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# Crystal Structure of 1,1′-Dihydroperoxy-cyclohexanylperoxide-1,1′

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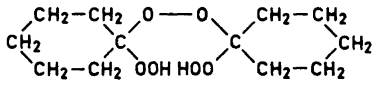
The crystals are monoclinic with cell dimensions $a=10.50_4$ Å, $b=6.99_1$ Å, $c=19.08_8$ Å and $\beta=107.7_8°$. The space group is $P2_1/c$ and the cell contains four molecules. The phase problem was solved three-dimensionally by means of a computer procedure based on direct methods. Full-matrix least squares refinement gave the *R*-value of 8.6 % for 1637 observed reflections. Rigid-body motion analysis including the **S**-tensor has been carried out. Mean values of O–O, C–O, and C–C distances are $1.47_7$ Å, $1.43_7$ Å, and $1.53_3$ Å, respectively. The average C–O–O angle for the hydroperoxy groups is 110.4° and the corresponding value for the peroxy bridge 107.9°. The asymmetric environments of the non-methylene carbon atoms resemble that observed for trimeric acetone peroxide, and may possibly be related to *intra*-molecular oxygen-hydrogen repulsions. Weak *inter*-molecular ($2.81_7$ Å) and *intra*-molecular ($2.90_4$ Å) hydrogen bonds are present, the *inter*-molecular bonds forming chains along *b*-axis. The conformation of the molecule is *cis*, and the dihedral angle C–O–O–C is 126.3°.

1,1′-Dihydroperoxycyclohexanylperoxide-1,1′




has been synthesized by T. Ledaal at this university by oxidation of cyclohexanone peroxide by means of hydrogen peroxide in the presence of $HClO_4$. No crystal structure determinations of compounds containing hydroperoxy groups have been reported. Structural information concerning covalent organic peroxides is also limited.[1–4] The crystal structure analysis of this compound was carried out in order to obtain information about the hydroperoxy group, specially its ability to form hydrogen bonds, and to determine the dihedral angle of the peroxy group.

## CRYSTAL DATA

The crystals belong to the monoclinic system and the systematic absences lead to the space group $P2_1/c$. The cell parameters, measured by means of a four circle diffractometer, and their estimated standard deviations are:

| | |
|---|---|
| $a = 10.504$ Å | $\sigma$(Å) = 0.003 |
| $b = 6.991$ Å | $\sigma$(Å) = 0.002 |
| $c = 19.088$ Å | $\sigma$(Å) = 0.002 |
| $\beta = 107.78°$ | $\sigma$(°) = 0.01 |

The unit cell contains four molecules ($\varrho_{calc}=1.30$ gcm$^{-3}$, $\varrho_{obs}=1.28$ gcm$^{-3}$).

Intensity data were obtained by photometric measurements of integrated Weissenberg diagrams corresponding to $0kl$, $h0l$, . . ., $h4l$ (Cu$K\alpha$-radiation). The diagrams were taken at room temperature, and due to instability four crystals were used. 1637 independent reflections were strong enough to be measured while 309 were given $(1/4)I_{min}$-values.

After cross-layer scaling the intensities were statistically put on absolute scale, and the overall temperature factor, $B=3.85$ Å$^2$, was used in the calculation of unitary structure factors, and as starting parameter in the isotropic refinement.

No corrections have been made for absorption or secondary extinction effects.

## DETERMINATION OF THE STRUCTURE

Solution of the phase problem was obtained by applying a set of FORTRAN IV programs for CDC 3300 [5] based on direct methods.[6-8] As to be expected from the $|U|$-distribution given in Table 1, the programmed systematic

*Table 1.* Distribution of $|U|$-values.

| Range of $\|U\|$ | Number of reflections |
|---|---|
| 0.00—0.01 | 62 |
| 0.01—0.02 | 281 |
| 0.02—0.03 | 97 |
| 0.03—0.04 | 138 |
| 0.04—0.05 | 102 |
| 0.05—0.06 | 110 |
| 0.06—0.07 | 117 |
| 0.07—0.08 | 103 |
| 0.08—0.09 | 111 |
| 0.09—0.10 | 88 |
| 0.10—0.15 | 378 |
| 0.15—0.20 | 190 |
| 0.20—0.25 | 96 |
| 0.25—0.30 | 31 |
| 0.30—0.35 | 21 |
| 0.35—0.40 | 7 |
| 0.40—0.50 | 4 |
| 0.50—1.00 | 0 |

application of Harker-Kasper inequalities gave no information about signs. A program, based on Sayre's sign relationship, which allows introduction of eight symbols for unknown signs, was used in deriving about 250 signs in terms of three unknowns. The corresponding eight three-dimensional Fourier syntheses were calculated and scanned for peaks larger than 2 e·Å$^{-3}$ followed by calculations of all distances less than 2 Å between peak maxima. The resulting eight lists of coordinates and distances were examined, and one of them contained the expected number of peaks, with roughly the same heights, and with reasonable distances between peak maxima.

## REFINEMENT

The $R$-factor corresponding to the coordinates thus obtained and the statistically determined overall temperature factor was $R=43.2$ % for the 500 largest structure factors. Using a program based on the minimum residual method,[9] this $R$-value was reduced to 14.2 %.

A full-matrix least squares refinement [5] was carried out. The weighting scheme No. 1:

$$\text{for } F_o \leqq \text{FB}, \quad W = \text{A1}(F_o)^{\text{B1}}$$
$$\text{for } F_o > \text{FB}, \quad W = \text{A2}(F_o)^{\text{B2}}$$

was adapted by taking:

$$\text{A1} = 10.0, \quad \text{A2} = 12.2, \quad \text{B1} = 0.0, \quad \text{B2} = -0.5 \text{ and } \text{FB} = 1.5.$$

The atomic form factors used were those of Hanson *et al.*[10] After two cycles of isotropic refinement, anisotropic thermal vibrational parameters were introduced for the oxygen and carbon atoms and three least squares cycles calculated. Positions of the 20 methylene hydrogen atoms were calculated assuming tetrahedral C—H bonds of length 1.03 Å. The scale factors of the individual layers were adjusted by structure factor calculations. An attempt to localize the hydroperoxy hydrogen atoms from a difference fourier map was unsuccessful. Isotropic temperature factors, $B=5.0$ Å$^2$, were applied for the methylene hydrogens, and their positional parameters only were refined. The final $R$-value for 1637 observed reflections was 8.6 %.

309 accidentally absent reflections had previously been given $(1/4)I_{\text{min}}$-values and had been scaled along with the rest of the data. Allowance for inclusion of these reflections in the refinement was made by applying weighting scheme No. 3 ($W=1/\sigma$). Satisfactory weight analysis was obtained by giving all unobserved reflections the same constant weight $W=\text{A1}/3$. The $R$-factor for all data was 9.5 %.

When checking the 250 signs originally determined no discrepancies were found.

*Table 2.* Fractional atomic coordinates for oxygen and carbon atoms with estimated standard deviations (multiplied by $10^5$).[a]

| Atom | $x$ | $y$ | $z$ |
|---|---|---|---|
| $O_1$ | 25570 | 19558 | 25861 |
| | 28 | 53 | 17 |
| $O_2$ | 30066 | 38712 | 28599 |
| | 26 | 47 | 15 |
| $O_3$ | 39499 | 27596 | 40646 |
| | 23 | 47 | 15 |
| $O_4$ | 53078 | 34336 | 41080 |
| | 22 | 46 | 14 |
| $O_5$ | 54315 | 14989 | 31287 |
| | 23 | 45 | 13 |
| $O_6$ | 55725 | 31622 | 26875 |
| | 27 | 53 | 16 |
| $C_1$ | 30194 | 40749 | 36147 |
| | 34 | 69 | 20 |
| $C_2$ | 16856 | 34926 | 37194 |
| | 38 | 82 | 28 |
| $C_3$ | 05744 | 48788 | 33164 |
| | 37 | 85 | 27 |
| $C_4$ | 09244 | 69300 | 35557 |
| | 42 | 86 | 27 |
| $C_5$ | 22294 | 75208 | 34130 |
| | 44 | 87 | 29 |
| $C_6$ | 33704 | 61562 | 37885 |
| | 39 | 74 | 25 |
| $C_7$ | 60092 | 18974 | 38956 |
| | 31 | 67 | 20 |
| $C_8$ | 74379 | 26463 | 40839 |
| | 33 | 78 | 24 |
| $C_9$ | 83658 | 10553 | 39541 |
| | 38 | 86 | 27 |
| $C_{10}$ | 82804 | −07473 | 43882 |
| | 38 | 86 | 26 |
| $C_{11}$ | 68472 | −15237 | 41671 |
| | 37 | 81 | 25 |
| $C_{12}$ | 58901 | 00160 | 42755 |
| | 35 | 71 | 22 |

[a] For numbering of atoms, see Fig. 1.

*Table 3.* Anisotropic thermal vibration parameters and their estimated standard deviations (multiplied by $10^5$).

| Atom | $B_{11}$ | $B_{22}$ | $B_{33}$ | $B_{12}$ | $B_{13}$ | $B_{23}$ |
|---|---|---|---|---|---|---|
| $O_1$ | 969 | 2045 | 428 | −368 | 257 | −366 |
| | 27 | 97 | 10 | 84 | 26 | 49 |
| $O_2$ | 876 | 1991 | 338 | −16 | 412 | 6 |
| | 24 | 93 | 8 | 75 | 22 | 42 |
| $O_3$ | 666 | 2064 | 362 | 194 | 415 | 286 |
| | 21 | 97 | 8 | 70 | 21 | 42 |
| $O_4$ | 636 | 1819 | 371 | 114 | 329 | −175 |
| | 21 | 92 | 8 | 68 | 21 | 41 |
| $O_5$ | 775 | 2017 | 292 | 107 | 251 | −11 |
| | 22 | 91 | 7 | 70 | 21 | 39 |
| $O_6$ | 1037 | 2880 | 350 | 620 | 541 | 606 |
| | 27 | 108 | 9 | 88 | 25 | 49 |
| $C_1$ | 756 | 1789 | 307 | 494 | 333 | 121 |
| | 31 | 134 | 10 | 103 | 29 | 58 |
| $C_2$ | 776 | 2113 | 470 | 451 | 564 | 433 |
| | 34 | 152 | 15 | 110 | 36 | 72 |
| $C_3$ | 747 | 2568 | 478 | 229 | 479 | 338 |
| | 33 | 168 | 15 | 121 | 36 | 80 |
| $C_4$ | 940 | 2525 | 418 | 977 | 434 | 205 |
| | 36 | 170 | 14 | 128 | 37 | 75 |
| $C_5$ | 1006 | 1975 | 489 | 570 | 473 | 81 |
| | 40 | 139 | 16 | 121 | 41 | 76 |
| $C_6$ | 869 | 1630 | 419 | 79 | 476 | −243 |
| | 34 | 133 | 13 | 109 | 34 | 65 |
| $C_7$ | 646 | 1571 | 315 | 198 | 238 | −84 |
| | 28 | 131 | 10 | 92 | 27 | 55 |
| $C_8$ | 638 | 2172 | 397 | −87 | 308 | −198 |
| | 30 | 155 | 13 | 102 | 31 | 67 |
| $C_9$ | 709 | 2857 | 454 | 375 | 423 | 321 |
| | 32 | 177 | 14 | 112 | 34 | 78 |
| $C_{10}$ | 793 | 2475 | 461 | 956 | 430 | 441 |
| | 33 | 168 | 15 | 117 | 35 | 76 |
| $C_{11}$ | 855 | 2026 | 397 | 547 | 367 | 61 |
| | 34 | 137 | 13 | 109 | 34 | 65 |
| $C_{12}$ | 747 | 1770 | 369 | 86 | 362 | 49 |
| | 29 | 130 | 11 | 104 | 30 | 61 |

The fractional atomic coordinates and the thermal vibration parameters arrived at are given in Tables 2, 3, and 4; the expression for the anisotropic vibrations being:

$$\exp[-(B_{11}h^2+B_{22}k^2+B_{33}l^2+B_{12}hk+B_{13}hl+B_{23}kl)]$$

*Table 4.* Fractional coordinates (multiplied by $10^3$) for hydrogen atoms. The estimated standard deviations range from 0.003 to 0.01.[a]

| Atom | $x$ | $y$ | $z$ |
|---|---|---|---|
| H2e | 149 | 215 | 355 |
| H2a | 185 | 356 | 424 |
| H3e | −039 | 449 | 338 |
| H3a | 028 | 477 | 271 |
| H4e | 028 | 790 | 333 |
| H4a | 110 | 704 | 410 |
| H5e | 246 | 882 | 364 |
| H5a | 214 | 748 | 284 |
| H6e | 417 | 625 | 365 |
| H6a | 369 | 629 | 434 |
| H8e | 740 | 388 | 378 |
| H8a | 772 | 306 | 463 |
| H9e | 936 | 149 | 418 |
| H9a | 810 | 078 | 337 |
| H10e | 891 | −196 | 434 |
| H10a | 872 | −027 | 499 |
| H11e | 688 | −278 | 447 |
| H11a | 657 | −213 | 363 |
| H12e | 504 | −047 | 408 |
| H12a | 614 | 037 | 481 |

[a] Referring to Fig. 1 the hydrogen atoms Hne and Hna are, respectively, equatorially and axially bonded to Cn.

In Table 5 calculated structure factors are compared with the observed values (and unobserved with $F_u=\frac{1}{2}F_o$ (min)).

## THERMAL MOTIONS

The principal axes of the thermal vibration ellipsoids for oxygen and carbon atoms were calculated from the temperature parameters given in Table 3. Root mean square amplitudes and the corresponding $B$-values for the atomic anisotropic thermal vibration along the principal axes together with the components of these axes along the crystal axes are given in Table 6. The thermal vibration parameters of Table 3 were applied in a rigid-body analysis including the S-tensor in order to account for correlations of libration and translation.[11] The results listed in Table 7 show that translational motion

*Table 5.* Observed [and unobserved with $F_u = \frac{1}{2}F_o(\min)$] and calculated structure factors on 10 times absolute scale.

| h | k | l | $F_o$ | $F_c$ |
|---|---|---|---|---|
| 0 | 0 | 2 | 415 | - 428 |
| 0 | 0 | 4 | 1283 | -1322 |
| 0 | 0 | 6 | 872 | - 916 |
| 0 | 0 | 8 | 140 | 139 |
| 0 | 0 | 10 | 154 | 163 |
| 0 | 0 | 12 | 190 | 203 |
| 0 | 0 | 14 | 39 | 29 |
| 0 | 0 | 16 | 67 | - 56 |
| 0 | 0 | 18 | 39 | - 40 |
| 0 | 0 | 22 | 38 | 39 |
| 0 | 1 | 1 | 88 | - 58 |
| 0 | 1 | 2 | 776 | 792 |
| 0 | 1 | 3 | 602 | - 638 |
| 0 | 1 | 4 | 26 | 25 |
| 0 | 1 | 5 | 131 | 135 |
| 0 | 1 | 6 | 117 | 115 |
| 0 | 1 | 7 | 254 | 269 |
| 0 | 1 | 8 | 762 | - 780 |
| 0 | 1 | 9 | 190 | 211 |
| 0 | 1 | 10 | 167 | 161 |
| 0 | 1 | 11 | 218 | - 210 |
| 0 | 1 | 12 | 190 | 182 |
| 0 | 1 | 13 | 50 | 50 |
| 0 | 1 | 14 | 138 | 129 |
| 0 | 1 | 15 | 33 | - 27 |
| 0 | 1 | 16 | 98 | - 79 |
| 0 | 1 | 17 | 61 | - 57 |
| 0 | 1 | 19 | 12 | 10 |
| 0 | 1 | 20 | 81 | - 68 |
| 0 | 1 | 21 | 7 | - 6 |
| 0 | 1 | 22 | 34 | 27 |
| 0 | 1 | 23 | 42 | 42 |
| 0 | 2 | 0 | 872 | - 893 |
| 0 | 2 | 1 | 254 | 253 |
| 0 | 2 | 2 | 300 | 285 |
| 0 | 2 | 3 | 242 | 237 |
| 0 | 2 | 4 | 233 | 209 |
| 0 | 2 | 5 | 368 | 342 |
| 0 | 2 | 6 | 408 | 399 |
| 0 | 2 | 7 | 119 | - 131 |
| 0 | 2 | 8 | 263 | - 253 |
| 0 | 2 | 9 | 115 | - 130 |
| 0 | 2 | 10 | 84 | - 80 |
| 0 | 2 | 11 | 88 | - 81 |
| 0 | 2 | 12 | 123 | - 140 |
| 0 | 2 | 13 | 116 | - 121 |
| 0 | 2 | 14 | 89 | 92 |
| 0 | 2 | 15 | 210 | 222 |
| 0 | 2 | 16 | 73 | 80 |
| 0 | 2 | 17 | 19 | - 24 |
| 0 | 2 | 18 | 40 | 49 |
| 0 | 2 | 19 | 8 | - 9 |
| 0 | 2 | 20 | 36 | - 42 |
| 0 | 2 | 21 | 41 | - 50 |
| 0 | 2 | 22 | 39 | - 31 |
| 0 | 3 | 1 | 275 | - 298 |
| 0 | 3 | 2 | 90 | 85 |
| 0 | 3 | 3 | 76 | - 65 |
| 0 | 3 | 4 | 511 | - 518 |
| 0 | 3 | 5 | 277 | 269 |
| 0 | 3 | 6 | 49 | 42 |
| 0 | 3 | 7 | 97 | 99 |
| 0 | 3 | 8 | 200 | 206 |
| 0 | 3 | 9 | 144 | - 151 |
| 0 | 3 | 10 | 76 | 64 |
| 0 | 3 | 11 | 156 | 156 |
| 0 | 3 | 12 | 60 | - 54 |
| 0 | 3 | 13 | 145 | - 134 |
| 0 | 3 | 14 | 50 | - 48 |
| 0 | 3 | 15 | 52 | - 49 |
| 0 | 3 | 16 | 54 | 54 |
| 0 | 3 | 17 | 72 | 64 |
| 0 | 3 | 18 | 33 | - 28 |
| 0 | 3 | 19 | 14 | 8 |
| 0 | 3 | 20 | 20 | 14 |
| 0 | 3 | 21 | 6 | - 5 |
| 0 | 4 | 0 | 236 | - 212 |
| 0 | 4 | 1 | 94 | 118 |
| 0 | 4 | 2 | 97 | 108 |
| 0 | 4 | 3 | 150 | - 184 |
| 0 | 4 | 4 | 59 | 68 |
| 0 | 4 | 5 | 98 | - 97 |
| 0 | 4 | 6 | 27 | 23 |
| 0 | 4 | 7 | 137 | 145 |
| 0 | 4 | 8 | 38 | - 43 |
| 0 | 4 | 9 | 117 | 128 |
| 0 | 4 | 10 | 126 | - 131 |
| 0 | 4 | 11 | 21 | - 20 |
| 0 | 4 | 12 | 196 | 181 |
| 0 | 4 | 13 | 86 | - 73 |
| 0 | 4 | 14 | 49 | - 40 |
| 0 | 4 | 15 | 91 | - 79 |
| 0 | 4 | 16 | 47 | - 35 |
| 0 | 4 | 17 | 29 | 30 |
| 0 | 4 | 18 | 13 | 9 |
| 0 | 4 | 19 | 7 | 6 |
| 0 | 4 | 20 | 22 | 22 |
| 0 | 5 | 1 | 9 | 4 |
| 0 | 5 | 2 | 105 | - 105 |
| 0 | 5 | 3 | 44 | 40 |
| 0 | 5 | 4 | 150 | 136 |
| 0 | 5 | 5 | 39 | - 32 |
| 0 | 5 | 6 | 111 | - 108 |
| 0 | 5 | 7 | 9 | - 8 |
| 0 | 5 | 8 | 9 | 9 |
| 0 | 5 | 9 | 83 | - 85 |
| 0 | 5 | 10 | 27 | - 24 |
| 0 | 5 | 11 | 84 | 84 |
| 0 | 5 | 12 | 21 | 17 |
| 0 | 5 | 13 | 51 | 45 |
| 0 | 5 | 14 | 27 | 23 |
| 0 | 5 | 16 | 20 | 23 |
| 0 | 5 | 17 | 18 | - 19 |
| 0 | 5 | 18 | 16 | - 14 |
| 0 | 5 | 19 | 5 | - 1 |
| 0 | 6 | 0 | 106 | 105 |
| 0 | 6 | 1 | 40 | - 35 |
| 0 | 6 | 2 | 39 | - 36 |
| 0 | 6 | 3 | 50 | 60 |
| 0 | 6 | 4 | 30 | 28 |
| 0 | 6 | 5 | 17 | - 20 |
| 0 | 6 | 6 | 56 | - 51 |
| 0 | 6 | 7 | 36 | 39 |
| 0 | 6 | 8 | 35 | - 38 |
| 0 | 6 | 9 | 60 | - 55 |
| 0 | 6 | 10 | 18 | 20 |
| 0 | 6 | 12 | 51 | 48 |
| 0 | 6 | 13 | 53 | 45 |
| 0 | 6 | 14 | 10 | - 7 |
| 0 | 6 | 15 | 28 | - 29 |
| 0 | 6 | 16 | 18 | 16 |
| 0 | 7 | 1 | 28 | - 20 |
| 0 | 7 | 2 | 26 | 28 |
| 0 | 7 | 4 | 22 | - 20 |
| 0 | 7 | 5 | 9 | 7 |
| 0 | 7 | 6 | 12 | - 5 |
| 0 | 7 | 7 | 48 | 40 |
| 0 | 7 | 8 | 14 | 8 |
| 0 | 7 | 9 | 32 | 24 |
| 0 | 7 | 10 | 8 | 5 |
| 0 | 7 | 11 | 52 | - 50 |
| 0 | 7 | 13 | 23 | - 20 |
| 0 | 8 | 0 | 59 | 45 |
| 0 | 8 | 2 | 13 | 12 |
| 0 | 8 | 3 | 34 | 27 |
| 0 | 8 | 4 | 57 | - 49 |
| 0 | 8 | 6 | 18 | 17 |
| 0 | 8 | 7 | 44 | - 41 |
| 0 | 8 | 8 | 36 | - 37 |
| 0 | 8 | 9 | 14 | 12 |
| 0 | 8 | 10 | 25 | 32 |
| 1 | 0 | -22 | 11 | - 19 |
| 1 | 0 | -20 | 24 | 23 |
| 1 | 0 | -18 | 74 | 70 |
| 1 | 0 | -16 | 26 | - 26 |
| 1 | 0 | -14 | 68 | 68 |
| 1 | 0 | -12 | 150 | 129 |
| 1 | 0 | -10 | 761 | - 804 |
| 1 | 0 | -8 | 185 | - 191 |
| 1 | 0 | -6 | 1013 | 1069 |
| 1 | 0 | -4 | 1048 | 1087 |
| 1 | 0 | -2 | 180 | - 204 |
| 1 | 0 | 0 | 964 | -1000 |
| 1 | 0 | 2 | 239 | 269 |
| 1 | 0 | 4 | 927 | - 950 |
| 1 | 0 | 6 | 457 | 470 |
| 1 | 0 | 8 | 258 | 293 |
| 1 | 0 | 12 | 244 | - 245 |
| 1 | 0 | 16 | 48 | 47 |
| 1 | 0 | 18 | 32 | 31 |
| 1 | 0 | 20 | 17 | 15 |
| 1 | 0 | 22 | 50 | - 44 |
| 1 | 1 | -22 | 37 | 26 |
| 1 | 1 | -20 | 45 | - 41 |
| 1 | 1 | -19 | 66 | - 67 |
| 1 | 1 | -18 | 40 | 32 |
| 1 | 1 | -16 | 77 | - 58 |
| 1 | 1 | -14 | 42 | 37 |
| 1 | 1 | -13 | 100 | 94 |
| 1 | 1 | -12 | 48 | 48 |
| 1 | 1 | -11 | 55 | 47 |
| 1 | 1 | -10 | 55 | 44 |
| 1 | 1 | -9 | 149 | - 151 |
| 1 | 1 | -8 | 310 | - 343 |
| 1 | 1 | -7 | 151 | 160 |
| 1 | 1 | -6 | 439 | 465 |
| 1 | 1 | -5 | 295 | 333 |
| 1 | 1 | -4 | 549 | - 584 |
| 1 | 1 | -3 | 878 | - 905 |
| 1 | 1 | -2 | 820 | 854 |
| 1 | 1 | -1 | 694 | - 721 |
| 1 | 1 | 0 | 10 | - 6 |
| 1 | 1 | 1 | 772 | 784 |
| 1 | 1 | 2 | 521 | - 544 |
| 1 | 1 | 3 | 379 | 411 |
| 1 | 1 | 4 | 285 | - 313 |
| 1 | 1 | 5 | 82 | 73 |
| 1 | 1 | 6 | 116 | 145 |
| 1 | 1 | 7 | 47 | 50 |
| 1 | 1 | 8 | 268 | 272 |
| 1 | 1 | 9 | 282 | - 302 |
| 1 | 1 | 10 | 127 | 123 |
| 1 | 1 | 11 | 148 | 149 |
| 1 | 1 | 12 | 36 | - 31 |
| 1 | 1 | 13 | 141 | - 134 |
| 1 | 1 | 14 | 194 | - 172 |
| 1 | 1 | 15 | 68 | 50 |
| 1 | 1 | 16 | 17 | - 11 |
| 1 | 1 | 17 | 45 | 40 |
| 1 | 1 | 18 | 67 | 51 |
| 1 | 1 | 20 | 74 | 48 |
| 1 | 1 | 21 | 22 | - 14 |
| 1 | 1 | 22 | 42 | - 36 |
| 1 | 2 | -19 | 56 | - 70 |
| 1 | 2 | -18 | 20 | 36 |
| 1 | 2 | -16 | 29 | - 38 |
| 1 | 2 | -15 | 137 | 155 |
| 1 | 2 | -14 | 90 | - 107 |
| 1 | 2 | -13 | 132 | 137 |
| 1 | 2 | -11 | 78 | - 64 |
| 1 | 2 | -10 | 113 | 114 |
| 1 | 2 | -9 | 158 | - 163 |
| 1 | 2 | -8 | 117 | 109 |
| 1 | 2 | -6 | 162 | - 179 |
| 1 | 2 | -5 | 116 | 109 |
| 1 | 2 | -4 | 33 | - 29 |
| 1 | 2 | -3 | 443 | 435 |
| 1 | 2 | -2 | 36 | - 33 |
| 1 | 2 | -1 | 131 | 120 |
| 1 | 2 | 1 | 113 | - 116 |
| 1 | 2 | 2 | 299 | - 275 |
| 1 | 2 | 3 | 234 | 212 |
| 1 | 2 | 4 | 30 | 16 |
| 1 | 2 | 5 | 381 | - 357 |
| 1 | 2 | 6 | 170 | - 177 |
| 1 | 2 | 7 | 204 | 192 |
| 1 | 2 | 8 | 81 | - 83 |
| 1 | 2 | 9 | 84 | - 81 |
| 1 | 2 | 10 | 144 | 160 |
| 1 | 2 | 11 | 73 | 83 |
| 1 | 2 | 12 | 142 | 166 |
| 1 | 2 | 13 | 49 | 63 |
| 1 | 2 | 14 | 109 | - 131 |
| 1 | 2 | 15 | 186 | - 195 |
| 1 | 2 | 16 | 29 | - 32 |
| 1 | 2 | 17 | 64 | 86 |
| 1 | 2 | 19 | 12 | 4 |
| 1 | 2 | 21 | 9 | 22 |
| 1 | 3 | -22 | 11 | - 13 |
| 1 | 3 | -21 | 22 | - 23 |
| 1 | 3 | -19 | 13 | - 13 |
| 1 | 3 | -16 | 104 | 88 |
| 1 | 3 | -15 | 64 | - 58 |
| 1 | 3 | -14 | 224 | - 200 |
| 1 | 3 | -13 | 128 | 112 |
| 1 | 3 | -11 | 170 | 168 |
| 1 | 3 | -10 | 29 | 31 |
| 1 | 3 | -9 | 22 | - 24 |
| 1 | 3 | -8 | 210 | 211 |
| 1 | 3 | -7 | 318 | - 307 |
| 1 | 3 | -6 | 111 | 91 |
| 1 | 3 | -5 | 432 | - 417 |
| 1 | 3 | -4 | 53 | - 52 |
| 1 | 3 | -3 | 405 | 393 |
| 1 | 3 | -2 | 158 | - 172 |
| 1 | 3 | -1 | 264 | 299 |
| 1 | 3 | 0 | 255 | - 268 |
| 1 | 3 | 1 | 76 | 64 |
| 1 | 3 | 2 | 275 | 275 |
| 1 | 3 | 3 | 281 | - 255 |
| 1 | 3 | 4 | 111 | 123 |
| 1 | 3 | 5 | 117 | 114 |
| 1 | 3 | 6 | 289 | - 279 |
| 1 | 3 | 7 | 188 | - 194 |
| 1 | 3 | 8 | 33 | 30 |
| 1 | 3 | 9 | 147 | 137 |
| 1 | 3 | 10 | 77 | 84 |
| 1 | 3 | 11 | 135 | - 125 |
| 1 | 3 | 12 | 77 | 73 |
| 1 | 3 | 13 | 233 | 211 |
| 1 | 3 | 14 | 87 | - 73 |
| 1 | 3 | 15 | 99 | - 88 |
| 1 | 3 | 17 | 27 | - 20 |
| 1 | 4 | -17 | 42 | 41 |
| 1 | 4 | -15 | 43 | - 54 |
| 1 | 4 | -14 | 101 | - 92 |
| 1 | 4 | -13 | 129 | - 120 |
| 1 | 4 | -12 | 68 | - 70 |
| 1 | 4 | -11 | 177 | 172 |
| 1 | 4 | -10 | 176 | 190 |
| 1 | 4 | -9 | 45 | - 48 |
| 1 | 4 | -8 | 98 | - 112 |
| 1 | 4 | -7 | 94 | 116 |
| 1 | 4 | -6 | 141 | 161 |
| 1 | 4 | -5 | 182 | - 219 |
| 1 | 4 | -4 | 24 | - 30 |
| 1 | 4 | -3 | 30 | 26 |
| 1 | 4 | -2 | 140 | - 161 |
| 1 | 4 | -1 | 127 | - 125 |
| 1 | 4 | 0 | 196 | 186 |
| 1 | 4 | 1 | 88 | 97 |
| 1 | 4 | 2 | 236 | - 206 |
| 1 | 4 | 3 | 172 | 157 |
| 1 | 4 | 5 | 66 | 73 |
| 1 | 4 | 6 | 139 | 149 |
| 1 | 4 | 7 | 70 | - 57 |
| 1 | 4 | 9 | 74 | - 74 |
| 1 | 4 | 10 | 145 | - 118 |
| 1 | 4 | 11 | 31 | - 44 |
| 1 | 4 | 12 | 44 | 43 |
| 1 | 4 | 13 | 71 | - 59 |
| 1 | 4 | 14 | 78 | 60 |
| 1 | 4 | 15 | 96 | 98 |
| 1 | 4 | 16 | 51 | - 38 |
| 2 | 0 | -22 | 30 | 27 |
| 2 | 0 | -18 | 77 | - 80 |
| 2 | 0 | -14 | 178 | - 182 |
| 2 | 0 | -12 | 210 | 220 |
| 2 | 0 | -10 | 306 | 310 |
| 2 | 0 | -8 | 544 | - 516 |
| 2 | 0 | -6 | 186 | 190 |
| 2 | 0 | -4 | 407 | 379 |
| 2 | 0 | -2 | 315 | - 313 |
| 2 | 0 | 0 | 444 | - 458 |
| 2 | 0 | 2 | 309 | 332 |
| 2 | 0 | 4 | 212 | - 209 |
| 2 | 0 | 6 | 165 | 165 |
| 2 | 0 | 8 | 136 | - 163 |
| 2 | 0 | 10 | 48 | 56 |
| 2 | 0 | 12 | 61 | 63 |
| 2 | 0 | 14 | 26 | - 28 |
| 2 | 0 | 18 | 47 | 50 |
| 2 | 0 | 20 | 37 | - 34 |
| 2 | 1 | -23 | 25 | - 18 |
| 2 | 1 | -22 | 15 | 10 |
| 2 | 1 | -20 | 80 | 63 |
| 2 | 1 | -18 | 97 | - 79 |
| 2 | 1 | -17 | 88 | 73 |
| 2 | 1 | -16 | 129 | - 108 |
| 2 | 1 | -15 | 110 | - 98 |
| 2 | 1 | -14 | 42 | 36 |
| 2 | 1 | -13 | 78 | 68 |
| 2 | 1 | -12 | 27 | 22 |
| 2 | 1 | -11 | 161 | 154 |
| 2 | 1 | -10 | 261 | 269 |
| 2 | 1 | -9 | 169 | - 176 |
| 2 | 1 | -8 | 18 | - 20 |
| 2 | 1 | -7 | 86 | - 91 |
| 2 | 1 | -6 | 130 | - 128 |
| 2 | 1 | -5 | 102 | - 113 |
| 2 | 1 | -4 | 151 | - 171 |
| 2 | 1 | -3 | 152 | 174 |
| 2 | 1 | -2 | 178 | - 165 |
| 2 | 1 | -1 | 102 | 109 |
| 2 | 1 | 0 | 41 | 29 |
| 2 | 1 | 1 | 40 | - 25 |
| 2 | 1 | 2 | 309 | 318 |
| 2 | 1 | 3 | 49 | 65 |
| 2 | 1 | 4 | 103 | - 111 |
| 2 | 1 | 5 | 110 | - 127 |
| 2 | 1 | 6 | 75 | 72 |
| 2 | 1 | 7 | 38 | - 34 |
| 2 | 1 | 8 | 84 | - 87 |
| 2 | 1 | 9 | 27 | 23 |
| 2 | 1 | 10 | 171 | - 166 |
| 2 | 1 | 12 | 154 | 155 |
| 2 | 1 | 13 | 151 | 130 |
| 2 | 1 | 14 | 109 | 95 |
| 2 | 1 | 15 | 136 | - 114 |
| 2 | 1 | 16 | 142 | - 121 |
| 2 | 1 | 17 | 37 | - 32 |
| 2 | 1 | 20 | 27 | 22 |
| 2 | 1 | 21 | 22 | 17 |
| 2 | 2 | -19 | 14 | 27 |
| 2 | 2 | -16 | 32 | - 41 |
| 2 | 2 | -15 | 59 | 72 |
| 2 | 2 | -14 | 81 | - 82 |
| 2 | 2 | -13 | 190 | - 195 |
| 2 | 2 | -12 | 52 | 59 |
| 2 | 2 | -11 | 91 | 87 |
| 2 | 2 | -10 | 89 | 82 |
| 2 | 2 | -9 | 249 | - 233 |
| 2 | 2 | -8 | 65 | 64 |
| 2 | 2 | -7 | 316 | 295 |
| 2 | 2 | -6 | 103 | - 99 |
| 2 | 2 | -5 | 46 | 59 |
| 2 | 2 | -4 | 208 | - 198 |
| 2 | 2 | -3 | 110 | 65 |
| 2 | 2 | -2 | 134 | 134 |
| 2 | 2 | -1 | 67 | 92 |
| 2 | 2 | 0 | 229 | 218 |
| 2 | 2 | 1 | 209 | - 210 |
| 2 | 2 | 2 | 272 | - 259 |
| 2 | 2 | 3 | 114 | - 109 |
| 2 | 2 | 4 | 169 | 181 |
| 2 | 2 | 5 | 481 | 493 |

*Table 5. Continued.*

| h | k | l | $F_o$ | $F_c$ |
|---|---|---|---|---|
| 2 | 2 | 6 | 86 | 89 |
| 2 | 2 | 7 | 298 | - 278 |
| 2 | 2 | 8 | 50 | - 64 |
| 2 | 2 | 9 | 45 | - 54 |
| 2 | 2 | 10 | 227 | - 229 |
| 2 | 2 | 11 | 62 | - 78 |
| 2 | 2 | 12 | 134 | 160 |
| 2 | 2 | 13 | 100 | 112 |
| 2 | 2 | 15 | 29 | 38 |
| 2 | 2 | 17 | 38 | - 61 |
| 2 | 2 | 18 | 18 | - 9 |
| 2 | 2 | 19 | 19 | 27 |
| 2 | 3 | -22 | 12 | - 10 |
| 2 | 3 | -21 | 42 | - 34 |
| 2 | 3 | -20 | 27 | 22 |
| 2 | 3 | -19 | 37 | 33 |
| 2 | 3 | -18 | 28 | - 25 |
| 2 | 3 | -17 | 70 | 59 |
| 2 | 3 | -15 | 147 | 129 |
| 2 | 3 | -14 | 25 | 24 |
| 2 | 3 | -13 | 276 | - 262 |
| 2 | 3 | -12 | 129 | - 122 |
| 2 | 3 | -11 | 92 | - 86 |
| 2 | 3 | -10 | 156 | 144 |
| 2 | 3 | -9 | 11 | 15 |
| 2 | 3 | -8 | 105 | 102 |
| 2 | 3 | -7 | 120 | 117 |
| 2 | 3 | -6 | 23 | - 17 |
| 2 | 3 | -5 | 393 | 374 |
| 2 | 3 | -4 | 62 | - 63 |
| 2 | 3 | -3 | 195 | - 209 |
| 2 | 3 | -2 | 123 | - 108 |
| 2 | 3 | -1 | 109 | - 110 |
| 2 | 3 | 0 | 163 | - 172 |
| 2 | 3 | 1 | 29 | - 23 |
| 2 | 3 | 2 | 212 | - 203 |
| 2 | 3 | 3 | 156 | - 161 |
| 2 | 3 | 4 | 301 | 308 |
| 2 | 3 | 5 | 113 | 122 |
| 2 | 3 | 6 | 45 | 51 |
| 2 | 3 | 7 | 243 | 227 |
| 2 | 3 | 8 | 26 | 25 |
| 2 | 3 | 9 | 193 | - 181 |
| 2 | 3 | 10 | 98 | - 94 |
| 2 | 3 | 11 | 106 | 100 |
| 2 | 3 | 13 | 118 | - 104 |
| 2 | 3 | 16 | 36 | - 26 |
| 2 | 3 | 18 | 31 | 24 |
| 2 | 3 | 19 | 31 | 24 |
| 2 | 3 | 20 | 20 | - 16 |
| 2 | 4 | -15 | 78 | 68 |
| 2 | 4 | -14 | 110 | 101 |
| 2 | 4 | -13 | 83 | 79 |
| 2 | 4 | -11 | 183 | - 190 |
| 2 | 4 | -10 | 74 | - 80 |
| 2 | 4 | -9 | 59 | 58 |
| 2 | 4 | -7 | 201 | - 235 |
| 2 | 4 | -5 | 298 | 331 |
| 2 | 4 | -3 | 30 | - 54 |
| 2 | 4 | -2 | 104 | - 98 |
| 2 | 4 | -1 | 114 | 103 |
| 2 | 4 | 0 | 77 | 66 |
| 2 | 4 | 1 | 187 | - 159 |
| 2 | 4 | 2 | 121 | 95 |
| 2 | 4 | 3 | 262 | 218 |
| 2 | 4 | 4 | 101 | - 78 |
| 2 | 4 | 5 | 167 | - 143 |
| 2 | 4 | 7 | 53 | 47 |
| 2 | 4 | 8 | 112 | 108 |
| 2 | 4 | 9 | 97 | - 91 |
| 2 | 4 | 12 | 143 | - 144 |
| 2 | 4 | 13 | 100 | 78 |
| 2 | 4 | 14 | 54 | 38 |
| 2 | 4 | 15 | 30 | 6 |
| 3 | 0 | -18 | 110 | 109 |
| 3 | 0 | -16 | 117 | - 115 |
| 3 | 0 | -14 | 71 | 73 |
| 3 | 0 | -12 | 254 | - 248 |
| 3 | 0 | -10 | 246 | 233 |
| 3 | 0 | -8 | 125 | - 117 |
| 3 | 0 | -6 | 444 | 466 |
| 3 | 0 | -4 | 364 | - 349 |
| 3 | 0 | -2 | 84 | 91 |
| 3 | 0 | 0 | 143 | - 150 |
| 3 | 0 | 2 | 247 | - 255 |
| 3 | 0 | 4 | 298 | 319 |
| 3 | 0 | 6 | 243 | - 282 |
| 3 | 0 | 8 | 247 | 258 |
| 3 | 0 | 10 | 120 | - 127 |
| 3 | 0 | 12 | 21 | 26 |
| 3 | 0 | 14 | 76 | 80 |
| 3 | 0 | 18 | 66 | - 65 |
| 3 | 0 | 20 | 19 | - 15 |
| 3 | 1 | -24 | 30 | - 32 |
| 3 | 1 | -21 | 36 | - 24 |
| 3 | 1 | -20 | 99 | - 77 |
| 3 | 1 | -19 | 31 | 22 |
| 3 | 1 | -18 | 68 | 58 |
| 3 | 1 | -16 | 95 | 78 |
| 3 | 1 | -15 | 125 | 120 |
| 3 | 1 | -13 | 178 | - 174 |
| 3 | 1 | -12 | 35 | 31 |
| 3 | 1 | -11 | 30 | 27 |
| 3 | 1 | -10 | 153 | - 160 |
| 3 | 1 | -9 | 37 | 43 |
| 3 | 1 | -8 | 86 | 81 |
| 3 | 1 | -7 | 93 | - 101 |
| 3 | 1 | -6 | 284 | - 289 |
| 3 | 1 | -5 | 230 | 254 |
| 3 | 1 | -4 | 425 | 451 |
| 3 | 1 | -3 | 511 | - 545 |
| 3 | 1 | -2 | 219 | - 247 |
| 3 | 1 | -1 | 43 | 51 |
| 3 | 1 | 0 | 559 | 587 |
| 3 | 1 | 1 | 497 | 533 |
| 3 | 1 | 2 | 752 | - 775 |
| 3 | 1 | 3 | 91 | - 96 |
| 3 | 1 | 4 | 142 | 166 |
| 3 | 1 | 5 | 73 | 78 |
| 3 | 1 | 6 | 28 | - 22 |
| 3 | 1 | 7 | 82 | 74 |
| 3 | 1 | 8 | 219 | 233 |
| 3 | 1 | 9 | 54 | - 48 |
| 3 | 1 | 10 | 51 | - 52 |
| 3 | 1 | 11 | 110 | - 112 |
| 3 | 1 | 12 | 126 | - 119 |
| 3 | 1 | 13 | 12 | 10 |
| 3 | 1 | 15 | 12 | - 16 |
| 3 | 1 | 16 | 87 | 69 |
| 3 | 1 | 17 | 54 | 45 |
| 3 | 1 | 18 | 55 | - 42 |
| 3 | 1 | 19 | 44 | 27 |
| 3 | 1 | 20 | 31 | 23 |
| 3 | 2 | -20 | 36 | - 47 |
| 3 | 2 | -19 | 43 | 61 |
| 3 | 2 | -18 | 52 | - 74 |
| 3 | 2 | -17 | 38 | - 46 |
| 3 | 2 | -16 | 129 | 142 |
| 3 | 2 | -15 | 20 | - 35 |
| 3 | 2 | -14 | 27 | 25 |
| 3 | 2 | -13 | 114 | 119 |
| 3 | 2 | -12 | 40 | 41 |
| 3 | 2 | -11 | 280 | - 273 |
| 3 | 2 | -10 | 193 | - 196 |
| 3 | 2 | -9 | 214 | 221 |
| 3 | 2 | -8 | 89 | - 92 |
| 3 | 2 | -7 | 155 | - 152 |
| 3 | 2 | -6 | 61 | 58 |
| 3 | 2 | -5 | 196 | 173 |
| 3 | 2 | -4 | 528 | 478 |
| 3 | 2 | -3 | 172 | 195 |
| 3 | 2 | -2 | 153 | - 140 |
| 3 | 2 | -1 | 114 | - 133 |
| 3 | 2 | 0 | 172 | 158 |
| 3 | 2 | 1 | 120 | 120 |
| 3 | 2 | 2 | 384 | - 346 |
| 3 | 2 | 3 | 315 | - 293 |
| 3 | 2 | 4 | 452 | - 379 |
| 3 | 2 | 5 | 86 | - 61 |
| 3 | 2 | 6 | 231 | 236 |
| 3 | 2 | 7 | 200 | 179 |
| 3 | 2 | 8 | 99 | 116 |
| 3 | 2 | 9 | 49 | - 57 |
| 3 | 2 | 10 | 23 | 24 |
| 3 | 2 | 11 | 88 | - 104 |
| 3 | 2 | 12 | 14 | - 14 |
| 3 | 2 | 13 | 75 | 94 |
| 3 | 2 | 14 | 20 | 25 |
| 3 | 2 | 15 | 37 | 63 |
| 3 | 2 | 16 | 66 | - 92 |
| 3 | 2 | 17 | 31 | - 43 |
| 3 | 2 | 19 | 10 | - 17 |
| 3 | 3 | -22 | 23 | 27 |
| 3 | 3 | -21 | 39 | 36 |
| 3 | 3 | -19 | 87 | - 74 |
| 3 | 3 | -18 | 24 | - 21 |
| 3 | 3 | -16 | 153 | - 146 |
| 3 | 3 | -15 | 166 | - 151 |
| 3 | 3 | -14 | 95 | 85 |
| 3 | 3 | -13 | 165 | 167 |
| 3 | 3 | -12 | 189 | 200 |
| 3 | 3 | -11 | 74 | 84 |
| 3 | 3 | -10 | 116 | 121 |
| 3 | 3 | -9 | 110 | 105 |
| 3 | 3 | -7 | 86 | - 85 |
| 3 | 3 | -6 | 287 | - 291 |
| 3 | 3 | -5 | 353 | - 367 |
| 3 | 3 | -4 | 132 | - 136 |
| 3 | 3 | -3 | 37 | 31 |
| 3 | 3 | -2 | 249 | 251 |
| 3 | 3 | -1 | 230 | 238 |
| 3 | 3 | 0 | 277 | 290 |
| 3 | 3 | 1 | 85 | 82 |
| 3 | 3 | 2 | 41 | - 47 |
| 3 | 3 | 3 | 10 | 16 |
| 3 | 3 | 4 | 272 | - 269 |
| 3 | 3 | 5 | 59 | - 61 |
| 3 | 3 | 6 | 180 | 161 |
| 3 | 3 | 7 | 38 | 31 |
| 3 | 3 | 8 | 42 | - 41 |
| 3 | 3 | 9 | 40 | - 46 |
| 3 | 3 | 10 | 136 | 127 |
| 3 | 3 | 11 | 81 | - 80 |
| 3 | 3 | 12 | 110 | - 101 |
| 3 | 3 | 13 | 44 | 30 |
| 3 | 3 | 14 | 25 | 17 |
| 3 | 3 | 15 | 34 | 38 |
| 3 | 3 | 16 | 29 | - 25 |
| 3 | 3 | 17 | 17 | - 16 |
| 3 | 3 | 19 | 22 | 20 |
| 3 | 4 | -15 | 32 | - 36 |
| 3 | 4 | -14 | 125 | - 127 |
| 3 | 4 | -13 | 63 | - 63 |
| 3 | 4 | -12 | 31 | - 21 |
| 3 | 4 | -11 | 42 | 40 |
| 3 | 4 | -10 | 57 | 66 |
| 3 | 4 | -8 | 68 | 75 |
| 3 | 4 | -7 | 64 | 79 |
| 3 | 4 | -6 | 51 | - 62 |
| 3 | 4 | -2 | 107 | - 102 |
| 3 | 4 | -1 | 28 | - 24 |
| 3 | 4 | 0 | 50 | 46 |
| 3 | 4 | 1 | 182 | 168 |
| 3 | 4 | 2 | 298 | 268 |
| 3 | 4 | 3 | 88 | - 73 |
| 3 | 4 | 4 | 174 | - 143 |
| 3 | 4 | 5 | 94 | - 94 |
| 3 | 4 | 6 | 27 | - 34 |
| 3 | 4 | 7 | 159 | - 135 |
| 3 | 4 | 8 | 197 | - 159 |
| 3 | 4 | 9 | 143 | 130 |
| 3 | 4 | 10 | 89 | 75 |
| 3 | 4 | 11 | 105 | 82 |
| 3 | 4 | 12 | 116 | 116 |
| 3 | 4 | 13 | 82 | - 96 |
| 3 | 4 | 14 | 60 | - 35 |
| 4 | 0 | -18 | 107 | - 109 |
| 4 | 0 | -16 | 15 | 16 |
| 4 | 0 | -14 | 24 | - 18 |
| 4 | 0 | -12 | 261 | 249 |
| 4 | 0 | -10 | 254 | - 229 |
| 4 | 0 | -8 | 138 | 126 |
| 4 | 0 | -6 | 270 | - 255 |
| 4 | 0 | -4 | 891 | 825 |
| 4 | 0 | -2 | 1187 | -1232 |
| 4 | 0 | 0 | 84 | 75 |
| 4 | 0 | 2 | 122 | 154 |
| 4 | 0 | 4 | 67 | 78 |
| 4 | 0 | 6 | 199 | 205 |
| 4 | 0 | 8 | 169 | - 183 |
| 4 | 0 | 10 | 20 | 19 |
| 4 | 0 | 12 | 42 | 51 |
| 4 | 0 | 14 | 34 | - 37 |
| 4 | 0 | 16 | 55 | - 43 |
| 4 | 1 | -22 | 30 | - 24 |
| 4 | 1 | -21 | 28 | 23 |
| 4 | 1 | -20 | 89 | 73 |
| 4 | 1 | -19 | 47 | 39 |
| 4 | 1 | -18 | 59 | - 49 |
| 4 | 1 | -17 | 46 | 36 |
| 4 | 1 | -16 | 16 | 15 |
| 4 | 1 | -15 | 153 | - 144 |
| 4 | 1 | -13 | 94 | 87 |
| 4 | 1 | -12 | 42 | 34 |
| 4 | 1 | -11 | 32 | 28 |
| 4 | 1 | -10 | 119 | - 122 |
| 4 | 1 | -9 | 84 | - 94 |
| 4 | 1 | -8 | 175 | 187 |
| 4 | 1 | -7 | 64 | - 66 |
| 4 | 1 | -6 | 72 | - 71 |
| 4 | 1 | -4 | 194 | - 192 |
| 4 | 1 | -3 | 261 | 315 |
| 4 | 1 | -2 | 288 | 311 |
| 4 | 1 | -1 | 30 | - 35 |
| 4 | 1 | 0 | 497 | - 534 |
| 4 | 1 | 1 | 346 | 367 |
| 4 | 1 | 2 | 353 | 381 |
| 4 | 1 | 3 | 98 | - 103 |
| 4 | 1 | 4 | 147 | - 185 |
| 4 | 1 | 5 | 161 | - 173 |
| 4 | 1 | 6 | 207 | 229 |
| 4 | 1 | 7 | 133 | - 139 |
| 4 | 1 | 9 | 79 | 75 |
| 4 | 1 | 10 | 80 | - 82 |
| 4 | 1 | 11 | 37 | 36 |
| 4 | 1 | 12 | 103 | - 96 |
| 4 | 1 | 13 | 12 | 6 |
| 4 | 1 | 14 | 35 | 34 |
| 4 | 1 | 15 | 86 | 72 |
| 4 | 1 | 16 | 72 | 52 |
| 4 | 1 | 17 | 47 | - 38 |
| 4 | 1 | 18 | 23 | 21 |
| 4 | 2 | -20 | 18 | - 22 |
| 4 | 2 | -19 | 30 | - 35 |
| 4 | 2 | -18 | 32 | 34 |
| 4 | 2 | -17 | 83 | 99 |
| 4 | 2 | -16 | 65 | - 70 |
| 4 | 2 | -15 | 46 | - 44 |
| 4 | 2 | -13 | 165 | - 176 |
| 4 | 2 | -12 | 92 | - 89 |
| 4 | 2 | -11 | 99 | 97 |
| 4 | 2 | -10 | 247 | 259 |
| 4 | 2 | -7 | 464 | 399 |
| 4 | 2 | -6 | 128 | 137 |
| 4 | 2 | -5 | 149 | - 130 |
| 4 | 2 | -4 | 376 | - 366 |
| 4 | 2 | -3 | 480 | - 450 |
| 4 | 2 | -2 | 250 | - 213 |
| 4 | 2 | -1 | 27 | 32 |
| 4 | 2 | 0 | 162 | - 168 |
| 4 | 2 | 1 | 203 | 210 |
| 4 | 2 | 2 | 370 | 328 |
| 4 | 2 | 3 | 151 | 143 |
| 4 | 2 | 4 | 91 | - 77 |
| 4 | 2 | 5 | 296 | - 272 |
| 4 | 2 | 6 | 43 | 53 |
| 4 | 2 | 7 | 33 | 43 |
| 4 | 2 | 8 | 83 | 79 |
| 4 | 2 | 9 | 23 | - 25 |
| 4 | 2 | 10 | 34 | - 33 |
| 4 | 2 | 11 | 143 | 179 |
| 4 | 2 | 12 | 79 | - 97 |
| 4 | 2 | 13 | 88 | - 108 |
| 4 | 2 | 15 | 19 | 31 |
| 4 | 2 | 17 | 11 | - 9 |
| 4 | 3 | -22 | 25 | - 31 |
| 4 | 3 | -21 | 18 | - 17 |
| 4 | 3 | -20 | 48 | - 40 |
| 4 | 3 | -19 | 54 | - 49 |
| 4 | 3 | -18 | 60 | 58 |
| 4 | 3 | -17 | 20 | 26 |
| 4 | 3 | -16 | 89 | 87 |
| 4 | 3 | -15 | 217 | 211 |
| 4 | 3 | -14 | 29 | - 31 |
| 4 | 3 | -13 | 46 | - 49 |
| 4 | 3 | -11 | 146 | - 156 |
| 4 | 3 | -10 | 134 | - 131 |
| 4 | 3 | -9 | 93 | - 96 |
| 4 | 3 | -8 | 11 | 14 |
| 4 | 3 | -7 | 130 | - 134 |
| 4 | 3 | -4 | 139 | 119 |
| 4 | 3 | -3 | 10 | - 18 |
| 4 | 3 | -2 | 61 | - 57 |
| 4 | 3 | -1 | 99 | 104 |
| 4 | 3 | 0 | 144 | - 147 |
| 4 | 3 | 1 | 20 | - 30 |
| 4 | 3 | 2 | 215 | 212 |
| 4 | 3 | 3 | 129 | - 124 |
| 4 | 3 | 4 | 16 | 22 |
| 4 | 3 | 5 | 108 | - 102 |
| 4 | 3 | 7 | 137 | 134 |
| 4 | 3 | 8 | 27 | 20 |
| 4 | 3 | 9 | 53 | - 50 |
| 4 | 3 | 10 | 102 | - 97 |
| 4 | 3 | 13 | 74 | 75 |
| 4 | 3 | 14 | 45 | - 41 |
| 4 | 3 | 15 | 67 | - 60 |
| 4 | 3 | 16 | 40 | 36 |
| 4 | 3 | 17 | 18 | 19 |
| 4 | 3 | 18 | 20 | 20 |
| 4 | 4 | -15 | 45 | - 58 |
| 4 | 4 | -14 | 32 | - 47 |
| 4 | 4 | -9 | 40 | 36 |
| 4 | 4 | -8 | 38 | - 24 |
| 4 | 4 | -6 | 66 | 72 |
| 4 | 4 | -5 | 24 | - 23 |
| 4 | 4 | -4 | 109 | - 130 |
| 4 | 4 | -3 | 268 | 268 |
| 4 | 4 | -2 | 156 | 134 |
| 4 | 4 | -1 | 254 | - 210 |
| 4 | 4 | 0 | 48 | - 37 |
| 4 | 4 | 1 | 81 | - 81 |
| 4 | 4 | 2 | 225 | - 191 |
| 4 | 4 | 3 | 26 | - 22 |
| 4 | 4 | 4 | 123 | 87 |
| 4 | 4 | 5 | 98 | 80 |
| 4 | 4 | 7 | 61 | - 46 |
| 4 | 4 | 8 | 178 | 141 |
| 4 | 4 | 9 | 78 | 68 |
| 4 | 4 | 10 | 88 | - 94 |
| 4 | 4 | 12 | 31 | - 28 |
| 4 | 4 | 13 | 42 | 30 |
| 5 | 0 | -22 | 54 | - 53 |
| 5 | 0 | -20 | 94 | - 88 |
| 5 | 0 | -18 | 153 | 142 |
| 5 | 0 | -16 | 90 | 82 |
| 5 | 0 | -14 | 196 | - 178 |
| 5 | 0 | -12 | 209 | 198 |
| 5 | 0 | -10 | 107 | 89 |
| 5 | 0 | -8 | 318 | - 334 |
| 5 | 0 | -6 | 202 | - 192 |
| 5 | 0 | -4 | 54 | - 56 |
| 5 | 0 | -2 | 503 | 505 |
| 5 | 0 | 0 | 23 | - 29 |
| 5 | 0 | 4 | 115 | - 115 |
| 5 | 0 | 6 | 76 | - 95 |
| 5 | 0 | 8 | 155 | 159 |
| 5 | 0 | 10 | 21 | 7 |
| 5 | 0 | 12 | 37 | - 36 |
| 5 | 0 | 14 | 55 | - 55 |
| 5 | 0 | 18 | 32 | 30 |
| 5 | 1 | -23 | 7 | 6 |
| 5 | 1 | -22 | 51 | 41 |
| 5 | 1 | -21 | 35 | 24 |
| 5 | 1 | -20 | 11 | 4 |
| 5 | 1 | -19 | 35 | - 24 |
| 5 | 1 | -18 | 55 | - 47 |
| 5 | 1 | -16 | 30 | - 24 |
| 5 | 1 | -15 | 48 | - 50 |
| 5 | 1 | -14 | 33 | 33 |
| 5 | 1 | -13 | 81 | - 70 |
| 5 | 1 | -12 | 15 | - 10 |
| 5 | 1 | -11 | 144 | 142 |
| 5 | 1 | -10 | 70 | 67 |
| 5 | 1 | -9 | 56 | 59 |
| 5 | 1 | -8 | 63 | - 71 |
| 5 | 1 | -7 | 284 | - 301 |
| 5 | 1 | -6 | 229 | 250 |
| 5 | 1 | -5 | 199 | 230 |
| 5 | 1 | -4 | 499 | - 503 |
| 5 | 1 | -3 | 394 | 397 |
| 5 | 1 | -2 | 183 | - 192 |
| 5 | 1 | -1 | 97 | - 99 |
| 5 | 1 | 0 | 485 | 481 |
| 5 | 1 | 1 | 333 | - 349 |
| 5 | 1 | 2 | 187 | 181 |
| 5 | 1 | 3 | 81 | - 61 |
| 5 | 1 | 4 | 38 | 27 |

*Table 5. Continued.*

| h | k | l | $F_o$ | $F_c$ |
|---|---|---|---|---|
| 5 | 1 | 5 | 81 | - 75 |
| 5 | 1 | 6 | 193 | - 193 |
| 5 | 1 | 7 | 244 | 252 |
| 5 | 1 | 8 | 187 | - 192 |
| 5 | 1 | 9 | 65 | - 59 |
| 5 | 1 | 10 | 103 | 90 |
| 5 | 1 | 11 | 20 | 19 |
| 5 | 1 | 12 | 114 | 103 |
| 5 | 1 | 13 | 11 | - 2 |
| 5 | 1 | 14 | 42 | 34 |
| 5 | 1 | 15 | 38 | - 34 |
| 5 | 1 | 16 | 63 | - 49 |
| 5 | 1 | 17 | 14 | 17 |
| 5 | 1 | 18 | 26 | - 24 |
| 5 | 2 | -18 | 37 | - 41 |
| 5 | 2 | -17 | 66 | - 72 |
| 5 | 2 | -16 | 91 | 95 |
| 5 | 2 | -15 | 14 | - 26 |
| 5 | 2 | -14 | 28 | 38 |
| 5 | 2 | -13 | 109 | 119 |
| 5 | 2 | -12 | 32 | - 35 |
| 5 | 2 | -10 | 50 | - 52 |
| 5 | 2 | -9 | 119 | 113 |
| 5 | 2 | -7 | 151 | - 146 |
| 5 | 2 | -6 | 92 | - 97 |
| 5 | 2 | -5 | 142 | - 135 |
| 5 | 2 | -4 | 75 | 73 |
| 5 | 2 | -3 | 61 | 61 |
| 5 | 2 | -2 | 104 | - 105 |
| 5 | 2 | -1 | 183 | 171 |
| 5 | 2 | 0 | 85 | - 72 |
| 5 | 2 | 1 | 80 | - 69 |
| 5 | 2 | 2 | 271 | 235 |
| 5 | 2 | 3 | 41 | - 45 |
| 5 | 2 | 4 | 114 | 112 |
| 5 | 2 | 5 | 137 | - 134 |
| 5 | 2 | 6 | 18 | - 16 |
| 5 | 2 | 7 | 42 | 44 |
| 5 | 2 | 8 | 137 | - 138 |
| 5 | 2 | 9 | 178 | 195 |
| 5 | 2 | 10 | 75 | - 86 |
| 5 | 2 | 11 | 78 | - 95 |
| 5 | 2 | 12 | 47 | 55 |
| 5 | 2 | 13 | 44 | 62 |
| 5 | 2 | 14 | 41 | 60 |
| 5 | 3 | -21 | 33 | 32 |
| 5 | 3 | -20 | 12 | 17 |
| 5 | 3 | -19 | 49 | 40 |
| 5 | 3 | -18 | 48 | - 53 |
| 5 | 3 | -17 | 20 | 8 |
| 5 | 3 | -16 | 120 | 107 |
| 5 | 3 | -15 | 75 | - 73 |
| 5 | 3 | -14 | 20 | 20 |
| 5 | 3 | -13 | 126 | - 128 |
| 5 | 3 | -12 | 59 | - 63 |
| 5 | 3 | -11 | 13 | 18 |
| 5 | 3 | -9 | 45 | 43 |
| 5 | 3 | -8 | 183 | - 181 |
| 5 | 3 | -7 | 409 | 419 |
| 5 | 3 | -6 | 44 | 49 |
| 5 | 3 | -5 | 125 | - 128 |
| 5 | 3 | -4 | 174 | 179 |
| 5 | 3 | -3 | 186 | - 190 |
| 5 | 3 | -2 | 125 | 142 |
| 5 | 3 | -1 | 307 | - 307 |
| 5 | 3 | 0 | 102 | - 92 |
| 5 | 3 | 1 | 226 | 241 |
| 5 | 3 | 2 | 162 | - 165 |
| 5 | 3 | 3 | 21 | 18 |
| 5 | 3 | 4 | 124 | 109 |
| 5 | 3 | 5 | 103 | 104 |
| 5 | 3 | 7 | 131 | - 131 |
| 5 | 3 | 8 | 14 | 15 |
| 5 | 3 | 9 | 104 | 99 |
| 5 | 3 | 10 | 85 | - 79 |
| 5 | 3 | 11 | 82 | - 74 |
| 5 | 3 | 12 | 20 | 10 |
| 5 | 3 | 14 | 25 | 25 |
| 5 | 3 | 15 | 22 | 19 |
| 5 | 3 | 17 | 20 | - 21 |
| 5 | 4 | -16 | 31 | 30 |
| 5 | 4 | -15 | 89 | 95 |
| 5 | 4 | -14 | 100 | 108 |
| 5 | 4 | -13 | 120 | - 134 |
| 5 | 4 | -11 | 69 | 71 |
| 5 | 4 | -10 | 52 | 58 |
| 5 | 4 | -8 | 122 | - 137 |
| 5 | 4 | -7 | 93 | 101 |
| 5 | 4 | -6 | 77 | - 95 |
| 5 | 4 | -4 | 92 | 103 |
| 5 | 4 | -3 | 75 | - 67 |
| 5 | 4 | -2 | 167 | - 142 |
| 5 | 4 | 0 | 260 | 280 |
| 5 | 4 | 1 | 161 | - 153 |
| 5 | 4 | 2 | 89 | 79 |
| 5 | 4 | 3 | 82 | 72 |
| 5 | 4 | 4 | 251 | - 200 |
| 5 | 4 | 5 | 101 | 91 |
| 5 | 4 | 6 | 82 | - 65 |
| 5 | 4 | 7 | 55 | 40 |
| 5 | 4 | 9 | 133 | - 102 |
| 5 | 4 | 10 | 76 | 46 |
| 5 | 4 | 11 | 90 | 64 |
| 5 | 4 | 12 | 41 | 35 |
| 6 | 0 | -20 | 44 | 55 |
| 6 | 0 | -16 | 162 | 156 |
| 6 | 0 | -14 | 134 | - 132 |
| 6 | 0 | -12 | 426 | - 392 |
| 6 | 0 | -10 | 431 | 380 |
| 6 | 0 | -8 | 159 | 132 |
| 6 | 0 | -6 | 20 | 29 |
| 6 | 0 | -4 | 223 | - 200 |
| 6 | 0 | -2 | 97 | - 101 |
| 6 | 0 | 0 | 138 | - 154 |
| 6 | 0 | 2 | 373 | 405 |
| 6 | 0 | 4 | 66 | - 76 |
| 6 | 0 | 6 | 87 | 87 |
| 6 | 0 | 8 | 101 | - 95 |
| 6 | 0 | 10 | 104 | - 115 |
| 6 | 0 | 12 | 29 | - 23 |
| 6 | 0 | 14 | 110 | 99 |
| 6 | 1 | -23 | 22 | 17 |
| 6 | 1 | -22 | 55 | - 48 |
| 6 | 1 | -21 | 41 | - 31 |
| 6 | 1 | -20 | 32 | - 26 |
| 6 | 1 | -19 | 88 | - 68 |
| 6 | 1 | -18 | 101 | 86 |
| 6 | 1 | -17 | 52 | 47 |
| 6 | 1 | -16 | 96 | - 84 |
| 6 | 1 | -15 | 99 | 91 |
| 6 | 1 | -14 | 177 | 175 |
| 6 | 1 | -13 | 144 | - 139 |
| 6 | 1 | -12 | 59 | - 65 |
| 6 | 1 | -11 | 28 | 28 |
| 6 | 1 | -10 | 162 | - 162 |
| 6 | 1 | -9 | 98 | 94 |
| 6 | 1 | -8 | 197 | - 208 |
| 6 | 1 | -7 | 111 | 115 |
| 6 | 1 | -6 | 262 | 267 |
| 6 | 1 | -5 | 111 | - 109 |
| 6 | 1 | -4 | 233 | 224 |
| 6 | 1 | -3 | 154 | - 155 |
| 6 | 1 | -2 | 65 | 62 |
| 6 | 1 | -1 | 36 | 41 |
| 6 | 1 | 0 | 112 | - 124 |
| 6 | 1 | 1 | 29 | - 23 |
| 6 | 1 | 2 | 100 | - 92 |
| 6 | 1 | 3 | 77 | 65 |
| 6 | 1 | 4 | 130 | - 128 |
| 6 | 1 | 5 | 27 | 23 |
| 6 | 1 | 6 | 42 | 40 |
| 6 | 1 | 7 | 44 | - 39 |
| 6 | 1 | 8 | 223 | 216 |
| 6 | 1 | 9 | 51 | 49 |
| 6 | 1 | 10 | 63 | - 56 |
| 6 | 1 | 11 | 84 | - 69 |
| 6 | 1 | 12 | 96 | - 86 |
| 6 | 1 | 13 | 49 | 40 |
| 6 | 1 | 15 | 24 | 22 |
| 6 | 1 | 16 | 40 | 32 |
| 6 | 2 | -19 | 29 | 36 |
| 6 | 2 | -17 | 51 | - 52 |
| 6 | 2 | -16 | 14 | - 19 |
| 6 | 2 | -15 | 78 | 82 |
| 6 | 2 | -13 | 42 | - 48 |
| 6 | 2 | -10 | 26 | - 25 |
| 6 | 2 | -9 | 91 | - 86 |
| 6 | 2 | -8 | 21 | 15 |
| 6 | 2 | -7 | 54 | 57 |
| 6 | 2 | -6 | 121 | - 118 |
| 6 | 2 | -5 | 255 | 235 |
| 6 | 2 | -4 | 23 | 17 |
| 6 | 2 | -3 | 210 | - 184 |
| 6 | 2 | -2 | 96 | 82 |
| 6 | 2 | -1 | 218 | - 195 |
| 6 | 2 | 0 | 294 | 271 |
| 6 | 2 | 1 | 51 | 58 |
| 6 | 2 | 2 | 244 | - 206 |
| 6 | 2 | 3 | 67 | - 69 |
| 6 | 2 | 4 | 69 | - 68 |
| 6 | 2 | 5 | 231 | 226 |
| 6 | 2 | 6 | 133 | - 130 |
| 6 | 2 | 7 | 20 | 35 |
| 6 | 2 | 8 | 171 | 169 |
| 6 | 2 | 9 | 25 | - 24 |
| 6 | 2 | 10 | 29 | 31 |
| 6 | 2 | 11 | 76 | - 87 |
| 6 | 2 | 13 | 50 | - 74 |
| 6 | 2 | 14 | 40 | - 67 |
| 6 | 2 | 15 | 61 | 65 |
| 6 | 2 | 17 | 10 | 23 |
| 6 | 3 | -21 | 10 | 15 |
| 6 | 3 | -20 | 35 | 36 |
| 6 | 3 | -19 | 21 | - 20 |
| 6 | 3 | -18 | 13 | 9 |
| 6 | 3 | -17 | 110 | - 102 |
| 6 | 3 | -16 | 25 | - 29 |
| 6 | 3 | -15 | 29 | 25 |
| 6 | 3 | -14 | 15 | 2 |
| 6 | 3 | -13 | 161 | 157 |
| 6 | 3 | -12 | 131 | - 128 |
| 6 | 3 | -11 | 47 | 52 |
| 6 | 3 | -10 | 14 | - 9 |
| 6 | 3 | -9 | 19 | - 18 |
| 6 | 3 | -8 | 260 | 254 |
| 6 | 3 | -7 | 342 | - 351 |
| 6 | 3 | -6 | 52 | - 46 |
| 6 | 3 | -5 | 94 | 98 |
| 6 | 3 | -4 | 33 | - 39 |
| 6 | 3 | -3 | 172 | 177 |
| 6 | 3 | -2 | 122 | - 114 |
| 6 | 3 | -1 | 25 | - 17 |
| 6 | 3 | 0 | 116 | 103 |
| 6 | 3 | 1 | 43 | 40 |
| 6 | 3 | 2 | 49 | 52 |
| 6 | 3 | 3 | 27 | - 17 |
| 6 | 3 | 5 | 110 | - 118 |
| 6 | 3 | 6 | 101 | - 110 |
| 6 | 3 | 7 | 99 | 87 |
| 6 | 3 | 8 | 69 | - 64 |
| 6 | 3 | 9 | 69 | - 63 |
| 6 | 3 | 10 | 47 | 34 |
| 6 | 3 | 11 | 24 | 28 |
| 6 | 3 | 12 | 26 | 29 |
| 6 | 3 | 13 | 31 | 30 |
| 6 | 3 | 14 | 87 | 72 |
| 6 | 3 | 16 | 26 | - 26 |
| 6 | 4 | -15 | 62 | - 67 |
| 6 | 4 | -14 | 31 | - 40 |
| 6 | 4 | -13 | 100 | 117 |
| 6 | 4 | -10 | 108 | - 120 |
| 6 | 4 | -9 | 148 | 173 |
| 6 | 4 | -8 | 53 | - 59 |
| 6 | 4 | -7 | 174 | - 169 |
| 6 | 4 | -6 | 123 | 148 |
| 6 | 4 | -5 | 203 | - 204 |
| 6 | 4 | -4 | 280 | 288 |
| 6 | 4 | -3 | 41 | - 28 |
| 6 | 4 | -2 | 88 | - 82 |
| 6 | 4 | -1 | 249 | 208 |
| 6 | 4 | 0 | 328 | - 342 |
| 6 | 4 | 1 | 30 | 26 |
| 6 | 4 | 2 | 31 | - 24 |
| 6 | 4 | 3 | 48 | - 49 |
| 6 | 4 | 4 | 104 | 101 |
| 6 | 4 | 5 | 55 | - 49 |
| 6 | 4 | 6 | 146 | 110 |
| 6 | 4 | 7 | 55 | 33 |
| 6 | 4 | 9 | 43 | 32 |
| 7 | 0 | -22 | 88 | 94 |
| 7 | 0 | -20 | 127 | - 119 |
| 7 | 0 | -18 | 41 | - 37 |
| 7 | 0 | -14 | 259 | 239 |
| 7 | 0 | -12 | 44 | - 49 |
| 7 | 0 | -10 | 116 | - 124 |
| 7 | 0 | -8 | 124 | - 129 |
| 7 | 0 | -6 | 121 | - 108 |
| 7 | 0 | -4 | 243 | 221 |
| 7 | 0 | -2 | 58 | 57 |
| 7 | 0 | 0 | 213 | 220 |
| 7 | 0 | 2 | 169 | - 173 |
| 7 | 0 | 6 | 253 | - 251 |
| 7 | 0 | 8 | 88 | 88 |
| 7 | 0 | 10 | 152 | 138 |
| 7 | 0 | 12 | 26 | - 35 |
| 7 | 0 | 14 | 36 | - 37 |
| 7 | 1 | -23 | 16 | 15 |
| 7 | 1 | -22 | 21 | 19 |
| 7 | 1 | -21 | 24 | 17 |
| 7 | 1 | -20 | 12 | 18 |
| 7 | 1 | -19 | 10 | - 17 |
| 7 | 1 | -18 | 37 | - 29 |
| 7 | 1 | -17 | 67 | - 60 |
| 7 | 1 | -16 | 32 | 28 |
| 7 | 1 | -15 | 90 | 86 |
| 7 | 1 | -14 | 189 | - 172 |
| 7 | 1 | -13 | 85 | 74 |
| 7 | 1 | -12 | 212 | 211 |
| 7 | 1 | -11 | 171 | - 174 |
| 7 | 1 | -10 | 44 | - 48 |
| 7 | 1 | -9 | 65 | 71 |
| 7 | 1 | -8 | 25 | 34 |
| 7 | 1 | -7 | 37 | - 43 |
| 7 | 1 | -6 | 114 | - 119 |
| 7 | 1 | -5 | 171 | 187 |
| 7 | 1 | -4 | 301 | 320 |
| 7 | 1 | -2 | 348 | - 361 |
| 7 | 1 | -1 | 285 | - 295 |
| 7 | 1 | 0 | 60 | 64 |
| 7 | 1 | 1 | 78 | 76 |
| 7 | 1 | 2 | 103 | 97 |
| 7 | 1 | 3 | 18 | - 16 |
| 7 | 1 | 4 | 11 | 13 |
| 7 | 1 | 5 | 11 | 16 |
| 7 | 1 | 6 | 113 | - 107 |
| 7 | 1 | 7 | 37 | 34 |
| 7 | 1 | 8 | 37 | - 31 |
| 7 | 1 | 9 | 76 | 70 |
| 7 | 1 | 10 | 111 | 91 |
| 7 | 1 | 11 | 45 | 38 |
| 7 | 1 | 12 | 27 | 27 |
| 7 | 1 | 13 | 24 | - 17 |
| 7 | 1 | 14 | 52 | - 43 |
| 7 | 1 | 15 | 18 | - 16 |
| 7 | 2 | -20 | 88 | 60 |
| 7 | 2 | -19 | 12 | - 9 |
| 7 | 2 | -18 | 23 | - 26 |
| 7 | 2 | -16 | 28 | - 39 |
| 7 | 2 | -15 | 139 | - 127 |
| 7 | 2 | -14 | 29 | - 29 |
| 7 | 2 | -13 | 217 | 210 |
| 7 | 2 | -12 | 35 | 44 |
| 7 | 2 | -11 | 96 | 80 |
| 7 | 2 | -9 | 79 | - 84 |
| 7 | 2 | -7 | 69 | - 76 |
| 7 | 2 | -6 | 18 | - 21 |
| 7 | 2 | -5 | 269 | - 239 |
| 7 | 2 | -3 | 213 | 196 |
| 7 | 2 | -2 | 79 | - 76 |
| 7 | 2 | -1 | 67 | - 53 |
| 7 | 2 | 1 | 196 | 183 |
| 7 | 2 | 2 | 212 | 182 |
| 7 | 2 | 3 | 117 | 110 |
| 7 | 2 | 4 | 79 | - 82 |
| 7 | 2 | 5 | 173 | - 179 |
| 7 | 2 | 6 | 48 | 40 |
| 7 | 2 | 7 | 80 | - 89 |
| 7 | 2 | 8 | 38 | - 41 |
| 7 | 2 | 9 | 42 | 50 |
| 7 | 2 | 10 | 43 | - 51 |
| 7 | 2 | 11 | 34 | 44 |
| 7 | 2 | 12 | 27 | - 38 |
| 7 | 2 | 14 | 38 | 72 |
| 7 | 3 | -18 | 22 | 17 |
| 7 | 3 | -17 | 81 | 70 |
| 7 | 3 | -16 | 37 | - 32 |
| 7 | 3 | -15 | 40 | - 43 |
| 7 | 3 | -14 | 14 | 3 |
| 7 | 3 | -13 | 143 | - 128 |
| 7 | 3 | -12 | 15 | - 22 |
| 7 | 3 | -11 | 66 | 66 |
| 7 | 3 | -8 | 68 | 81 |
| 7 | 3 | -7 | 121 | 110 |
| 7 | 3 | -6 | 105 | 96 |
| 7 | 3 | -5 | 47 | - 44 |
| 7 | 3 | -4 | 108 | - 97 |
| 7 | 3 | -3 | 65 | 64 |
| 7 | 3 | -2 | 19 | 18 |
| 7 | 3 | -1 | 48 | 50 |
| 7 | 3 | 0 | 63 | - 55 |
| 7 | 3 | 1 | 77 | - 78 |
| 7 | 3 | 2 | 62 | 53 |
| 7 | 3 | 3 | 78 | 74 |
| 7 | 3 | 4 | 110 | - 109 |
| 7 | 3 | 5 | 72 | - 63 |
| 7 | 3 | 6 | 32 | 37 |
| 7 | 3 | 10 | 99 | 94 |
| 7 | 3 | 11 | 32 | 32 |
| 7 | 3 | 14 | 51 | - 50 |
| 7 | 4 | -16 | 40 | 40 |
| 7 | 4 | -15 | 66 | 77 |
| 7 | 4 | -14 | 61 | - 67 |
| 7 | 4 | -12 | 32 | - 37 |
| 7 | 4 | -11 | 78 | - 93 |
| 7 | 4 | -10 | 141 | 179 |
| 7 | 4 | -9 | 71 | - 75 |
| 7 | 4 | -8 | 45 | 56 |
| 7 | 4 | -6 | 134 | - 169 |
| 7 | 4 | -5 | 82 | 108 |
| 7 | 4 | -4 | 54 | - 69 |
| 7 | 4 | -2 | 62 | 60 |
| 7 | 4 | -1 | 44 | - 51 |
| 7 | 4 | 0 | 109 | - 101 |
| 7 | 4 | 1 | 71 | - 58 |
| 7 | 4 | 2 | 162 | 137 |
| 7 | 4 | 3 | 32 | 28 |
| 7 | 4 | 4 | 84 | 74 |
| 7 | 4 | 5 | 104 | 93 |
| 7 | 4 | 7 | 43 | 27 |
| 7 | 4 | 8 | 29 | - 44 |
| 8 | 0 | -20 | 177 | 169 |
| 8 | 0 | -16 | 84 | - 82 |
| 8 | 0 | -14 | 186 | - 171 |
| 8 | 0 | -12 | 37 | 34 |
| 8 | 0 | -10 | 74 | 68 |
| 8 | 0 | -8 | 232 | 219 |
| 8 | 0 | -6 | 243 | - 220 |
| 8 | 0 | -4 | 149 | 133 |
| 8 | 0 | -2 | 129 | 110 |
| 8 | 0 | 0 | 222 | - 211 |
| 8 | 0 | 2 | 78 | 71 |
| 8 | 0 | 4 | 51 | - 49 |
| 8 | 0 | 12 | 64 | 59 |
| 8 | 0 | 14 | 18 | - 21 |
| 8 | 1 | -22 | 49 | - 65 |
| 8 | 1 | -19 | 15 | - 16 |
| 8 | 1 | -18 | 115 | 99 |
| 8 | 1 | -17 | 11 | 11 |
| 8 | 1 | -16 | 14 | 17 |
| 8 | 1 | -15 | 37 | - 37 |
| 8 | 1 | -14 | 126 | - 121 |
| 8 | 1 | -13 | 12 | - 15 |
| 8 | 1 | -12 | 121 | - 114 |
| 8 | 1 | -11 | 137 | 145 |
| 8 | 1 | -10 | 121 | 133 |
| 8 | 1 | -8 | 95 | 92 |
| 8 | 1 | -6 | 79 | 76 |
| 8 | 1 | -5 | 190 | - 191 |
| 8 | 1 | -4 | 105 | - 120 |
| 8 | 1 | -3 | 33 | - 32 |
| 8 | 1 | -2 | 41 | 40 |
| 8 | 1 | -1 | 104 | - 98 |
| 8 | 1 | 0 | 300 | - 301 |
| 8 | 1 | 1 | 87 | 82 |
| 8 | 1 | 2 | 97 | 110 |
| 8 | 1 | 3 | 216 | 235 |
| 8 | 1 | 4 | 224 | 220 |
| 8 | 1 | 6 | 55 | - 52 |
| 8 | 1 | 7 | 110 | - 106 |
| 8 | 1 | 8 | 43 | - 42 |
| 8 | 1 | 9 | 73 | - 69 |
| 8 | 1 | 10 | 29 | - 22 |
| 8 | 1 | 11 | 40 | 40 |
| 8 | 1 | 13 | 19 | - 16 |
| 8 | 2 | -20 | 39 | - 53 |
| 8 | 2 | -18 | 28 | 31 |
| 8 | 2 | -17 | 45 | 44 |
| 8 | 2 | -16 | 48 | 51 |
| 8 | 2 | -15 | 91 | 87 |
| 8 | 2 | -14 | 28 | 40 |
| 8 | 2 | -13 | 97 | - 93 |
| 8 | 2 | -12 | 60 | - 57 |

*Table 5. Continued.*

| h | k | l | $F_o$ | $F_c$ |
|---|---|---|---|---|
| 8 | 2 | -10 | 78 | - 80 |
| 8 | 2 | -9 | 139 | - 141 |
| 8 | 2 | -8 | 136 | - 140 |
| 8 | 2 | -7 | 109 | - 115 |
| 8 | 2 | -6 | 113 | 124 |
| 8 | 2 | -5 | 374 | 345 |
| 8 | 2 | -4 | 289 | 260 |
| 8 | 2 | -3 | 81 | 81 |
| 8 | 2 | -2 | 63 | 46 |
| 8 | 2 | -1 | 57 | - 48 |
| 8 | 2 | 0 | 182 | - 176 |
| 8 | 2 | 1 | 316 | - 294 |
| 8 | 2 | 2 | 56 | - 48 |
| 8 | 2 | 3 | 138 | 118 |
| 8 | 2 | 4 | 48 | - 35 |
| 8 | 2 | 5 | 91 | 85 |
| 8 | 2 | 7 | 14 | 25 |
| 8 | 2 | 8 | 58 | 61 |
| 8 | 2 | 9 | 104 | - 121 |
| 8 | 2 | 10 | 29 | 34 |
| 8 | 2 | 11 | 22 | 30 |
| 8 | 2 | 12 | 16 | - 29 |
| 8 | 3 | -20 | 9 | 14 |
| 8 | 3 | -19 | 15 | - 19 |
| 8 | 3 | -18 | 47 | - 47 |
| 8 | 3 | -17 | 25 | - 21 |
| 8 | 3 | -16 | 39 | - 42 |
| 8 | 3 | -15 | 36 | 38 |
| 8 | 3 | -13 | 84 | 71 |
| 8 | 3 | -12 | 136 | 131 |
| 8 | 3 | -11 | 87 | - 87 |
| 8 | 3 | -10 | 15 | 20 |
| 8 | 3 | -9 | 100 | 94 |
| 8 | 3 | -8 | 72 | - 70 |
| 8 | 3 | -7 | 169 | - 159 |
| 8 | 3 | -6 | 35 | - 32 |
| 8 | 3 | -5 | 41 | 43 |
| 8 | 3 | -4 | 32 | - 41 |
| 8 | 3 | -3 | 66 | 74 |
| 8 | 3 | -2 | 111 | 111 |
| 8 | 3 | -1 | 29 | - 25 |
| 8 | 3 | 0 | 15 | - 25 |
| 8 | 3 | 1 | 21 | - 28 |
| 8 | 3 | 2 | 87 | - 96 |
| 8 | 3 | 3 | 62 | - 71 |
| 8 | 3 | 5 | 14 | 17 |
| 8 | 3 | 6 | 28 | 31 |
| 8 | 3 | 7 | 99 | 93 |
| 8 | 3 | 8 | 56 | 58 |
| 8 | 3 | 9 | 73 | 63 |
| 8 | 3 | 10 | 29 | - 27 |
| 8 | 3 | 11 | 111 | - 114 |
| 8 | 4 | -14 | 29 | 38 |
| 8 | 4 | -12 | 53 | - 76 |
| 8 | 4 | -8 | 32 | 41 |
| 8 | 4 | -7 | 78 | 83 |
| 8 | 4 | -5 | 159 | - 189 |
| 8 | 4 | -4 | 84 | - 109 |
| 8 | 4 | -3 | 55 | 55 |
| 8 | 4 | -2 | 55 | 63 |
| 8 | 4 | -1 | 64 | 77 |
| 8 | 4 | 0 | 191 | 181 |
| 8 | 4 | 1 | 123 | 110 |
| 8 | 4 | 2 | 83 | - 71 |
| 8 | 4 | 3 | 62 | - 59 |
| 8 | 4 | 4 | 43 | - 21 |
| 8 | 4 | 5 | 51 | - 37 |
| 8 | 4 | 6 | 63 | - 95 |
| 8 | 4 | 7 | 46 | - 69 |
| 9 | 0 | -22 | 20 | 22 |
| 9 | 0 | -20 | 68 | - 79 |
| 9 | 0 | -18 | 128 | - 121 |
| 9 | 0 | -16 | 95 | 90 |
| 9 | 0 | -14 | 65 | 64 |
| 9 | 0 | -12 | 54 | 45 |
| 9 | 0 | -10 | 77 | - 60 |
| 9 | 0 | -8 | 58 | - 59 |
| 9 | 0 | -6 | 100 | 87 |
| 9 | 0 | -4 | 48 | 47 |
| 9 | 0 | -2 | 34 | 36 |
| 9 | 0 | 0 | 122 | - 113 |
| 9 | 0 | 2 | 227 | - 214 |
| 9 | 0 | 4 | 166 | 149 |
| 9 | 0 | 6 | 106 | 108 |
| 9 | 0 | 10 | 32 | - 31 |
| 9 | 0 | 12 | 26 | - 23 |
| 9 | 1 | -22 | 11 | 25 |
| 9 | 1 | -21 | 10 | - 13 |
| 9 | 1 | -20 | 12 | 14 |
| 9 | 1 | -18 | 109 | - 100 |
| 9 | 1 | -17 | 52 | 47 |
| 9 | 1 | -16 | 54 | - 44 |
| 9 | 1 | -15 | 97 | 84 |
| 9 | 1 | -14 | 67 | 57 |
| 9 | 1 | -13 | 49 | - 44 |
| 9 | 1 | -12 | 106 | 100 |
| 9 | 1 | -11 | 102 | - 98 |
| 9 | 1 | -10 | 189 | 191 |
| 9 | 1 | -9 | 38 | 38 |
| 9 | 1 | -8 | 175 | - 169 |
| 9 | 1 | -7 | 122 | - 128 |
| 9 | 1 | -6 | 285 | - 312 |
| 9 | 1 | -5 | 79 | - 62 |
| 9 | 1 | -4 | 14 | - 24 |
| 9 | 1 | -3 | 185 | 173 |
| 9 | 1 | -2 | 287 | 283 |
| 9 | 1 | -1 | 186 | 166 |

| h | k | l | $F_o$ | $F_c$ |
|---|---|---|---|---|
| 9 | 1 | 0 | 135 | 145 |
| 9 | 1 | 1 | 83 | - 77 |
| 9 | 1 | 2 | 128 | - 121 |
| 9 | 1 | 3 | 34 | 33 |
| 9 | 1 | 4 | 136 | - 129 |
| 9 | 1 | 5 | 108 | - 94 |
| 9 | 1 | 6 | 89 | 73 |
| 9 | 1 | 7 | 10 | 15 |
| 9 | 1 | 8 | 46 | - 31 |
| 9 | 1 | 9 | 49 | 41 |
| 9 | 1 | 10 | 52 | 45 |
| 9 | 2 | -20 | 27 | 42 |
| 9 | 2 | -19 | 17 | 22 |
| 9 | 2 | -17 | 34 | 34 |
| 9 | 2 | -16 | 56 | - 53 |
| 9 | 2 | -15 | 46 | - 52 |
| 9 | 2 | -14 | 74 | - 75 |
| 9 | 2 | -13 | 61 | - 63 |
| 9 | 2 | -12 | 57 | - 55 |
| 9 | 2 | -11 | 14 | - 21 |
| 9 | 2 | -10 | 221 | 215 |
| 9 | 2 | -9 | 126 | 127 |
| 9 | 2 | -8 | 140 | 138 |
| 9 | 2 | -7 | 48 | 49 |
| 9 | 2 | -6 | 96 | - 100 |
| 9 | 2 | -5 | 138 | - 136 |
| 9 | 2 | -4 | 141 | - 129 |
| 9 | 2 | -2 | 14 | - 14 |
| 9 | 2 | -1 | 106 | 87 |
| 9 | 2 | 0 | 89 | - 67 |
| 9 | 2 | 2 | 119 | 114 |
| 9 | 2 | 3 | 47 | - 49 |
| 9 | 2 | 4 | 41 | 37 |
| 9 | 2 | 6 | 58 | - 58 |
| 9 | 2 | 7 | 54 | - 65 |
| 9 | 2 | 9 | 38 | 55 |
| 9 | 3 | -18 | 24 | 31 |
| 9 | 3 | -17 | 19 | - 14 |
| 9 | 3 | -15 | 13 | 18 |
| 9 | 3 | -13 | 50 | - 55 |
| 9 | 3 | -12 | 47 | - 47 |
| 9 | 3 | -11 | 42 | 44 |
| 9 | 3 | -10 | 59 | 58 |
| 9 | 3 | -9 | 49 | - 50 |
| 9 | 3 | -8 | 25 | 25 |
| 9 | 3 | -7 | 91 | 87 |
| 9 | 3 | -5 | 29 | - 38 |
| 9 | 3 | -4 | 44 | - 44 |
| 9 | 3 | -3 | 43 | - 36 |
| 9 | 3 | -2 | 108 | - 110 |
| 9 | 3 | -1 | 77 | - 74 |
| 9 | 3 | 0 | 102 | 95 |
| 9 | 3 | 1 | 98 | 94 |
| 9 | 3 | 3 | 70 | 63 |
| 9 | 3 | 4 | 27 | 26 |
| 9 | 3 | 5 | 18 | 14 |
| 9 | 3 | 7 | 95 | - 89 |
| 9 | 3 | 8 | 21 | 24 |
| 9 | 3 | 9 | 13 | - 22 |
| 9 | 4 | -11 | 58 | - 77 |
| 9 | 4 | -10 | 59 | - 78 |
| 9 | 4 | -8 | 53 | 61 |
| 9 | 4 | -5 | 115 | 131 |
| 9 | 4 | -4 | 62 | 63 |
| 9 | 4 | -3 | 53 | - 63 |
| 9 | 4 | -2 | 53 | - 52 |
| 9 | 4 | -1 | 22 | 16 |
| 9 | 4 | 0 | 30 | - 36 |
| 9 | 4 | 1 | 41 | - 37 |
| 9 | 4 | 2 | 40 | 23 |
| 10 | 0 | -18 | 15 | 17 |
| 10 | 0 | -16 | 47 | - 43 |
| 10 | 0 | -14 | 159 | 142 |
| 10 | 0 | -12 | 140 | - 125 |
| 10 | 0 | -10 | 65 | 59 |
| 10 | 0 | -6 | 129 | - 107 |
| 10 | 0 | -2 | 33 | 23 |
| 10 | 0 | 0 | 36 | - 21 |
| 10 | 0 | 2 | 136 | 116 |
| 10 | 0 | 4 | 35 | - 34 |
| 10 | 0 | 6 | 12 | - 14 |
| 10 | 1 | -20 | 72 | - 76 |
| 10 | 1 | -19 | 36 | 29 |
| 10 | 1 | -18 | 84 | 81 |
| 10 | 1 | -17 | 69 | - 61 |
| 10 | 1 | -16 | 35 | 28 |
| 10 | 1 | -14 | 60 | 58 |
| 10 | 1 | -13 | 43 | - 42 |
| 10 | 1 | -12 | 89 | - 89 |
| 10 | 1 | -11 | 47 | - 38 |
| 10 | 1 | -10 | 134 | - 135 |
| 10 | 1 | -9 | 72 | 67 |
| 10 | 1 | -8 | 66 | 68 |
| 10 | 1 | -7 | 54 | 52 |
| 10 | 1 | -6 | 96 | 102 |
| 10 | 1 | -5 | 35 | 30 |
| 10 | 1 | -3 | 55 | - 44 |
| 10 | 1 | 1 | 49 | - 38 |
| 10 | 1 | 2 | 63 | - 57 |
| 10 | 1 | 4 | 45 | 43 |
| 10 | 1 | 5 | 72 | 63 |
| 10 | 1 | 7 | 26 | - 21 |
| 10 | 1 | 8 | 35 | 26 |
| 10 | 2 | -18 | 42 | - 48 |
| 10 | 2 | -16 | 45 | 43 |
| 10 | 2 | -14 | 79 | 74 |
| 10 | 2 | -13 | 41 | - 35 |

| h | k | l | $F_o$ | $F_c$ |
|---|---|---|---|---|
| 10 | 2 | -12 | 19 | 18 |
| 10 | 2 | -11 | 47 | - 49 |
| 10 | 2 | -10 | 116 | - 99 |
| 10 | 2 | -9 | 118 | 110 |
| 10 | 2 | -8 | 24 | 26 |
| 10 | 2 | -7 | 24 | 34 |
| 10 | 2 | -6 | 58 | - 58 |
| 10 | 2 | -4 | 65 | 70 |
| 10 | 2 | -3 | 24 | - 35 |
| 10 | 2 | -2 | 28 | - 19 |
| 10 | 2 | -1 | 66 | - 63 |
| 10 | 2 | 0 | 14 | 10 |
| 10 | 2 | 1 | 88 | 81 |
| 10 | 2 | 2 | 47 | - 49 |
| 10 | 2 | 3 | 61 | - 57 |
| 10 | 2 | 4 | 78 | 76 |
| 10 | 2 | 6 | 34 | - 40 |
| 10 | 2 | 7 | 17 | 25 |
| 10 | 3 | -14 | 31 | 32 |
| 10 | 3 | -13 | 30 | 31 |
| 10 | 3 | -12 | 64 | 55 |
| 10 | 3 | -11 | 48 | - 48 |
| 10 | 3 | -10 | 97 | - 88 |
| 10 | 3 | -9 | 23 | 28 |
| 10 | 3 | -8 | 33 | - 32 |
| 10 | 3 | -6 | 36 | - 36 |
| 10 | 3 | -5 | 58 | - 48 |
| 10 | 3 | -4 | 73 | 62 |
| 10 | 3 | -3 | 92 | 84 |
| 10 | 3 | -1 | 13 | - 18 |
| 10 | 3 | 0 | 18 | - 12 |
| 10 | 3 | 2 | 39 | 39 |
| 10 | 3 | 3 | 20 | 22 |
| 10 | 3 | 4 | 22 | - 22 |
| 10 | 3 | 5 | 74 | - 80 |
| 10 | 3 | 8 | 13 | 7 |
| 10 | 4 | -9 | 27 | - 36 |
| 10 | 4 | -8 | 39 | - 40 |
| 10 | 4 | -7 | 62 | 70 |
| 10 | 4 | -5 | 39 | 41 |
| 10 | 4 | -4 | 10 | - 9 |
| 10 | 4 | -3 | 55 | - 48 |
| 10 | 4 | -2 | 38 | 63 |
| 11 | 0 | -18 | 27 | 36 |
| 11 | 0 | -16 | 18 | 22 |
| 11 | 0 | -14 | 70 | - 67 |
| 11 | 0 | -10 | 27 | - 25 |
| 11 | 0 | -8 | 113 | 90 |
| 11 | 0 | -6 | 61 | - 50 |
| 11 | 0 | -4 | 31 | 29 |
| 11 | 0 | -2 | 81 | - 64 |
| 11 | 0 | 4 | 53 | 53 |
| 11 | 0 | 6 | 28 | 30 |
| 11 | 1 | -18 | 36 | - 39 |
| 11 | 1 | -17 | 18 | - 22 |
| 11 | 1 | -16 | 73 | 63 |
| 11 | 1 | -15 | 38 | - 36 |
| 11 | 1 | -14 | 52 | - 48 |
| 11 | 1 | -13 | 82 | 76 |
| 11 | 1 | -10 | 30 | - 32 |
| 11 | 1 | -8 | 15 | 23 |
| 11 | 1 | -7 | 35 | - 28 |
| 11 | 1 | -5 | 106 | - 99 |
| 11 | 1 | -4 | 58 | 50 |
| 11 | 1 | -3 | 138 | 124 |
| 11 | 1 | -2 | 33 | - 36 |
| 11 | 1 | 0 | 40 | - 33 |
| 11 | 1 | 1 | 14 | 12 |
| 11 | 1 | 2 | 13 | 16 |
| 11 | 1 | 3 | 43 | - 35 |
| 11 | 1 | 5 | 35 | - 35 |
| 11 | 1 | 6 | 39 | 38 |
| 11 | 2 | -16 | 33 | - 35 |
| 11 | 2 | -13 | 30 | 5 |
| 11 | 2 | -11 | 86 | 73 |
| 11 | 2 | -9 | 61 | - 63 |
| 11 | 2 | -7 | 74 | 67 |
| 11 | 2 | -5 | 101 | - 87 |
| 11 | 2 | -4 | 25 | - 25 |
| 11 | 2 | -2 | 57 | 51 |
| 11 | 2 | -1 | 17 | 24 |
| 11 | 2 | 0 | 35 | - 40 |
| 11 | 2 | 1 | 37 | - 36 |
| 11 | 2 | 3 | 57 | 61 |
| 11 | 3 | -16 | 7 | - 12 |
| 11 | 3 | -15 | 36 | 41 |
| 11 | 3 | -13 | 14 | - 10 |
| 11 | 3 | -11 | 11 | - 10 |
| 11 | 3 | -10 | 11 | 12 |
| 11 | 3 | -9 | 31 | - 33 |
| 11 | 3 | -8 | 34 | - 36 |
| 11 | 3 | -7 | 24 | - 28 |
| 11 | 3 | -4 | 12 | - 5 |
| 11 | 3 | -3 | 29 | - 23 |
| 11 | 3 | -2 | 47 | 45 |
| 11 | 3 | -1 | 11 | 15 |
| 11 | 3 | 0 | 30 | - 35 |
| 11 | 3 | 1 | 74 | - 73 |
| 11 | 3 | 2 | 37 | 48 |
| 11 | 3 | 3 | 61 | 61 |
| 11 | 3 | 4 | 13 | 18 |
| 12 | 0 | -16 | 24 | 26 |
| 12 | 0 | -14 | 30 | 34 |
| 12 | 0 | -12 | 52 | - 49 |
| 12 | 0 | -10 | 28 | - 24 |
| 12 | 0 | -8 | 119 | 97 |
| 12 | 0 | -6 | 71 | - 64 |

| h | k | l | $F_o$ | $F_c$ |
|---|---|---|---|---|
| 12 | 0 | -4 | 174 | - 145 |
| 12 | 0 | -2 | 91 | 78 |
| 12 | 0 | 0 | 68 | 56 |
| 12 | 0 | 2 | 46 | 48 |
| 12 | 1 | -15 | 30 | 31 |
| 12 | 1 | -14 | 23 | 16 |
| 12 | 1 | -13 | 50 | - 48 |
| 12 | 1 | -12 | 11 | - 9 |
| 12 | 1 | -11 | 19 | - 17 |
| 12 | 1 | -10 | 9 | 4 |
| 12 | 1 | -9 | 9 | 5 |
| 12 | 1 | -8 | 9 | 5 |
| 12 | 1 | -7 | 74 | 68 |
| 12 | 1 | -6 | 13 | 14 |
| 12 | 1 | -5 | 25 | 22 |
| 12 | 1 | -4 | 32 | - 30 |
| 12 | 1 | 0 | 36 | 28 |
| 12 | 1 | 1 | 94 | - 90 |
| 12 | 1 | 2 | 26 | - 23 |
| 12 | 2 | -15 | 25 | 31 |
| 12 | 2 | -14 | 25 | - 23 |
| 12 | 2 | -11 | 33 | - 35 |
| 12 | 2 | -10 | 10 | 14 |
| 12 | 2 | -9 | 70 | 63 |
| 12 | 2 | -8 | 15 | - 10 |
| 12 | 2 | -7 | 76 | - 71 |
| 12 | 2 | -6 | 31 | - 31 |
| 12 | 2 | -4 | 18 | - 18 |
| 12 | 2 | -3 | 26 | - 23 |
| 12 | 2 | -2 | 32 | 31 |
| 12 | 2 | -1 | 69 | 62 |
| 12 | 2 | 1 | 16 | - 14 |
| 12 | 2 | 2 | 9 | 13 |
| 12 | 3 | -12 | 41 | - 51 |
| 12 | 3 | -11 | 23 | - 29 |
| 12 | 3 | -10 | 30 | - 33 |
| 12 | 3 | -9 | 43 | 48 |
| 12 | 3 | -7 | 24 | 29 |
| 12 | 3 | -6 | 60 | 66 |
| 12 | 3 | -5 | 30 | - 41 |
| 12 | 3 | -3 | 32 | 41 |
| 12 | 3 | -2 | 16 | 18 |
| 12 | 3 | -1 | 39 | - 39 |
| 13 | 0 | -12 | 23 | 29 |
| 13 | 0 | -10 | 37 | - 38 |
| 13 | 0 | -8 | 32 | - 37 |
| 13 | 0 | -2 | 58 | 52 |
| 13 | 1 | -12 | 44 | - 62 |
| 13 | 1 | -11 | 32 | - 37 |
| 13 | 1 | -10 | 18 | 19 |
| 13 | 1 | -8 | 52 | 61 |
| 13 | 1 | -7 | 42 | 41 |
| 13 | 1 | -6 | 28 | 24 |
| 13 | 1 | -5 | 27 | - 28 |
| 13 | 1 | -4 | 55 | - 57 |
| 13 | 1 | -3 | 56 | - 65 |
| 13 | 1 | -2 | 18 | - 30 |
| 13 | 2 | -9 | 54 | - 46 |
| 13 | 2 | -8 | 27 | 27 |
| 13 | 2 | -6 | 31 | 36 |

UNOBSERVED

| h | k | l | $F_m$ | $F_c$ |
|---|---|---|---|---|
| 0 | 0 | 20 | 6 | - 6 |
| 0 | 1 | 18 | 6 | - 0 |
| 0 | 3 | 22 | 3 | - 12 |
| 0 | 6 | 11 | 5 | 2 |
| 0 | 6 | 17 | 2 | - 1 |
| 0 | 7 | 3 | 5 | - 3 |
| 0 | 7 | 12 | 4 | - 0 |
| 0 | 8 | 1 | 4 | - 3 |
| 0 | 8 | 5 | 4 | 6 |
| 1 | 0 | 10 | 6 | - 17 |
| 1 | 0 | 14 | 8 | 19 |
| 1 | 1 | -23 | 4 | - 9 |
| 1 | 1 | -21 | 5 | - 11 |
| 1 | 1 | -17 | 6 | 7 |
| 1 | 1 | -15 | 6 | - 0 |
| 1 | 1 | 19 | 6 | - 2 |
| 1 | 2 | -21 | 6 | - 14 |
| 1 | 2 | -20 | 7 | 20 |
| 1 | 2 | -17 | 8 | - 20 |
| 1 | 2 | -12 | 7 | 0 |
| 1 | 2 | 18 | 7 | 19 |
| 1 | 2 | 20 | 6 | 0 |
| 1 | 3 | -20 | 6 | 8 |
| 1 | 3 | -18 | 7 | 5 |
| 1 | 3 | -17 | 8 | - 13 |
| 1 | 3 | -12 | 7 | - 7 |
| 1 | 3 | 14 | 8 | - 1 |
| 1 | 3 | 18 | 7 | - 3 |
| 1 | 3 | 19 | 6 | 0 |
| 1 | 3 | 20 | 5 | 4 |
| 1 | 3 | 21 | 4 | - 7 |
| 1 | 4 | -16 | 17 | 33 |
| 1 | 4 | 4 | 10 | 18 |
| 1 | 4 | 8 | 14 | - 11 |
| 2 | 0 | -20 | 8 | 13 |
| 2 | 0 | -16 | 8 | 12 |
| 2 | 0 | 16 | 8 | 11 |
| 2 | 1 | -21 | 5 | - 1 |
| 2 | 1 | -19 | 6 | 6 |

*Table 5. Continued.*

| h | k | l | $F_o$ | $F_c$ |
|---|---|---|---|---|
| 2 | 1 | 11 | 6 | - 7 |
| 2 | 2 | -21 | 9 | 11 |
| 2 | 2 | -20 | 7 | - 1 |
| 2 | 2 | -18 | 8 | - 9 |
| 2 | 2 | -17 | 8 | 19 |
| 2 | 2 | 14 | 8 | 29 |
| 2 | 2 | 16 | 8 | 1 |
| 2 | 2 | 20 | 5 | 2 |
| 2 | 2 | 21 | 4 | 11 |
| 2 | 3 | -16 | 8 | - 9 |
| 2 | 3 | 12 | 8 | 16 |
| 2 | 3 | 14 | 8 | 11 |
| 2 | 3 | 15 | 8 | 5 |
| 2 | 3 | 17 | 7 | 2 |
| 2 | 4 | -17 | 16 | 5 |
| 2 | 4 | -16 | 17 | 11 |
| 2 | 4 | -12 | 17 | - 7 |
| 2 | 4 | -8 | 14 | 11 |
| 2 | 4 | -6 | 12 | - 31 |
| 2 | 4 | -4 | 10 | 29 |
| 2 | 4 | 6 | 14 | - 27 |
| 2 | 4 | 10 | 17 | 12 |
| 2 | 4 | 11 | 17 | - 10 |
| 3 | 0 | -22 | 6 | - 2 |
| 3 | 0 | -20 | 8 | - 13 |
| 3 | 0 | 16 | 8 | 0 |
| 3 | 1 | -23 | 4 | 6 |
| 3 | 1 | -22 | 5 | - 5 |
| 3 | 1 | -17 | 6 | - 5 |
| 3 | 1 | 14 | 6 | 1 |
| 3 | 1 | 15 | 6 | - 4 |
| 3 | 2 | -21 | 6 | - 9 |
| 3 | 2 | 18 | 6 | 20 |
| 3 | 2 | 20 | 4 | 5 |
| 3 | 3 | -20 | 7 | 10 |
| 3 | 3 | -17 | 8 | 9 |
| 3 | 3 | 18 | 6 | - 7 |
| 3 | 4 | -17 | 16 | 18 |
| 3 | 4 | -16 | 17 | 18 |
| 3 | 4 | -9 | 15 | - 16 |
| 3 | 4 | -5 | 12 | - 24 |
| 3 | 4 | -4 | 11 | - 2 |
| 3 | 4 | -3 | 11 | - 1 |
| 4 | 0 | -22 | 6 | 4 |
| 4 | 0 | -20 | 8 | 1 |
| 4 | 0 | 18 | 6 | - 6 |
| 4 | 1 | -23 | 4 | 2 |
| 4 | 1 | -14 | 6 | 0 |
| 4 | 1 | -5 | 4 | 6 |
| 4 | 1 | 8 | 6 | 7 |
| 4 | 2 | -21 | 6 | - 1 |
| 4 | 2 | -14 | 8 | - 9 |
| 4 | 2 | -9 | 6 | - 8 |
| 4 | 2 | -8 | 6 | 8 |
| 4 | 2 | 14 | 8 | 7 |
| 4 | 2 | 16 | 7 | 9 |
| 4 | 2 | 18 | 5 | - 5 |
| 4 | 2 | 19 | 4 | - 15 |
| 4 | 3 | -12 | 7 | - 6 |
| 4 | 3 | -6 | 6 | 12 |
| 4 | 3 | 8 | 7 | - 20 |
| 4 | 3 | 11 | 8 | 11 |
| 4 | 3 | 12 | 8 | 18 |
| 4 | 4 | -17 | 16 | - 5 |
| 4 | 4 | -16 | 17 | 11 |
| 4 | 4 | -13 | 17 | 12 |
| 4 | 4 | -12 | 17 | 38 |
| 4 | 4 | -11 | 17 | 15 |
| 4 | 4 | -10 | 16 | 17 |
| 4 | 4 | -7 | 14 | - 23 |
| 4 | 4 | -6 | 16 | 9 |
| 4 | 4 | 11 | 17 | - 16 |
| 5 | 0 | 2 | 6 | 8 |
| 5 | 0 | 16 | 7 | - 8 |
| 5 | 1 | -17 | 6 | - 1 |
| 5 | 2 | -21 | 6 | 22 |
| 5 | 2 | -20 | 7 | 6 |
| 5 | 2 | -19 | 7 | - 7 |
| 5 | 2 | -11 | 7 | 2 |
| 5 | 2 | -8 | 6 | - 12 |
| 5 | 2 | 16 | 6 | 12 |
| 5 | 2 | 17 | 5 | 2 |
| 5 | 2 | 18 | 4 | - 23 |
| 5 | 3 | -22 | 5 | 9 |
| 5 | 3 | -10 | 7 | - 11 |
| 5 | 3 | 6 | 7 | - 7 |
| 5 | 3 | 13 | 7 | 3 |
| 5 | 3 | 16 | 5 | 11 |
| 5 | 4 | -17 | 16 | - 11 |
| 5 | 4 | -12 | 17 | 17 |
| 5 | 4 | -9 | 16 | 12 |
| 5 | 4 | -5 | 15 | - 28 |
| 5 | 4 | -1 | 15 | 0 |
| 5 | 4 | 8 | 17 | 24 |
| 5 | 4 | 13 | 15 | - 20 |
| 6 | 0 | -22 | 6 | - 16 |
| 6 | 0 | -18 | 8 | - 10 |
| 6 | 0 | 16 | 6 | 3 |
| 6 | 1 | 14 | 5 | - 3 |
| 6 | 2 | -21 | 6 | - 8 |
| 6 | 2 | -20 | 7 | 11 |
| 6 | 2 | -18 | 7 | - 6 |
| 6 | 2 | -14 | 8 | 12 |
| 6 | 2 | -12 | 8 | 9 |
| 6 | 2 | -11 | 7 | 3 |
| 6 | 2 | 12 | 7 | 35 |
| 6 | 2 | 16 | 5 | - 31 |
| 6 | 3 | -22 | 4 | 12 |
| 6 | 3 | 4 | 8 | 31 |
| 6 | 3 | 15 | 5 | 1 |
| 6 | 4 | -17 | 15 | - 11 |
| 6 | 4 | -16 | 16 | 18 |
| 6 | 4 | -12 | 17 | 16 |
| 6 | 4 | -11 | 17 | - 12 |
| 6 | 4 | 8 | 17 | 14 |
| 6 | 4 | 10 | 16 | - 4 |
| 6 | 4 | 11 | 15 | - 36 |
| 7 | 0 | -16 | 8 | - 6 |
| 7 | 0 | 4 | 8 | 14 |
| 7 | 0 | 16 | 4 | 11 |
| 7 | 1 | -3 | 6 | 21 |
| 7 | 2 | -21 | 5 | 8 |
| 7 | 2 | -17 | 8 | - 12 |
| 7 | 2 | -10 | 8 | 15 |
| 7 | 2 | -8 | 7 | 7 |
| 7 | 2 | -4 | 7 | - 2 |
| 7 | 2 | 0 | 7 | 9 |
| 7 | 2 | 13 | 6 | - 27 |
| 7 | 2 | 15 | 4 | 9 |
| 7 | 3 | -22 | 3 | 4 |
| 7 | 3 | -21 | 5 | 9 |
| 7 | 3 | -20 | 6 | - 5 |
| 7 | 3 | -19 | 6 | 14 |
| 7 | 3 | -10 | 8 | - 25 |
| 7 | 3 | -9 | 8 | 10 |
| 7 | 3 | 7 | 8 | 8 |
| 7 | 3 | 8 | 6 | - 16 |
| 7 | 3 | 12 | 7 | 16 |
| 7 | 3 | 13 | 6 | - 4 |
| 7 | 3 | 14 | 6 | - 23 |
| 7 | 4 | -13 | 17 | - 11 |
| 7 | 4 | -7 | 17 | 28 |
| 7 | 4 | -3 | 17 | - 1 |
| 7 | 4 | 6 | 17 | - 6 |
| 8 | 0 | -22 | 5 | - 3 |
| 8 | 0 | -18 | 7 | - 12 |
| 8 | 0 | 6 | 8 | 9 |
| 8 | 0 | 8 | 8 | - 2 |
| 8 | 0 | 10 | 7 | 3 |
| 8 | 1 | -21 | 4 | 11 |
| 8 | 1 | -20 | 5 | 8 |
| 8 | 1 | -9 | 6 | 1 |
| 8 | 1 | -7 | 6 | 2 |
| 8 | 1 | 5 | 6 | - 2 |
| 8 | 1 | 12 | 5 | 2 |
| 8 | 1 | 14 | 3 | 6 |
| 8 | 2 | -21 | 5 | - 12 |
| 8 | 2 | -19 | 6 | 7 |
| 8 | 2 | -11 | 8 | - 8 |
| 8 | 2 | 6 | 8 | - 5 |
| 8 | 3 | -21 | 4 | 9 |
| 8 | 3 | -14 | 8 | 1 |
| 8 | 3 | 4 | 8 | 15 |
| 8 | 3 | 12 | 4 | 13 |
| 8 | 4 | -15 | 15 | 7 |
| 8 | 4 | -13 | 16 | 9 |
| 8 | 4 | -11 | 17 | 10 |
| 8 | 4 | -10 | 17 | 20 |
| 8 | 4 | -9 | 17 | - 34 |
| 8 | 4 | -6 | 17 | - 34 |
| 9 | 0 | 8 | 7 | 0 |
| 9 | 1 | -19 | 5 | 9 |
| 9 | 1 | 11 | 4 | 3 |
| 9 | 1 | 12 | 3 | - 1 |
| 9 | 2 | -18 | 6 | - 11 |
| 9 | 2 | -3 | 8 | 1 |
| 9 | 2 | 1 | 8 | 4 |
| 9 | 2 | 5 | 7 | 16 |
| 9 | 2 | 8 | 6 | 14 |
| 9 | 2 | 10 | 5 | 4 |
| 9 | 2 | 11 | 4 | - 20 |
| 9 | 3 | -20 | 4 | 3 |
| 9 | 3 | -19 | 5 | 14 |
| 9 | 3 | -16 | 6 | 3 |
| 9 | 3 | -14 | 7 | 2 |
| 9 | 3 | -6 | 8 | - 7 |
| 9 | 3 | 2 | 8 | - 9 |
| 9 | 3 | 6 | 7 | 23 |
| 9 | 4 | -13 | 15 | - 1 |
| 9 | 4 | -12 | 15 | - 20 |
| 9 | 4 | -9 | 17 | - 27 |
| 9 | 4 | -7 | 17 | 40 |
| 9 | 4 | -6 | 17 | 1 |
| 9 | 4 | 3 | 15 | - 25 |
| 10 | 0 | -20 | 4 | 5 |
| 10 | 0 | -8 | 8 | 16 |
| 10 | 0 | -6 | 8 | - 3 |
| 10 | 0 | 8 | 6 | 4 |
| 10 | 0 | 10 | 4 | - 11 |
| 10 | 1 | -15 | 6 | - 9 |
| 10 | 1 | -4 | 6 | - 9 |
| 10 | 1 | -2 | 6 | - 21 |
| 10 | 1 | -1 | 6 | 2 |
| 10 | 1 | 0 | 6 | 0 |
| 10 | 1 | 3 | 6 | - 8 |
| 10 | 1 | 4 | 5 | - 4 |
| 10 | 1 | 9 | 3 | - 3 |
| 10 | 2 | -20 | 3 | - 11 |
| 10 | 2 | -19 | 4 | - 3 |
| 10 | 2 | -17 | 6 | 7 |
| 10 | 2 | -15 | 6 | - 2 |
| 10 | 2 | -5 | 8 | - 11 |
| 10 | 2 | 5 | 6 | 8 |
| 10 | 2 | 8 | 5 | - 8 |
| 10 | 2 | 9 | 4 | 9 |
| 10 | 3 | -19 | 3 | - 13 |
| 10 | 3 | -18 | 4 | 1 |
| 10 | 3 | -17 | 5 | 5 |
| 10 | 3 | -16 | 6 | 7 |
| 10 | 3 | -15 | 6 | 4 |
| 10 | 3 | -7 | 7 | - 14 |
| 10 | 3 | -2 | 7 | 8 |
| 10 | 3 | 1 | 7 | - 3 |
| 10 | 3 | 6 | 5 | - 8 |
| 10 | 3 | 7 | 4 | 23 |
| 10 | 4 | -6 | 15 | - 9 |
| 11 | 0 | -12 | 7 | 3 |
| 11 | 0 | 0 | 7 | - 2 |
| 11 | 0 | 2 | 7 | - 13 |
| 11 | 1 | -12 | 5 | - 0 |
| 11 | 1 | -11 | 6 | - 5 |
| 11 | 1 | -9 | 6 | 9 |
| 11 | 1 | -6 | 6 | 10 |
| 11 | 1 | -1 | 6 | 15 |
| 11 | 1 | 4 | 4 | 0 |
| 11 | 2 | -18 | 3 | 6 |
| 11 | 2 | -17 | 4 | - 0 |
| 11 | 2 | -15 | 5 | 3 |
| 11 | 2 | -14 | 6 | 35 |
| 11 | 2 | -12 | 6 | 12 |
| 11 | 2 | -10 | 7 | - 11 |
| 11 | 2 | -8 | 7 | - 2 |
| 11 | 2 | -6 | 7 | - 10 |
| 11 | 2 | -3 | 7 | - 0 |
| 11 | 2 | 2 | 6 | 9 |
| 11 | 2 | 4 | 5 | - 6 |
| 11 | 2 | 5 | 4 | - 16 |
| 11 | 2 | 6 | 4 | 1 |
| 11 | 3 | -17 | 2 | - 19 |
| 11 | 3 | -14 | 5 | - 13 |
| 11 | 3 | -12 | 6 | 6 |
| 11 | 3 | -6 | 7 | 7 |
| 12 | 1 | -16 | 3 | - 5 |
| 12 | 1 | -3 | 5 | - 9 |
| 12 | 1 | -2 | 5 | 6 |
| 12 | 1 | -1 | 4 | 4 |
| 12 | 1 | 3 | 3 | - 9 |
| 12 | 2 | -13 | 5 | 3 |
| 12 | 2 | -12 | 5 | - 0 |
| 12 | 2 | -5 | 6 | 11 |
| 12 | 2 | 0 | 5 | - 2 |
| 12 | 3 | -14 | 1 | 10 |
| 12 | 3 | -13 | 3 | 19 |
| 12 | 3 | -8 | 5 | 5 |
| 12 | 3 | -4 | 5 | 2 |
| 12 | 3 | 0 | 3 | - 2 |
| 13 | 0 | -6 | 5 | 5 |
| 13 | 0 | -4 | 4 | - 2 |
| 13 | 1 | -9 | 3 | - 0 |
| 13 | 2 | -7 | 3 | 16 |

*Table 6.* The principal axes of the thermal vibration ellipsoids given by the components of a unit vector in fractional coordinates $e_x$, $e_y$, $e_z$; the corresponding r.m.s. amplitudes, and the $B$-values.

| Atom | $e_x$ | $e_y$ | $e_z$ | $(\bar{u}^2)^{\frac{1}{2}}$(Å) | $B$(Å$^2$) |
|---|---|---|---|---|---|
| $O_1$ | .005 | .045 | −.049 | .283 | 6.31 |
| | .048 | −.088 | .005 | .232 | 4.26 |
| | .063 | .104 | .025 | .205 | 3.32 |
| $O_2$ | .043 | .023 | .054 | .240 | 4.53 |
| | .010 | −.142 | .008 | .221 | 3.85 |
| | .090 | .006 | −.008 | .207 | 3.38 |
| $O_3$ | .029 | .070 | .048 | .256 | 5.16 |
| | .016 | −.125 | .027 | .210 | 3.49 |
| | −.095 | .000 | .002 | .178 | 2.49 |

*Table 6. Continued.*

| | | | | | |
|---|---|---|---|---|---|
| | .017 | −.035 | .053 | .252 | 5.02 |
| $O_4$ | .027 | .136 | .015 | .207 | 3.37 |
| | .095 | −.032 | .004 | .178 | 2.51 |
| | .013 | .060 | −.045 | .226 | 4.04 |
| $O_5$ | .020 | .126 | .026 | .221 | 3.84 |
| | .098 | −.033 | .018 | .196 | 3.04 |
| | .037 | .112 | .032 | .298 | 6.99 |
| $O_6$ | .080 | −.078 | .027 | .219 | 3.79 |
| | .048 | .044 | −.035 | .206 | 3.36 |
| | .044 | .073 | .046 | .234 | 4.28 |
| $C_1$ | .035 | .094 | −.029 | .219 | 3.77 |
| | .083 | −.079 | .008 | .183 | 2.64 |
| | .053 | .059 | .050 | .294 | 6.84 |
| $C_2$ | .011 | .126 | −.023 | .218 | 3.77 |
| | .093 | −.037 | .002 | .183 | 2.65 |
| | .027 | .065 | .049 | .292 | 6.74 |
| $C_3$ | .003 | .126 | −.025 | .243 | 4.65 |
| | .097 | −.022 | .004 | .189 | 2.82 |
| | 0.46 | .080 | .044 | .274 | 5.92 |
| $C_4$ | .031 | .090 | −.032 | .256 | 5.19 |
| | .083 | −.078 | .008 | .192 | 2.90 |
| | .027 | .015 | .055 | .288 | 6.54 |
| $C_5$ | .075 | .087 | −.002 | .241 | 4.57 |
| | .061 | −.113 | .006 | .194 | 2.98 |
| | .034 | −.025 | .054 | .267 | 5.63 |
| $C_6$ | .082 | .077 | .003 | .209 | 3.45 |
| | −.046 | .119 | .009 | .191 | 2.88 |
| | .002 | −.028 | .052 | .236 | 4.41 |
| $C_7$ | .035 | .132 | .015 | .198 | 3.10 |
| | .094 | −.049 | .011 | .178 | 2.51 |
| | .013 | −.047 | .051 | .264 | 5.49 |
| $C_8$ | .003 | .135 | .018 | .225 | 4.01 |
| | .100 | .002 | .010 | .180 | 2.57 |
| | .020 | .094 | .041 | .287 | 6.52 |
| $C_9$ | .001 | −.106 | .035 | .254 | 5.11 |
| | .098 | −.018 | .008 | .186 | 2.73 |
| | .035 | .084 | .044 | .290 | 6.66 |
| $C_{10}$ | .028 | .098 | −.031 | .250 | 4.94 |
| | .090 | −.063 | .011 | .177 | 2.47 |
| | .017 | −.008 | .054 | .261 | 5.37 |
| $C_{11}$ | .057 | .118 | .007 | .235 | 4.35 |
| | .081 | −.081 | .005 | .191 | 2.88 |
| | .020 | .007 | .055 | .245 | 4.73 |
| $C_{12}$ | .007 | .143 | −.002 | .208 | 3.43 |
| | .098 | −.012 | .006 | .193 | 2.95 |

*Table 7.* Results of the rigid-body analysis.

a) In the orthogonal system, $J_1\ J_2\ J_3$, defined by $J_1||a$, $J_2||b$, $J_3||c^*$. (E.s.d. of components of **L** are given in parentheses in units of last place shown).

$$\mathbf{L} = \begin{Bmatrix} 163\ (16) & -95\ (11) & -44\ (7) \\ & 101\ (9) & 43\ (7) \\ & & 62\ (5) \end{Bmatrix} \times 10^{-1}(^\circ)^2$$

| | r.m.s. amplitude | Direction cosines ($\times 10^3$) | | |
|---|---|---|---|---|
| | | $J_1$ | $J_2$ | $J_3$ |
| **L** | 5.0° | 761 | −572 | 306 |
| | 2.2° | 520 | 257 | −814 |
| | 1.6° | 387 | 779 | 494 |
| **T** [a] | 0.23 Å | −069 | −038 | 997 |
| | 0.20 » | 199 | −980 | −023 |
| | 0.18 » | 978 | 197 | 075 |

b) In the orthogonal system, $L_1$, $L_2$, $L_3$, defined by the principal axes of the libration tensor **L**.

Displacement of libration axes from intersecting (Å)

| | |
|---|---|
| Parallel to $L_1$ | −0.19 |
| » » $L_2$ | −0.67 |
| » » $L_3$ | 0.11 |

Effective screw translations (Å)

| | |
|---|---|
| Parallel to $L_1$ | 0.004 |
| » » $L_2$ | −0.014 |
| » » $L_3$ | 0.008 |

$\left(\overline{\Delta U_{ij}^2}\right)^{\frac{1}{2}} = 0.0035$ Å$^2$

[a] **T** is the *reduced* translation tensor.

*Table 8.* Corrections in fractional atomic coordinates due to libration compared with estimated standard deviations in coordinates. ($\sigma$'s and $\Delta$'s are multiplied by $10^5$).

| Atom | $\Delta x$ | $\sigma(x)$ | $\Delta y$ | $\sigma(y)$ | $\Delta z$ | $\sigma(z)$ |
|---|---|---|---|---|---|---|
| $O_1$ | −58 | 28 | − 83 | 53 | −41 | 17 |
| $O_2$ | −25 | 26 | − 3 | 47 | −26 | 15 |
| $O_3$ | −15 | 23 | − 16 | 47 | 22 | 15 |
| $O_4$ | 25 | 22 | 40 | 46 | 21 | 14 |
| $O_5$ | 6 | 23 | − 31 | 45 | −28 | 13 |
| $O_6$ | 29 | 27 | 29 | 53 | −44 | 16 |
| $C_1$ | −22 | 34 | 8 | 69 | 9 | 20 |
| $C_2$ | −62 | 38 | − 43 | 82 | 16 | 28 |
| $C_3$ | −72 | 37 | − 21 | 85 | 6 | 27 |
| $C_4$ | −40 | 42 | 61 | 86 | 21 | 27 |
| $C_5$ | − 2 | 44 | 111 | 87 | 11 | 29 |
| $C_6$ | 10 | 39 | 91 | 74 | 20 | 25 |
| $C_7$ | 25 | 31 | 0 | 67 | 5 | 20 |
| $C_8$ | 68 | 33 | 60 | 78 | 10 | 24 |
| $C_9$ | 72 | 38 | 24 | 86 | − 3 | 27 |
| $C_{10}$ | 49 | 38 | − 40 | 86 | 12 | 26 |
| $C_{11}$ | 5 | 37 | −101 | 81 | 5 | 25 |
| $C_{12}$ | 0 | 35 | − 68 | 71 | 17 | 22 |

is reasonably isotropic, while libration is more anisotropic, with the primary motion corresponding to an r.m.s. amplitude of 5.0°. The r.m.s. discrepancy between observed and calculated $U_{ij}$ serves as a measure of the applicability of the analysis and thus of the rigidity of the molecule. The value of Table 7, 0.0035 Å$^2$, supports the assumption of regarding the molecule as an oscillating rigid body, and the fractional coordinates were accordingly corrected for librational effects.[12] Table 8 shows that all corrections are less than three times the corresponding standard deviations of the coordinates.

## DISCUSSION

Interatomic distances and angles (corrected for librational effects) may be found in Figs. 1, 2, and 3. The standard deviations, given in parentheses (in units of last place shown), have been calculated from the correlation matrix corresponding to the last full-matrix least squares refinement cycle without taking into account the e.s.d.'s of the cell parameters. The largest correction

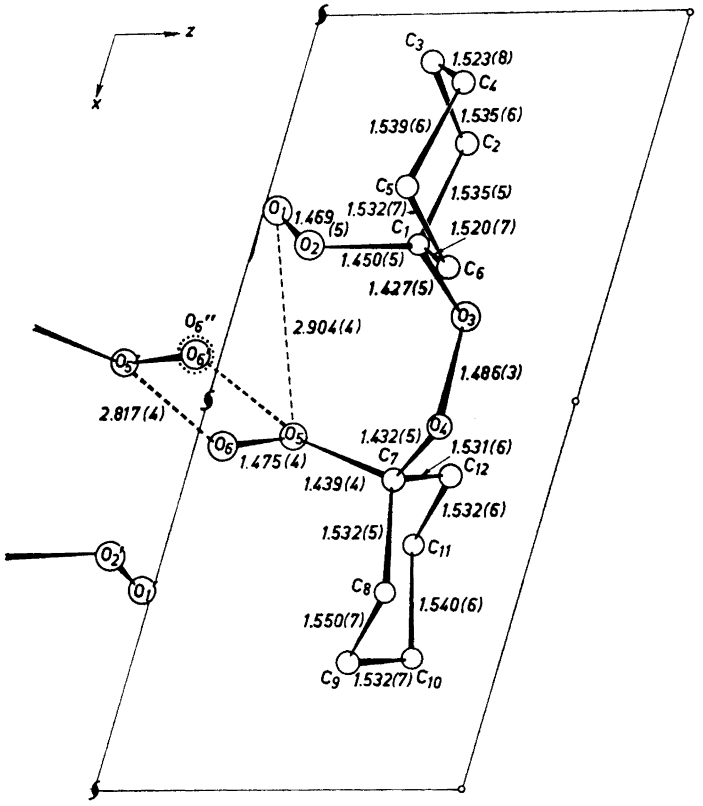



*Fig. 1.* Schematical drawing of the molecule showing interatomic distances.

for libration in distances and angles are $1.6 \times \sigma_d$ and $0.6 \times \sigma_a$, where $\sigma_d$ and $\sigma_a$ are the corresponding standard deviations. The C—H distances arrived at range from 0.91 Å to 1.14 Å with estimated standard deviations of about 0.06 Å.

From Fig. 1 it may be seen that the three O—O bond distances as well as the four C—O bond lengths, respectively, are equal within probable limits of error. The corresponding mean values, $1.47_7$ Å and $1.43_7$ Å, agree closely with earlier findings.[13–17] The C—C bond lengths are also normal, with mean value $1.53_3$ Å.

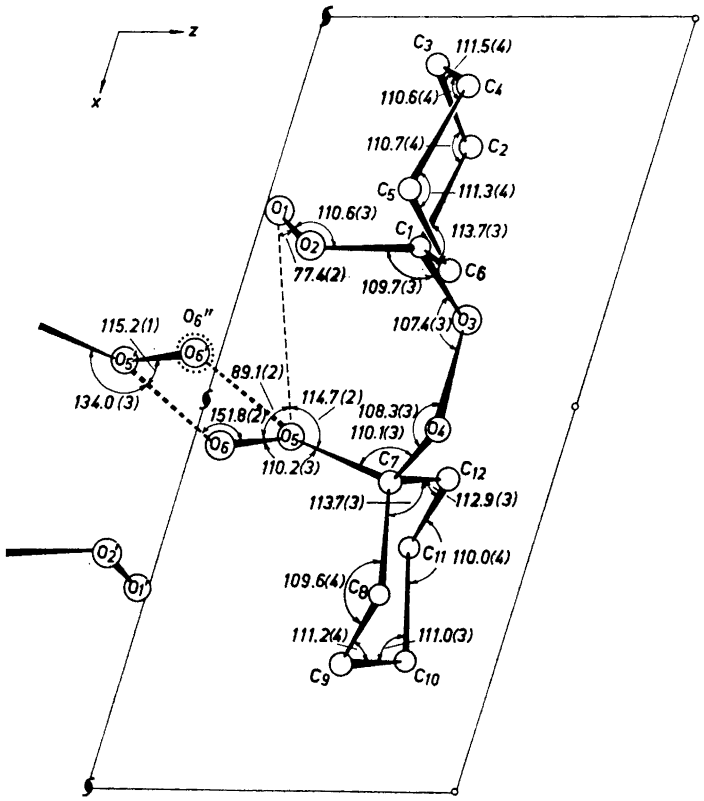



*Fig. 2.* Schematical drawing of the molecule showing bond angles.

The angles (Fig. 2) $C_1—O_2—O_1$ (110.6°) and $C_7—O_5—O_6$ (110.2°) are equal and significantly larger than $C_1—O_3—O_4$ (107.4°) and $C_7—O_4—O_3$ (108.3°). The larger C—O—O angles correspond to the values obtained for dibenzoyl peroxide [4] (109° and 111°), while the smaller agree with those found in trimeric and dimeric peroxides.[13–17]

The arrangements around the carbon atoms $C_1$ and $C_7$ are asymmetric as shown in Fig. 3 (a) and (b). The angles $C_2—C_1—O_3$ (103.6°), $C_6—C_1—O_2$

(104.0°), $C_8-C_7-O_4$ (103.2°), and $C_{12}-C_7-O_5$ (104.3°) are considerably smaller, (about 9° in average), than $C_2-C_1-O_2$ (111.8°), $C_7-C_1-O_3$ (114.2°), $C_8-C_7-O_5$ (112.9°), and $C_{12}-C_7-O_4$ (112.9°). The kind of asymmetry resembles what was observed for trimeric acetone peroxide,[17] and the distortions may roughly be described as "rotations" (*ca.* 6°) about axes through $C_1$

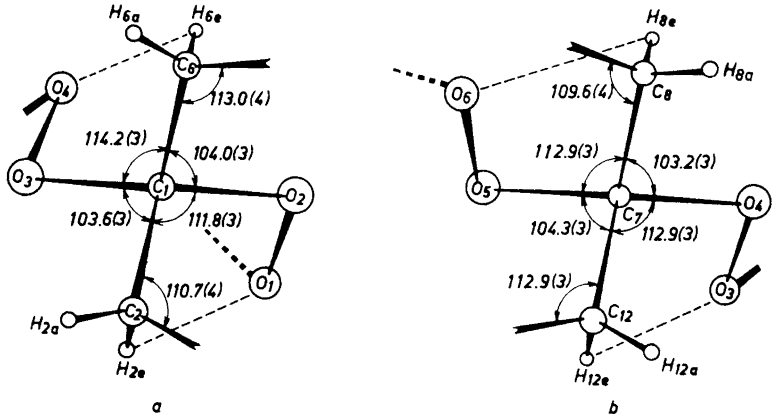



*Fig. 3.* Schematical drawings showing bond angles and the asymmetric environments of the carbon atoms $C_1$ and $C_7$.

and $C_7$ normal to the paper plane (Fig. 3). In dimeric peroxides the corresponding axes of "rotation" are normal to the C—C—C planes.

The cyclohexane rings are also slightly distorted; the angles $C_1-C_2-C_3$ (110.7°) and $C_7-C_8-C_9$ (109.6°) being *possibly significantly* smaller than $C_1-C_6-C_5$ (113.0°) and $C_7-C_{12}-C_{11}$ (112.9°). As pointed out elsewhere,[13,17] it seems reasonable to relate the effects to *intra*-molecular oxygen-hydrogen repulsions (see Fig. 3). The angles $C_2-C_1-C_6$ and $C_8-C_7-C_{12}$ are both equal to 113.7° while the rest of the C—C—C angles have normal cyclohexane values (110.8° in average with standard deviation 0.3°).

The conformation of the molecule with respect to the hydroperoxy groups is *cis*, and the dihedral angle $C_1-O_3-O_4-C_7$ is found to be 126.3° (3), which is 35° larger than the dibenzoyl peroxide value.[4]

As mentioned above, the hydroperoxy hydrogen atoms could not be localized in the difference Fourier map. The solid state infrared spectrum (nujol) recorded in the region 3200 $cm^{-1}$ to 3600 $cm^{-1}$, containing two bands, at 3385 $cm^{-1}$ and 3420 $cm^{-1}$, predicts two different kinds of hydrogen bonds, since $\nu_{OH}$ for hydroperoxides should be in the region 3530 $cm^{-1}$ to 3560 $cm^{-1}$.[18] In Fig. 1 the dotted lines from $O_6$ to $O_5'$, and from $O_5$ to $O_6''$ in a neighbouring cell, indicate *inter*-molecular hydrogen bonds of length $2.81_7$ Å, forming helical chains in direction of the *b*-axis. Since the shortest *inter*-molecular $O_1-O$ distance, $O_1-O_6''$, is about 3.42 Å, the hydrogen bond associated with the $O_2O_1H$-group has to be *intra*-molecular. The distance $O_1-O_5$ and $O_1-O_6$ of lengths $2.90_4$ Å and $3.23_8$ Å, respectively, together with the corre-

sponding angles, $O_2—O_1—O_5$ (77.4°) and $O_2—O_1—O_6$ (62.1°), point out $O_1—O_5$ as a weak *intra*-molecular hydrogen bond. The extreme values of the O—O—O angles, (77.4° and 151.8°), show that the hydrogen bonds in this compound are far from linear. The angles of bond direction at the oxygen atom $O_5$, which are accepting *both* the hydrogens, are closer to normal values: $O_1—O_5—O_6$ (89.1°), $O_1—O_5—C_7$ (114.7°), $O_6''—O_5—O_6$ (115.2°), and $O_6''—O_5—C_7$ (134.0°).

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