CRUICKSHANK, D. W. J. & ROBERTSON, A. P. (1953). *Acta Cryst.* **6**, 698.
DEGRÈVE, Y., MEUNIER-PIRET, J., MEERSSCHE, M. VAN & PIRET, P. (1967). *Acta Cryst.* **23**, 119.
DODGE, R. P. & SCHOMAKER, V. (1965). *J. Organometal. Chem.* **3**, 274.
HELM, D. VAN DER & PATTERSON, A. L. (1962). *Programs ICR* 1, 4, 6. Institute for Cancer Research, Philadelphia.
HOCK, A. A. & MILLS, O. S. (1961). *Acta Cryst.* **14**, 139.
HOWELLS, E. R., PHILIPS, D. C. & ROGERS, D. (1950). *Acta Cryst.* **3**, 210.
*International Tables for X-ray Crystallography* (1962). Vol. III. Birmingham: Kynoch Press.
JAMES, R. W. (1958). *The Optical Principles of the Diffraction of X-rays*, p. 608. London: Bell.
KING, G. S. D. (1962). *Acta Cryst.* **15**, 243.
KING, G. S. D. (1963). 1620 *Least Squares Refinement Program ERA* 302. Union Carbide European Research Associates, Bruxelles 18.
MAIN, P. & WOOLFSON, M. M. (1963). *Acta Cryst.* **16**, 731.
MEUNIER-PIRET, J., PIRET, P. & MEERSSCHE, M. VAN (1965). *Acta Cryst.* **19**, 85.
MILLS, O. S. & REDHOUSE, A. D. (1966). *Chem. Comm.* p. 444.
PARRISH, W. (1960). *Acta Cryst.* **13**, 838.
PAULING, L. (1960). *The Nature of the Chemical Bond.* Ithaca: Cornell Univ. Press.
PIRET, P., MEUNIER-PIRET, J. & MEERSSCHE, M. VAN (1965). *Acta Cryst.* **19**, 78.
ROBERTSON, J. M. (1953). *Organic Crystals and Molecules.* Ithaca: Cornell Univ. Press.
SANDS, D. E. (1963). *Z. Kristallogr.* **119**, 245.
*Tables of Interatomic Distances and Configuration in Molecules and Ions*, Supplement 1956–1959 (1965). London: The Chemical Society.
VAND, V., EILAND, P. F. & PEPINSKY, R. (1957). *Acta Cryst.* **10**, 303.
WILSON, A. J. C. (1942). *Nature, Lond.* **150**, 151.

*Acta Cryst.* (1969). B**25**, 532

# The Crystal Structure of *N*-Acetyl-*N'*-phenylselenourea

BY M. PEREZ-RODRIGUEZ AND LÓPEZ-CASTRO

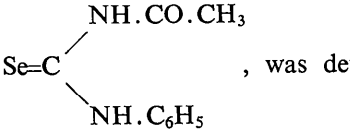
*División de Ciencias Matemáticas, Médicas y de la Naturaleza, C.S.I.C. Departamento de Optica, Universidad de Sevilla, Spain*

(*Received* 5 *March* 1968)

The crystal structure of *N*-acetyl-*N'*-phenylselenourea, $C_6H_5.NH.CSe.NH.CO.CH_3$, was determined by single-crystal methods. The monoclinic unit cell is, $a=10{\cdot}22$, $b=22{\cdot}42$, $c=9{\cdot}33$ Å, $\beta=113{\cdot}40$, $Z=8$, space group $P2_1/c$. The structure was determined by three-dimensional Patterson and Fourier syntheses from visual inspection of intensity data made with Cu $K\alpha$ radiation. Isotropic and anisotropic refinement was carried out by differential syntheses, as far as is reasonable with the existing data. The final $R$ value is 0·116. Each molecule consists of three planar parts, the $SeC(NH)_2$ group, the acetyl group and the phenyl group.

## Introduction

The crystal structure of *N*-acetyl-*N'*-phenylselenourea,



, was determined as part of a study of selenourea and some *N*-substituted selenoureas. The principal aim of the investigation was to obtain information about the carbon double bond.

Work was first begun on selenourea and the location of the selenium atoms was under way when Dr C. Calvo, Canada, informed us of his investigation of this compound, which was almost complete. Attention was therefore turned to other compounds such as *N*-phenyl-*N'*-benzoylselenourea (Perez-Rodriguez & Cubero, 1963; Hope, 1965) and *N*-acetyl-*N'*-phenylselenourea.

## Experimental

The crystals of *N*-acetyl-*N'*-phenylselenourea were supplied by Dr Pino, University of Seville. They were prepared according to the procedure given by Douglas (1928). Yellow prismatic crystals were obtained after recrystallization from alcoholic solution.

The unit-cell dimensions were measured from oscillation and Weissenberg photographs. For the intensity measurements a crystal of $0{\cdot}15\times0{\cdot}12\times0{\cdot}16$ mm was used. Equi-inclination multiple-film Weissenberg photographs were taken from the zero to the fourth layer about the $c$ axis and at the zero level about the $a$ axis. Out of 2641 non-symmetry related reflexions accesible to film observation, 1275 reflexions were observed. The intensities were corrected for Lorentz and polarization effects in the usual way. No absorption correction was made ($\mu=53{\cdot}6$ cm$^{-1}$). The non-equa-

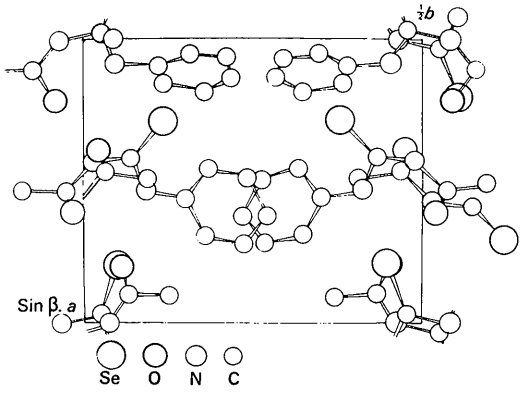



Fig. 1. The structure of *N*-acetyl-*N'*-phenylselenourea projected down [001].

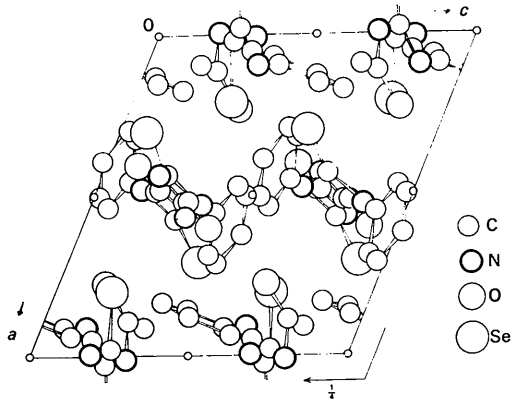



Fig. 2. The structure projected down [010].

torial intensities were corrected for spot extension factors (Phillips, 1956). For the *hk*0 reflexions the approximate scale factor was obtained by Wilson's (1942) method and the remaining observations were correlated with these. During refinement the scale factor was one of the parameters and in the last calculation the scale for the different layers was adjusted to allow comparison between calculated and observed structure factors.

*Crystal data*

$a = 10{\cdot}22 \pm 0{\cdot}03$, $b = 22{\cdot}42 \pm 0{\cdot}06$, $c = 9{\cdot}33 \pm 0{\cdot}03$ Å, $\beta = 113{\cdot}4 \pm 0{\cdot}5°$, $V = 1962{\cdot}1$ Å$^3$, $F(000) = 960$. $Z = 8$, $D_x =$

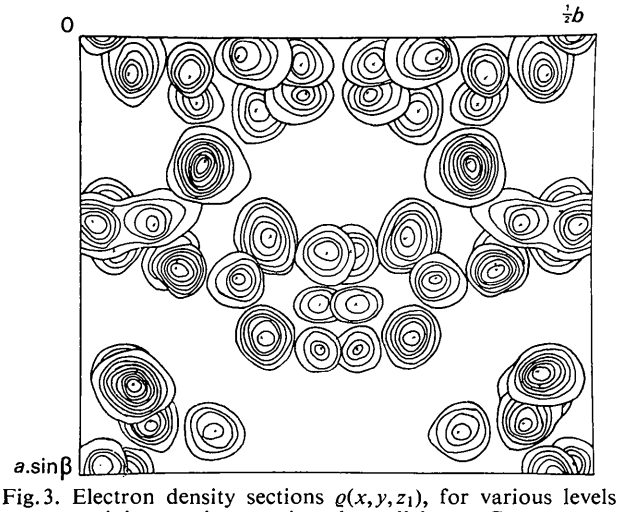



Fig. 3. Electron density sections $\varrho(x,y,z_1)$, for various levels $z_1$ containing maxima, projected parallel to c. Contours are drawn on an arbitrary scale. Intervals for the light atoms are one fifth those for selenium. The final locations for the atoms are indicated by crosses.

Table 1. *Final atomic coordinates and standard deviations* (Å)

| | *x* | σ(*x*) | *y* | σ(*y*) | *z* | σ(*z*) |
|---|---|---|---|---|---|---|
| Se(1) | 0·2925 | 0·0020 | 0·1192 | 0·0014 | 0·0778 | 0·0033 |
| C(1) | 0·4317 | 0·024 | 0·0728 | 0·022 | 0·2303 | 0·022 |
| N(1) | 0·4241 | 0·014 | 0·0105 | 0·009 | 0·1834 | 0·044 |
| N(2) | −0·4702 | 0·010 | 0·0909 | 0·008 | 0·3479 | 0·017 |
| C(2) | −0·4467 | 0·017 | 0·1499 | 0·011 | 0·3928 | 0·031 |
| C(3) | 0·4599 | 0·022 | 0·1825 | 0·021 | 0·4469 | 0·032 |
| C(4) | 0·4927 | 0·023 | 0·2389 | 0·021 | 0·4980 | 0·052 |
| C(5) | −0·3846 | 0·025 | 0·2328 | 0·023 | 0·0240 | 0·052 |
| C(6) | −0·2866 | 0·025 | 0·2336 | 0·016 | 0·4726 | 0·033 |
| C(7) | −0·3110 | 0·015 | 0·1755 | 0·011 | 0·4158 | 0·029 |
| C(8) | −0·4885 | 0·014 | −0·0327 | 0·013 | 0·2778 | 0·033 |
| C(9) | 0·4837 | 0·026 | −0·0942 | 0·013 | 0·1987 | 0·030 |
| O(1) | 0·3985 | 0·055 | 0·4749 | 0·005 | 0·0954 | 0·037 |
| Se(2) | −0·2050 | 0·0017 | 0·0513 | 0·0015 | 0·1744 | 0·0034 |
| C(10) | −0·0202 | 0·017 | 0·0199 | 0·011 | 0·2523 | 0·028 |
| N(3) | 0·0079 | 0·012 | 0·4651 | 0·010 | 0·3041 | 0·022 |
| N(4) | 0·0900 | 0·011 | 0·0472 | 0·005 | 0·3549 | 0·010 |
| C(11) | 0·0932 | 0·013 | 0·1063 | 0·013 | 0·4177 | 0·030 |
| C(12) | 0·0516 | 0·017 | 0·1540 | 0·016 | 0·3181 | 0·031 |
| C(13) | 0·0631 | 0·023 | 0·2147 | 0·022 | 0·3910 | 0·048 |
| C(14) | 0·1248 | 0·015 | 0·2820 | 0·013 | 0·0434 | 0·036 |
| C(15) | 0·1689 | 0·023 | 0·3310 | 0·015 | 0·1488 | 0·031 |
| C(16) | 0·1538 | 0·016 | 0·3909 | 0·015 | 0·0687 | 0·026 |
| C(17) | −0·1136 | 0·009 | 0·4315 | 0·012 | 0·2640 | 0·019 |
| C(18) | 0·0959 | 0·020 | −0·1315 | 0·017 | 0·1651 | 0·033 |
| O(2) | 0·2363 | 0·020 | −0·0529 | 0·012 | 0·3417 | 0·040 |

Table 2. *Thermal parameters* (Å²)

| | $B_{11}$ | $B_{22}$ | $B_{33}$ | $B_{12}$ | $B_{23}$ | $B_{13}$ |
|---|---|---|---|---|---|---|
| Se(1) | 4·52 | 3·56 | 3·23 | 0·16 | −0·38 | 0·50 |
| C(1) | 4·38 | 7·41 | 3·51 | 0·60 | 0·80 | 1·00 |
| N(1) | 3·77 | 3·62 | 6·00 | −0·23 | 0·50 | 0·70 |
| N(2) | 5·60 | 6·23 | 2·70 | 0 | −0·50 | 0·80 |
| C(2) | 4·92 | 3·57 | 2·97 | 0·08 | 0·18 | 1·00 |
| C(3) | 4·96 | 6·64 | 2·36 | 0·16 | −0·55 | 0·80 |
| C(4) | 7·03 | 4·43 | 6·35 | 0·03 | −0·24 | 1·33 |
| C(5) | 8·70 | 3·90 | 3·85 | −0·50 | 0·40 | 1·00 |
| C(6) | 9·00 | 8·00 | 7·00 | −1·00 | −0·50 | 1·00 |
| C(7) | 6·85 | 4·89 | 8·38 | −0·50 | −0·40 | 1·00 |
| C(8) | 2·41 | 3·64 | 1·17 | −0·40 | −0·80 | 1·00 |
| C(9) | 6·39 | 4·74 | 4·71 | −0·01 | −1·00 | 0·47 |
| O(1) | 5·97 | 4·95 | 5·13 | −0·36 | −1·07 | 1·00 |
| Se(2) | 3·56 | 4·51 | 4·41 | 0·42 | −1·00 | 1·00 |
| C(10) | 3·48 | 4·53 | 3·21 | 0·59 | 0·88 | 1·00 |
| N(3) | 4·44 | 4·25 | 2·38 | 0·51 | 0·80 | 1·00 |
| N(4) | 3·33 | 4·83 | 0·14 | −0·16 | −0·80 | 1·00 |
| C(11) | 4·26 | 5·15 | 2·55 | 0·81 | 0·86 | 0·27 |
| C(12) | 6·57 | 5·27 | 6·06 | 0·60 | 0·80 | 1·00 |
| C(13) | 4·89 | 5·16 | 4·03 | 0·80 | 0·24 | 1·00 |
| C(14) | 5·04 | 5·09 | 2·91 | −0·50 | 0·80 | 1·00 |
| C(15) | 7·37 | 7·67 | 2·97 | 0·15 | 0·42 | 1·00 |
| C(16) | 3·27 | 5·85 | 7·80 | −0·90 | −0·60 | 1·00 |
| C(17) | 3·46 | 4·30 | 1·23 | −0·51 | −0·80 | 1·00 |
| C(18) | 6·29 | 5·19 | 5·23 | −0·39 | −0·31 | 0·90 |
| O(2) | 5·25 | 7·56 | 6·63 | 0·78 | −0·68 | 0·90 |

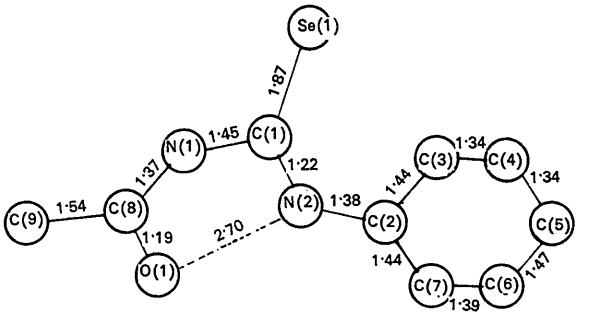
1·63 g.cm$^{-3}$, $D_m$ = 1·7 g.cm$^{-3}$ (flotation). The systematic absences are: $0k0$ absent for $k$ odd and $h0l$ for $l$ odd, so that the space group is uniquely determined as $P2_1/c$. The absorption coefficient for Cu $K\alpha$ radiation is 53·6 cm$^{-1}$.

### Structure determination

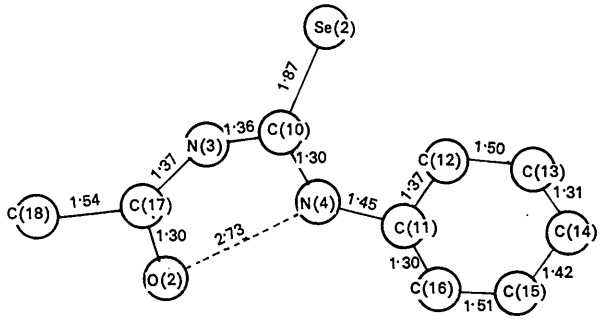
Twenty-six atoms other than hydrogen were to be located, two selenium [designated Se(1) and Se(2)], four nitrogen N(1)···N(4), two oxygen O(1) and O(2), and eighteen carbon atoms. The carbon atoms were designated: C(1) and C(10) the carbon atoms of the selenourea groups; C(2) and C(11) the carbon atoms of the two phenyl groups attached to N(2) and N(4) respectively; C(3)···C(7) and C(12)···C(16) the remaining atoms of the two rings; C(8) and C(9) the acetyl group attached to N(1); C(17) and C(18) the acetyl group attached to N(3). It proved necessary to use a three-dimensional Patterson synthesis to obtain trial coordinates for the selenium atom. The three-dimensional Patterson synthesis showed outstanding maxima, which were attributed to selenium–selenium vectors.

Table 3. *Hydrogen atomic parameters*

| | $x$ | $y$ | $z$ | $B$(Å²) |
|---|---|---|---|---|
| H(3) | 0·366 | 0·167 | 0·450 | 3·00 |
| H(4) | 0·408 | 0·267 | 0·520 | 3·00 |
| H(5) | 0·615 | 0·308 | 0·560 | 3·00 |
| H(6) | 0·815 | 0·241 | 0·500 | 3·00 |
| H(7) | 0·773 | 0·158 | 0·390 | 3·00 |
| H[N(1)] | 0·340 | −0·008 | 0·150 | 3·00 |
| H[N(2)] | 0·605 | 0·063 | 0·350 | 3·00 |
| H(12) | −0·030 | 0·147 | 0·140 | 3·00 |
| H(13) | 0·030 | 0·243 | 0·320 | 3·00 |
| H(14) | 0·133 | 0·258 | 0·590 | 3·00 |
| H(15) | 0·233 | 0·183 | 0·820 | 3·00 |
| H(16) | 0·183 | 0·083 | 0·630 | 3·00 |
| H[N(3)] | −0·067 | −0·050 | 0·100 | 3·00 |
| H[N(4)] | 0·166 | 0·023 | 0·380 | 3·00 |




(*a*)




(*b*)

Fig. 4. Bond lengths.

Table 4. *Observed and calculated structure factors*

| H | K | L | FOBS | FCAL |
|---|---|---|---|---|
| | 4 | | 45.0 | 26.0- |
| | 6 | | 81.8 | 76.5- |
| | 8 | | 19.0 | 13.9 |
| | 10 | | 84.6 | 79.8- |
| | 12 | | 99.2 | 105.8- |
| | 14 | | 64.1 | 60.4- |
| | 16 | | 35.7 | 35.2 |
| | 18 | | 59.9 | 57.5 |
| | 20 | | 7.4 | 3.6- |
| | 22 | | 7.4 | 3.7- |
| | 24 | | 11.7 | 9.6 |
| | 26 | | 5.8 | 8.0 |
| | 28 | | 15.6 | 14.2- |
| 1 | 1 | | 37.5 | 43.0- |
| 1 | 2 | | 25.9 | 30.3 |
| 1 | | | 20.0 | 17.3- |
| 1 | 3 | | 12.7 | 12.6- |
| 1 | 4 | | 4.5 | 6.5 |
| 1 | 5 | | 166.0 | 181.6 |
| 1 | 6 | | 11.3 | 4.1 |
| 1 | 7 | | 138.7 | 143.4 |
| 1 | 8 | | 56.1 | 55.6- |
| 1 | 9 | | 12.1 | 17.1- |
| 1 | 10 | | 56.6 | 49.8- |
| 1 | 11 | | 129.0 | 132.2- |
| 1 | 12 | | 63.9 | 49.1- |
| 1 | 13 | | 45.0 | 46.2- |
| 1 | 14 | | 10.5 | 13.0 |
| 1 | 17 | | 24.7 | 26.5- |
| 1 | 18 | | 20.0 | 18.1 |
| 1 | 19 | | 40.5 | 41.5- |
| 1 | 20 | | 15.0 | 15.0 |
| 1 | 23 | | 45.4 | 43.4 |
| 1 | 25 | | 19.1 | 15.4 |
| 2 | | | 26.2 | 31.1- |
| 2 | 1 | | 37.4 | 33.7- |
| 2 | 2 | | 19.5 | 21.3- |
| 2 | 3 | | 132.1 | 130.6 |
| 2 | 4 | | 76.6 | 83.6 |
| 2 | 5 | | 46.1 | 41.4 |
| 2 | 6 | | 49.8 | 49.1 |
| 2 | 7 | | 32.0 | 30.0 |
| 2 | 8 | | 9.9 | 12.6 |
| 2 | 9 | | 44.1 | 41.9 |
| 2 | 10 | | 46.8 | 45.0 |
| 2 | 11 | | 21.8 | 21.4 |
| 2 | 12 | | 93.6 | 91.3 |
| 2 | 13 | | 35.3 | 35.7- |
| 2 | 14 | | 24.9 | 28.2 |
| 2 | 15 | | 34.8 | 40.7- |
| 2 | 16 | | 73.9 | 72.2- |
| 2 | 17 | | 30.5 | 26.9 |
| 2 | 18 | | 66.7 | 64.1- |
| 2 | 19 | | 23.2 | 21.7 |
| 2 | 24 | | 13.8 | 15.3- |
| 2 | 27 | | 10.8 | 9.3 |
| 2 | 28 | | 10.8 | 13.7 |
| 3 | | | 72.2 | 67.0- |
| 3 | 1 | | 29.5 | 27.3- |
| 3 | 2 | | 62.0 | 53.1- |
| 3 | 3 | | 12.2 | 13.3- |
| 3 | 4 | | 29.5 | 34.3- |
| 3 | 5 | | 149.8 | 158.1- |
| 3 | 6 | | 62.4 | 57.6 |
| 3 | 7 | | 143.2 | 139.6- |
| 3 | 8 | | 113.2 | 108.6 |
| 3 | 9 | | 10.1 | 5.9- |
| 3 | 10 | | 52.6 | 53.2 |
| 3 | 11 | | 33.1 | 34.1 |
| 3 | 12 | | 15.6 | 19.2- |
| 3 | 13 | | 16.2 | 11.0 |
| 3 | 14 | | 9.7 | 9.8- |
| 3 | 16 | | 8.6 | 11.2 |
| 3 | 17 | | 32.0 | 34.4 |
| 3 | 18 | | 9.4 | 8.5- |
| 3 | 19 | | 17.8 | 20.2 |
| 3 | 20 | | 35.1 | 40.0- |
| 3 | 21 | | 9.7 | 9.8- |
| 3 | 22 | | 25.8 | 23.0- |
| 3 | 23 | | 28.3 | 25.3- |
| 3 | 25 | | 13.5 | 13.5- |
| 3 | 26 | | 14.3 | 13.1 |
| 4 | | | 74.8 | 80.0 |
| 4 | 1 | | 67.4 | 67.9- |
| 4 | 2 | | 49.0 | 47.3 |
| 4 | 3 | | 116.6 | 121.8- |
| 4 | 4 | | 13.3 | 15.0- |
| 4 | 5 | | 32.2 | 32.3- |
| 4 | 6 | | 17.0 | 14.2- |
| 4 | 7 | | 21.4 | 22.2 |
| 4 | 9 | | 28.6 | 32.1- |
| 4 | 10 | | 27.4 | 26.1- |
| 4 | 11 | | 24.0 | 13.9- |
| 4 | 12 | | 33.4 | 34.1- |
| 4 | 13 | | 73.6 | 70.6 |
| 4 | 14 | | 32.9 | 31.5- |
| 4 | 15 | | 60.5 | 63.6 |
| 4 | 17 | | 38.6 | 34.8 |
| 4 | 21 | | 5.3 | 13.4- |
| 4 | 25 | | 3.9 | 8.0- |
| 4 | 27 | | 14.7 | 16.4- |
| 5 | | | 11.8 | 15.2- |
| 5 | 2 | | 87.4 | 79.2 |
| 5 | 3 | | 12.1 | 14.3 |
| 5 | 4 | | 102.3 | 106.2 |
| 5 | 5 | | 11.1 | 8.6 |
| 5 | 6 | | 27.0 | 23.4 |
| 5 | 8 | | 84.6 | 89.5- |
| 5 | 10 | | 67.6 | 66.9- |
| 5 | 14 | | 14.6 | 13.6 |
| 5 | 16 | | 9.5 | 13.0- |
| 5 | 17 | | 11.7 | 11.4- |
| 5 | 19 | | 9.6 | 11.0- |
| 5 | 20 | | 31.2 | 32.9 |
| 5 | 22 | | 11.5 | 18.1 |
| 5 | 24 | | 13.1 | 10.8- |
| 5 | 26 | | 11.0 | 12.9- |
| 6 | 1 | | 34.5 | 48.8 |
| 6 | 2 | | 11.9 | 6.7- |
| 6 | 3 | | 76.1 | 76.2 |
| 6 | 5 | | 41.3 | 37.8 |
| 6 | 9 | | 28.6 | 28.8 |
| 6 | 11 | | 26.0 | 29.5 |
| 6 | 13 | | 39.7 | 38.7- |
| 6 | 14 | | 11.6 | 16.1- |
| 6 | 15 | | 62.8 | 64.4- |
| 6 | 17 | | 15.3 | 13.5- |
| 6 | 19 | | 21.6 | 21.4 |
| 7 | 2 | | 25.4 | 24.5- |
| 7 | 3 | | 14.6 | 9.3 |
| 7 | 4 | | 40.6 | 43.8- |
| 7 | 5 | | 28.5 | 24.9 |
| 7 | 6 | | 15.6 | 15.2 |
| 7 | 7 | | 13.8 | 16.8 |
| 7 | 8 | | 66.0 | 64.9 |
| 7 | 10 | | 44.6 | 46.9 |
| 7 | 20 | | 30.4 | 27.2- |
| 7 | 22 | | 18.8 | 19.4- |
| 7 | 23 | | 8.8 | 11.0 |
| 8 | | | 34.3 | 33.7- |
| 8 | 1 | | 32.3 | 30.3- |
| 8 | 2 | | 9.4 | 8.9- |
| 8 | 3 | | 56.4 | 54.6- |
| 8 | 4 | | 18.8 | 21.4 |
| 8 | 5 | | 9.4 | 8.3- |
| 8 | 9 | | 15.6 | 14.0- |
| 8 | 10 | | 15.6 | 9.4 |
| 8 | 11 | | 9.7 | 9.9- |
| 8 | 12 | | 9.6 | 12.5 |
| 8 | 13 | | 16.3 | 18.9 |
| 8 | 15 | | 22.4 | 23.7 |
| 8 | 16 | | 19.2 | 18.3- |
| 8 | 18 | | 14.6 | 17.0- |
| 9 | | | 17.0 | 5.7 |
| 9 | 2 | | 17.6 | 19.5 |
| 9 | 4 | | 16.2 | 16.9 |
| 9 | 5 | | 19.5 | 22.5- |
| 9 | 7 | | 27.8 | 27.0- |
| 9 | 8 | | 28.7 | 30.4- |
| 9 | 10 | | 19.2 | 19.8- |
| 9 | 11 | | 20.3 | 20.4 |
| 9 | 13 | | 12.9 | 10.4 |
| 9 | 15 | | 8.0 | 6.6 |
| 9 | 17 | | 9.4 | 9.6 |
| 10 | | | 42.9 | 42.5 |
| 10 | 2 | | 26.8 | 26.2 |
| 10 | 3 | | 12.1 | 14.4 |
| 10 | 10 | | 14.5 | 15.3- |
| 10 | 12 | | 22.1 | 24.0- |
| 10 | 14 | | 9.8 | 11.1- |
| 10 | 15 | | 11.5 | 12.0- |
| 10 | 16 | | 6.1 | 11.2 |
| 11 | 5 | | 20.9 | 23.1 |
| 11 | 7 | | 14.6 | 17.0 |
| 11 | 11 | | 8.4 | 14.3- |
| 12 | | | 7.8 | 16.0- |
| | 1 | 1 | 28.7 | 20.6 |
| | 2 | 1 | 100.4 | 127.5- |
| | 3 | 1 | 45.5 | 43.0 |
| | 4 | 1 | 48.7 | 50.0- |
| | 5 | 1 | 122.1 | 117.5- |
| | 6 | 1 | 33.6 | 21.1- |
| | 7 | 1 | 43.0 | 43.8 |
| | 8 | 1 | 17.2 | 15.1- |
| | 9 | 1 | 44.2 | 38.8 |
| | 10 | 1 | 10.2 | 17.5- |
| | 11 | 1 | 44.6 | 48.1- |
| | 12 | 1 | 27.0 | 28.8 |
| | 13 | 1 | 57.8 | 59.7- |
| | 14 | 1 | 47.1 | 49.0 |
| | 15 | 1 | 44.2 | 42.0 |
| | 16 | 1 | 32.8 | 37.8 |
| | 17 | 1 | 47.5 | 51.7 |
| | 20 | 1 | 23.3 | 23.8- |
| | 21 | 1 | 13.9 | 14.4- |
| | 22 | 1 | 19.2 | 17.4- |
| | 24 | 1 | 13.1 | 11.6- |
| | 25 | 1 | 22.1 | 18.3 |
| | 26 | 1 | 20.5 | 18.9- |
| | 28 | 1 | 15.5 | 15.1- |
| 1 | 1 | 1 | 14.3 | 18.3 |
| 1 | 2 | 1 | 12.9 | 9.8- |
| 1 | 3 | 1 | 70.1 | 74.6 |
| 1 | 5 | 1 | 81.4 | 86.1 |
| 1 | 6 | 1 | 66.8 | 71.9 |
| 1 | 7 | 1 | 37.6 | 42.2- |
| 1 | 9 | 1 | 133.0 | 151.3- |
| 1 | 10 | 1 | 62.4 | 61.3- |
| 1 | 11 | 1 | 19.0 | 23.1- |
| 1 | 12 | 1 | 30.7 | 32.1- |
| 1 | 13 | 1 | 13.2 | 6.4 |
| 1 | 14 | 1 | 23.1 | 22.6 |
| 1 | 15 | 1 | 25.5 | 21.3- |
| 1 | 16 | 1 | 22.4 | 16.8 |
| 1 | 17 | 1 | 15.8 | 14.7- |
| 1 | 21 | 1 | 37.8 | 40.5 |
| 1 | 23 | 1 | 16.6 | 5.6 |
| 1 | 24 | 1 | 1.1 | 14.4 |
| 2 | 1 | 1 | 62.8 | 60.6- |
| 2 | 2 | 1 | 148.4 | 175.6 |
| 2 | 3 | 1 | 65.1 | 69.7 |
| 2 | 4 | 1 | 86.3 | 103.1 |
| 2 | 5 | 1 | 51.7 | 53.3 |
| 2 | 6 | 1 | 20.9 | 13.8- |
| 2 | 7 | 1 | 20.5 | 15.0- |
| 2 | 9 | 1 | 33.0 | 30.3- |
| 2 | 10 | 1 | 66.3 | 68.7 |
| 2 | 11 | 1 | 28.1 | 34.3 |
| 2 | 13 | 1 | 31.8 | 28.2 |
| 2 | 14 | 1 | 85.7 | 94.6- |
| 2 | 16 | 1 | 61.6 | 68.2- |
| 2 | 20 | 1 | 17.4 | 18.8 |
| 2 | 21 | 1 | 12.1 | 13.0 |
| 2 | 22 | 1 | 14.5 | 11.4- |
| 2 | 28 | 1 | 12.8 | 11.3 |
| 3 | 1 | 1 | 17.6 | 16.1- |
| 3 | 2 | 1 | 55.5 | 65.5 |
| 3 | 3 | 1 | 87.0 | 94.3- |
| 3 | 4 | 1 | 37.3 | 35.5 |
| 3 | 5 | 1 | 56.3 | 59.7- |
| 3 | 6 | 1 | 35.4 | 38.8 |
| 3 | 7 | 1 | 66.9 | 73.7 |
| 3 | 8 | 1 | 8.5 | 3.0- |
| 3 | 9 | 1 | 111.1 | 124.6 |
| 3 | 10 | 1 | 38.7 | 37.5 |
| 3 | 11 | 1 | 13.4 | 12.4 |
| 3 | 13 | 1 | 35.4 | 35.9- |
| 3 | 14 | 1 | 28.1 | 31.9- |
| 3 | 15 | 1 | 17.5 | 15.1- |
| 3 | 16 | 1 | 29.6 | 30.9- |
| 3 | 19 | 1 | 24.6 | 29.8- |
| 3 | 21 | 1 | 31.0 | 37.5- |
| 3 | 25 | 1 | 18.5 | 19.6 |
| 4 | 1 | 1 | 37.4 | 41.4- |
| 4 | 2 | 1 | 97.9 | 106.7- |
| 4 | 3 | 1 | 15.9 | 15.1 |
| 4 | 4 | 1 | 20.9 | 26.8- |
| 4 | 5 | 1 | 12.1 | 8.1 |
| 4 | 6 | 1 | 29.1 | 29.9 |
| 4 | 7 | 1 | 25.3 | 30.1 |
| 4 | 9 | 1 | 42.3 | 45.1 |
| 4 | 10 | 1 | 34.5 | 35.9- |
| 4 | 11 | 1 | 41.3 | 30.0 |
| 4 | 14 | 1 | 45.1 | 57.0 |
| 4 | 16 | 1 | 34.1 | 38.3 |
| 4 | 18 | 1 | 35.0 | 33.7- |
| 4 | 20 | 1 | 21.2 | 20.9- |
| 4 | 21 | 1 | 19.6 | 18.1- |
| 4 | 26 | 1 | 14.0 | 12.7- |
| 5 | 1 | 1 | 13.2 | 13.1- |
| 5 | 2 | 1 | 26.4 | 28.2- |
| 5 | 3 | 1 | 45.2 | 54.6 |
| 5 | 4 | 1 | 55.4 | 60.5- |
| 5 | 5 | 1 | 43.4 | 52.0 |
| 5 | 6 | 1 | 41.1 | 46.4- |
| 5 | 7 | 1 | 51.0 | 55.2- |
| 5 | 9 | 1 | 46.0 | 56.6- |
| 5 | 12 | 1 | 31.0 | 31.5 |
| 5 | 13 | 1 | 24.4 | 24.5 |
| 5 | 15 | 1 | 19.5 | 18.0- |
| 5 | 17 | 1 | 17.5 | 15.7- |
| 5 | 21 | 1 | 29.8 | 31.5 |
| 5 | 22 | 1 | 20.0 | 19.9- |
| 5 | 25 | 1 | 12.3 | 12.0- |
| 6 | 1 | 1 | 40.3 | 80.3 |
| 6 | 2 | 1 | 33.2 | 64.5 |
| 6 | 3 | 1 | 33.7 | 36.5 |
| 6 | 4 | 1 | 23.7 | 24.4 |
| 6 | 5 | 1 | 18.6 | 19.6- |
| 6 | 6 | 1 | 13.3 | 14.8- |
| 6 | 7 | 1 | 19.2 | 20.3- |
| 6 | 9 | 1 | 19.5 | 23.7- |
| 6 | 10 | 1 | 28.2 | 35.4 |
| 6 | 11 | 1 | 32.9 | 39.9- |
| 6 | 13 | 1 | 27.1 | 34.1- |
| 6 | 14 | 1 | 11.7 | 17.2- |
| 6 | 16 | 1 | 19.1 | 21.0- |
| 6 | 17 | 1 | 22.6 | 22.6 |
| 7 | 1 | 1 | 37.1 | 41.5 |
| 7 | 4 | 1 | 24.3 | 24.5 |
| 7 | 5 | 1 | 25.7 | 23.0- |
| 7 | 6 | 1 | 65.1 | 56.7 |
| 7 | 8 | 1 | 21.9 | 20.2 |
| 7 | 10 | 1 | 26.4 | 29.3- |
| 7 | 12 | 1 | 22.7 | 28.8- |
| 7 | 13 | 1 | 19.1 | 17.5- |
| 7 | 14 | 1 | 17.1 | 16.8- |
| 7 | 16 | 1 | 19.7 | 17.5- |
| 7 | 17 | 1 | 25.1 | 14.8 |
| 8 | 1 | 1 | 31.9 | 38.5- |
| 8 | 3 | 1 | 11.8 | 9.3- |
| 8 | 4 | 1 | 17.4 | 15.5 |
| 8 | 5 | 1 | 17.4 | 19.6 |
| 8 | 6 | 1 | 22.9 | 26.3 |
| 8 | 8 | 1 | 10.4 | 11.2 |
| 8 | 11 | 1 | 21.7 | 27.3 |
| 9 | 4 | 1 | 21.7 | 25.9- |
| 9 | 6 | 1 | 32.3 | 37.2- |
| - 1 | 2 | 1 | 71.1 | 69.1 |
| - 1 | 3 | 1 | 33.7 | 20.3- |
| - 1 | 4 | 1 | 57.8 | 55.3- |
| - 1 | 5 | 1 | 31.4 | 32.5- |
| - 1 | 6 | 1 | 161.1 | 176.3- |
| - 1 | 7 | 1 | 72.3 | 62.9 |
| - 1 | 8 | 1 | 53.2 | 59.6- |
| - 1 | 9 | 1 | 32.3 | 33.2 |
| - 1 | 10 | 1 | 19.4 | 22.4 |
| - 1 | 11 | 1 | 27.9 | 30.2 |
| - 1 | 12 | 1 | 27.6 | 30.1 |
| - 1 | 13 | 1 | 11.3 | 8.6 |
| - 1 | 14 | 1 | 22.5 | 23.3- |
| - 1 | 15 | 1 | 10.1 | 13.5 |
| - 1 | 16 | 1 | 10.6 | 7.4 |
| - 1 | 17 | 1 | 7.8 | 9.8- |
| - 1 | 18 | 1 | 57.0 | 67.1 |
| - 1 | 19 | 1 | 37.1 | 33.3- |
| - 1 | 21 | 1 | 15.0 | 18.0- |
| - 1 | 22 | 1 | 31.5 | 28.3- |
| - 1 | 23 | 1 | 16.5 | 10.5- |
| - 1 | 24 | 1 | 24.7 | 25.4- |
| - 1 | 28 | 1 | 12.4 | 11.4 |
| - 2 | 1 | 1 | 138.3 | 140.4- |
| - 2 | 2 | 1 | 100.2 | 91.6- |
| - 2 | 3 | 1 | 21.8 | 21.1 |
| - 2 | 4 | 1 | 78.5 | 68.1 |
| - 2 | 5 | 1 | 76.7 | 66.3 |
| - 2 | 6 | 1 | 70.4 | 68.7 |
| - 2 | 8 | 1 | 46.8 | 47.1 |
| - 2 | 9 | 1 | 32.4 | 30.3- |
| - 2 | 10 | 1 | 18.1 | 11.4 |
| - 2 | 11 | 1 | 41.9 | 46.8 |
| - 2 | 13 | 1 | 69.4 | 71.2 |
| - 2 | 14 | 1 | 25.5 | 22.1- |
| - 2 | 15 | 1 | 19.5 | 17.6- |
| - 2 | 16 | 1 | 23.0 | 23.2- |
| - 2 | 17 | 1 | 54.1 | 60.2- |
| - 2 | 19 | 1 | 26.1 | 23.4- |
| - 2 | 20 | 1 | 27.1 | 21.5- |
| - 2 | 21 | 1 | 11.7 | 9.2 |
| - 2 | 25 | 1 | 14.8 | 16.0- |
| - 3 | 1 | 1 | 118.9 | 111.8 |
| - 3 | 2 | 1 | 142.3 | 127.7- |
| - 3 | 3 | 1 | 61.3 | 45.9- |
| - 3 | 4 | 1 | 113.5 | 97.8 |
| - 3 | 5 | 1 | 37.0 | 30.1- |
| - 3 | 6 | 1 | 123.1 | 109.4 |
| - 3 | 7 | 1 | 13.6 | 13.6- |
| - 3 | 8 | 1 | 71.9 | 66.0 |
| - 3 | 9 | 1 | 19.5 | 18.4 |
| - 3 | 11 | 1 | 24.8 | 23.8- |
| - 3 | 12 | 1 | 65.6 | 60.9- |
| - 3 | 13 | 1 | 15.2 | 12.1- |
| - 3 | 14 | 1 | 10.3 | 9.8- |
| - 3 | 15 | 1 | 10.8 | 5.1 |
| - 3 | 16 | 1 | 11.1 | 5.0 |

Table 4 (*cont.*)

| H | K | L | FOBS | FCAL |
|---|---|---|---|---|
| - 3 | 17 | 1 | 27.9 | 27.5 |
| - 3 | 18 | 1 | 43.9 | 45.0- |
| - 3 | 20 | 1 | 19.5 | 18.0- |
| - 3 | 22 | 1 | 31.0 | 32.3 |
| - 3 | 24 | 1 | 30.0 | 27.6 |
| - 4 | 1 | 1 | 154.5 | 158.4 |
| - 4 | 2 | 1 | 40.6 | 36.4 |
| - 4 | 3 | 1 | 91.4 | 18.7- |
| - 4 | 4 | 1 | 19.7 | 23.1 |
| - 4 | 5 | 1 | 93.4 | 76.9- |
| - 4 | 8 | 1 | 12.1 | 4.9 |
| - 4 | 9 | 1 | 15.5 | 15.3- |
| - 4 | 10 | 1 | 28.7 | 27.7 |
| - 4 | 11 | 1 | 79.7 | 78.2- |
| - 4 | 12 | 1 | 26.8 | 26.1 |
| - 4 | 13 | 1 | 83.3 | 81.0- |
| - 4 | 14 | 1 | 29.7 | 28.7- |
| - 4 | 16 | 1 | 36.6 | 33.4- |
| - 4 | 17 | 1 | 30.3 | 34.1 |
| - 4 | 18 | 1 | 21.0 | 16.9 |
| - 4 | 19 | 1 | 35.3 | 37.0 |
| - 5 | 1 | 1 | 12.9 | 10.4 |
| - 5 | 2 | 1 | 28.2 | 18.3 |
| - 5 | 3 | 1 | 14.6 | 18.0 |
| - 5 | 4 | 1 | 53.3 | 48.2- |
| - 5 | 5 | 1 | 59.6 | 52.4 |
| - 5 | 6 | 1 | 97.0 | 91.1- |
| - 5 | 7 | 1 | 74.8 | 67.7- |
| - 5 | 8 | 1 | 41.6 | 38.7- |
| - 5 | 9 | 1 | 46.6 | 42.0- |
| - 5 | 10 | 1 | 45.0 | 37.2 |
| - 5 | 12 | 1 | 41.1 | 37.9 |
| - 5 | 13 | 1 | 37.7 | 31.5 |
| - 5 | 14 | 1 | 16.1 | 13.2 |
| - 5 | 15 | 1 | 11.5 | 11.0- |
| - 5 | 18 | 1 | 17.3 | 16.1 |
| - 5 | 19 | 1 | 20.9 | 17.1 |
| - 5 | 21 | 1 | 24.0 | 24.5 |
| - 5 | 22 | 1 | 16.8 | 17.7- |
| - 5 | 24 | 1 | 22.7 | 20.2- |
| - 5 | 25 | 1 | 12.5 | 11.7- |
| - 6 | 1 | 1 | 72.6 | 68.0- |
| - 6 | 2 | 1 | 61.9 | 54.5- |
| - 6 | 3 | 1 | 21.5 | 18.7- |
| - 6 | 4 | 1 | 25.8 | 24.2- |
| - 6 | 5 | 1 | 22.2 | 19.3 |
| - 6 | 6 | 1 | 29.6 | 25.3 |
| - 6 | 7 | 1 | 10.3 | 11.3 |
| - 6 | 10 | 1 | 30.1 | 25.7- |
| - 6 | 11 | 1 | 22.4 | 23.2 |
| - 6 | 12 | 1 | 16.1 | 12.8 |
| - 6 | 13 | 1 | 31.5 | 26.2 |
| - 6 | 14 | 1 | 37.1 | 38.7 |
| - 6 | 16 | 1 | 18.6 | 16.9 |
| - 6 | 17 | 1 | 37.3 | 34.7- |
| - 6 | 18 | 1 | 23.8 | 20.7- |
| - 7 | 1 | 1 | 31.0 | 26.2- |
| - 7 | 2 | 1 | 15.9 | 13.4 |
| - 7 | 3 | 1 | 44.6 | 42.0- |
| - 7 | 4 | 1 | 28.6 | 24.1 |
| - 7 | 5 | 1 | 23.2 | 21.4- |
| - 7 | 6 | 1 | 32.3 | 33.6 |
| - 7 | 7 | 1 | 44.8 | 38.1 |
| - 7 | 8 | 1 | 14.0 | 12.9 |
| - 7 | 9 | 1 | 55.3 | 63.4 |
| - 7 | 11 | 1 | 11.7 | 13.9 |
| - 7 | 12 | 1 | 11.8 | 18.7- |
| - 7 | 16 | 1 | 20.7 | 18.0- |
| - 7 | 13 | 1 | 17.6 | 13.6- |
| - 7 | 18 | 1 | 23.5 | 16.8- |
| - 7 | 19 | 1 | 14.1 | 13.6- |
| - 7 | 21 | 1 | 18.9 | 20.6- |
| - 8 | 2 | 1 | 75.5 | 70.3 |
| - 8 | 6 | 1 | 19.4 | 18.6 |
| - 8 | 4 | 1 | 52.5 | 47.7 |
| - 8 | 9 | 1 | 19.1 | 15.8- |
| - 8 | 10 | 1 | 23.1 | 21.6 |
| - 8 | 14 | 1 | 37.0 | 38.3- |
| - 8 | 16 | 1 | 24.3 | 25.2- |
| - 9 | 3 | 1 | 26.3 | 26.3 |
| - 9 | 5 | 1 | 20.7 | 14.9 |
| - 9 | 7 | 1 | 27.7 | 27.6- |
| - 9 | 9 | 1 | 39.1 | 41.6- |
| - 9 | 11 | 1 | 14.3 | 13.1- |
| -10 | 1 | 1 | 14.7 | 16.3 |
| -10 | 2 | 1 | 17.1 | 20.1- |
| -10 | 4 | 1 | 22.4 | 22.4- |
| -10 | 5 | 1 | 17.0 | 13.1- |
| -10 | 14 | 1 | 24.7 | 23.9 |
| -10 | 16 | 1 | 18.4 | 18.1 |
| -11 | 1 | 1 | 18.3 | 16.8- |
| -11 | 3 | 1 | 19.2 | 20.2- |
| -11 | 6 | 1 | 20.9 | 20.5- |
| -11 | 9 | 1 | 18.7 | 18.9 |
| | | 2 | 32.7 | 35.6- |
| | 1 | 2 | 17.6 | 22.2- |
| | 2 | 2 | 170.7 | 222.8- |
| | 3 | 2 | 95.8 | 112.3- |
| | 4 | 2 | 40.6 | 50.3- |
| | 5 | 2 | 70.3 | 70.8- |
| | 6 | 2 | 20.3 | 17.7- |
| | 7 | 2 | 6.0 | 1.6- |
| | 8 | 2 | 107.5 | 119.7 |
| | 9 | 2 | 53.7 | 56.0- |
| | 10 | 2 | 58.2 | 64.6 |
| | 11 | 2 | 36.0 | 43.8- |
| | 13 | 2 | 47.3 | 49.4 |
| | 14 | 2 | 16.5 | 15.6- |
| | 15 | 2 | 70.6 | 76.8 |
| | 16 | 2 | 16.9 | 19.3 |
| | 18 | 2 | 8.2 | 9.2 |
| | 19 | 2 | 40.2 | 40.7- |
| | 20 | 2 | 27.0 | 30.2- |
| | 21 | 2 | 15.7 | 13.9- |
| | 22 | 2 | 16.9 | 15.0- |
| | 23 | 2 | 6.7 | 7.2 |
| | 26 | 2 | 13.5 | 10.9 |
| | 27 | 2 | 15.4 | 17.7- |
| 1 | | 2 | 117.4 | 111.4- |
| 1 | 1 | 2 | 40.0 | 43.5- |
| 1 | 2 | 2 | 92.0 | 93.0 |
| 1 | 3 | 2 | 108.6 | 113.8- |
| 1 | 4 | 2 | 76.5 | 89.1 |
| 1 | 5 | 2 | 7.6 | 3.3- |
| 1 | 6 | 2 | 53.6 | 57.6- |
| 1 | 9 | 2 | 33.9 | 29.8 |
| 1 | 10 | 2 | 26.5 | 38.0- |
| 1 | 11 | 2 | 12.1 | 12.5 |
| 1 | 13 | 2 | 33.9 | 40.8 |
| 1 | 14 | 2 | 26.0 | 27.2 |
| 1 | 15 | 2 | 43.0 | 48.3 |
| 1 | 16 | 2 | 20.9 | 28.2- |
| 1 | 17 | 2 | 20.9 | 18.5 |
| 1 | 20 | 2 | 39.5 | 49.1 |
| 1 | 22 | 2 | 24.2 | 28.2 |
| 1 | 26 | 2 | 17.1 | 17.3- |
| 1 | 27 | 2 | 9.4 | 7.5- |
| 2 | | 2 | 86.4 | 78.4 |
| 2 | 1 | 2 | 87.1 | 86.3 |
| 2 | 2 | 2 | 75.4 | 66.9 |
| 2 | 3 | 2 | 147.0 | 139.1 |
| 2 | 4 | 2 | 47.6 | 47.1 |
| 2 | 5 | 2 | 36.0 | 36.3- |
| 2 | 6 | 2 | 16.2 | 17.6- |
| 2 | 7 | 2 | 20.3 | 24.8- |
| 2 | 8 | 2 | 63.0 | 70.5- |
| 2 | 9 | 2 | 21.0 | 31.9 |
| 2 | 10 | 2 | 54.6 | 65.7- |
| 2 | 11 | 2 | 32.8 | 39.1 |
| 2 | 12 | 2 | 27.1 | 33.6- |
| 2 | 13 | 2 | 24.8 | 31.9- |
| 2 | 15 | 2 | 49.1 | 62.8- |
| 2 | 17 | 2 | 15.3 | 16.3- |
| 2 | 18 | 2 | 20.3 | 30.1 |
| 2 | 20 | 2 | 30.6 | 33.1 |
| 2 | 27 | 2 | 16.3 | 15.5 |
| 3 | | 2 | 53.7 | 51.9 |
| 3 | 1 | 2 | 15.3 | 8.6 |
| 3 | 2 | 2 | 34.7 | 29.5- |
| 3 | 3 | 2 | 46.6 | 45.1 |
| 3 | 4 | 2 | 94.3 | 90.9- |
| 3 | 5 | 2 | 84.2 | 89.7 |
| 3 | 6 | 2 | 31.6 | 29.3- |
| 3 | 7 | 2 | 90.6 | 94.4 |
| 3 | 8 | 2 | 33.9 | 40.3 |
| 3 | 9 | 2 | 23.5 | 25.4 |
| 3 | 10 | 2 | 23.5 | 27.2 |
| 3 | 11 | 2 | 39.9 | 39.3- |
| 3 | 12 | 2 | 31.2 | 39.1- |
| 3 | 13 | 2 | 35.5 | 39.3- |
| 3 | 14 | 2 | 21.7 | 27.7- |
| 3 | 15 | 2 | 30.6 | 33.1- |
| 3 | 16 | 2 | 20.3 | 26.1 |
| 3 | 17 | 2 | 23.0 | 28.7- |
| 3 | 18 | 2 | 19.6 | 23.9 |
| 3 | 22 | 2 | 13.3 | 11.6- |
| 3 | 23 | 2 | 14.3 | 14.0 |
| 3 | 24 | 2 | 15.3 | 14.2 |
| 3 | 26 | 2 | 10.9 | 12.5 |
| 4 | | 2 | 86.1 | 78.9- |
| 4 | 1 | 2 | 14.3 | 13.6- |
| 4 | 2 | 2 | 62.4 | 56.6- |
| 4 | 3 | 2 | 51.5 | 55.2- |
| 4 | 5 | 2 | 36.4 | 33.3 |
| 4 | 6 | 2 | 21.7 | 24.5 |
| 4 | 7 | 2 | 51.2 | 49.5 |
| 4 | 8 | 2 | 19.5 | 19.3 |
| 4 | 9 | 2 | 18.8 | 22.0- |
| 4 | 10 | 2 | 36.0 | 31.2 |
| 4 | 11 | 2 | 34.8 | 35.8- |
| 4 | 12 | 2 | 53.5 | 62.1 |
| 4 | 13 | 2 | 26.0 | 26.8 |
| 4 | 14 | 2 | 29.2 | 31.6 |
| 4 | 15 | 2 | 27.6 | 29.1 |
| 4 | 16 | 2 | 20.9 | 20.7- |
| 4 | 17 | 2 | 18.0 | 14.3- |
| 4 | 18 | 2 | 22.3 | 23.7- |
| 4 | 19 | 2 | 26.5 | 28.3- |
| 4 | 23 | 2 | 17.1 | 17.5 |
| 5 | | 2 | 66.9 | 55.5- |
| 5 | 1 | 2 | 14.3 | 12.1- |
| 5 | 2 | 2 | 27.1 | 23.2- |
| 5 | 3 | 2 | 35.1 | 25.9- |
| 5 | 4 | 2 | 18.8 | 22.0 |
| 5 | 5 | 2 | 71.8 | 68.7- |
| 5 | 6 | 2 | 15.3 | 10.7 |
| 5 | 7 | 2 | 59.9 | 63.6- |
| 5 | 8 | 2 | 24.8 | 31.8- |
| 5 | 11 | 2 | 30.2 | 33.0 |
| 5 | 12 | 2 | 23.0 | 25.5 |
| 5 | 17 | 2 | 18.0 | 16.7 |
| 5 | 19 | 2 | 18.8 | 15.1 |
| 5 | 24 | 2 | 23.0 | 6.5- |
| 6 | | 2 | 94.4 | 92.8 |
| 6 | 2 | 2 | 23.0 | 17.7 |
| 6 | 4 | 2 | 35.3 | 37.5- |
| 6 | 5 | 2 | 30.6 | 31.5- |
| 6 | 6 | 2 | 27.1 | 28.3- |
| 6 | 7 | 2 | 35.3 | 38.4- |
| 6 | 10 | 2 | 17.1 | 18.9- |
| 6 | 11 | 2 | 21.0 | 22.3 |
| 6 | 12 | 2 | 27.8 | 29.9- |
| 6 | 13 | 2 | 18.0 | 16.3 |
| 6 | 16 | 2 | 30.1 | 29.6 |
| 6 | 18 | 2 | 23.0 | 27.2 |
| 7 | | 2 | 31.6 | 31.5 |
| 7 | 1 | 2 | 18.8 | 21.3- |
| 7 | 2 | 2 | 20.3 | 15.4 |
| 7 | 5 | 2 | 32.5 | 36.0 |
| 7 | 7 | 2 | 39.9 | 47.2 |
| 7 | 8 | 2 | 14.3 | 10.3- |
| 7 | 10 | 2 | 19.6 | 19.0- |
| 7 | 11 | 2 | 33.4 | 36.3- |
| 7 | 12 | 2 | 27.1 | 27.5- |
| 7 | 20 | 2 | 12.1 | 4.3 |
| 8 | | 2 | 43.6 | 46.4- |
| 8 | 2 | 2 | 21.2 | 21.6- |
| 8 | 4 | 2 | 21.2 | 18.6 |
| 8 | 5 | 2 | 23.6 | 25.7 |
| 8 | 11 | 2 | 16.3 | 12.8- |
| 8 | 12 | 2 | 24.2 | 27.7 |
| 8 | 13 | 2 | 13.3 | 13.1- |
| 8 | 14 | 2 | 19.6 | 20.0 |
| 8 | 15 | 2 | 16.3 | 15.8- |
| 8 | 16 | 2 | 14.3 | 13.0- |
| 9 | | 2 | 24.2 | 25.9- |
| 9 | 2 | 2 | 17.9 | 22.2- |
| 9 | 6 | 2 | 17.1 | 19.7 |
| 9 | 7 | 2 | 16.3 | 12.6- |
| - 1 | 2 | 2 | 60.0 | 56.4- |
| - 1 | 3 | 2 | 176.7 | 152.1 |
| - 1 | 4 | 2 | 159.4 | 146.9- |
| -1 | 1 | 2 | 47.3 | 58.7 |
| - 1 | 5 | 2 | 46.3 | 52.0 |
| - 1 | 6 | 2 | 17.1 | 17.6 |
| - 1 | 8 | 2 | 147.0 | 142.0 |
| - 1 | 9 | 2 | 79.1 | 81.2 |
| - 1 | 10 | 2 | 133.2 | 145.2 |
| - 1 | 11 | 2 | 82.7 | 89.0 |
| - 1 | 12 | 2 | 18.8 | 19.9 |
| - 1 | 13 | 2 | 40.6 | 48.4- |
| - 1 | 15 | 2 | 44.3 | 53.5- |
| - 1 | 19 | 2 | 21.7 | 25.8 |
| - 1 | 20 | 2 | 39.9 | 42.1- |
| - 1 | 22 | 2 | 18.0 | 25.9- |
| - 1 | 23 | 2 | 15.3 | 18.5- |
| - 1 | 27 | 2 | 12.1 | 11.5 |
| - 2 | | 2 | 236.1 | 240.7- |
| - 2 | 1 | 2 | 197.0 | 182.8 |
| - 2 | 2 | 2 | 160.1 | 139.5- |
| - 2 | 3 | 2 | 221.0 | 193.5 |
| - 2 | 4 | 2 | 50.2 | 48.8 |
| - 2 | 5 | 2 | 144.0 | 118.5 |
| - 2 | 6 | 2 | 10.9 | 3.5 |
| - 2 | 7 | 2 | 9.4 | 6.4 |
| - 2 | 8 | 2 | 79.4 | 77.6- |
| - 2 | 9 | 2 | 16.9 | 18.9 |
| - 2 | 10 | 2 | 30.6 | 25.1- |
| - 2 | 12 | 2 | 39.5 | 47.8 |
| - 2 | 13 | 2 | 60.7 | 69.1- |
| - 2 | 14 | 2 | 19.6 | 23.8 |
| - 2 | 15 | 2 | 46.3 | 58.1- |
| - 2 | 17 | 2 | 26.5 | 34.3- |
| - 2 | 20 | 2 | 14.3 | 21.6 |
| - 2 | 21 | 2 | 18.0 | 14.0 |
| - 2 | 22 | 2 | 21.0 | 21.2 |
| - 2 | 27 | 2 | 10.9 | 12.4 |
| - 3 | | 2 | 139.8 | 103.1 |
| - 3 | 2 | 2 | 158.6 | 141.6 |
| - 3 | 3 | 2 | 84.9 | 76.9- |
| - 3 | 4 | 2 | 32.9 | 27.6 |
| - 3 | 5 | 2 | 61.6 | 67.7 |
| - 3 | 6 | 2 | 43.3 | 31.7- |
| - 3 | 7 | 2 | 97.0 | 86.3 |
| - 3 | 8 | 2 | 82.7 | 76.0- |
| - 3 | 9 | 2 | 35.9 | 34.4- |
| - 3 | 10 | 2 | 68.5 | 66.1- |
| - 3 | 11 | 2 | 53.7 | 52.7- |
| - 3 | 12 | 2 | 15.3 | 19.9- |
| - 3 | 15 | 2 | 21.6 | 25.9 |
| - 3 | 16 | 2 | 12.1 | 11.4 |
| - 3 | 17 | 2 | 17.1 | 14.8- |
| - 3 | 20 | 2 | 17.9 | 21.9 |
| - 3 | 22 | 2 | 17.9 | 18.8 |
| - 3 | 23 | 2 | 19.5 | 20.0 |
| - 3 | 27 | 2 | 16.3 | 19.0- |
| - 4 | 1 | 2 | 17.1 | 5.8- |
| - 4 | 2 | 2 | 24.8 | 17.0- |
| - 4 | 3 | 2 | 49.4 | 54.3- |
| - 4 | 4 | 2 | 92.2 | 81.0- |
| - 4 | 5 | 2 | 69.7 | 67.2- |
| - 4 | 6 | 2 | 44.6 | 37.6- |
| - 4 | 7 | 2 | 65.5 | 56.7- |
| - 4 | 8 | 2 | 13.3 | 14.0 |
| - 4 | 9 | 2 | 13.3 | 11.4- |
| - 4 | 10 | 2 | 21.0 | 16.9- |
| - 4 | 11 | 2 | 35.1 | 33.9 |
| - 4 | 12 | 2 | 47.3 | 44.9- |
| - 4 | 13 | 2 | 49.1 | 48.7 |
| - 4 | 15 | 2 | 56.6 | 54.6 |
| - 4 | 16 | 2 | 83.3 | 82.1 |
| - 4 | 17 | 2 | 33.4 | 32.3 |
| - 4 | 18 | 2 | 23.6 | 32.8 |
| - 4 | 23 | 2 | 20.3 | 15.3- |
| - 5 | | 2 | 143.6 | 117.4- |
| - 5 | 1 | 2 | 24.2 | 12.3- |
| - 5 | 2 | 2 | 20.3 | 20.2- |
| - 5 | 3 | 2 | 39.5 | 36.5- |
| - 5 | 4 | 2 | 22.3 | 17.0- |
| - 5 | 5 | 2 | 104.9 | 93.7- |
| - 5 | 7 | 2 | 77.4 | 79.8- |
| - 5 | 8 | 2 | 24.2 | 24.1 |
| - 5 | 9 | 2 | 18.0 | 9.7 |
| - 5 | 10 | 2 | 34.3 | 32.9 |
| - 5 | 11 | 2 | 58.2 | 56.4 |
| - 5 | 12 | 2 | 50.3 | 48.8 |
| - 5 | 13 | 2 | 20.2 | 15.4 |
| - 5 | 14 | 2 | 26.5 | 22.9 |
| - 5 | 16 | 2 | 17.1 | 19.1- |
| - 5 | 17 | 2 | 13.3 | 16.6 |
| - 5 | 18 | 2 | 12.6 | 30.1- |
| - 5 | 23 | 2 | 26.0 | 27.8- |
| - 6 | | 2 | 141.7 | 132.3- |
| - 6 | 1 | 2 | 52.0 | 43.6- |
| - 6 | 2 | 2 | 52.3 | 46.2- |
| - 6 | 4 | 2 | 32.5 | 28.4 |
| - 6 | 5 | 2 | 67.3 | 64.9 |
| - 6 | 6 | 2 | 25.4 | 25.0 |
| - 6 | 7 | 2 | 71.8 | 66.4 |
| - 6 | 10 | 2 | 29.7 | 25.1 |
| - 6 | 11 | 2 | 18.0 | 16.5- |
| - 6 | 12 | 2 | 52.0 | 54.3 |
| - 6 | 14 | 2 | 18.8 | 18.7 |
| - 6 | 18 | 2 | 24.2 | 25.9- |
| - 6 | 23 | 2 | 14.4 | 12.5 |
| - 7 | | 2 | 64.7 | 54.2 |
| - 7 | 1 | 2 | 18.0 | 16.9- |
| - 7 | 4 | 2 | 46.3 | 47.7- |
| - 7 | 5 | 2 | 53.6 | 53.4 |
| - 7 | 6 | 2 | 16.3 | 16.4- |
| - 7 | 7 | 2 | 48.2 | 54.8 |
| - 7 | 11 | 2 | 34.3 | 34.6- |
| - 7 | 12 | 2 | 32.1 | 31.0- |
| - 7 | 13 | 2 | 17.1 | 16.1- |
| - 7 | 14 | 2 | 25.6 | 24.6- |
| - 7 | 18 | 2 | 13.3 | 15.4 |
| - 7 | 23 | 2 | 20.9 | 18.9 |
| - 8 | | 2 | 50.3 | 60.0 |
| - 8 | 2 | 2 | 28.2 | 28.5 |
| - 8 | 3 | 2 | 23.0 | 29.4 |
| - 8 | 7 | 2 | 18.8 | 22.2- |
| - 8 | 8 | 2 | 15.4 | 14.3- |
| - 8 | 10 | 2 | 27.6 | 21.0- |
| - 8 | 11 | 2 | 21.0 | 23.1 |
| - 8 | 12 | 2 | 30.2 | 25.5- |
| - 8 | 15 | 2 | 13.3 | 18.3- |
| - 8 | 16 | 2 | 15.4 | 18.2 |
| - 8 | 18 | 2 | 31.6 | 28.5 |
| - 9 | 5 | 2 | 21.0 | 28.4- |

Table 4 (*cont.*)

| H | K | L | FOBS | FCAL |
|---|---|---|---|---|
| - 9 | 8 | 2 | 26.0 | 29.9- |
| - 9 | 13 | 2 | 23.0 | 22.7 |
| -10 | | 2 | 18.0 | 21.2- |
| -10 | 2 | 2 | 21.7 | 24.1- |
| -10 | 3 | 2 | 14.3 | 20.1- |
| -10 | 8 | 2 | 13.3 | 17.5 |
| -10 | 10 | 2 | 17.1 | 16.7 |
| -11 | 3 | 2 | 20.3 | 21.5 |
| -11 | 5 | 2 | 16.3 | 14.2 |
| -11 | 8 | 2 | 17.1 | 18.4 |
| -11 | 10 | 2 | 17.1 | 14.6 |
| -12 | 3 | 2 | 13.3 | 16.9 |
| -12 | 5 | 2 | 12.1 | 11.8 |
| | 1 | 3 | 59.5 | 65.0- |
| | 2 | 3 | 108.9 | 134.7- |
| | 3 | 3 | 55.7 | 61.9- |
| | 4 | 3 | 19.5 | 20.3 |
| | 5 | 3 | 10.2 | 13.1- |
| | 6 | 3 | 80.7 | 85.7 |
| | 7 | 3 | 35.0 | 39.0 |
| | 8 | 3 | 39.5 | 38.7 |
| | 9 | 3 | 22.0 | 24.3 |
| | 10 | 3 | 30.6 | 42.1- |
| | 11 | 3 | 40.3 | 33.9 |
| | 12 | 3 | 18.3 | 16.3- |
| | 13 | 3 | 11.4 | 15.4 |
| | 14 | 3 | 41.2 | 41.7 |
| | 15 | 3 | 13.8 | 12.3- |
| | 16 | 3 | 29.3 | 33.0 |
| | 17 | 3 | 21.6 | 25.8- |
| | 18 | 3 | 20.8 | 24.9- |
| | 19 | 3 | 12.2 | 18.1- |
| | 20 | 3 | 12.2 | 12.5- |
| | 21 | 3 | 17.9 | 18.9- |
| | 22 | 3 | 17.1 | 16.9 |
| | 24 | 3 | 20.4 | 18.8 |
| 1 | 1 | 3 | 55.7 | 71.7- |
| 1 | 2 | 3 | 17.5 | 22.8- |
| 1 | 3 | 3 | 13.5 | 17.6 |
| 1 | 4 | 3 | 76.7 | 94.8- |
| 1 | 5 | 3 | 82.0 | 92.7 |
| 1 | 6 | 3 | 69.5 | 77.5- |
| 1 | 7 | 3 | 24.2 | 23.4- |
| 1 | 8 | 3 | 25.4 | 36.2- |
| 1 | 9 | 3 | 50.0 | 47.4- |
| 1 | 11 | 3 | 54.8 | 61.7 |
| 1 | 12 | 3 | 34.7 | 42.5 |
| 1 | 13 | 3 | 72.4 | 81.5 |
| 1 | 14 | 3 | 32.3 | 40.4 |
| 1 | 17 | 3 | 28.8 | 30.3- |
| 1 | 25 | 3 | 18.3 | 18.4- |
| 2 | 1 | 3 | 30.4 | 35.5 |
| 2 | 2 | 3 | 17.2 | 18.2- |
| 2 | 3 | 3 | 28.3 | 18.5- |
| 2 | 4 | 3 | 35.4 | 38.2- |
| 2 | 5 | 3 | 47.8 | 49.0- |
| 2 | 6 | 3 | 91.6 | 109.2- |
| 2 | 7 | 3 | 21.5 | 28.0- |
| 2 | 8 | 3 | 44.9 | 48.1- |
| 2 | 9 | 3 | 16.3 | 19.9- |
| 2 | 10 | 3 | 47.7 | 52.0 |
| 2 | 11 | 3 | 40.8 | 41.5- |
| 2 | 12 | 3 | 37.2 | 44.3 |
| 2 | 13 | 3 | 21.7 | 27.1- |
| 2 | 17 | 3 | 29.0 | 28.0 |
| 2 | 18 | 3 | 37.3 | 41.0 |
| 2 | 24 | 3 | 23.3 | 20.3- |
| 3 | 1 | 3 | 91.9 | 95.0 |
| 3 | 2 | 3 | 30.3 | 31.5- |
| 3 | 4 | 3 | 33.6 | 28.1 |
| 3 | 5 | 3 | 38.9 | 46.9- |
| 3 | 6 | 3 | 60.1 | 68.6 |
| 3 | 10 | 3 | 33.2 | 29.1- |
| 3 | 11 | 3 | 41.6 | 51.7- |
| 3 | 13 | 3 | 25.3 | 23.0- |
| 3 | 14 | 3 | 30.6 | 26.1 |
| 3 | 15 | 3 | 20.4 | 20.4 |
| 3 | 17 | 3 | 35.5 | 39.2 |
| 3 | 22 | 3 | 23.7 | 21.3 |
| 4 | 1 | 3 | 66.1 | 69.4- |
| 4 | 2 | 3 | 29.7 | 30.5- |
| 4 | 4 | 3 | 34.8 | 43.8 |
| 4 | 5 | 3 | 29.7 | 35.3 |
| 4 | 6 | 3 | 51.2 | 61.6 |
| 4 | 8 | 3 | 24.2 | 24.6 |
| 4 | 9 | 3 | 31.3 | 34.9- |
| 4 | 10 | 3 | 37.2 | 39.5- |
| 4 | 11 | 3 | 28.3 | 27.0 |
| 4 | 12 | 3 | 34.8 | 32.3- |
| 4 | 13 | 3 | 28.8 | 30.4 |
| 4 | 14 | 3 | 20.4 | 17.1- |
| 4 | 17 | 3 | 25.9 | 24.7- |
| 5 | 1 | 3 | 69.4 | 71.2- |
| 5 | 2 | 3 | 72.2 | 72.6 |
| 5 | 3 | 3 | 31.9 | 34.9- |
| 5 | 4 | 3 | 32.2 | 32.1 |
| 5 | 6 | 3 | 25.0 | 26.2- |
| 5 | 7 | 3 | 22.7 | 21.2 |
| 5 | 9 | 3 | 28.4 | 25.4 |
| 5 | 10 | 3 | 36.5 | 27.7 |
| 5 | 11 | 3 | 36.5 | 31.0 |
| 5 | 12 | 3 | 28.9 | 30.2 |
| 5 | 13 | 3 | 36.3 | 42.1 |
| 5 | 16 | 3 | 23.6 | 10.2- |
| 5 | 17 | 3 | 25.8 | 20.0- |
| 6 | 2 | 3 | 20.1 | 20.1- |
| 6 | 3 | 3 | 28.8 | 30.1- |
| 6 | 4 | 3 | 31.0 | 30.8- |
| 6 | 5 | 3 | 25.8 | 26.1- |
| 6 | 6 | 3 | 33.2 | 38.6- |
| 6 | 7 | 3 | 33.5 | 39.2 |
| 6 | 8 | 3 | 25.8 | 23.9- |
| 6 | 9 | 3 | 35.5 | 39.5 |
| 6 | 13 | 3 | 19.5 | 25.4- |
| 6 | 16 | 3 | 17.5 | 9.3 |
| 7 | 2 | 3 | 31.0 | 29.1- |
| 7 | 9 | 3 | 19.8 | 23.2- |
| 7 | 14 | 3 | 29.7 | 26.6 |
| 8 | 2 | 3 | 19.0 | 19.4 |
| 8 | 3 | 3 | 27.0 | 27.3 |
| 8 | 5 | 3 | 18.7 | 15.3 |
| 8 | 7 | 3 | 18.3 | 18.3- |
| 8 | 9 | 3 | 29.9 | 27.5- |
| - 1 | 4 | 3 | 20.1 | 26.8 |
| - 1 | 5 | 3 | 53.0 | 50.0- |
| - 1 | 7 | 3 | 49.4 | 55.4 |
| - 1 | 1 | 3 | 20.4 | 28.0 |
| - 1 | 2 | 3 | 95.5 | 115.3 |
| - 1 | 3 | 3 | 43.3 | 52.6- |
| - 1 | 8 | 3 | 50.3 | 53.1 |
| - 1 | 9 | 3 | 56.8 | 64.3 |
| - 1 | 10 | 3 | 19.1 | 16.7 |
| - 1 | 12 | 3 | 21.9 | 22.3- |
| - 1 | 13 | 3 | 44.7 | 49.5- |
| - 1 | 14 | 3 | 42.5 | 48.9- |
| - 1 | 16 | 3 | 45.5 | 43.2- |
| - 1 | 17 | 3 | 37.4 | 38.3 |
| - 1 | 25 | 3 | 22.4 | 20.5 |
| - 2 | 1 | 3 | 42.9 | 52.0 |
| - 2 | 2 | 3 | 122.0 | 117.3 |
| - 2 | 3 | 3 | 87.7 | 82.4 |
| - 2 | 4 | 3 | 38.7 | 39.9 |
| - 2 | 5 | 3 | 64.6 | 49.1 |
| - 2 | 6 | 3 | 35.9 | 33.1- |
| - 2 | 7 | 3 | 61.8 | 57.5- |
| - 2 | 8 | 3 | 26.1 | 18.3 |
| - 2 | 9 | 3 | 85.0 | 78.6- |
| - 2 | 10 | 3 | 38.0 | 33.4 |
| - 2 | 11 | 3 | 34.5 | 39.7- |
| - 2 | 14 | 3 | 39.7 | 43.1- |
| - 2 | 15 | 3 | 24.5 | 20.0- |
| - 2 | 16 | 3 | 22.4 | 23.2- |
| - 2 | 17 | 3 | 20.1 | 16.6- |
| - 2 | 18 | 3 | 43.0 | 38.9 |
| - 2 | 19 | 3 | 26.5 | 27.8 |
| - 2 | 20 | 3 | 26.5 | 27.1 |
| - 2 | 21 | 3 | 34.7 | 34.3 |
| - 3 | 1 | 3 | 47.8 | 34.9- |
| - 3 | 2 | 3 | 93.1 | 83.4- |
| - 3 | 3 | 3 | 16.7 | 18.8 |
| - 3 | 4 | 3 | 17.5 | 15.8- |
| - 3 | 5 | 3 | 58.7 | 46.4 |
| - 3 | 7 | 3 | 69.1 | 62.9- |
| - 3 | 8 | 3 | 39.9 | 32.6 |
| - 3 | 9 | 3 | 41.2 | 45.5- |
| - 3 | 10 | 3 | 48.0 | 44.2- |
| - 3 | 14 | 3 | 45.9 | 48.5 |
| - 3 | 16 | 3 | 52.3 | 48.0 |
| - 3 | 18 | 3 | 20.5 | 17.4- |
| - 3 | 19 | 3 | 20.5 | 20.0 |
| - 3 | 21 | 3 | 27.0 | 29.9 |
| - 4 | 1 | 3 | 69.1 | 57.7 |
| - 4 | 2 | 3 | 49.4 | 45.7- |
| - 4 | 3 | 3 | 60.0 | 58.5- |
| - 4 | 4 | 3 | 61.6 | 53.3- |
| - 4 | 5 | 3 | 109.6 | 82.4- |
| - 4 | 6 | 3 | 30.4 | 30.1- |
| - 4 | 7 | 3 | 73.7 | 57.9 |
| - 4 | 8 | 3 | 26.1 | 24.1- |
| - 4 | 9 | 3 | 102.5 | 95.1 |
| - 4 | 10 | 3 | 22.6 | 20.5- |
| - 4 | 13 | 3 | 23.4 | 17.1- |
| - 4 | 14 | 3 | 43.2 | 40.9 |
| - 4 | 15 | 3 | 29.9 | 23.9 |
| - 4 | 16 | 3 | 40.5 | 35.8 |
| - 4 | 21 | 3 | 41.1 | 38.0- |
| - 5 | 1 | 3 | 66.3 | 58.0- |
| - 5 | 2 | 3 | 111.2 | 98.4 |
| - 5 | 3 | 3 | 83.9 | 75.8- |
| - 5 | 4 | 3 | 36.8 | 40.4 |
| - 5 | 5 | 3 | 17.5 | 8.2 |
| - 5 | 6 | 3 | 25.3 | 24.6- |
| - 5 | 7 | 3 | 20.4 | 17.6 |
| - 5 | 9 | 3 | 81.6 | 75.0 |
| - 5 | 10 | 3 | 66.6 | 63.5 |
| - 5 | 11 | 3 | 36.0 | 34.4 |
| - 5 | 12 | 3 | 26.4 | 21.5 |
| - 5 | 14 | 3 | 34.3 | 31.9- |
| - 5 | 16 | 3 | 28.8 | 27.4- |
| - 5 | 18 | 3 | 20.4 | 13.3 |
| - 5 | 19 | 3 | 28.5 | 24.9- |
| - 5 | 21 | 3 | 21.2 | 21.0- |
| - 5 | 22 | 3 | 18.7 | 14.5- |
| - 6 | 1 | 3 | 24.8 | 32.4- |
| - 6 | 2 | 3 | 44.6 | 39.2 |
| - 6 | 3 | 3 | 25.1 | 21.0 |
| - 6 | 4 | 3 | 28.9 | 29.9 |
| - 6 | 5 | 3 | 38.1 | 38.5 |
| - 6 | 6 | 3 | 34.1 | 33.7 |
| - 6 | 7 | 3 | 22.7 | 13.9- |
| - 6 | 9 | 3 | 26.2 | 24.4- |
| - 6 | 11 | 3 | 29.1 | 27.0 |
| - 6 | 12 | 3 | 25.6 | 25.8- |
| - 6 | 13 | 3 | 39.6 | 41.8 |
| - 6 | 14 | 3 | 20.1 | 22.2- |
| - 6 | 16 | 3 | 20.4 | 22.3- |
| - 6 | 17 | 3 | 26.1 | 28.8- |
| - 6 | 18 | 3 | 23.0 | 17.4- |
| - 6 | 22 | 3 | 15.9 | 17.2 |
| - 7 | 1 | 3 | 35.5 | 41.0 |
| - 7 | 3 | 3 | 21.2 | 17.4 |
| - 7 | 6 | 3 | 55.1 | 54.4 |
| - 7 | 9 | 3 | 22.7 | 21.0- |
| - 7 | 10 | 3 | 25.9 | 21.5- |
| - 7 | 11 | 3 | 31.0 | 31.9- |
| - 7 | 12 | 3 | 20.4 | 14.6- |
| - 7 | 13 | 3 | 26.4 | 22.2- |
| - 8 | 1 | 3 | 25.1 | 29.3 |
| - 8 | 4 | 3 | 55.9 | 53.8- |
| - 8 | 5 | 3 | 23.0 | 22.2- |
| - 8 | 6 | 3 | 47.5 | 51.2- |
| - 8 | 8 | 3 | 26.1 | 26.4- |
| - 9 | 1 | 3 | 31.3 | 35.3- |
| - 9 | 4 | 3 | 20.4 | 23.2- |
| - 9 | 5 | 3 | 20.4 | 17.0 |
| - 9 | 6 | 3 | 26.4 | 30.2- |
| - 9 | 11 | 3 | 19.8 | 23.2 |
| - 9 | 13 | 3 | 18.6 | 21.0 |
| -10 | 1 | 3 | 28.4 | 30.9- |
| | | 4 | 68.2 | 76.6- |
| | 1 | 4 | 30.0 | 35.9- |
| | 2 | 4 | 34.5 | 38.6- |
| | 3 | 4 | 11.6 | 19.9- |
| | 4 | 4 | 56.2 | 66.1 |
| | 5 | 4 | 73.5 | 86.1 |
| | 6 | 4 | 12.0 | 11.7- |
| | 7 | 4 | 103.8 | 122.9 |
| | 8 | 4 | 12.0 | 8.8 |
| | 9 | 4 | 20.6 | 22.0- |
| | 11 | 4 | 66.7 | 72.6- |
| | 12 | 4 | 32.2 | 33.7 |
| | 13 | 4 | 13.5 | 14.1- |
| | 14 | 4 | 6.7 | 9.2 |
| | 16 | 4 | 17.5 | 13.1- |
| | 17 | 4 | 1..7 | 22.5- |
| | 18 | 4 | 21.0 | 23.7- |
| | 19 | 4 | 18.7 | 23.8- |
| | 20 | 4 | 10.5 | 10.8- |
| | 21 | 4 | 14.2 | 12.4 |
| | 23 | 4 | 32.2 | 32.0 |
| | 25 | 4 | 11.2 | 12.8 |
| 1 | | 4 | 138.7 | 161.9- |
| 1 | 1 | 4 | 19.2 | 21.5 |
| 1 | 2 | 4 | 28.2 | 33.3- |
| 1 | 3 | 4 | 16.9 | 21.7 |
| 1 | 4 | 4 | 19.2 | 19.5 |
| 1 | 6 | 4 | 42.0 | 51.2 |
| 1 | 7 | 4 | 53.1 | 71.7- |
| 1 | 10 | 4 | 39.8 | 52.4 |
| 1 | 11 | 4 | 33.5 | 40.7 |
| 1 | 12 | 4 | 60.1 | 82.3 |
| 1 | 14 | 4 | 28.9 | 35.7 |
| 1 | 16 | 4 | 31.8 | 35.6- |
| 1 | 18 | 4 | 43.2 | 43.5- |
| 2 | | 4 | 38.0 | 38.1 |
| 2 | 1 | 4 | 16.2 | 13.5 |
| 2 | 4 | 4 | 44.4 | 54.6- |
| 2 | 5 | 4 | 78.0 | 87.0- |
| 2 | 7 | 4 | 48.2 | 59.2- |
| 2 | 8 | 4 | 37.5 | 48.8 |
| 2 | 11 | 4 | 30.1 | 37.1 |
| 2 | 12 | 4 | 18.9 | 21.0- |
| 2 | 16 | 4 | 25.9 | 27.0 |
| 2 | 19 | 4 | 19.2 | 23.1 |
| 2 | 20 | 4 | 25.1 | 28.1- |
| 2 | 22 | 4 | 22.8 | 21.4- |
| 2 | 23 | 4 | 27.7 | 23.0- |
| 2 | 25 | 4 | 16.2 | 10.7- |
| 3 | | 4 | 96.1 | 97.9 |
| 3 | 1 | 4 | 37.8 | 40.0- |
| 3 | 2 | 4 | 47.0 | 45.7 |
| 3 | 3 | 4 | 48.1 | 53.4- |
| 3 | 4 | 4 | 17.0 | 21.4- |
| 3 | 5 | 4 | 17.0 | 22.1 |
| 3 | 6 | 4 | 25.7 | 22.9- |
| 3 | 9 | 4 | 32.1 | 40.7- |
| 3 | 11 | 4 | 24.8 | 24.6- |
| 3 | 12 | 4 | 25.6 | 26.9- |
| 3 | 13 | 4 | 23.1 | 19.9 |
| 3 | 15 | 4 | 30.8 | 39.8 |
| 3 | 16 | 4 | 27.0 | 27.1 |
| 3 | 18 | 4 | 22.8 | 24.0 |
| 3 | 22 | 4 | 17.8 | 7.5 |
| 3 | 23 | 4 | 18.1 | 14.4 |
| 4 | | 4 | 23.4 | 19.7- |
| 4 | 1 | 4 | 25.7 | 28.8 |
| 4 | 2 | 4 | 31.5 | 32.4 |
| 4 | 3 | 4 | 32.5 | 25.6 |
| 4 | 4 | 4 | 52.8 | 60.5 |
| 4 | 5 | 4 | 43.7 | 55.9 |
| 4 | 7 | 4 | 27.2 | 30.5 |
| 4 | 8 | 4 | 32.7 | 42.1- |
| 4 | 10 | 4 | 30.3 | 37.0- |
| 4 | 13 | 4 | 28.5 | 29.5- |
| 4 | 16 | 4 | 23.1 | 21.9- |
| 5 | 1 | 4 | 33.9 | 30.4 |
| 5 | 3 | 4 | 49.5 | 50.8 |
| 5 | 4 | 4 | 19.9 | 14.6- |
| - 1 | 0 | 4 | 101.5 | 140.2 |
| - 1 | 1 | 4 | 32.9 | 41.1- |
| - 1 | 2 | 4 | 63.1 | 77.9 |
| - 1 | 3 | 4 | 25.7 | 24.1 |
| - 1 | 4 | 4 | 40.4 | 59.7- |
| - 2 | 0 | 4 | 74.9 | 89.4 |
| - 2 | 1 | 4 | 11.1 | 13.3 |
| 5 | 10 | 4 | 30.8 | 34.6 |
| 5 | 11 | 4 | 19.9 | 21.4 |
| 5 | 13 | 4 | .. 0 | 34.3- |
| 5 | 15 | 4 | 29.4 | 34.9- |
| 5 | 19 | 4 | 17.8 | 18.0 |
| 6 | 2 | 4 | 28.5 | 24.2- |
| 6 | 3 | 4 | 28.5 | 26.2- |
| 6 | 4 | 4 | 26.1 | 22.8- |
| 6 | 8 | 4 | 48.4 | 52.9 |
| 6 | 10 | 4 | 29.2 | 25.4 |
| 7 | 1 | 4 | 19.2 | 25.3- |
| 7 | 3 | 4 | 40.9 | 43.8- |
| 7 | 4 | 4 | 20.6 | 22.0 |
| 7 | 5 | 4 | 28.7 | 23.2- |
| 7 | 8 | 4 | 25.1 | 24.3- |
| 7 | 15 | 4 | 26.1 | 28.0 |
| 8 | 4 | 4 | 25.4 | 25.1 |
| 8 | 5 | 4 | 25.4 | 18.6- |
| 8 | 8 | 4 | 27.7 | 25.6- |
| 8 | 10 | 4 | 25.7 | 23.3- |
| - 1 | 5 | 4 | 30.1 | 23.6 |
| - 1 | 8 | 4 | 17.7 | 16.2 |
| - 1 | 9 | 4 | 34.3 | 30.7- |
| - 1 | 10 | 4 | 21.9 | 23.9- |
| - 1 | 11 | 4 | 16.1 | 23.8- |
| - 1 | 12 | 4 | 63.6 | 76.7- |
| - 1 | 13 | 4 | 23.1 | 22.0- |
| - 1 | 14 | 4 | 28.0 | 25.1- |
| - 1 | 16 | 4 | 19.6 | 32.8 |
| - 1 | 18 | 4 | 30.8 | 33.7 |
| - 2 | 4 | 4 | 59.8 | 66.1 |
| - 2 | 5 | 4 | 99.3 | 110.9- |
| - 2 | 6 | 4 | 27.0 | 24.7- |
| - 2 | 7 | 4 | 106.8 | 111.0- |
| - 2 | 8 | 4 | 60.6 | 65.0- |
| - 2 | 9 | 4 | 25.4 | 23.4 |
| - 2 | 10 | 4 | 52.9 | 45.0- |
| - 2 | 11 | 4 | 72.0 | 81.4 |
| - 2 | 16 | 4 | 19.6 | 12.6 |
| - 2 | 17 | 4 | 35.1 | 31.7 |
| - 2 | 18 | 4 | 25.9 | 21.6 |
| - 2 | 19 | 4 | 34.6 | 40.8 |
| - 2 | 23 | 4 | 24.2 | 24.3- |
| - 3 | | 4 | 100.5 | 133.7- |
| - 3 | 1 | 4 | 45.1 | 44.5- |
| - 3 | 2 | 4 | 32.4 | 28.7- |
| - 3 | 3 | 4 | 111.9 | 93.7- |
| - 3 | 4 | 4 | 52.5 | 46.0 |
| - 3 | 5 | 4 | 94.8 | 90.9- |
| - 3 | 6 | 4 | 39.9 | 40.1 |
| - 3 | 7 | 4 | 90.9 | 85.8- |
| - 3 | 8 | 4 | 35.4 | 31.0- |
| - 3 | 9 | 4 | 57.7 | 54.9- |
| - 3 | 10 | 4 | 20.3 | 10.7- |
| - 3 | 12 | 4 | 52.6 | 53.3 |
| - 3 | 13 | 4 | 40.9 | 41.9 |
| - 3 | 14 | 4 | 32.4 | 31.0 |
| - 3 | 15 | 4 | 48.2 | 54.2 |
| - 3 | 16 | 4 | 35.0 | 40.1- |
| - 3 | 18 | 4 | 25.9 | 24.8- |
| - 4 | | 4 | 39.8 | 22.1 |
| - 4 | 1 | 4 | 42.8 | 37.4- |
| - 4 | 2 | 4 | 41.9 | 32.4- |
| - 2 | 2 | 4 | 64.2 | 75.4 |
| - 2 | 5 | 4 | 30.4 | 33.3- |

Table 4 (*cont.*)

| H | K | L | FOBS | FCAL |
|---|---|---|---|---|
| -4 | 3 | 4 | 83·4 | 65·0- |
| -4 | 4 | 4 | 34·3 | 25·1- |
| -4 | 5 | 4 | 24·0 | 25·0 |
| -4 | 6 | 4 | 69·0 | 59·2 |
| -4 | 7 | 4 | 59·7 | 58·9 |
| -4 | 8 | 4 | 89·4 | 83·2 |
| -4 | 10 | 4 | 56·7 | 52·6 |
| -4 | 12 | 4 | 17·4 | 11·2 |
| -4 | 14 | 4 | 27·0 | 25·8- |
| -4 | 20 | 4 | 30·8 | 32·2- |
| -5 | 1 | 4 | 87·0 | 61·8 |
| -5 | 3 | 4 | 148·1 | 114·3 |
| -5 | 4 | 4 | 51·7 | 38·8- |
| -5 | 5 | 4 | 27·9 | 21·9 |
| -5 | 6 | 4 | 15·3 | 7·1 |
| -5 | 8 | 4 | 32·5 | 32·6 |
| -5 | 9 | 4 | 19·5 | 14·0 |
| -5 | 11 | 4 | 18·2 | 12·6- |
| -5 | 12 | 4 | 26·4 | 24·7- |
| -5 | 13 | 4 | 52·5 | 50·2- |
| -5 | 15 | 4 | 50·0 | 47·8- |
| -6 | | 4 | 54·6 | 46·5 |
| -6 | 2 | 4 | 85·2 | 72·7 |
| -6 | 3 | 4 | 22·8 | 24·2 |
| -6 | 4 | 4 | 79·7 | 68·2 |
| -6 | 8 | 4 | 66·4 | 65·0- |
| -6 | 10 | 4 | 52·2 | 55·1- |
| -6 | 11 | 4 | 19·2 | 15·3- |
| -6 | 12 | 4 | 19·6 | 9·0- |
| -6 | 13 | 4 | 28·0 | 27·1- |
| -6 | 15 | 4 | 34·7 | 32·7- |
| -6 | 20 | 4 | 40·2 | 30·3 |
| -7 | | 4 | 36·5 | 32·4 |
| -7 | 1 | 4 | 30·5 | 29·9- |
| -7 | 2 | 4 | 25·2 | 24·6 |
| -7 | 3 | 4 | 51·2 | 44·6- |
| -7 | 5 | 4 | 18·1 | 11·5- |
| -7 | 6 | 4 | 21·6 | 19·1- |
| -7 | 8 | 4 | 24·6 | 23·0- |
| -7 | 9 | 4 | 27·5 | 26·9- |
| -7 | 10 | 4 | 24·2 | 25·7- |
| -7 | 11 | 4 | 42·5 | 34·6- |
| -7 | 13 | 4 | 25·9 | 25·9 |
| -7 | 15 | 4 | 44·1 | 40·7 |
| -8 | | 4 | 45·3 | 42·4 |
| -8 | 1 | 4 | 29·4 | 22·5- |
| -8 | 2 | 4 | 24·9 | 15·8- |
| -8 | 3 | 4 | 22·2 | 19·6- |
| -8 | 4 | 4 | 44·4 | 36·9- |
| -8 | 5 | 4 | 41·4 | 34·7- |
| -8 | 7 | 4 | 32·5 | 27·2- |
| -8 | 8 | 4 | 35·5 | 41·3 |
| -8 | 10 | 4 | 26·0 | 26·1 |
| -8 | 20 | 4 | 27·0 | 18·5- |
| -9 | | 4 | 30·6 | 34·7- |
| -9 | 1 | 4 | 19·9 | 22·1 |
| -9 | 3 | 4 | 26·0 | 26·7 |
| -9 | 10 | 4 | 29·2 | 27·6 |
| | 1 | 5 | 58·5 | 50·5 |
| | 2 | 5 | 14·8 | 17·0- |
| | 3 | 5 | 53·9 | 55·8 |
| | 4 | 5 | 52·0 | 60·2 |
| | 5 | 5 | 48·3 | 41·9 |

| H | K | L | FOBS | FCAL |
|---|---|---|---|---|
| | 6 | 5 | 75·3 | 76·4 |
| | 7 | 5 | 33·4 | 38·8- |
| | 8 | 5 | 11·1 | 15·6 |
| | 9 | 5 | 57·6 | 57·3- |
| | 10 | 5 | 30·6 | 31·0- |
| | 12 | 5 | 39·0 | 35·8- |
| | 13 | 5 | 12·0 | 13·0 |
| | 15 | 5 | 12·0 | 8·3- |
| | 17 | 5 | 18·6 | 18·9- |
| | 18 | 5 | 34·4 | 33·3- |
| | 19 | 5 | 14·8 | 14·5 |
| | 21 | 5 | 26·0 | 25·3 |
| | 22 | 5 | 17·6 | 18·5 |
| | 24 | 5 | 18·6 | 15·6 |
| | 25 | 5 | 13·9 | 12·9- |
| | | 6 | 14·8 | 4·4- |
| | 1 | 6 | 15·8 | 16·7- |
| | 2 | 6 | 17·6 | 22·5 |
| | 3 | 6 | 15·8 | 14·0- |
| | 4 | 6 | 69·7 | 64·1 |
| | 5 | 6 | 19·5 | 18·0- |
| | 6 | 6 | 18·6 | 12·3- |
| | 8 | 6 | 69·7 | 58·9- |
| | 10 | 6 | 60·4 | 61·7- |
| | 11 | 6 | 14·8 | 13·0- |
| | 12 | 6 | 13·9 | 13·9 |
| | 13 | 6 | 13·0 | 18·8 |
| | 14 | 6 | 13·0 | 12·4 |
| | 16 | 6 | 11·1 | 9·8- |
| | 20 | 6 | 40·2 | 34·2 |
| | 22 | 6 | 35·3 | 29·0 |
| | 1 | 7 | 33·4 | 37·9- |
| | 3 | 7 | 14·8 | 17·1 |
| | 4 | 7 | 27·9 | 31·2- |
| | 5 | 7 | 27·9 | 36·6 |
| | 6 | 7 | 36·2 | 41·5- |
| | 8 | 7 | 18·6 | 21·4- |
| | 9 | 7 | 21·3 | 19·6- |
| | 10 | 7 | 15·8 | 16·1 |
| | 11 | 7 | 8·3 | 12·0 |
| | 12 | 7 | 16·7 | 20·0 |
| | 13 | 7 | 16·7 | 20·1 |
| | 16 | 7 | 14·8 | 13·2 |
| | 17 | 7 | 13·0 | 16·4- |
| | 21 | 7 | 8·3 | 9·8 |
| | 22 | 7 | 11·1 | 10·7- |
| | | 8 | 39·0 | 40·5- |
| | 2 | 8 | 18·6 | 13·6- |
| | 3 | 8 | 11·1 | 15·7 |
| | 4 | 8 | 19·5 | 22·8 |
| | 5 | 8 | 15·8 | 17·7- |
| | 7 | 8 | 20·4 | 19·9- |
| | 8 | 8 | 8·3 | 10·1- |
| | 9 | 8 | 10·2 | 12·6 |
| | 11 | 8 | 26·9 | 28·5 |
| | 12 | 8 | 26·9 | 29·9 |
| | 14 | 8 | 17·6 | 16·6 |
| | 17 | 8 | 10·2 | 7·3 |
| | 18 | 8 | 11·1 | 13·6- |
| | 1 | 9 | 12·0 | 17·0- |
| | 2 | 9 | 23·7 | 26·0 |
| | 7 | 9 | 18·6 | 7·3- |
| | 10 | 9 | 12·0 | 13·0 |
| | 12 | 9 | 11·1 | 3·7 |
| | 13 | 9 | 14·8 | 11·2 |
| | 3 | 10 | 17·6 | 24·6 |
| | 7 | 10 | 9·3 | 4·0- |
| | 10 | 10 | 10·7 | 3·1 |

A three-dimensional minimum function (Buerger, 1951) was then calculated with sections of the vector Se(1)–Se(1′) ($\frac{36}{60}$, $\frac{14}{60}$, $\frac{9}{60}$). They led to the location of twelve possible positions for the light atoms. In assigning positions to the light atoms, the criterion was that the positions were consistent with vectors in the three-dimensional Patterson function and maxima in the minimum three-dimensional function, as well as with the chemical model.

Structure factors calculated for the observed reflexions using the coordinates of two selenium and twelve light atoms gave $R=0{\cdot}41$. Successive three-dimensional Fourier syntheses and structure factor calculations were used to locate the remaining atoms and the structure found is depicted in Figs. 1 and 2. For the first calculation of (*hkl*) structure factors and the complete structure, $R$ was 0·36. After coordinate corrections deduced from the Fourier syntheses $R$ fell to 0·24. The temperature factor used for all the atoms was 2·0 Å$^2$. A three-dimensional difference synthesis was calculated. The results confirmed the previous positions for all twenty-six atoms. Fig. 3 shows the electron density sections $\varrho(x,y,z_1)$, for various layers $z_1$ containing maxima, projected parallel to **c**.

Refinement was carried out by differential syntheses. When isotropic refinement had been completed the value of $R$ was 0·16. Anisotropic refinement was then started and was continued until the largest shift in a coordinate was less than the corresponding standard deviation. The value of $R$ at this stage was 0·120.

The atomic coordinates are shown in Table 1, as fractions of the unit-cell edges with the corresponding standard deviations. Table 2 shows the thermal parameters.

Positions for the ten hydrogen atoms of the two phenyl groups and the four attached to the nitrogen atoms were calculated from the positions of the carbon and nitrogen atoms, assuming 1·0 Å for the C–H and N–H distances. The hydrogen positions are given in Table 3. The hydrogen atoms are designated by the numbers of the carbon atoms to which they are attached. The hydrogen atoms of the two selenourea groups are H[N(1)], H[N(2)], H[N(3)] and H[N(4)] respectively, indicating the N atoms to which they are attached. In the final structure factors calculation these hydrogen atoms were included with temperature coefficients of 3·0 Å$^2$, but no hydrogen parameters were refined.

A comparison of observed and calculated structure factors is given in Table 4. The parameters used in the calculation of the $F_c$'s are those listed in Tables 1, 2 and 3. The $R$ value is 0·116.

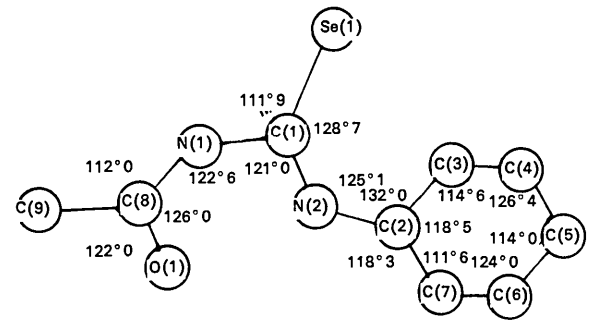
The structure factors, differential syntheses and all Fourier summations were calculated by use of a program written for the IBM 7070 computer (The Crystallography Laboratory, University of Pittsburgh). The atomic form factors were taken from *International*

Table 5. *Interatomic distances*

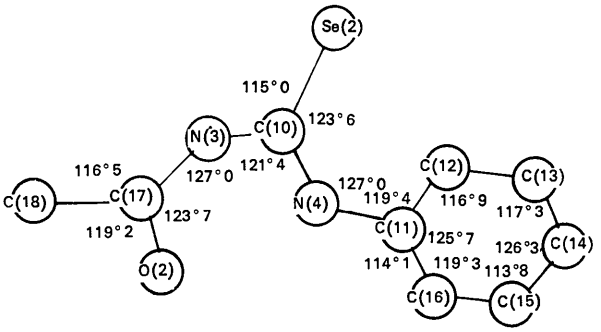
| | | | |
|---|---|---|---|
| Se(1) —C(1) | 1·87 ± 0·03 Å | Se(2) —C(10) | 1·87 ± 0·03 Å |
| C(1)—N(1) | 1·45 ± 0·05 | C(10)—N(3) | 1·36 ± 0·04 |
| C(1)—N(2) | 1·22 ± 0·03 | C(10)—N(4) | 1·30 ± 0·03 |
| N(2)—C(2) | 1·38 ± 0·04 | N(4)—C(11) | 1·45 ± 0·03 |
| C(2)—C(3) | 1·44 ± 0·04 | C(11)—C(12) | 1·37 ± 0·04 |
| C(3)—C(4) | 1·34 ± 0·06 | C(12)—C(13) | 1·50 ± 0·05 |
| C(4)—C(5) | 1·34 ± 0·07 | C(13)—C(14) | 1·31 ± 0·06 |
| C(5)—C(6) | 1·47 ± 0·06 | C(14)—C(15) | 1·42 ± 0·05 |
| C(6)—C(7) | 1·39 ± 0·04 | C(15)—C(16) | 1·51 ± 0·04 |
| C(7)—C(2) | 1·44 ± 0·04 | C(16)—C(11) | 1·30 ± 0·04 |
| N(1)—C(8) | 1·37 ± 0·04 | N(3)—C(17) | 1·37 ± 0·03 |
| C(8)—C(9) | 1·54 ± 0·04 | C(17)—C(18) | 1·54 ± 0·04 |
| C(8)—O(1) | 1·19 ± 0·06 | C(17)—O(2) | 1·30 ± 0·04 |
| O(1)···N(2) | 2·70 ± 0·06 | O(2)···N(4) | 2·73 ± 0·04 |

*Tables for X-ray Crystallography* (1962). The isotropic temperature factors are of the form: $\exp\left(-B\frac{\sin^2\theta}{\lambda^2}\right)$, and the anisotropic factors of the form:

$$\exp\left[-\tfrac{1}{4}(B_{11}h^2a^{*2}+B_{22}k^2b^{*2}+B_{33}l^2c^{*2}+2B_{12}hka^*b^*+2B_{23}klb^*c^*+2B_{13}hla^*c^*)\right].$$




(*a*)




(*b*)

Fig. 5. Bond angles.

The $R$ index is defined by

$$R=\frac{\Sigma\,||F_o|-|F_c||}{\Sigma\,F_o}.$$

## Description of the structure

In Figs. 1 and 2 are shown two projections of the structure along the $b$ axis and the $c$ axis respectively. Fig. 3 shows the electron density sections $\varrho(x,y,z_1)$, for various levels $z_1$ containing maxima, projected parallel to **c**. Bond distances are given in Table 5 and Figs. 4(*a*) and (*b*), and bond angles in Table 6 and Figs. 5(*a*) and (*b*).

Each molecule consists of three planar parts, (I) the selenourea group, (II) the phenyl group and (III) the *N*-acetyl group. The parameters defining the three planes are given in Table 7 together with individual deviations from the planes for the molecule (*a*), and in Table 8 for the molecule (*b*).

Table 7. *Coefficients in the expression* $Ax+By+Cz=D$ *referred to crystallographic axes and distances from planes* [*molecule* (*a*)]

| | *A* | *B* | *C* | *D* |
|---|---|---|---|---|
| I(*a*) | 0·8605 | 0·1591 | −0·7858 | 2·4096 |
| II(*a*) | 0·0713 | −0·3787 | 0·8185 | 2·1627 |
| III(*a*) | 0·9002 | 0·1902 | −0·7170 | 2·7172 |

| | Deviation from plane | |
|---|---|---|
| Se(1) | 0·011 Å | I |
| C(1) | −0·042 | I |
| N(1) | 0·013 | I |
| N(2) | 0·018 | I |
| C(2) | −0·032 | II |
| C(3) | 0·035 | II |
| C(4) | −0·028 | II |
| C(5) | 0·018 | II |
| C(6) | −0·017 | II |
| C(7) | 0·024 | II |
| N(1) | 0·002 | III |
| C(8) | −0·009 | III |
| C(9) | 0·002 | III |
| O(10) | 0·004 | III |

Table 6. *Bond angles*

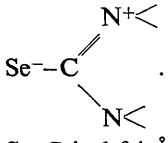
| | | | |
|---|---|---|---|
| Se(1)–C(1)–N(1) | 111·9 ± 0·2° | Se(2)–C(10)–N(3) | 115·0 ± 0·2° |
| Se(1)–C(1)–N(2) | 126·7 ± 0·3 | Se(2)–C(10)–N(4) | 123·6 ± 0·2 |
| N(1)–C(1)–N(2) | 121·0 ± 0·3 | N(3)–C(10)–N(4) | 121·4 ± 0·2 |
| C(1)–N(2)–C(2) | 125·1 ± 0·4 | C(10)–N(4)–C(11) | 127·0 ± 0·3 |
| N(2)–C(2)–C(3) | 122·0 ± 0·3 | N(4)–C(11)–C(12) | 119·4 ± 0·2 |
| C(2)–C(3)–C(4) | 119·6 ± 0·2 | C(11)–C(12)–C(13) | 116·9 ± 0·2 |
| C(3)–C(4)–C(5) | 126·4 ± 0·2 | C(12)–C(13)–C(14) | 117·3 ± 0·2 |
| C(4)–C(5)–C(6) | 114·0 ± 0·2 | C(14)–C(15)–C(16) | 113·6 ± 0·2 |
| C(5)–C(6)–C(7) | 124·0 ± 0·2 | C(13)–C(14)–C(15) | 126·3 ± 0·2 |
| C(6)–C(7)–C(2) | 116·6 ± 0·2 | C(15)–C(16)–C(11) | 119·3 ± 0·2 |
| C(7)–C(2)–C(3) | 118·5 ± 0·2 | C(16)–C(11)–C(12) | 125·7 ± 0·2 |
| N(2)–C(2)–C(7) | 118·3 ± 0·3 | N(4)–C(11)–C(16) | 114·1 ± 0·2 |
| C(1)–N(1)–C(8) | 122·6 ± 0·3 | C(10)–N(3)–C(17) | 127·0 ± 0·2 |
| N(1)–C(8)–C(9) | 112·0 ± 0·2 | N(3)–C(17)–C(18) | 116·5 ± 0·2 |
| N(1)–C(8)–O(1) | 126·0 ± 0·3 | N(3)–C(17)–O(2) | 123·7 ± 0·2 |
| C(9)–C(8)–O(1) | 122·0 ± 0·2 | C(18)–C(17)–O(2) | 119·2 ± 0·2 |

Table 8. *Coefficients in the expression* $Ax+By+Cz=D$ *referred to crystallographic axes and distances from planes* [*molecule* (*b*)]

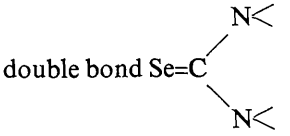
| | *A* | *B* | *C* | *D* |
|---|---|---|---|---|
| I(*b*) | −0·5070 | −0·4365 | 0·8834 | 1·9952 |
| II(*b*) | 0·9964 | 0·0834 | −0·4105 | −0·4286 |
| III(*b*) | −0·5512 | −0·3882 | 0·8967 | 1·9730 |

| | Deviation from plane | |
|---|---|---|
| Se(2) | 0·002 Å | I |
| C(10) | −0·006 | I |
| N(3) | 0·002 | I |
| N(4) | 0·002 | I |
| C(11) | −0·024 | II |
| C(12) | 0·023 | II |
| C(13) | −0·025 | II |
| C(14) | 0·026 | II |
| C(15) | −0·020 | II |
| C(16) | 0·021 | II |
| N(3) | 0·014 | III |
| C(17) | −0·042 | III |
| C(18) | 0·012 | III |
| O(2) | 0·015 | III |

The observed value, 1·87 Å, for the Se–C bond indicates a considerable contribution by the structure



. The sum of the covalent bond radii for Se–C is 1·94 Å for the single bond, and 1·74 Å for the double bond



The N(2)–H···O(1) and N(4)–H···O(2) hydrogen bonds, 2·70 and 2·73 Å respectively, are consistent with the assumption of a positive charge placed on the NH group. It is suggested that the possibility of the NH group forming a hydrogen bond may account for the difference between the bond distances C(1)–N(2) and C(1)–N(1) for the molecule (*a*) and the bond distances C(10)–N(4) and C(10)–N(3) for the molecule (*b*).

We are very grateful to Dr Sagrario Martinez Carrera for making crystallographic programs available to us and also for help in running them. Our thanks to Dr M. Cubero for her helpful discussions and suggestions during the course of this work.

### References

BUERGER, M. J. (1951). *Acta Cryst.* **4**, 531.
DOUGLAS, I. B. (1928). *Ann. Chim.* **9** (10), 113.
HOPE, H. (1965). *Acta Cryst.* **18**, 259.
*International Tables for X-ray Crystallography* (1962). Vol. III. Birmingham: Kynoch Press.
PEREZ-RODRIGUEZ, M. & CUBERO, M. (1963). *Anales de la Universidad Hispalense.*
PHILLIPS, D. C. (1956). *Acta Cryst.* **9**, 819.
WILSON, A. J. C. (1942). *Nature, Lond.* **150**, 151.

*Acta Cryst.* (1969). B**25**, 540

## The Crystal Structure of Trisethylsulphonylmethane

BY D. R. MCGREGOR AND J. C. SPEAKMAN
*Chemistry Department, The University, Glasgow W.2, Scotland*

(*Received* 1 *April* 1968)

Trisethylsulphonylmethane (TESM) crystallizes with six molecules in a unit cell belonging to the hexagonal system with $a=14·97$, $c=9·81$ Å. The space group is $R3c$, and the required molecular symmetry 3. The crystal structure has been determined and refined to $R=0·085$ for 636 independent reflexions whose intensities were measured on an automatic diffractometer. The structure resembles that of trismethylsulphonylmethane (TMSM), but the crystals are not isomorphous. They differ in the manner of lateral packing of very similar stacks of molecules along **c**. The crystals of TESM are also free from the disorder which gives rise to spectacular diffuse scattering from TMSM. These differences are discussed. The principal bond-lengths, with standard deviations in parentheses are as follows: C–S = 1·834 (4); S–O (mean) = 1·442 (7); S–$CH_2$ = 1·785 (10); $H_2C$–$CH_3$ = 1·496 (15) Å.

### Introduction

The crystal structure of trismethylsulphonylmethane (TMSM, I) has been studied by Silverton, Gibson & Abrahams (1965). This study was motivated not only by the interesting chemical properties of TMSM, but also by the remarkable diffuse reflexions observed in its X-ray diffraction patterns (Abrahams & Speakman, 1956). Dr Gibson presented us with a sample of the analogous trisethylsulphonylmethane (TESM, II). Interest quickened when we found that this compound crystallizes in the same trigonal space group as TMSM, with similar unit-cell dimensions, but that its X-ray photographs were free from diffuse reflexions.