| Se(6) | Se(6a) | C(3a) | 88.0(5) |
| Se(6a) | Se(6) | C(5) | 89.0(5) |
| Se(1) | C(2) | C(3) | 126.7(1.5) |
| C(2) | C(3) | C(3a) | 118.6(1.7) |
| C(2) | C(3) | C(6) | 121.5(1.5) |
| C(6) | C(3) | C(3a) | 119.9(1.4) |
| Se(6a) | C(3a) | C(3) | 119.5(1.2) |
| Se(6a) | C(3a) | C(4) | 119.1(1.3) |
| C(3) | C(3a) | C(4) | 121.4(1.7) |
| C(3a) | C(4) | C(5) | 121.4(1.7) |
| C(3a) | C(4) | C(8) | 119.6(1.4) |
| C(5) | C(4) | C(8) | 118.9(1.4) |
| Se(6) | C(5) | C(4) | 122.5(1.3) |
| C(3) | C(6) | C(7) | 108.8(1.9) |
| C(6) | C(7) | C(8) | 109.8(1.5) |
| C(4) | C(8) | C(7) | 105.8(1.9) |

*Comparison with related molecules.* Fig. 1a shows that the 3,4-trimethylene-6a-selenaselenophthene molecule is nearly symmetric about a plane perpendicular to the molecular plane and passing through Se(6a), C(3a), and C(7).

If one takes the average of corresponding bond lengths ($l$) in the two halves of 3,4-trimethylene-6a-selenaselenophthene, one gets the values given in Ia.

There are no significant deviations between the C-C and C-Se bond lengths in structure Ia and the corresponding C-C and C-Se bond lengths in the average structure of 6a-selenaselenophthene (II).[2] However, the Se-Se bonds in Ia, 2.556(3) Å, are significantly shorter than the Se-Se bonds in II, 2.583(3) Å, and the shortening of the Se-Se bonds seems to be due to the presence of the 3,4-trimethylene bridge.

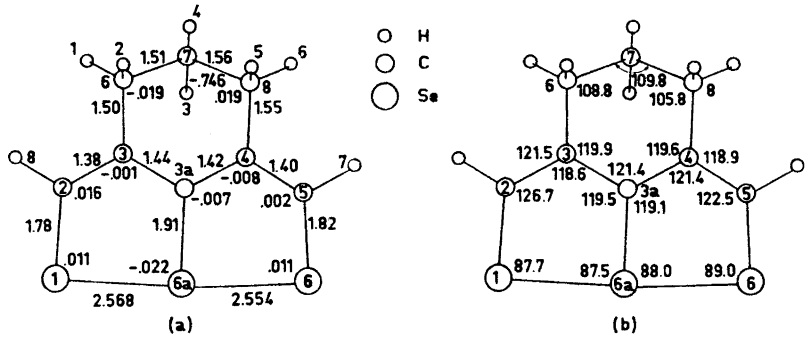
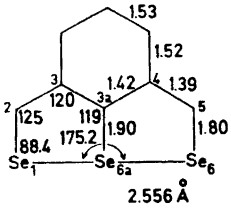
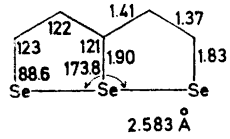



*Fig. 1.* (a) Bond lengths (Å) in the 3,4-trimethylene-6a-selenaselenophthene molecule, and atomic distances (Å) from the least squares plane of the atoms of the 6a-selenaselenophthene system and carbons C(6) and C(8). (b) Bond angles (°).

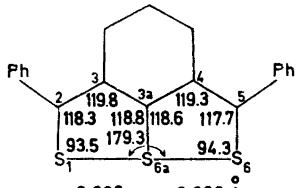
Support for this idea derives from a comparison of the structures Ia and II with the structures of 2,5-diphenyl-3,4-trimethylene-6a-thiathiophthene (III)[3] and 2,5-diphenyl-6a-thiathiophthene (IV).[4] The sum of the Se-Se bond lengths in Ia, 5.112 Å, is 0.054 Å shorter than the sum of the Se-Se bond lengths



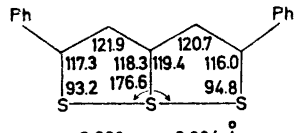

(Ia)




(II)




(III)




(IV)

in II, 5.166 Å, and similarly the sum of the S-S bond lengths in III, 4.617 Å, is 0.049 Å shorter than the sum of the S-S bond lengths in IV, 4.666 Å.

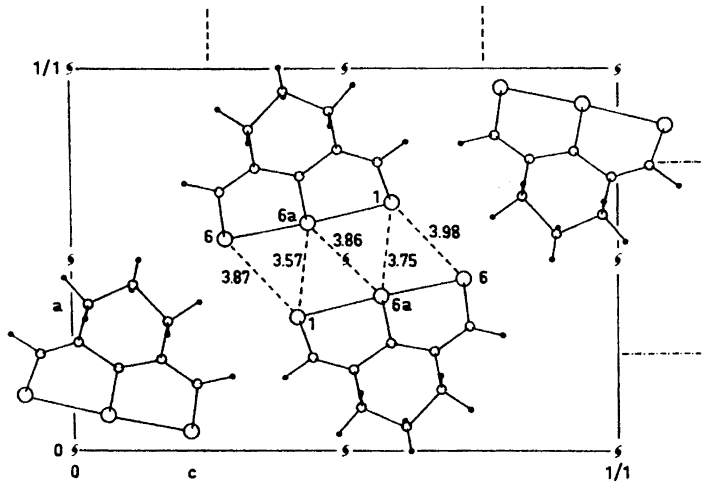



*Fig. 2.* The arrangement of 3,4-trimethylene-6a-selenaselenophthene molecules in the crystal as seen along the *b*-axis. Atomic distances are given in Å units.

A comparison of bond angles in Ia and II shows that the bond angle at Se(1) is almost the same in the two compounds, while the bond angle at C(2) is greater, and the bond angles at C(3) and C(3a) are smaller in Ia than in II. Similar equalities and differences in bond angles are found for structures III and IV.

The arrangement of 3,4-trimethylene-6a-selenaselenophthene molecules in the unit cell, as seen along the *b* axis, is shown in Fig. 2. Intermolecular atomic distances shorter than corresponding van der Waals distances are given in the figure.

*Table 3.* Atomic coordinates in fractions of corresponding cell edges. The standard deviations given in parentheses refer to the last digits of the respective values.

| Atom | $x$ | $y$ | $z$ |
|---|---|---|---|
| Se(1) | 0.14332(17) | 0.02769(87) | −0.08708(9) |
| Se(6a) | 0.09320(13) | 0.00000 | 0.06329(9) |
| Se(6) | 0.05284(18) | 0.00969(90) | 0.2143(11) |
| C(2) | 0.2553(17) | 0.2633(55) | −0.0613(11) |
| C(3) | 0.2832(13) | 0.3543(43) | 0.0148(8) |
| C(3a) | 0.2159(16) | 0.2557(47) | 0.0816(10) |
| C(4) | 0.2392(14) | 0.3435(43) | 0.1613(8) |
| C(5) | 0.1726(16) | 0.2498(52) | 0.2264(9) |
| C(6) | 0.3816(15) | 0.5508(56) | 0.0289(11) |
| C(7) | 0.4323(15) | 0.4980(72) | 0.1110(9) |
| C(8) | 0.3378(15) | 0.5536(64) | 0.1770(10) |
| H(1) | 0.454 | 0.499 | −0.010 |
| H(2) | 0.348 | 0.737 | 0.025 |
| H(3) | 0.430 | 0.265 | 0.113 |
| H(4) | 0.496 | 0.520 | 0.123 |
| H(5) | 0.303 | 0.728 | 0.176 |
| H(6) | 0.384 | 0.487 | 0.231 |
| H(7) | 0.196 | 0.317 | 0.288 |
| H(8) | 0.308 | 0.329 | −0.110 |

*Table 4.* Temperature parameters $U_{ij}$ (Å²) for selenium and carbon. The expression used is $\exp[-2\pi^2(h^2a^{*2}U_{11} + \cdots + 2hka^*b^*U_{12} + \cdots)]$. All values are multiplied by $10^4$. Standard deviations in parentheses refer to the last digits of the respective values. Isotropic temperature factors $\exp[-8\pi^2U(\sin^2\theta/\lambda^2]$ with $U = 0.0375$ Å² were used for the hydrogen atoms.

| | $U_{11}$ | $U_{22}$ | $U_{33}$ | $U_{12}$ | $U_{23}$ | $U_{13}$ |
|---|---|---|---|---|---|---|
| Se(1) | 446(9) | 432(15) | 271(6) | 82(16) | −92(14) | −68(6) |
| Se(6a) | 300(6) | 232(12) | 340(7) | −20(12) | −7(12) | −13(6) |
| Se(6) | 500(10) | 437(15) | 373(8) | −11(18) | 28(19) | 150(7) |
| C(2) | 415(95) | 343(146) | 340(95) | 133(103) | −19(101) | 33(79) |
| C(3) | 299(68) | 281(116) | 91(56) | 32(72) | 24(63) | −21(54) |
| C(3a) | 475(94) | 74(114) | 212(75) | −75(90) | −53(77) | 19(66) |
| C(4) | 315(74) | 203(119) | 104(64) | −99(72) | −37(65) | −52(55) |
| C(5) | 490(95) | 402(135) | 186(66) | 34(100) | −36(84) | −8(72) |
| C(6) | 340(72) | 152(147) | 484(81) | −49(89) | −8(102) | 142(65) |
| C(7) | 403(80) | 599(176) | 335(77) | −397(142) | 252(133) | −58(65) |
| C(8) | 418(86) | 445(191) | 350(71) | 1(121) | −17(120) | 76(67) |

*Table 5.* Observed and calculated structure factors for 3,4-trimethylene-6a-selenaselenophthene. The values given are ten times the absolute values. Unobserved reflections are marked with a minus sign.

| H | K | L | F(O) | F(C) | H | K | L | F(O) | F(C) | H | K | L | F(O) | F(C) | H | K | L | F(O) | F(C) | H | K | L | F(O) | F(C) |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 2 | 0 | 0 | 394 | 491 | 5 | 0 | 4 | 414 | 414 | 10 | 0 | 0 | 79 | 69 | 3 | 1 | 8 | 1030 | 1080 | 8 | 1 | 9 | 270 | 302 |
| 4 | 0 | 0 | 1151 | 1165 | 5 | 0 | 5 | 314 | 300 | 11 | 0 | 1 | 117 | 93 | 3 | 1 | 9 | 229 | 214 | 8 | 1 | 10 | 626 | 625 |
| 6 | 0 | 0 | 752 | 763 | 5 | 0 | 6 | 405 | 420 | 11 | 0 | 2 | 118 | 95 | 3 | 1 | 10 | 103 | 101 | 8 | 1 | 11 | 79 | 73 |
| 8 | 0 | 0 | 134 | 114 | 5 | 0 | 7 | 683 | 711 | 11 | 0 | 3 | 938 | 965 | 3 | 1 | 11 | 224 | 230 | 8 | 1 | 12 | 110 | 104 |
| 10 | 0 | 0 | 370 | 341 | 5 | 0 | 8 | 1033 | 1099 | 11 | 0 | 4 | 959 | 966 | 3 | 1 | 12 | 147 | 136 | 8 | 1 | 13 | 131 | 106 |
| 12 | 0 | 0 | 61 | 83 | 5 | 0 | 9 | 302 | 493 | 11 | 0 | 5 | -68 | 77 | 3 | 1 | 13 | 491 | 985 | 8 | 1 | 14 | 124 | 104 |
| 14 | 0 | 0 | 84 | 67 | 5 | 0 | 11 | 96 | 89 | 11 | 0 | 6 | -67 | 33 | 3 | 1 | 14 | 360 | 366 | 8 | 1 | 15 | 432 | 383 |
| 0 | 0 | 4 | 743 | 617 | 5 | 0 | 11 | 149 | 114 | 11 | 0 | 7 | -66 | 88 | 3 | 1 | 15 | 415 | 377 | 8 | 1 | 16 | 429 | 426 |
| 6 | 0 | 4 | 112 | 76 | 5 | 0 | 12 | 93 | 75 | 11 | 0 | 8 | -64 | 49 | 3 | 1 | 16 | 370 | 301 | 8 | 1 | 17 | 92 | 81 |
| 8 | 0 | 4 | 1515 | 1546 | 5 | 0 | 13 | 367 | 338 | 11 | 0 | 9 | 436 | 384 | 3 | 1 | 17 | -65 | 25 | 9 | 1 | 1 | 90 | 93 |
| 0 | 0 | 6 | 1393 | 1567 | 5 | 0 | 14 | 435 | 399 | 11 | 0 | 10 | 142 | 177 | 3 | 1 | 18 | 348 | 316 | 9 | 1 | 2 | 99 | 94 |
| 2 | 0 | 10 | 560 | 509 | 5 | 0 | 15 | 334 | 303 | 11 | 0 | 11 | 148 | 109 | 3 | 1 | 19 | 163 | 145 | 9 | 1 | 3 | 255 | 245 |
| 4 | 0 | 12 | 277 | 250 | 5 | 0 | 16 | 364 | 365 | 11 | 0 | 12 | 113 | 110 | 3 | 1 | 20 | 129 | 141 | 9 | 1 | 4 | 701 | 699 |
| 6 | 0 | 14 | 873 | 880 | 5 | 0 | 17 | 300 | 249 | 12 | 0 | 1 | -62 | 50 | 4 | 1 | 1 | 517 | 439 | 9 | 1 | 5 | 176 | 166 |
| 8 | 0 | 16 | 374 | 330 | 5 | 0 | 18 | 320 | 295 | 12 | 0 | 2 | 210 | 180 | 4 | 1 | 2 | 488 | 448 | 9 | 1 | 6 | 184 | 163 |
| 0 | 0 | 18 | 123 | 127 | 6 | 0 | 1 | 312 | 322 | 12 | 0 | 3 | 624 | 562 | 4 | 1 | 3 | 191 | 169 | 9 | 1 | 7 | -70 | 65 |
| 0 | 0 | 20 | 177 | 176 | 6 | 0 | 2 | 362 | 355 | 12 | 0 | 4 | 168 | 119 | 4 | 1 | 4 | 608 | 606 | 9 | 1 | 8 | 291 | 257 |
| 1 | 0 | 1 | 467 | 466 | 6 | 0 | 3 | 467 | 460 | 12 | 0 | 5 | 144 | 100 | 4 | 1 | 5 | 153 | 130 | 9 | 1 | 9 | 445 | 402 |
| 1 | 0 | 3 | 426 | 387 | 6 | 0 | 4 | 367 | 333 | 12 | 0 | 6 | 139 | 140 | 4 | 1 | 6 | 344 | 415 | 9 | 1 | 10 | 367 | 330 |
| 1 | 0 | 4 | 657 | 617 | 6 | 0 | 5 | 306 | 296 | 12 | 0 | 7 | -58 | 71 | 4 | 1 | 7 | 451 | 401 | 9 | 1 | 11 | 456 | 388 |
| 1 | 0 | 5 | 94 | 77 | 6 | 0 | 6 | 407 | 407 | 12 | 0 | 8 | 157 | 135 | 4 | 1 | 8 | 530 | 475 | 9 | 1 | 12 | -64 | 49 |
| 1 | 0 | 6 | 581 | 564 | 6 | 0 | 7 | 433 | 464 | 12 | 0 | 9 | 149 | 125 | 4 | 1 | 9 | 433 | 487 | 9 | 1 | 13 | -60 | 36 |
| 1 | 0 | 8 | 543 | 466 | 6 | 0 | 8 | 409 | 451 | 12 | 0 | 10 | 149 | 108 | 4 | 1 | 10 | 193 | 154 | 9 | 1 | 14 | -55 | 25 |
| 1 | 0 | 9 | 191 | 214 | 6 | 0 | 9 | 538 | 506 | 12 | 0 | 11 | 165 | 177 | 4 | 1 | 11 | 392 | 392 | 9 | 1 | 15 | 195 | 157 |
| 1 | 0 | 10 | 420 | 374 | 6 | 0 | 10 | 499 | 455 | 13 | 0 | 1 | 165 | 151 | 4 | 1 | 12 | 565 | 528 | 10 | 1 | 1 | 92 | 96 |
| 1 | 0 | 11 | 209 | 180 | 6 | 0 | 11 | 208 | 201 | 13 | 0 | 2 | 143 | 142 | 4 | 1 | 13 | 512 | 500 | 10 | 1 | 2 | 92 | 85 |
| 1 | 0 | 12 | 490 | 453 | 6 | 0 | 12 | 349 | 324 | 13 | 0 | 3 | -53 | 67 | 4 | 1 | 14 | 574 | 543 | 10 | 1 | 3 | 952 | 947 |
| 1 | 0 | 13 | 614 | 592 | 6 | 0 | 13 | -67 | 10 | 13 | 0 | 4 | 364 | 404 | 4 | 1 | 15 | 461 | 445 | 10 | 1 | 4 | 101 | 85 |
| 1 | 0 | 14 | 341 | 370 | 6 | 0 | 14 | -69 | 177 | 13 | 0 | 5 | 121 | 119 | 4 | 1 | 16 | 134 | 111 | 10 | 1 | 5 | 370 | 384 |
| 1 | 0 | 15 | 742 | 666 | 6 | 0 | 15 | 158 | 166 | 14 | 0 | 1 | -71 | 30 | 4 | 1 | 17 | -63 | 46 | 10 | 1 | 6 | -71 | 63 |
| 1 | 0 | 16 | 187 | 142 | 6 | 0 | 16 | 268 | 269 | 14 | 0 | 2 | -70 | 48 | 4 | 1 | 18 | 383 | 377 | 10 | 1 | 7 | 90 | 78 |
| 1 | 0 | 17 | 170 | 150 | 6 | 0 | 17 | 170 | 158 | 14 | 0 | 3 | -69 | 112 | 4 | 1 | 19 | 330 | 333 | 10 | 1 | 8 | -69 | 82 |
| 1 | 0 | 18 | 265 | 247 | 6 | 0 | 18 | 265 | 272 | 14 | 0 | 4 | 84 | 81 | 4 | 1 | 20 | -56 | 81 | 10 | 1 | 9 | 307 | 287 |
| 1 | 0 | 19 | 170 | 144 | 6 | 0 | 19 | 156 | 180 | 14 | 0 | 5 | 130 | 155 | 5 | 1 | 1 | 587 | 537 | 10 | 1 | 10 | 184 | 157 |
| 1 | 0 | 20 | 359 | 420 | 7 | 0 | 1 | 403 | 405 | 4 | 1 | 0 | 1276 | 1204 | 5 | 1 | 2 | 478 | 403 | 10 | 1 | 11 | 531 | 486 |
| 2 | 0 | 1 | 467 | 436 | 7 | 0 | 2 | 191 | 192 | 6 | 1 | 0 | 244 | 209 | 5 | 1 | 3 | 391 | 337 | 10 | 1 | 12 | 96 | 73 |
| 2 | 0 | 2 | 697 | 697 | 7 | 0 | 3 | 129 | 118 | 8 | 1 | 0 | 160 | 155 | 5 | 1 | 4 | 692 | 679 | 10 | 1 | 13 | 149 | 147 |
| 2 | 0 | 3 | 872 | 915 | 7 | 0 | 4 | 739 | 695 | 10 | 1 | 0 | 109 | 110 | 5 | 1 | 5 | 1140 | 1295 | 10 | 1 | 14 | -66 | 50 |
| 2 | 0 | 4 | 541 | 506 | 7 | 0 | 5 | 604 | 767 | 12 | 1 | 0 | 211 | 188 | 5 | 1 | 6 | 531 | 517 | 10 | 1 | 15 | 63 | 77 |
| 2 | 0 | 5 | 500 | 529 | 7 | 0 | 6 | 116 | 124 | 14 | 1 | 0 | 75 | 83 | 5 | 1 | 7 | 331 | 315 | 11 | 1 | 1 | -68 | 91 |
| 2 | 0 | 6 | 365 | 382 | 7 | 0 | 7 | 239 | 255 | 0 | 1 | 1 | 1228 | 1203 | 5 | 1 | 8 | 146 | 137 | 11 | 1 | 2 | 451 | 404 |
| 2 | 0 | 7 | 605 | 586 | 7 | 0 | 8 | 356 | 407 | 0 | 1 | 1 | 1176 | 1008 | 5 | 1 | 9 | 216 | 227 | 11 | 1 | 3 | -69 | 19 |
| 2 | 0 | 8 | 454 | 431 | 7 | 0 | 9 | 192 | 202 | 0 | 1 | 2 | 802 | 670 | 5 | 1 | 10 | 181 | 192 | 11 | 1 | 4 | 307 | 262 |
| 2 | 0 | 9 | 478 | 450 | 7 | 0 | 10 | 440 | 424 | 0 | 1 | 3 | 203 | 162 | 5 | 1 | 11 | 657 | 754 | 11 | 1 | 5 | -68 | 55 |
| 2 | 0 | 10 | 192 | 184 | 7 | 0 | 11 | 208 | 240 | 0 | 1 | 11 | 85 | 50 | 5 | 1 | 12 | 491 | 531 | 11 | 1 | 6 | -67 | 23 |
| 2 | 0 | 11 | 471 | 431 | 7 | 0 | 12 | 203 | 184 | 0 | 1 | 13 | 1254 | 1445 | 5 | 1 | 13 | 165 | 171 | 11 | 1 | 7 | 160 | 141 |
| 2 | 0 | 12 | 675 | 662 | 7 | 0 | 13 | -66 | 7 | 0 | 1 | 15 | 491 | 424 | 5 | 1 | 14 | 284 | 260 | 11 | 1 | 8 | -64 | 35 |
| 2 | 0 | 13 | 751 | 1211 | 7 | 0 | 14 | -65 | 63 | 0 | 1 | 17 | 134 | 119 | 5 | 1 | 15 | 277 | 271 | 11 | 1 | 9 | 234 | 218 |
| 2 | 0 | 14 | 467 | 570 | 7 | 0 | 15 | 159 | 163 | 0 | 1 | 19 | 496 | 504 | 5 | 1 | 16 | 165 | 130 | 11 | 1 | 10 | 519 | 492 |
| 2 | 0 | 15 | 207 | 227 | 7 | 0 | 16 | 140 | 95 | 0 | 1 | 21 | 207 | 325 | 5 | 1 | 17 | 186 | 175 | 11 | 1 | 11 | -53 | 25 |
| 2 | 0 | 16 | -58 | 31 | 7 | 0 | 17 | 272 | 271 | 1 | 1 | 1 | 1019 | 1159 | 5 | 1 | 18 | 171 | 155 | 11 | 1 | 12 | 194 | 195 |
| 2 | 0 | 17 | 119 | 102 | 7 | 0 | 18 | 154 | 160 | 1 | 1 | 2 | 651 | 624 | 5 | 1 | 19 | 259 | 243 | 11 | 1 | 13 | 99 | 105 |
| 2 | 0 | 18 | 247 | 211 | 8 | 0 | 1 | 349 | 288 | 1 | 1 | 3 | 50 | 22 | 6 | 1 | 1 | 828 | 763 | 12 | 1 | 1 | -61 | 53 |
| 2 | 0 | 19 | 524 | 510 | 8 | 0 | 2 | 614 | 653 | 1 | 1 | 4 | 451 | 390 | 6 | 1 | 2 | 974 | 972 | 12 | 1 | 2 | 217 | 170 |
| 3 | 0 | 1 | 747 | 796 | 8 | 0 | 3 | 961 | 1187 | 1 | 1 | 5 | 609 | 629 | 6 | 1 | 3 | 772 | 755 | 12 | 1 | 3 | 396 | 372 |
| 3 | 0 | 2 | 736 | 800 | 8 | 0 | 4 | 430 | 469 | 1 | 1 | 6 | 1393 | 1419 | 6 | 1 | 4 | 615 | 579 | 12 | 1 | 4 | -61 | 71 |
| 3 | 0 | 3 | 474 | 490 | 8 | 0 | 5 | 477 | 520 | 1 | 1 | 7 | 1329 | 1361 | 6 | 1 | 5 | 804 | 874 | 12 | 1 | 5 | 282 | 261 |
| 3 | 0 | 4 | 476 | 461 | 8 | 0 | 6 | 104 | 86 | 1 | 1 | 8 | 267 | 244 | 6 | 1 | 6 | 516 | 507 | 12 | 1 | 6 | 132 | 142 |
| 3 | 0 | 5 | 1230 | 1227 | 8 | 0 | 7 | 113 | 101 | 1 | 1 | 9 | -51 | 48 | 6 | 1 | 7 | -58 | 54 | 12 | 1 | 7 | -56 | 37 |
| 3 | 0 | 6 | 1304 | 1296 | 8 | 0 | 8 | 147 | 133 | 1 | 1 | 10 | 404 | 448 | 6 | 1 | 8 | 306 | 305 | 12 | 1 | 8 | 168 | 143 |
| 3 | 0 | 7 | 481 | 466 | 8 | 0 | 9 | 431 | 484 | 1 | 1 | 11 | 209 | 180 | 6 | 1 | 9 | 549 | 604 | 12 | 1 | 9 | -50 | 40 |
| 3 | 0 | 8 | 415 | 420 | 8 | 0 | 10 | 140 | 125 | 1 | 1 | 12 | 658 | 667 | 6 | 1 | 10 | 221 | 233 | 12 | 1 | 10 | 297 | 311 |
| 3 | 0 | 9 | 169 | 160 | 8 | 0 | 11 | 723 | 697 | 1 | 1 | 13 | 495 | 503 | 6 | 1 | 11 | 385 | 406 | 12 | 1 | 11 | 230 | 251 |
| 3 | 0 | 10 | 270 | 276 | 8 | 0 | 12 | 448 | 432 | 1 | 1 | 14 | 513 | 533 | 6 | 1 | 12 | 602 | 621 | 13 | 1 | 1 | 125 | 119 |
| 3 | 0 | 11 | 547 | 562 | 8 | 0 | 13 | -58 | 60 | 1 | 1 | 15 | 202 | 176 | 6 | 1 | 13 | 238 | 295 | 13 | 1 | 2 | 114 | 86 |
| 3 | 0 | 12 | 706 | 772 | 8 | 0 | 14 | 273 | 145 | 1 | 1 | 16 | -70 | 46 | 6 | 1 | 14 | 172 | 135 | 13 | 1 | 3 | 216 | 222 |
| 3 | 0 | 13 | 426 | 429 | 8 | 0 | 15 | -58 | 15 | 1 | 1 | 17 | 216 | 187 | 6 | 1 | 15 | 238 | 202 | 13 | 1 | 4 | -50 | 27 |
| 3 | 0 | 14 | 636 | 626 | 8 | 0 | 16 | 56 | 60 | 1 | 1 | 18 | 162 | 65 | 6 | 1 | 16 | 100 | 102 | 13 | 1 | 5 | 109 | 109 |
| 3 | 0 | 15 | 178 | 121 | 8 | 0 | 17 | 234 | 101 | 1 | 1 | 19 | -55 | 45 | 6 | 1 | 17 | -55 | 31 | 13 | 1 | 6 | -46 | 40 |
| 3 | 0 | 16 | -57 | 87 | 9 | 0 | 1 | 57 | 67 | 1 | 1 | 20 | 462 | 514 | 6 | 1 | 18 | 221 | 225 | 13 | 1 | 7 | -43 | 36 |
| 3 | 0 | 17 | 135 | 141 | 9 | 0 | 2 | 636 | 691 | 2 | 1 | 1 | 1128 | 1182 | 6 | 1 | 19 | 113 | 130 | 13 | 1 | 8 | 109 | 109 |
| 3 | 0 | 18 | 122 | 83 | 9 | 0 | 3 | 238 | 219 | 2 | 1 | 2 | 737 | 715 | 7 | 1 | 1 | 417 | 362 | 13 | 1 | 9 | 212 | 201 |
| 3 | 0 | 19 | 230 | 220 | 9 | 0 | 4 | 848 | 949 | 2 | 1 | 3 | 166 | 136 | 7 | 1 | 2 | 921 | 962 | 14 | 1 | 1 | 109 | 118 |
| 3 | 0 | 20 | 402 | 427 | 9 | 0 | 5 | 447 | 450 | 2 | 1 | 4 | 180 | 138 | 7 | 1 | 3 | 447 | 426 | 14 | 1 | 2 | 201 | 238 |
| 4 | 0 | 1 | 1102 | 1172 | 9 | 0 | 6 | 183 | 167 | 2 | 1 | 5 | 702 | 658 | 7 | 1 | 4 | 616 | 630 | 14 | 1 | 3 | 195 | 227 |
| 4 | 0 | 2 | 865 | 910 | 9 | 0 | 7 | 206 | 174 | 2 | 1 | 6 | 1258 | 1471 | 7 | 1 | 5 | 573 | 564 | 14 | 1 | 4 | 84 | 102 |
| 4 | 0 | 3 | 417 | 444 | 9 | 0 | 8 | 419 | 393 | 2 | 1 | 7 | 255 | 203 | 7 | 1 | 6 | 419 | 424 | 14 | 1 | 5 | 88 | 102 |
| 4 | 0 | 4 | 382 | 407 | 9 | 0 | 9 | 622 | 614 | 2 | 1 | 8 | 961 | 994 | 7 | 1 | 7 | 145 | 143 | 4 | 2 | 0 | 1437 | 1312 |
| 4 | 0 | 5 | 859 | 563 | 9 | 0 | 10 | 486 | 444 | 2 | 1 | 9 | 535 | 496 | 7 | 1 | 8 | 747 | 833 | 4 | 2 | 0 | 1477 | 1373 |
| 4 | 0 | 6 | 1040 | 1163 | 9 | 0 | 11 | 133 | 124 | 2 | 1 | 10 | 211 | 202 | 7 | 1 | 9 | 580 | 663 | 6 | 2 | 0 | 577 | 565 |
| 4 | 0 | 7 | 444 | 467 | 9 | 0 | 12 | 307 | 273 | 2 | 1 | 11 | 68 | 68 | 7 | 1 | 10 | 238 | 237 | 8 | 2 | 0 | 180 | 159 |
| 4 | 0 | 8 | 534 | 550 | 9 | 0 | 13 | -61 | 22 | 2 | 1 | 12 | 270 | 264 | 7 | 1 | 11 | 78 | 58 | 10 | 2 | 0 | 232 | 214 |
| 4 | 0 | 9 | 666 | 663 | 9 | 0 | 14 | 159 | 145 | 2 | 1 | 13 | 344 | 378 | 7 | 1 | 12 | 274 | 244 | 12 | 2 | 0 | -54 | 34 |
| 4 | 0 | 10 | -56 | 11 | 9 | 0 | 15 | 160 | 129 | 2 | 1 | 14 | 507 | 560 | 7 | 1 | 13 | 163 | 146 | 0 | 2 | 2 | 332 | 266 |
| 4 | 0 | 11 | -55 | 23 | 9 | 0 | 16 | 67 | 77 | 2 | 1 | 15 | 384 | 394 | 7 | 1 | 14 | 249 | 241 | 0 | 2 | 4 | 130 | 114 |
| 4 | 0 | 12 | 407 | 486 | 10 | 0 | 1 | 186 | 170 | 2 | 1 | 16 | 213 | 192 | 7 | 1 | 15 | 218 | 190 | 0 | 2 | 6 | 1336 | 1273 |
| 4 | 0 | 13 | 430 | 450 | 10 | 0 | 2 | 483 | 494 | 2 | 1 | 17 | 115 | 94 | 7 | 1 | 16 | 206 | 205 | 0 | 2 | 8 | 1003 | 948 |
| 4 | 0 | 14 | 143 | 115 | 10 | 0 | 3 | 242 | 188 | 2 | 1 | 18 | -61 | 16 | 7 | 1 | 17 | 354 | 333 | 0 | 2 | 10 | 423 | 414 |
| 4 | 0 | 15 | 422 | 357 | 10 | 0 | 4 | -70 | 49 | 2 | 1 | 19 | 122 | 130 | 7 | 1 | 18 | 40 | 70 | 0 | 2 | 12 | -67 | 40 |
| 4 | 0 | 16 | -56 | 22 | 10 | 0 | 5 | 415 | 403 | 2 | 1 | 20 | 123 | 119 | 8 | 1 | 1 | 611 | 577 | 0 | 2 | 14 | 611 | 597 |
| 4 | 0 | 17 | -63 | 33 | 10 | 0 | 6 | -70 | 73 | 3 | 1 | 1 | 1346 | 1409 | 8 | 1 | 2 | 567 | 521 | 0 | 2 | 16 | 210 | 192 |
| 4 | 0 | 18 | 163 | 153 | 10 | 0 | 7 | -69 | 43 | 3 | 1 | 2 | 815 | 818 | 8 | 1 | 3 | 75 | 70 | 0 | 2 | 18 | -55 | 87 |
| 4 | 0 | 19 | 159 | 147 | 10 | 0 | 8 | 191 | 139 | 3 | 1 | 3 | 224 | 190 | 8 | 1 | 4 | 192 | 187 | 1 | 2 | 1 | 1184 | 1150 |
| 4 | 0 | 20 | 131 | 88 | 10 | 0 | 9 | -67 | 56 | 3 | 1 | 4 | 214 | 193 | 8 | 1 | 5 | 444 | 403 | 1 | 2 | 2 | 252 | 248 |
| 5 | 0 | 1 | 859 | 874 | 10 | 0 | 10 | 522 | 566 | 3 | 1 | 5 | 69 | 51 | 8 | 1 | 6 | 87 | 80 | 1 | 2 | 3 | 245 | 197 |
| 5 | 0 | 2 | 1137 | 1274 | 10 | 0 | 11 | 125 | 114 | 3 | 1 | 6 | 112 | 94 | 8 | 1 | 7 | 110 | 112 | 1 | 2 | 4 | 229 | 217 |
| 5 | 0 | 3 | 365 | 352 | 10 | 0 | 12 | -59 | 23 | 3 | 1 | 7 | 1329 | 1570 | 8 | 1 | 8 | 214 | 215 | 1 | 2 | 5 | 118 | 120 |

*Table 5. Continued.*

| H | K | L | F(o) | F(c) |
|---|---|---|---|---|
| 1 | 2 | 4 | 665 | 645 |
| 1 | 2 | 7 | 1418 | 1529 |
| 1 | 2 | 8 | 467 | 367 |
| 1 | 2 | 9 | 161 | 161 |
| 1 | 2 | 10 | 217 | 228 |
| 1 | 2 | 11 | 145 | 145 |
| 1 | 2 | 12 | 431 | 398 |
| 1 | 2 | 13 | 471 | 466 |
| 1 | 2 | 14 | 610 | 662 |
| 1 | 2 | 15 | 380 | 353 |
| 1 | 2 | 16 | 135 | 188 |
| 1 | 2 | 17 | 143 | 158 |
| 1 | 2 | 18 | 171 | 149 |
| 1 | 2 | 19 | 149 | 135 |
| 2 | 2 | 1 | 249 | 263 |
| 2 | 2 | 4 | 342 | 485 |
| 2 | 2 | 5 | 557 | 545 |
| 2 | 2 | 6 | 506 | 546 |
| 2 | 2 | 7 | 563 | 513 |
| 2 | 2 | 8 | 374 | 363 |
| 2 | 2 | 9 | 620 | 664 |
| 2 | 2 | 10 | 432 | 383 |
| 2 | 2 | 11 | 245 | 257 |
| 2 | 2 | 12 | 259 | 259 |
| 2 | 2 | 13 | 149 | 137 |
| 2 | 2 | 14 | 367 | 351 |
| 2 | 2 | 15 | 274 | 331 |
| 2 | 2 | 16 | 472 | 442 |
| 2 | 2 | 17 | 201 | 244 |
| 2 | 2 | 18 | -05 | 33 |
| 2 | 2 | 19 | -31 | 41 |
| 3 | 2 | 0 | 468 | 440 |
| 3 | 2 | 1 | 229 | 240 |
| 3 | 2 | 2 | 375 | 400 |
| 3 | 2 | 3 | 578 | 582 |
| 3 | 2 | 4 | 808 | 745 |
| 3 | 2 | 5 | 444 | 368 |
| 3 | 2 | 6 | 134 | 147 |
| 3 | 2 | 7 | 1041 | 1080 |
| 3 | 2 | 8 | 134 | 147 |
| 3 | 2 | 9 | 1041 | 1080 |
| 3 | 2 | 10 | 952 | 1001 |
| 3 | 2 | 11 | 132 | 119 |
| 3 | 2 | 12 | 315 | 340 |
| 3 | 2 | 13 | 256 | 261 |
| 3 | 2 | 14 | 134 | 158 |
| 3 | 2 | 15 | 208 | 228 |
| 3 | 2 | 16 | 505 | 513 |
| 3 | 2 | 17 | 228 | 216 |
| 3 | 2 | 18 | 301 | 283 |
| 3 | 2 | 19 | 86 | 70 |
| 4 | 2 | 0 | -04 | 4 |
| 4 | 2 | 1 | 377 | 418 |
| 4 | 2 | 2 | 470 | 459 |
| 4 | 2 | 3 | 805 | 866 |
| 4 | 2 | 4 | 805 | 803 |
| 4 | 2 | 5 | 616 | 670 |
| 4 | 2 | 6 | 125 | 132 |
| 4 | 2 | 7 | 146 | 143 |
| 4 | 2 | 8 | 565 | 563 |
| 4 | 2 | 9 | 474 | 456 |
| 4 | 2 | 10 | 210 | 204 |
| 4 | 2 | 11 | 313 | 276 |
| 4 | 2 | 12 | 167 | 145 |
| 4 | 2 | 13 | 126 | 123 |
| 4 | 2 | 14 | 100 | 104 |
| 4 | 2 | 15 | 134 | 154 |
| 5 | 2 | 1 | 764 | 760 |
| 5 | 2 | 2 | 926 | 924 |
| 5 | 2 | 3 | 131 | 138 |
| 5 | 2 | 4 | 282 | 284 |
| 5 | 2 | 5 | 385 | 381 |
| 5 | 2 | 6 | 518 | 547 |
| 5 | 2 | 7 | 792 | 812 |
| 5 | 2 | 8 | 800 | 1034 |
| 5 | 2 | 9 | 359 | 427 |
| 5 | 2 | 10 | -54 | 26 |
| 5 | 2 | 11 | 120 | 120 |
| 5 | 2 | 12 | 226 | 212 |
| 5 | 2 | 13 | 402 | 393 |
| 5 | 2 | 14 | 197 | 194 |
| 5 | 2 | 15 | 244 | 236 |
| 5 | 2 | 16 | 246 | 234 |
| 5 | 2 | 17 | 191 | 186 |
| 5 | 2 | 18 | 176 | 190 |
| 6 | 2 | 1 | 640 | 589 |
| 6 | 2 | 2 | -58 | 13 |
| 6 | 2 | 3 | 282 | 264 |
| 6 | 2 | 4 | 372 | 409 |
| 6 | 2 | 5 | 212 | 213 |
| 6 | 2 | 6 | 243 | 258 |
| 6 | 2 | 7 | 162 | 171 |
| 6 | 2 | 8 | 238 | 269 |
| 6 | 2 | 9 | 317 | 355 |
| 6 | 2 | 10 | 348 | 372 |
| 6 | 2 | 11 | 378 | 368 |
| 6 | 2 | 12 | 385 | 360 |
| 6 | 2 | 13 | -66 | 86 |
| 6 | 2 | 14 | 434 | 494 |
| 6 | 2 | 15 | 435 | 448 |
| 6 | 2 | 16 | 238 | 236 |
| 6 | 2 | 17 | 97 | 88 |
| 6 | 2 | 18 | 257 | 310 |
| 7 | 2 | 1 | 54 | 79 |
| 7 | 2 | 2 | 206 | 195 |
| 7 | 2 | 3 | 129 | 119 |
| 7 | 2 | 4 | 795 | 831 |
| 7 | 2 | 5 | 629 | 695 |
| 7 | 2 | 6 | 71 | 102 |
| 7 | 2 | 7 | 192 | 228 |
| 7 | 2 | 8 | 170 | 210 |
| 7 | 2 | 9 | 86 | 76 |
| 7 | 2 | 10 | 348 | 306 |
| 7 | 2 | 11 | 629 | 584 |
| 7 | 2 | 12 | 323 | 270 |
| 7 | 2 | 13 | -63 | 45 |
| 7 | 2 | 14 | 120 | 113 |
| 7 | 2 | 15 | 215 | 206 |
| 7 | 2 | 16 | 111 | 109 |
| 7 | 2 | 17 | 261 | 280 |
| 8 | 2 | 1 | 123 | 269 |
| 8 | 2 | 2 | 424 | 436 |
| 8 | 2 | 3 | 765 | 826 |
| 8 | 2 | 4 | 470 | 456 |
| 8 | 2 | 5 | 514 | 480 |
| 8 | 2 | 6 | 143 | 129 |
| 8 | 2 | 7 | 69 | 76 |
| 8 | 2 | 8 | -09 | 17 |
| 8 | 2 | 9 | 298 | 270 |
| 8 | 2 | 10 | 87 | 93 |
| 8 | 2 | 11 | 501 | 476 |
| 8 | 2 | 12 | 338 | 319 |
| 8 | 2 | 13 | 145 | 154 |
| 8 | 2 | 14 | 125 | 121 |
| 9 | 2 | 1 | 108 | 103 |
| 9 | 2 | 2 | 541 | 543 |
| 9 | 2 | 3 | 234 | 257 |
| 9 | 2 | 4 | 700 | 664 |
| 9 | 2 | 5 | 299 | 277 |
| 9 | 2 | 6 | 156 | 144 |
| 9 | 2 | 7 | 169 | 138 |
| 9 | 2 | 8 | 234 | 246 |
| 9 | 2 | 9 | 441 | 399 |
| 9 | 2 | 10 | 389 | 376 |
| 9 | 2 | 11 | -62 | 17 |
| 9 | 2 | 12 | 223 | 206 |
| 9 | 2 | 13 | -35 | 33 |
| 9 | 2 | 14 | 135 | 142 |
| 9 | 2 | 15 | 124 | 123 |
| 10 | 2 | 1 | 135 | 152 |
| 10 | 2 | 2 | 377 | 406 |
| 10 | 2 | 3 | 404 | 474 |
| 10 | 2 | 4 | -03 | 8 |
| 10 | 2 | 5 | 224 | 295 |
| 10 | 2 | 6 | 111 | 117 |
| 10 | 2 | 7 | -06 | 20 |
| 10 | 2 | 8 | 204 | 186 |
| 10 | 2 | 9 | 152 | 137 |
| 10 | 2 | 10 | 508 | 510 |
| 10 | 2 | 11 | 224 | 208 |
| 10 | 2 | 12 | -30 | 52 |
| 10 | 2 | 13 | 56 | 59 |
| 11 | 2 | 1 | 110 | 125 |
| 11 | 2 | 2 | -04 | 81 |
| 11 | 2 | 3 | 263 | 264 |
| 11 | 2 | 4 | 166 | 161 |
| 11 | 2 | 5 | 178 | 148 |
| 11 | 2 | 6 | -62 | 60 |
| 11 | 2 | 7 | 97 | 98 |
| 11 | 2 | 8 | 81 | 82 |
| 11 | 2 | 9 | 387 | 398 |
| 11 | 2 | 10 | 120 | 112 |
| 11 | 2 | 11 | 137 | 122 |
| 11 | 2 | 12 | 62 | 68 |
| 12 | 2 | 1 | 71 | 83 |
| 12 | 2 | 2 | 225 | 225 |
| 12 | 2 | 3 | 478 | 514 |
| 12 | 2 | 4 | 94 | 93 |
| 12 | 2 | 5 | 151 | 143 |
| 12 | 2 | 6 | 113 | 103 |
| 12 | 2 | 7 | -48 | 44 |
| 12 | 2 | 8 | 91 | 90 |
| 12 | 2 | 9 | 210 | 228 |
| 13 | 2 | 1 | 121 | 133 |
| 13 | 2 | 2 | 210 | 231 |
| 13 | 2 | 3 | 130 | 125 |
| 13 | 2 | 4 | 384 | 459 |
| 13 | 2 | 5 | 125 | 159 |
| 13 | 2 | 6 | 36 | 46 |
| 0 | 3 | 0 | 1600 | 1708 |
| 0 | 3 | 0 | 898 | 858 |
| 0 | 3 | 0 | 248 | 240 |
| 0 | 3 | 0 | 273 | 265 |
| 0 | 3 | 0 | 146 | 134 |
| 0 | 3 | 0 | 113 | 118 |
| 0 | 3 | 1 | 743 | 630 |
| 0 | 3 | 3 | 632 | 546 |
| 0 | 3 | 5 | 663 | 597 |
| 0 | 3 | 7 | 642 | 609 |
| 0 | 3 | 9 | 235 | 237 |
| 0 | 3 | 11 | -00 | 76 |
| 0 | 3 | 13 | 945 | 854 |
| 0 | 3 | 15 | 122 | 118 |
| 0 | 3 | 17 | 102 | 79 |
| 1 | 3 | 2 | 547 | 489 |
| 1 | 3 | 3 | 54 | 30 |
| 1 | 3 | 4 | 254 | 245 |
| 1 | 3 | 5 | 365 | 341 |
| 1 | 3 | 6 | 879 | 867 |
| 1 | 3 | 7 | 705 | 697 |
| 1 | 3 | 8 | 234 | 253 |
| 1 | 3 | 9 | 187 | 178 |
| 1 | 3 | 10 | 240 | 230 |
| 1 | 3 | 11 | 193 | 203 |
| 1 | 3 | 12 | 465 | 481 |
| 1 | 3 | 13 | 403 | 392 |
| 1 | 3 | 14 | 409 | 388 |
| 1 | 3 | 15 | 169 | 142 |
| 1 | 3 | 16 | -08 | 45 |
| 1 | 3 | 17 | 134 | 149 |
| 2 | 3 | 1 | 660 | 671 |
| 2 | 3 | 2 | 414 | 382 |
| 2 | 3 | 3 | 82 | 47 |
| 2 | 3 | 4 | 204 | 193 |
| 2 | 3 | 5 | 522 | 474 |
| 2 | 3 | 6 | 878 | 957 |
| 2 | 3 | 7 | 149 | 143 |
| 2 | 3 | 8 | 604 | 727 |
| 2 | 3 | 9 | 397 | 419 |
| 2 | 3 | 10 | 137 | 175 |
| 2 | 3 | 11 | -78 | 49 |
| 2 | 3 | 12 | 161 | 134 |
| 2 | 3 | 13 | 376 | 376 |
| 2 | 3 | 14 | 440 | 423 |
| 2 | 3 | 15 | 132 | 178 |
| 2 | 3 | 16 | 139 | 132 |
| 2 | 3 | 17 | 76 | 72 |
| 3 | 3 | 1 | 772 | 720 |
| 3 | 3 | 2 | 522 | 501 |
| 3 | 3 | 3 | 79 | 61 |
| 3 | 3 | 4 | 171 | 131 |
| 3 | 3 | 5 | 174 | 172 |
| 3 | 3 | 6 | 130 | 110 |
| 3 | 3 | 7 | 982 | 1100 |
| 3 | 3 | 8 | 615 | 674 |
| 3 | 3 | 9 | 149 | 110 |
| 3 | 3 | 10 | -75 | 28 |
| 3 | 3 | 11 | 228 | 223 |
| 3 | 3 | 12 | 90 | 101 |
| 3 | 3 | 13 | 342 | 328 |
| 3 | 3 | 14 | 308 | 300 |
| 3 | 3 | 15 | 363 | 347 |
| 3 | 3 | 16 | 294 | 292 |
| 3 | 3 | 17 | -96 | 30 |
| 4 | 3 | 0 | 145 | 102 |
| 4 | 3 | 1 | 414 | 365 |
| 4 | 3 | 2 | 180 | 170 |
| 4 | 3 | 3 | 100 | 80 |
| 4 | 3 | 4 | 455 | 461 |
| 4 | 3 | 5 | 239 | 234 |
| 4 | 3 | 6 | 235 | 246 |
| 4 | 3 | 7 | 221 | 215 |
| 4 | 3 | 8 | 279 | 309 |
| 4 | 3 | 9 | 231 | 240 |
| 4 | 3 | 10 | 108 | 84 |
| 4 | 3 | 11 | 274 | 251 |
| 4 | 3 | 12 | 396 | 395 |
| 4 | 3 | 13 | 393 | 393 |
| 4 | 3 | 14 | 401 | 383 |
| 4 | 3 | 15 | 358 | 344 |
| 4 | 3 | 16 | 100 | 85 |
| 5 | 3 | 1 | 225 | 197 |
| 5 | 3 | 2 | 351 | 335 |
| 5 | 3 | 3 | 272 | 249 |
| 5 | 3 | 4 | 519 | 502 |
| 5 | 3 | 5 | 755 | 676 |
| 5 | 3 | 6 | 396 | 410 |
| 5 | 3 | 7 | 174 | 137 |
| 5 | 3 | 8 | -75 | 34 |
| 5 | 3 | 9 | 108 | 96 |
| 5 | 3 | 10 | 89 | 88 |
| 5 | 3 | 11 | 500 | 495 |
| 5 | 3 | 12 | 377 | 326 |
| 5 | 3 | 13 | -74 | 57 |
| 5 | 3 | 14 | 169 | 168 |
| 5 | 3 | 15 | 145 | 129 |
| 5 | 3 | 16 | -56 | 34 |
| 5 | 3 | 17 | 124 | 137 |
| 6 | 3 | 1 | 551 | 554 |
| 6 | 3 | 2 | 645 | 735 |
| 6 | 3 | 3 | 406 | 511 |
| 6 | 3 | 4 | 305 | 305 |
| 6 | 3 | 5 | 464 | 532 |
| 6 | 3 | 6 | 325 | 326 |
| 6 | 3 | 7 | 88 | 102 |
| 6 | 3 | 8 | 163 | 155 |
| 6 | 3 | 9 | 359 | 347 |
| 6 | 3 | 10 | 154 | 169 |
| 6 | 3 | 11 | 373 | 347 |
| 6 | 3 | 12 | 404 | 429 |
| 6 | 3 | 13 | 196 | 210 |
| 6 | 3 | 14 | 92 | 76 |
| 6 | 3 | 15 | 156 | 168 |
| 6 | 3 | 16 | 108 | 126 |
| 7 | 3 | 1 | 365 | 372 |
| 7 | 3 | 2 | 621 | 658 |
| 7 | 3 | 3 | 253 | 252 |
| 7 | 3 | 4 | 368 | 376 |
| 7 | 3 | 5 | 347 | 371 |
| 7 | 3 | 6 | 287 | 308 |
| 7 | 3 | 7 | 152 | 143 |
| 7 | 3 | 8 | 503 | 545 |
| 7 | 3 | 9 | 494 | 492 |
| 7 | 3 | 10 | 215 | 212 |
| 7 | 3 | 11 | -71 | 14 |
| 7 | 3 | 12 | 271 | 262 |
| 7 | 3 | 13 | 163 | 156 |
| 7 | 3 | 14 | 132 | 129 |
| 7 | 3 | 15 | 111 | 107 |
| 8 | 3 | 1 | 322 | 339 |
| 8 | 3 | 2 | 308 | 291 |
| 8 | 3 | 3 | 82 | 73 |
| 8 | 3 | 4 | 82 | 82 |
| 8 | 3 | 5 | 340 | 303 |
| 8 | 3 | 6 | 196 | 194 |
| 8 | 3 | 7 | 111 | 100 |
| 8 | 3 | 8 | 207 | 244 |
| 8 | 3 | 9 | 237 | 235 |
| 8 | 3 | 10 | 446 | 478 |
| 8 | 3 | 11 | 97 | 87 |
| 8 | 3 | 12 | 110 | 111 |
| 8 | 3 | 13 | 105 | 125 |
| 8 | 3 | 14 | 84 | 72 |
| 9 | 3 | 1 | 114 | 112 |
| 9 | 3 | 2 | 105 | 70 |
| 9 | 3 | 3 | 234 | 233 |
| 9 | 3 | 4 | 441 | 424 |
| 9 | 3 | 5 | 111 | 109 |
| 9 | 3 | 6 | 120 | 106 |
| 9 | 3 | 7 | 131 | 146 |
| 9 | 3 | 8 | 204 | 192 |
| 9 | 3 | 9 | 271 | 255 |
| 9 | 3 | 10 | 266 | 293 |
| 9 | 3 | 11 | 225 | 200 |
| 9 | 3 | 12 | 88 | 91 |
| 10 | 3 | 1 | -74 | 2 |
| 10 | 3 | 2 | -74 | 56 |
| 10 | 3 | 3 | 610 | 633 |
| 10 | 3 | 4 | 128 | 108 |
| 10 | 3 | 5 | 240 | 272 |
| 10 | 3 | 6 | -71 | 61 |
| 10 | 3 | 7 | -68 | 59 |
| 10 | 3 | 8 | -65 | 7 |
| 10 | 3 | 9 | 180 | 188 |
| 10 | 3 | 10 | 89 | 74 |
| 10 | 3 | 11 | 272 | 313 |
| 11 | 3 | 1 | -63 | 58 |
| 11 | 3 | 2 | 201 | 270 |
| 11 | 3 | 3 | 82 | 86 |
| 11 | 3 | 4 | 498 | 558 |
| 11 | 3 | 5 | 105 | 132 |
| 11 | 3 | 6 | 82 | 85 |
| 11 | 3 | 7 | 95 | 84 |
| 11 | 3 | 8 | -50 | 38 |
| 11 | 3 | 9 | 88 | 88 |
| 12 | 3 | 1 | 65 | 74 |
| 12 | 3 | 2 | 175 | 196 |
| 12 | 3 | 3 | 239 | 270 |
| 12 | 3 | 4 | 61 | 60 |
| 12 | 3 | 5 | 139 | 147 |
| 12 | 3 | 6 | 82 | 89 |
| 2 | 4 | 0 | 474 | 443 |
| 2 | 4 | 0 | 609 | 578 |
| 2 | 4 | 0 | 425 | 430 |
| 8 | 4 | 0 | 126 | 141 |
| 10 | 4 | 0 | 159 | 164 |
| 0 | 4 | 2 | 243 | 207 |
| 0 | 4 | 4 | 97 | 85 |
| 0 | 4 | 6 | 825 | 930 |
| 0 | 4 | 8 | 717 | 691 |
| 0 | 4 | 10 | 181 | 185 |
| 0 | 4 | 12 | 137 | 137 |
| 0 | 4 | 14 | 467 | 477 |
| 0 | 4 | 16 | 144 | 172 |
| 1 | 4 | 1 | 601 | 677 |
| 1 | 4 | 2 | 130 | 138 |
| 1 | 4 | 3 | 123 | 111 |
| 1 | 4 | 4 | 215 | 212 |
| 1 | 4 | 5 | 58 | 114 |
| 1 | 4 | 6 | 336 | 320 |
| 1 | 4 | 7 | 759 | 885 |
| 1 | 4 | 8 | 251 | 265 |
| 1 | 4 | 9 | 119 | 138 |
| 1 | 4 | 10 | 139 | 132 |
| 1 | 4 | 11 | 138 | 136 |
| 1 | 4 | 12 | 200 | 244 |
| 1 | 4 | 13 | 344 | 311 |
| 1 | 4 | 14 | 226 | 216 |
| 1 | 4 | 15 | 229 | 232 |
| 1 | 4 | 16 | 83 | 87 |
| 2 | 4 | 1 | 317 | 322 |
| 2 | 4 | 2 | 215 | 202 |
| 2 | 4 | 3 | 307 | 310 |
| 2 | 4 | 4 | 254 | 235 |
| 2 | 4 | 5 | 418 | 446 |
| 2 | 4 | 6 | -75 | 19 |
| 2 | 4 | 7 | 286 | 281 |
| 2 | 4 | 8 | 148 | 117 |
| 2 | 4 | 9 | 158 | 144 |
| 2 | 4 | 10 | -83 | 30 |
| 2 | 4 | 11 | 147 | 117 |
| 2 | 4 | 12 | 268 | 250 |
| 2 | 4 | 13 | 340 | 363 |
| 2 | 4 | 14 | 173 | 170 |
| 2 | 4 | 15 | 112 | 110 |
| 3 | 4 | 1 | 346 | 341 |
| 3 | 4 | 2 | 426 | 443 |
| 3 | 4 | 3 | 203 | 186 |
| 3 | 4 | 4 | 132 | 140 |
| 3 | 4 | 5 | 498 | 535 |
| 3 | 4 | 6 | 518 | 508 |
| 3 | 4 | 7 | 166 | 167 |
| 3 | 4 | 8 | 81 | 78 |
| 3 | 4 | 9 | 106 | 99 |
| 3 | 4 | 10 | 125 | 134 |
| 3 | 4 | 11 | 279 | 273 |
| 3 | 4 | 12 | 429 | 380 |
| 3 | 4 | 13 | 234 | 207 |
| 3 | 4 | 14 | 247 | 240 |
| 3 | 4 | 15 | 74 | 60 |
| 4 | 4 | 1 | 507 | 491 |
| 4 | 4 | 2 | 415 | 422 |
| 4 | 4 | 3 | 134 | 120 |
| 4 | 4 | 4 | 195 | 187 |
| 4 | 4 | 5 | 376 | 411 |
| 4 | 4 | 6 | 373 | 374 |
| 4 | 4 | 7 | 115 | 120 |
| 4 | 4 | 8 | 273 | 264 |
| 4 | 4 | 9 | 336 | 367 |
| 4 | 4 | 10 | 132 | 150 |
| 4 | 4 | 11 | 129 | 119 |
| 4 | 4 | 12 | 264 | 230 |
| 4 | 4 | 13 | 217 | 248 |
| 4 | 4 | 14 | 155 | 151 |
| 4 | 4 | 15 | 131 | 140 |
| 5 | 4 | 1 | 399 | 401 |
| 5 | 4 | 2 | 421 | 486 |
| 5 | 4 | 3 | 136 | 107 |
| 5 | 4 | 4 | 134 | 121 |
| 5 | 4 | 5 | 196 | 199 |
| 5 | 4 | 6 | 227 | 242 |
| 5 | 4 | 7 | 399 | 413 |
| 5 | 4 | 8 | 529 | 547 |
| 5 | 4 | 9 | 338 | 331 |
| 5 | 4 | 10 | 79 | 90 |
| 5 | 4 | 11 | 124 | 123 |
| 5 | 4 | 12 | 93 | 93 |
| 5 | 4 | 13 | 174 | 162 |
| 5 | 4 | 14 | 157 | 160 |
| 6 | 4 | 1 | 362 | 363 |
| 6 | 4 | 2 | 178 | 170 |
| 6 | 4 | 3 | 124 | 148 |
| 6 | 4 | 4 | 131 | 141 |
| 6 | 4 | 5 | 175 | 177 |
| 6 | 4 | 6 | 266 | 268 |
| 6 | 4 | 7 | 107 | 121 |
| 6 | 4 | 8 | 312 | 290 |
| 6 | 4 | 9 | 256 | 255 |
| 6 | 4 | 10 | 269 | 254 |
| 6 | 4 | 11 | 177 | 180 |
| 6 | 4 | 12 | 136 | 162 |
| 7 | 4 | 1 | 146 | 102 |
| 7 | 4 | 2 | -88 | 73 |
| 7 | 4 | 3 | -88 | 40 |
| 7 | 4 | 4 | 470 | 447 |
| 7 | 4 | 5 | 325 | 295 |
| 7 | 4 | 6 | -63 | 70 |
| 7 | 4 | 7 | 227 | 210 |
| 7 | 4 | 8 | 194 | 190 |
| 7 | 4 | 9 | 123 | 81 |
| 7 | 4 | 10 | 223 | 210 |
| 7 | 4 | 11 | 254 | 263 |
| 7 | 4 | 12 | 138 | 134 |
| 8 | 4 | 1 | 145 | 109 |
| 8 | 4 | 2 | 325 | 300 |
| 8 | 4 | 3 | 563 | 575 |
| 8 | 4 | 4 | 185 | 158 |
| 8 | 4 | 5 | 388 | 363 |
| 8 | 4 | 6 | -76 | 82 |
| 8 | 4 | 7 | -76 | 62 |
| 8 | 4 | 8 | -72 | 60 |
| 9 | 4 | 9 | 202 | 204 |
| 9 | 4 | 10 | -01 | 54 |
| 9 | 4 | 11 | 248 | 321 |
| 9 | 4 | 1 | 182 | 186 |
| 9 | 4 | 2 | 385 | 374 |
| 9 | 4 | 3 | 212 | 208 |
| 9 | 4 | 4 | 378 | 458 |
| 9 | 4 | 5 | 242 | 246 |
| 9 | 4 | 6 | 156 | 156 |
| 9 | 4 | 7 | 85 | 80 |
| 9 | 4 | 8 | 156 | 167 |
| 9 | 4 | 9 | 223 | 235 |
| 10 | 4 | 1 | 123 | 133 |
| 10 | 4 | 2 | 237 | 239 |
| 10 | 4 | 3 | 99 | 90 |
| 10 | 4 | 4 | -59 | 64 |
| 10 | 4 | 5 | 162 | 153 |
| 10 | 4 | 6 | 92 | 90 |
| 11 | 4 | 1 | 73 | 90 |
| 11 | 4 | 2 | -44 | 63 |
| 11 | 4 | 3 | 124 | 143 |

## EXPERIMENTAL

The unit cell dimensions for crystals of 3,4-trimethylene-6a-selenaselenophthene were determined from high-order reflections on *h*0*l* and 0*kl* Weissenberg photographs, where lead nitrate powder lines had been superimposed for reference. A least squares procedure on 41 measured $2\theta$-values gave $a = 11.437(3)$ Å, $b = 4.860(5)$ Å, and $c = 16.589(4)$ Å.

Four molecules per unit cell give a calculated density of 2.456 g/cm$^3$ as compared with the density 2.45 g/cm$^3$, found by flotation.

The intensities of the *h*0*l*–*h*4*l* and 0*kl* reflections were estimated visually from Weissenberg photographs taken with Ni-filtered Cu$K\alpha$ radiation ($\mu = 159.4$ cm$^{-1}$). 0*kl* reflections from the zero layer about *a* were used for scaling only.

Lp corrections and absorption corrections were applied, the latter according to a procedure of Coppens *et al.*[5]

The hydrogen positions were estimated and included in the structure factor calculations, but not refined.

The scattering factors used for selenium, carbon, and hydrogen in the structure factor calculations were those given in the International Tables.[6] The selenium scattering curve was corrected for anomalous dispersion, using the $\Delta f'$ and $\Delta f''$ values given by Cromer.[7]

The final atomic coordinates are listed in Table 3, the temperature parameters in Table 4. The final list of structure factors is given in Table 5.

An analysis of the thermal parameters of the S and C atoms, assuming the molecule a rigid body was carried out according to the method of Schomaker and Trueblood.[8] The Se–Se, Se–C, and C–C bond lengths have been corrected for rigid body libration according to Cruickshank's formula.[9] The corrected bond lengths are listed in the first column of Table 1.

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