## 1276. *The Crystal Structure of Trimethyl-(8-quinolinolato)-platinum*(IV)

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A three-dimensional *X*-ray crystal structure analysis has been carried out on the complex, $Me_3(C_9H_6NO)Pt$. All measurements were made at 120 ± 5°K. In an orthorhombic unit cell, $a = 15{\cdot}23$, $b = 16{\cdot}09$, $c = 9{\cdot}48$ Å all ±0·02 Å, space group $P2_12_12_1$, there are eight formula units, now shown to be four dimeric molecules. The platinum atoms were located from Patterson projections, and the other atoms, excluding hydrogen, by Fourier difference syntheses. After refinement by least-squares, allowing for anisotropic vibration of the platinum atoms and individual isotropic vibration parameters for the other atoms, $R$ is 0·10.

The dimer is formed by a symmetrical pair of oxygen bridges between the Pt atoms, with Pt–O = 2·24 ± 0·03 Å and a separation of 3·384 ± 0·003 Å between the platinum atoms. Each platinum atom is six-co-ordinated, by the two oxygen atoms, one nitrogen (Pt–N = 2·13 ± 0·05 Å), and three methyl groups in the usual *cis* configuration (Pt–C = 2·06 ± 0·05 Å). The halves of the molecule are related (within experimental error) by a non-crystallographic two-fold axis.

Structural studies [1-3] on complexes of trimethylplatinum(IV) have, so far, all shown that the platinum atom is six-co-ordinated with the methyl groups in the *cis* configuration. Trimethyl-(8-quinolinolato)platinium(IV) has been prepared [4] and shown to have a molecular weight which varies with solvent and temperature. An *X*-ray crystal structure analysis was undertaken to establish its stereochemistry. As reported briefly,[5] it is dimeric in the solid state, maintaining six-co-ordination round the platinum atoms.

### Methods and Results

Our preliminary findings were that the space group was non-centrosymmetric with two platinum atoms in the asymmetric unit. Approximate calculations by Cruickshank's [6] method

[1] A. G. Swallow and M. R. Truter; A. C. Hazell and M. R. Truter, *Proc. Roy. Soc.*, 1960, *A*, **254**, 205, 218.
[2] A. G. Swallow and M. R. Truter, *Proc. Roy. Soc.*, 1962, *A*, **266**, 527.
[3] A. Robson and M. R. Truter, *J.*, 1965, 630.
[4] K. Kite and M. R. Truter, *J.*, 1966, to be published.
[5] J. E. Lydon, M. R. Truter, and R. C. Watling, *Proc. Chem. Soc.*, 1964, 193.
[6] D. W. J. Cruickshank, *Acta Cryst.*, 1960, **13**, 774.

indicated that, even with measurements made at 120°K, we could not hope for a precision greater than about ±0·05 Å in the positions of the carbon atoms; clearly, to ensure unequivocal location of the light atoms (other than hydrogen) a low-temperature technique was required.

*Crystal Data.*—$C_{12}H_{15}NOPt$, $M = 384{\cdot}4$. Orthorhombic, $a = 15{\cdot}23$, $b = 16{\cdot}09$, $c = 9{\cdot}48$ Å all ±0·02 Å at 120 ± 5°K, $U = 2323$ Å$^3$, $D_c = 2{\cdot}20$, $D_m = 2{\cdot}17$ (by flotation), $Z = 8$, $F(000) = 1440$. Space group $P2_12_12_1$ ($D_2^4$, No. 19) uniquely determined. Cu $K_\alpha$ radiation, single-crystal oscillation and Weissenberg photographs; absorption coefficient $\mu = 226$ cm.$^{-1}$; absorption corrections applied. No molecular symmetry required; two formula units, shown by structure analysis to be one dimeric molecule, in the asymmetric unit.

*Structure Determination.*—As there are two formula units in the asymmetric unit, it was necessary to locate two platinum atoms, designated Pt(1) and Pt(2) (Figure 1), and associated with each platinum atom three methyl groups, one oxygen atom, one nitrogen atom, and the nine carbon atoms of the 8-quinolinolato-ligand.

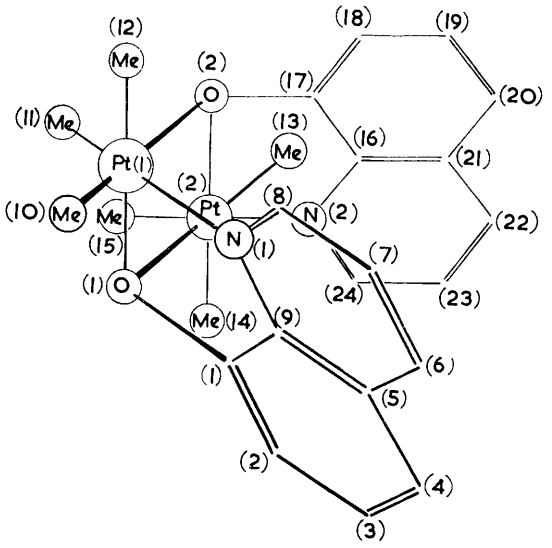



FIGURE 1. One dimeric molecule, showing the numbering of the atoms

The platinum atoms were located from Patterson projections down the three principal axes. For three-dimensional work the co-ordinates were chosen to correspond to the origin in " International Tables." [7] Structure factors were calculated and gave an $R$ value of 0·16, showing that the platinum atoms were correctly located. The shortest Pt–Pt distance was 3·4 Å, indicating that the asymmetric unit consisted of a dimeric molecule probably with two bridges between the Pt atoms. A three-dimensional Fourier difference synthesis was calculated. In the resulting electron-density map, 12 peaks were readily assigned to one complete 8-quinolinolato-ligand [O(1), N(1), and C(1)—C(9) inclusive] and to O(2), with O(1) and O(2) occupying the bridging positions. Addition of these twelve atoms reduced $R$ to 0·148. Although no more atoms were clearly shown in the electron-density map, the positions of another seven could be deduced on the assumption that the arrangement about each platinum atom was octahedral. Addition of these seven atoms, all treated as carbon atoms, reduced $R$ to 0·119; a further difference synthesis revealed the remaining nine carbon atoms, C(16)—C(24), and indicated which of the seven was N(2). Both 8-hydroxyquinoline molecules are on the same side of the bridges joining the Pt atoms. One molecule is shown in Figure 1 and the structure as a whole in projection in Figure 2.

Refinement was carried out allowing for anisotropic thermal vibration of the platinum atoms and individual isotropic thermal parameters of the other atoms. (No attempt was made to locate hydrogen atoms.) After four cycles of refinement, $R$ fell to 0·10, and the most significant shift, 0·06 Å, in $x$ for C(14), was 0·8 of the corresponding standard deviation. Each cycle

[7] " International Tables for X-ray Crystallography, vol. I," Kynoch Press, Birmingham, 1952.

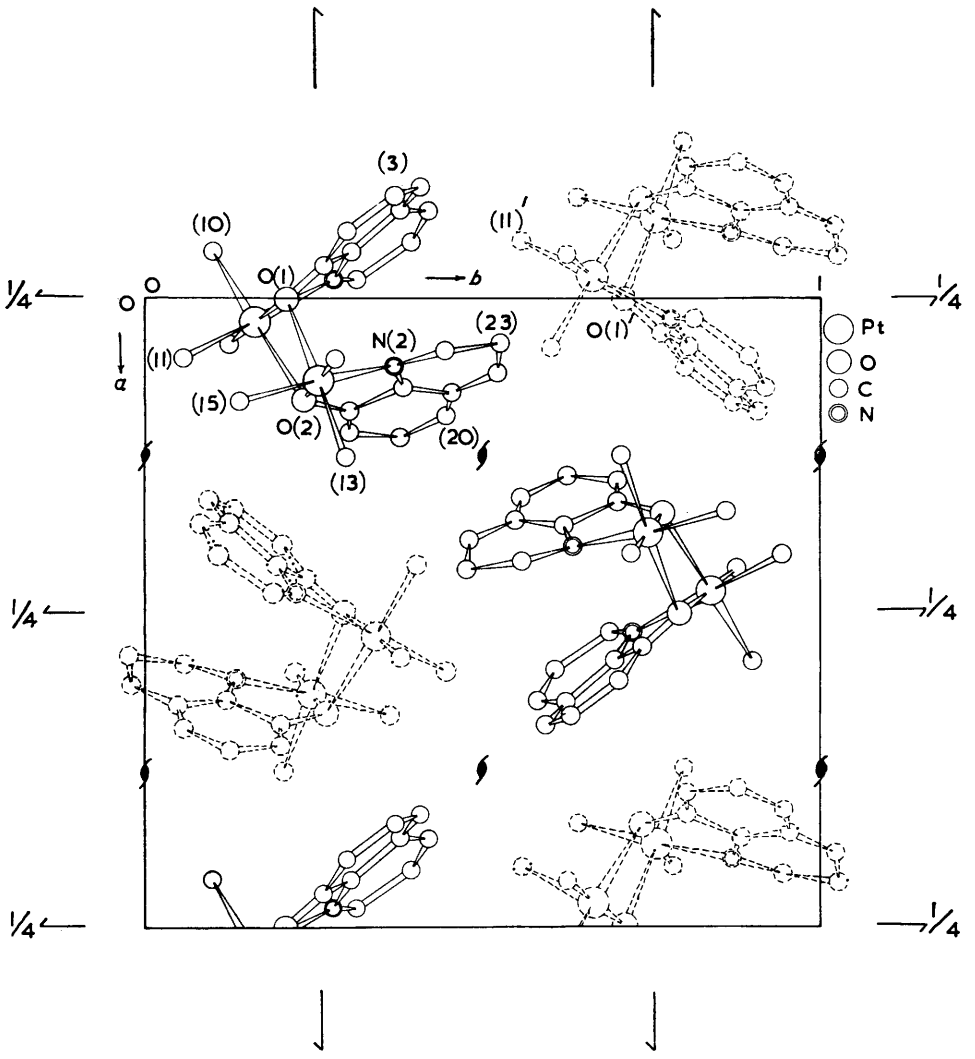



FIGURE 2. The structure projected down [001]

took 13 hours on the computer, and, as further refinement was unlikely to lead to chemically significant improvements in the accuracy of the bond lengths, it was left at this stage.

*Results.*—Table 1 shows the final atomic co-ordinates with their standard deviations, $\sigma$, and the isotropic vibration parameters, $\bar{U}$, with their standard deviations. For the platinum atoms an average value, $\bar{U} = [(U_{11}^2 + U_{22}^2 + U_{33}^2)/3]^{\frac{1}{2}}$ is shown for comparison with those of the light atoms. The values of the anisotropic vibration parameters in $Å^2 \times 10^4$ are:

| | $U_{11}$ | $\sigma$ | $U_{22}$ | $\sigma$ | $U_{33}$ | $\sigma$ | $U_{12}$ | $\sigma$ | $U_{23}$ | $\sigma$ | $U_{13}$ | $\sigma$ |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| Pt(1) | 240 | 6 | 149 | 6 | 191 | 7 | −20 | 6 | 19 | 8 | −1 | 8 |
| Pt(2) | 261 | 7 | 150 | 6 | 199 | 7 | −21 | 7 | 34 | 8 | −34 | 8 |

In Table 2 the observed and calculated structure amplitudes are shown, and also the real and imaginary parts of the calculated structure factors.

Table 3 gives a list of the bond lengths and their standard deviations, and Table 4 lists the bond angles and their standard deviations. The molecule found has a two-fold axis of symmetry along the line through the mid-point between the platinum atoms (1·274, 3·377, 1·279) with

TABLE 1

Atomic co-ordinates and their standard deviations, in Å, and isotropic vibration parameters, $U_{iso}$, and their standard deviation, in Å$^2$

| | $x$ | $\sigma(x)$ | $y$ | $\sigma(y)$ | $z$ | $\sigma(z)$ | $U_{iso}$ | $\sigma(U)$ |
|---|---|---|---|---|---|---|---|---|
| Pt(1) | 0·564 | 0·002 | 2·616 | 0·002 | −0·058 | 0·002 | 0·020 | — |
| Pt(2) | 1·984 | 0·002 | 4·139 | 0·002 | 2·616 | 0·002 | 0·020 | — |
| O(1) | 0·00 | 0·03 | 3·38 | 0·03 | 1·95 | 0·03 | 0·020 | 0·006 |
| O(2) | 2·46 | 0·04 | 3·79 | 0·04 | 0·47 | 0·04 | 0·050 | 0·010 |
| N(1) | −0·47 | 0·03 | 4·50 | 0·03 | −0·48 | 0·03 | 0·016 | 0·006 |
| N(2) | 1·62 | 0·03 | 5·95 | 0·04 | 1·67 | 0·04 | 0·026 | 0·008 |
| C(1) | −0·83 | 0·05 | 4·27 | 0·05 | 1·90 | 0·05 | 0·039 | 0·011 |
| C(2) | −1·64 | 0·05 | 4·83 | 0·05 | 3·04 | 0·06 | 0·041 | 0·012 |
| C(3) | −2·51 | 0·05 | 5·98 | 0·05 | 2·85 | 0·05 | 0·043 | 0·012 |
| C(4) | −2·72 | 0·05 | 6·58 | 0·05 | 1·64 | 0·05 | 0·035 | 0·011 |
| C(5) | −1·97 | 0·06 | 6·09 | 0·06 | 0·46 | 0·06 | 0·048 | 0·012 |
| C(6) | −2·13 | 0·05 | 6·77 | 0·05 | −0·79 | 0·05 | 0·033 | 0·010 |
| C(7) | −1·38 | 0·05 | 6·36 | 0·05 | −1·70 | 0·05 | 0·043 | 0·011 |
| C(8) | −0·48 | 0·05 | 5·06 | 0·05 | −1·60 | 0·05 | 0·044 | 0·011 |
| C(9) | −1·14 | 0·03 | 4·93 | 0·04 | 0·59 | 0·04 | 0·014 | 0·007 |
| C(10) | −1·17 | 0·03 | 1·63 | 0·04 | −0·42 | 0·04 | 0·017 | 0·007 |
| C(11) | 1·42 | 0·04 | 0·91 | 0·04 | 0·53 | 0·04 | 0·023 | 0·008 |
| C(12) | 1·11 | 0·05 | 2·00 | 0·05 | −1·96 | 0·06 | 0·045 | 0·012 |
| C(13) | 3·85 | 0·06 | 4·79 | 0·06 | 3·02 | 0·06 | 0·050 | 0·014 |
| C(14) | 1·25 | 0·09 | 4·54 | 0·09 | 4·61 | 0·09 | 0·102 | 0·025 |
| C(15) | 2·48 | 0·04 | 2·25 | 0·04 | 3·44 | 0·05 | 0·022 | 0·008 |
| C(16) | 2·13 | 0·04 | 6·17 | 0·04 | 0·37 | 0·04 | 0·019 | 0·007 |
| C(17) | 2·72 | 0·04 | 4·86 | 0·04 | −0·15 | 0·04 | 0·025 | 0·008 |
| C(18) | 3·22 | 0·03 | 4·86 | 0·04 | −1·41 | 0·04 | 0·014 | 0·007 |
| C(19) | 3·34 | 0·04 | 6·08 | 0·04 | −2·14 | 0·05 | 0·029 | 0·009 |
| C(20) | 2·82 | 0·05 | 7·19 | 0·05 | −1·70 | 0·05 | 0·033 | 0·010 |
| C(21) | 2·25 | 0·04 | 7·33 | 0·04 | −0·39 | 0·04 | 0·023 | 0·008 |
| C(22) | 1·78 | 0·06 | 8·42 | 0·06 | 0·22 | 0·07 | 0·060 | 0·015 |
| C(23) | 1·07 | 0·04 | 8·49 | 0·04 | 1·44 | 0·04 | 0·020 | 0·008 |
| C(24) | 1·27 | 0·05 | 7·16 | 0·05 | 2·21 | 0·05 | 0·036 | 0·010 |

direction cosines −0·3, 0·9, −0·3. Tables 3 and 4 are arranged to display the agreement between the corresponding dimensions in the halves of the molecule. The platinum–platinum distance in the dimer is 3·389 ± 0·003 Å.

Planes were calculated through the atoms of the 8-quinolinolato-ligands, with the results shown in Table 5. The platinum–oxygen bridge system is non-planar; the angle between the normals to the two planes III and IV in Table 5 is 12·6°.

All the intermolecular distances of less than 3·5 Å were calculated; those found were 3·45 Å between C(3) and the methyl group C(11)′, and 3·40 Å between C(23) and O(1)′ (see Figure 2).

## DISCUSSION

The structure analysis has solved the stereochemical problem. In the solid at 120°K, and probably also at room temperature, the complex is dimeric. The structure as found satisfies the criteria for correctness [1] in that co-ordinates obtained by a mathematical process lead to reasonable bond lengths and no improbably short van der Waals separations. The methyl carbon atom, C(14), is the least satisfactorily located both in its distance from the platinum atom and in its large temperature factor, and this is reflected in the large standard deviations.

The platinum atom displays its usual six-co-ordination, achieved here by three methyl groups in the *cis* configuration, one nitrogen atom, and two oxygen atoms in a double bridge. Some caution is required in the discussion of the bond lengths because the structure, having heavy atoms in a non-centrosymmetrical space group, is one in which parameter interaction is likely to be of importance. Our method of refinement (block diagonal) does not allow for the effect of changes in the parameters of one atom on those of the other atoms, so that the standard deviations quoted so far are minimum values. Some assessment of the probable error can be made by comparing the lengths of the chemically

TABLE 2

Observed and calculated structure amplitudes

| h | k | l | $F_o$ | $F_c$ | h | k | l | $F_o$ | $F_c$ | h | k | l | $F_o$ | $F_c$ | h | k | l | $F_o$ | $F_c$ | h | k | l | $F_o$ | $F_c$ |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 0 | 0 | 6 | 139 | 133 | 0 | 13 | 1 | 58 | 64 | | | 11 | 48 | 41 | | | 2 | 95 | 95 | | | 12 | 47 | 38 |
| | | 8 | 119 | 112 | | | 3 | 141 | 139 | | | 12 | 77 | 78 | | | 3 | 114 | 114 | 2 | 4 | 0 | 105 | 102 |
| | | 10 | 96 | 85 | | | 6 | 50 | 40 | 1 | 5 | 0 | 66 | 71 | | | 4 | 50 | 40 | | | 1 | 57 | 58 |
| | | 12 | 50 | 29 | | | 7 | 163 | 154 | | | 1 | 173 | 187 | | | 5 | 121 | 141 | | | 2 | 136 | 134 |
| 0 | 1 | 1 | 255 | 363 | 0 | 14 | 0 | 137 | 134 | | | 2 | 75 | 65 | | | 6 | 79 | 88 | | | 3 | 90 | 78 |
| | | 3 | 251 | 322 | | | 1 | 75 | 82 | | | 3 | 151 | 139 | | | 7 | 55 | 53 | | | 4 | 118 | 113 |
| | | 4 | 46 | 31 | | | 2 | 59 | 75 | | | 4 | 88 | 85 | 1 | 14 | 1 | 108 | 90 | | | 5 | 195 | 204 |
| | | 5 | 76 | 63 | | | 3 | 71 | 56 | | | 5 | 178 | 170 | | | 2 | 175 | 188 | | | 6 | 83 | 84 |
| | | 7 | 227 | 239 | | | 4 | 95 | 106 | | | 6 | 61 | 50 | | | 3 | 63 | 55 | | | 7 | 108 | 113 |
| | | 9 | 51 | 46 | | | 5 | 61 | 54 | | | 7 | 64 | 56 | | | 4 | 102 | 92 | | | 8 | 89 | 92 |
| | | 11 | 140 | 151 | 0 | 15 | 1 | 61 | 42 | | | 8 | 100 | 104 | | | 5 | 78 | 96 | | | 9 | 142 | 162 |
| 0 | 2 | 1 | 48 | 42 | | | 4 | 43 | 47 | | | 9 | 73 | 71 | | | 6 | 132 | 140 | | | 10 | 52 | 49 |
| | | 2 | 140 | 133 | | | 5 | 74 | 89 | | | 10 | 24 | 27 | | | 8 | 93 | 96 | | | 11 | 72 | 61 |
| | | 3 | 15 | 15 | | | 6 | 35 | 31 | | | 11 | 36 | 37 | | | 9 | 66 | 52 | | | 12 | 58 | 48 |
| | | 4 | 270 | 288 | | | 8 | 66 | 78 | 1 | 6 | 0 | 98 | 93 | 1 | 15 | 1 | 149 | 145 | 2 | 5 | 0 | 137 | 146 |
| | | 5 | 79 | 66 | 0 | 16 | 1 | 77 | 82 | | | 1 | 160 | 160 | | | 2 | 70 | 71 | | | 1 | 190 | 212 |
| | | 7 | 53 | 54 | | | 2 | 151 | 186 | | | 2 | 44 | 32 | | | 3 | 115 | 113 | | | 2 | 261 | 276 |
| | | 8 | 82 | 83 | | | 3 | 64 | 56 | | | 3 | 143 | 125 | | | 4 | 74 | 70 | | | 3 | 171 | 172 |
| | | 9 | 43 | 28 | | | 5 | 52 | 49 | | | 4 | 147 | 140 | | | 5 | 108 | 131 | | | 4 | 103 | 102 |
| | | 10 | 57 | 61 | | | 6 | 107 | 121 | | | 5 | 119 | 114 | | | 6 | 54 | 59 | | | 5 | 149 | 143 |
| | | 11 | 48 | 42 | 0 | 17 | 1 | 141 | 128 | | | 6 | 96 | 79 | | | 7 | 50 | 51 | | | 6 | 164 | 172 |
| 0 | 3 | 1 | 121 | 114 | | | 2 | 41 | 28 | | | 7 | 45 | 44 | | | 8 | 61 | 64 | | | 7 | 132 | 142 |
| | | 2 | 23 | 17 | | | 3 | 74 | 72 | | | 8 | 99 | 101 | 1 | 16 | 1 | 78 | 69 | | | 8 | 38 | 40 |
| | | 3 | 122 | 106 | | | 4 | 36 | 39 | | | 9 | 62 | 47 | | | 2 | 128 | 129 | | | 9 | 76 | 77 |
| | | 4 | 113 | 111 | | | 5 | 125 | 145 | | | 10 | 59 | 59 | | | 3 | 42 | 32 | | | 10 | 52 | 41 |
| | | 5 | 189 | 178 | | | 6 | 36 | 48 | | | 11 | 57 | 56 | | | 4 | 45 | 41 | | | 11 | 76 | 80 |
| | | 6 | 22 | 14 | 0 | 18 | 1 | 88 | 78 | 1 | 7 | 0 | 90 | 88 | | | 5 | 68 | 91 | 2 | 6 | 0 | 182 | 211 |
| | | 7 | 154 | 142 | | | 2 | 146 | 160 | | | 1 | 186 | 199 | | | 6 | 75 | 78 | | | 1 | 139 | 156 |
| | | 8 | 72 | 61 | | | 3 | 57 | 71 | | | 2 | 39 | 29 | 1 | 17 | 0 | 49 | 53 | | | 2 | 187 | 195 |
| | | 9 | 99 | 115 | | | 4 | 52 | 45 | | | 3 | 181 | 172 | | | 1 | 71 | 60 | | | 3 | 37 | 20 |
| | | 11 | 86 | 78 | 0 | 19 | 1 | 77 | 57 | | | 4 | 112 | 99 | | | 2 | 60 | 60 | | | 4 | 190 | 172 |
| | | 12 | 48 | 43 | 0 | 20 | 0 | 77 | 62 | | | 5 | 118 | 115 | | | 3 | 47 | 48 | | | 5 | 204 | 212 |
| 0 | 4 | 0 | 79 | 79 | | | 1 | 64 | 68 | | | 6 | 75 | 68 | | | 4 | 63 | 68 | | | 6 | 147 | 147 |
| | | 1 | 64 | 55 | | | 2 | 45 | 49 | | | 7 | 112 | 107 | | | 5 | 47 | 48 | | | 7 | 64 | 59 |
| | | 2 | 270 | 319 | 1 | 0 | 1 | 223 | 261 | | | 8 | 129 | 128 | | | 6 | 36 | 26 | | | 8 | 91 | 110 |
| | | 4 | 68 | 59 | | | 2 | 96 | 82 | | | 9 | 60 | 50 | 1 | 18 | 0 | 124 | 104 | | | 9 | 144 | 155 |
| | | 5 | 74 | 52 | | | 3 | 175 | 189 | | | 10 | 43 | 43 | | | 1 | 59 | 57 | | | 10 | 98 | 86 |
| | | 6 | 191 | 194 | | | 4 | 122 | 132 | | | 11 | 71 | 67 | | | 3 | 37 | 39 | | | 11 | 61 | 38 |
| | | 7 | 49 | 53 | | | 5 | 78 | 62 | 1 | 8 | 0 | 252 | 282 | | | 4 | 80 | 80 | 2 | 7 | 0 | 112 | 123 |
| | | 8 | 29 | 36 | | | 6 | 114 | 105 | | | 1 | 134 | 139 | | | 5 | 42 | 46 | | | 1 | 138 | 145 |
| | | 10 | 60 | 52 | | | 7 | 80 | 76 | | | 2 | 147 | 160 | 1 | 19 | 0 | 69 | 61 | | | 2 | 229 | 256 |
| | | 11 | 47 | 29 | | | 8 | 89 | 86 | | | 3 | 118 | 120 | | | 1 | 107 | 91 | | | 3 | 162 | 160 |
| | | 12 | 68 | 69 | | | 10 | 104 | 96 | | | 4 | 205 | 196 | | | 3 | 95 | 102 | | | 4 | 75 | 73 |
| 0 | 5 | 1 | 193 | 228 | | | 12 | 48 | 50 | | | 5 | 77 | 63 | | | 4 | 53 | 57 | | | 5 | 115 | 104 |
| | | 2 | 100 | 81 | 1 | 1 | 1 | 165 | 192 | | | 6 | 161 | 147 | 1 | 20 | 0 | 114 | 139 | | | 6 | 142 | 136 |
| | | 3 | 110 | 105 | | | 2 | 101 | 99 | | | 7 | 84 | 72 | | | 1 | 39 | 37 | | | 7 | 125 | 105 |
| | | 4 | 69 | 59 | | | 3 | 190 | 196 | | | 8 | 139 | 150 | | | 2 | 43 | 43 | | | 9 | 73 | 69 |
| | | 5 | 282 | 305 | | | 4 | 76 | 69 | | | 10 | 107 | 104 | 2 | 0 | 1 | 113 | 121 | | | 11 | 67 | 60 |
| | | 6 | 69 | 54 | | | 5 | 142 | 143 | | | 11 | 43 | 38 | | | 2 | 217 | 247 | 2 | 8 | 0 | 91 | 76 |
| | | 9 | 194 | 221 | | | 6 | 132 | 121 | 1 | 9 | 0 | 92 | 90 | | | 3 | 185 | 209 | | | 1 | 78 | 66 |
| | | 10 | 24 | 15 | | | 7 | 89 | 82 | | | 1 | 204 | 221 | | | 4 | 196 | 203 | | | 2 | 67 | 49 |
| 0 | 6 | 0 | 57 | 53 | | | 8 | 57 | 42 | | | 2 | 53 | 40 | | | 6 | 153 | 155 | | | 3 | 59 | 54 |
| | | 3 | 118 | 105 | | | 9 | 78 | 74 | | | 3 | 210 | 226 | | | 7 | 204 | 213 | | | 4 | 88 | 74 |
| | | 6 | 264 | 261 | | | 10 | 108 | 109 | | | 4 | 102 | 95 | | | 8 | 107 | 96 | | | 5 | 138 | 134 |
| | | 10 | 81 | 90 | | | 11 | 44 | 41 | | | 5 | 128 | 115 | | | 9 | 81 | 70 | | | 6 | 79 | 61 |
| 0 | 7 | 1 | 168 | 165 | 1 | 2 | 0 | 110 | 122 | | | 6 | 85 | 83 | | | 10 | 91 | 91 | | | 7 | 79 | 92 |
| | | 2 | 126 | 120 | | | 1 | 186 | 210 | | | 7 | 154 | 159 | | | 11 | 122 | 124 | | | 8 | 54 | 45 |
| | | 3 | 77 | 74 | | | 2 | 248 | 259 | | | 8 | 67 | 73 | | | 12 | 64 | 58 | | | 9 | 96 | 115 |
| | | 4 | 37 | 14 | | | 3 | 184 | 182 | | | 9 | 72 | 56 | 2 | 1 | 1 | 199 | 236 | | | 10 | 60 | 56 |
| | | 5 | 254 | 229 | | | 4 | 205 | 203 | | | 10 | 80 | 77 | | | 2 | 112 | 116 | | | 11 | 82 | 77 |
| | | 6 | 109 | 93 | | | 5 | 101 | 90 | | | 11 | 96 | 88 | | | 3 | 122 | 131 | 2 | 9 | 0 | 204 | 238 |
| | | 9 | 179 | 193 | | | 6 | 160 | 176 | 1 | 10 | 0 | 172 | 177 | | | 4 | 245 | 277 | | | 1 | 84 | 76 |
| 0 | 8 | 0 | 147 | 134 | | | 7 | 66 | 57 | | | 1 | 111 | 116 | | | 5 | 169 | 185 | | | 2 | 144 | 145 |
| | | 1 | 87 | 71 | | | 8 | 156 | 161 | | | 2 | 104 | 94 | | | 6 | 49 | 39 | | | 3 | 66 | 63 |
| | | 2 | 255 | 247 | | | 9 | 43 | 39 | | | 3 | 110 | 108 | | | 7 | 91 | 78 | | | 4 | 136 | 131 |
| | | 3 | 67 | 67 | | | 10 | 124 | 124 | | | 4 | 166 | 165 | | | 8 | 104 | 110 | | | 5 | 56 | 40 |
| | | 4 | 99 | 90 | | | 12 | 82 | 79 | | | 5 | 52 | 45 | | | 9 | 87 | 90 | | | 6 | 74 | 71 |
| | | 6 | 144 | 126 | 1 | 3 | 0 | 68 | 68 | | | 6 | 110 | 105 | | | 10 | 49 | 48 | | | 9 | 39 | 35 |
| 0 | 9 | 2 | 41 | 32 | | | 2 | 83 | 81 | | | 7 | 82 | 76 | | | 11 | 66 | 60 | 2 | 10 | 0 | 100 | 93 |
| | | 3 | 125 | 129 | | | 3 | 264 | 266 | | | 8 | 103 | 94 | 2 | 2 | 0 | 106 | 126 | | | 1 | 70 | 59 |
| | | 5 | 73 | 60 | | | 4 | 87 | 74 | | | 10 | 94 | 88 | | | 1 | 43 | 33 | | | 2 | 116 | 117 |
| | | 6 | 98 | 77 | | | 5 | 247 | 249 | 1 | 11 | 0 | 81 | 73 | | | 2 | 126 | 108 | | | 3 | 138 | 129 |
| | | 10 | 79 | 72 | | | 6 | 101 | 93 | | | 1 | 133 | 126 | | | 3 | 154 | 147 | | | 4 | 100 | 89 |
| 0 | 10 | 0 | 249 | 258 | | | 7 | 139 | 135 | | | 2 | 64 | 65 | | | 4 | 107 | 97 | | | 5 | 58 | 50 |
| | | 1 | 82 | 76 | | | 8 | 87 | 85 | | | 3 | 107 | 109 | | | 5 | 130 | 125 | | | 6 | 102 | 107 |
| | | 3 | 87 | 79 | | | 9 | 133 | 140 | | | 4 | 69 | 54 | | | 6 | 76 | 74 | | | 7 | 109 | 119 |
| | | 4 | 238 | 226 | | | 10 | 71 | 68 | | | 5 | 72 | 65 | | | 7 | 166 | 178 | | | 8 | 78 | 84 |
| 0 | 11 | 1 | 135 | 128 | | | 11 | 82 | 79 | | | 6 | 87 | 89 | | | 8 | 48 | 34 | | | 9 | 77 | 77 |
| | | 2 | 46 | 26 | | | 12 | 58 | 59 | | | 7 | 84 | 79 | | | 9 | 99 | 103 | | | 10 | 80 | 70 |
| | | 3 | 228 | 213 | 1 | 4 | 0 | 109 | 127 | | | 8 | 46 | 40 | | | 10 | 55 | 51 | 2 | 11 | 0 | 226 | 245 |
| | | 5 | 64 | 37 | | | 1 | 188 | 217 | | | 10 | 83 | 80 | | | 11 | 109 | 121 | | | 1 | 164 | 161 |
| | | 6 | 80 | 83 | | | 2 | 180 | 170 | 1 | 12 | 1 | 81 | 74 | | | 12 | 40 | 37 | | | 2 | 63 | 62 |
| | | 7 | 236 | 208 | | | 3 | 166 | 149 | | | 2 | 95 | 102 | 2 | 3 | 2 | 189 | 185 | | | 3 | 157 | 155 |
| 0 | 12 | 0 | 209 | 213 | | | 4 | 195 | 187 | | | 3 | 99 | 92 | | | 3 | 70 | 63 | | | 4 | 161 | 170 |
| | | 1 | 93 | 87 | | | 5 | 139 | 132 | | | 4 | 65 | 58 | | | 4 | 172 | 159 | | | 5 | 122 | 122 |
| | | 2 | 58 | 34 | | | 6 | 169 | 164 | | | 5 | 53 | 56 | | | 5 | 52 | 33 | | | 7 | 87 | 109 |
| | | 3 | 100 | 91 | | | 7 | 28 | 19 | | | 6 | 80 | 85 | | | 6 | 121 | 102 | | | 8 | 62 | 61 |
| | | 4 | 208 | 215 | | | 8 | 131 | 146 | | | 7 | 64 | 68 | | | 7 | 46 | 39 | | | 9 | 79 | 86 |
| | | 6 | 51 | 36 | | | 9 | 41 | 42 | | | 8 | 57 | 57 | | | 8 | 59 | 49 | 2 | 12 | 0 | 130 | 122 |
| | | 8 | 100 | 131 | | | 10 | 100 | 109 | 1 | 13 | 1 | 162 | 161 | | | 10 | 46 | 38 | | | 1 | 44 | 26 |

TABLE 2 (*Continued*)

| h | k | l | $F_o$ | $F_c$ | h | k | l | $F_o$ | $F_c$ | h | k | l | $F_o$ | $F_c$ | h | k | l | $F_o$ | $F_c$ | h | k | l | $F_o$ | $F_c$ |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | 2 | 142 | 139 | | | 6 | 172 | 163 | 3 | 12 | 0 | 73 | 74 | | | 2 | 59 | 39 | | | 6 | 66 | 71 |
| | | 3 | 135 | 140 | | | 7 | 150 | 145 | | | 1 | 122 | 121 | | | 3 | 136 | 120 | 4 | 16 | 1 | 111 | 99 |
| | | 4 | 128 | 122 | | | 8 | 124 | 121 | | | 2 | 63 | 56 | | | 4 | 47 | 43 | | | 3 | 88 | 86 |
| | | 5 | 64 | 47 | | | 9 | 94 | 86 | | | 3 | 82 | 87 | | | 5 | 151 | 140 | | | 4 | 109 | 115 |
| | | 6 | 119 | 123 | | | 10 | 106 | 99 | | | 4 | 85 | 87 | | | 6 | 46 | 26 | | | 5 | 55 | 69 |
| | | 8 | 103 | 106 | | | 11 | 72 | 69 | | | 5 | 90 | 95 | | | 7 | 156 | 158 | 4 | 17 | 0 | 119 | 95 |
| 2 | 13 | 0 | 109 | 122 | | | 12 | 73 | 70 | | | 6 | 76 | 71 | | | 9 | 104 | 98 | | | 1 | 61 | 52 |
| | | 1 | 115 | 112 | 3 | 4 | 0 | 143 | 144 | | | 9 | 66 | 54 | | | 10 | 44 | 37 | | | 2 | 61 | 76 |
| | | 2 | 75 | 70 | | | 1 | 181 | 188 | 3 | 13 | 1 | 99 | 83 | | | 11 | 92 | 96 | | | 3 | 88 | 93 |
| | | 3 | 103 | 98 | | | 2 | 124 | 110 | | | 2 | 109 | 126 | 4 | 4 | 0 | 214 | 250 | | | 4 | 93 | 93 |
| | | 4 | 134 | 126 | | | 3 | 200 | 195 | | | 3 | 115 | 112 | | | 1 | 130 | 158 | | | 6 | 63 | 77 |
| | | 5 | 106 | 95 | | | 4 | 198 | 193 | | | 4 | 51 | 46 | | | 2 | 133 | 110 | 4 | 18 | 0 | 157 | 122 |
| | | 6 | 50 | 40 | | | 5 | 164 | 150 | | | 6 | 81 | 81 | | | 3 | 119 | 112 | | | 1 | 99 | 96 |
| | | 7 | 66 | 63 | | | 6 | 139 | 126 | | | 7 | 106 | 104 | | | 4 | 234 | 237 | | | 3 | 83 | 93 |
| | | 8 | 66 | 55 | | | 7 | 110 | 101 | | | 8 | 80 | 82 | | | 5 | 81 | 73 | | | 4 | 86 | 96 |
| | | 9 | 55 | 53 | | | 8 | 134 | 138 | 3 | 14 | 0 | 97 | 129 | | | 6 | 60 | 48 | | | 5 | 56 | 68 |
| 2 | 14 | 2 | 57 | 38 | | | 9 | 81 | 73 | | | 1 | 121 | 125 | | | 7 | 85 | 81 | 4 | 19 | 0 | 62 | 58 |
| | | 3 | 65 | 64 | | | 10 | 98 | 87 | | | 2 | 51 | 44 | | | 8 | 98 | 102 | | | 2 | 37 | 36 |
| | | 4 | 80 | 79 | | | 11 | 21 | 23 | | | 3 | 96 | 89 | | | 9 | 28 | 42 | | | 3 | 54 | 57 |
| | | 5 | 65 | 68 | 3 | 5 | 0 | 76 | 56 | | | 4 | 117 | 119 | | | 10 | 40 | 49 | | | 4 | 61 | 60 |
| | | 6 | 60 | 53 | | | 1 | 139 | 141 | | | 5 | 124 | 124 | | | 11 | 50 | 53 | 4 | 20 | 0 | 51 | 53 |
| | | 7 | 74 | 84 | | | 2 | 120 | 110 | | | 6 | 78 | 65 | 4 | 5 | 0 | 186 | 222 | | | 1 | 53 | 61 |
| | | 8 | 64 | 65 | | | 3 | 130 | 125 | | | 8 | 89 | 89 | | | 1 | 93 | 96 | 5 | 0 | 1 | 162 | 181 |
| 2 | 15 | 0 | 101 | 101 | | | 4 | 88 | 77 | 3 | 15 | 1 | 110 | 98 | | | 2 | 136 | 126 | | | 2 | 44 | 41 |
| | | 1 | 105 | 97 | | | 5 | 134 | 131 | | | 2 | 104 | 109 | | | 3 | 219 | 211 | | | 3 | 72 | 74 |
| | | 2 | 94 | 111 | | | 6 | 148 | 150 | | | 3 | 116 | 128 | | | 4 | 165 | 161 | | | 4 | 119 | 114 |
| | | 3 | 73 | 70 | | | 7 | 86 | 75 | | | 4 | 52 | 47 | | | 5 | 55 | 45 | | | 5 | 97 | 93 |
| | | 4 | 67 | 62 | | | 8 | 70 | 64 | | | 5 | 63 | 52 | | | 6 | 120 | 122 | | | 6 | 72 | 54 |
| | | 5 | 52 | 55 | | | 9 | 32 | 43 | | | 6 | 87 | 94 | | | 7 | 166 | 194 | | | 8 | 118 | 110 |
| | | 6 | 55 | 68 | | | 10 | 100 | 98 | | | 7 | 102 | 100 | | | 8 | 74 | 81 | 5 | 1 | 0 | 101 | 104 |
| 2 | 16 | 0 | 96 | 105 | | | 11 | 50 | 52 | | | 8 | 56 | 57 | | | 9 | 63 | 56 | | | 1 | 186 | 201 |
| | | 1 | 70 | 46 | 3 | 6 | 1 | 152 | 151 | 3 | 16 | 0 | 94 | 104 | | | 10 | 68 | 78 | | | 2 | 134 | 132 |
| | | 2 | 80 | 85 | | | 2 | 86 | 88 | | | 1 | 88 | 82 | 4 | 6 | 2 | 64 | 58 | | | 3 | 132 | 134 |
| | | 4 | 94 | 97 | | | 3 | 144 | 140 | | | 3 | 72 | 69 | | | 3 | 196 | 179 | | | 4 | 128 | 160 |
| | | 5 | 59 | 77 | | | 4 | 126 | 118 | | | 4 | 83 | 91 | | | 4 | 243 | 242 | | | 5 | 129 | 137 |
| | | 6 | 74 | 83 | | | 5 | 92 | 79 | | | 5 | 67 | 82 | | | 5 | 134 | 125 | | | 6 | 104 | 107 |
| 2 | 17 | 0 | 49 | 30 | | | 6 | 60 | 47 | | | 6 | 40 | 30 | 4 | 7 | 0 | 125 | 130 | | | 7 | 58 | 49 |
| | | 1 | 131 | 127 | | | 7 | 77 | 68 | 3 | 17 | 0 | 48 | 38 | | | 1 | 81 | 94 | | | 8 | 110 | 113 |
| | | 2 | 117 | 127 | | | 8 | 128 | 97 | | | 1 | 67 | 48 | | | 2 | 137 | 109 | | | 9 | 49 | 49 |
| | | 3 | 116 | 119 | 3 | 7 | 0 | 96 | 85 | | | 2 | 56 | 56 | | | 3 | 163 | 159 | | | 10 | 72 | 64 |
| | | 5 | 62 | 87 | | | 1 | 168 | 192 | | | 3 | 56 | 57 | | | 4 | 156 | 145 | | | 11 | 42 | 46 |
| | | 6 | 61 | 70 | | | 2 | 45 | 52 | | | 6 | 48 | 56 | | | 6 | 74 | 56 | 5 | 2 | 0 | 105 | 92 |
| 2 | 18 | 0 | 105 | 96 | | | 3 | 126 | 118 | 3 | 18 | 1 | 74 | 58 | 4 | 8 | 1 | 80 | 92 | | | 1 | 223 | 252 |
| | | 1 | 72 | 53 | | | 4 | 153 | 151 | | | 2 | 57 | 82 | | | 2 | 138 | 134 | | | 2 | 60 | 61 |
| | | 2 | 80 | 80 | | | 5 | 140 | 130 | | | 3 | 77 | 80 | | | 3 | 78 | 71 | | | 3 | 169 | 174 |
| | | 4 | 78 | 88 | | | 6 | 98 | 92 | 3 | 19 | 0 | 87 | 97 | | | 4 | 171 | 152 | | | 4 | 123 | 115 |
| | | 5 | 45 | 68 | | | 7 | 49 | 37 | | | 1 | 80 | 79 | | | 5 | 85 | 68 | | | 5 | 168 | 170 |
| 2 | 19 | 0 | 62 | 36 | | | 8 | 107 | 112 | | | 3 | 39 | 42 | | | 6 | 50 | 39 | | | 6 | 92 | 90 |
| | | 1 | 82 | 85 | | | 9 | 77 | 72 | | | 4 | 62 | 70 | 4 | 9 | 0 | 36 | 19 | | | 7 | 127 | 130 |
| | | 2 | 69 | 76 | | | 10 | 105 | 99 | 3 | 20 | 0 | 44 | 20 | | | 1 | 71 | 49 | | | 8 | 113 | 127 |
| | | 3 | 62 | 70 | 3 | 8 | 0 | 86 | 73 | | | 1 | 50 | 59 | | | 2 | 69 | 59 | | | 9 | 73 | 74 |
| | | 4 | 36 | 30 | | | 1 | 187 | 205 | | | 2 | 75 | 106 | | | 3 | 54 | 40 | | | 10 | 75 | 79 |
| 3 | 0 | 1 | 196 | 222 | | | 2 | 201 | 211 | 4 | 0 | 0 | 196 | 228 | | | 4 | 80 | 74 | | | 11 | 67 | 71 |
| | | 2 | 55 | 45 | | | 3 | 165 | 160 | | | 1 | 117 | 120 | | | 6 | 51 | 39 | 5 | 3 | 0 | 214 | 224 |
| | | 3 | 99 | 94 | | | 4 | 138 | 125 | | | 2 | 238 | 277 | 4 | 10 | 0 | 106 | 106 | | | 1 | 195 | 197 |
| | | 4 | 28 | 26 | | | 5 | 123 | 112 | | | 3 | 117 | 121 | | | 1 | 156 | 155 | | | 2 | 203 | 184 |
| | | 5 | 155 | 141 | | | 6 | 131 | 130 | | | 4 | 58 | 55 | | | 2 | 191 | 221 | | | 3 | 185 | 176 |
| | | 6 | 100 | 99 | | | 7 | 129 | 118 | | | 5 | 143 | 134 | | | 3 | 116 | 104 | | | 4 | 215 | 209 |
| | | 8 | 83 | 86 | | | 8 | 100 | 104 | | | 6 | 169 | 187 | | | 4 | 52 | 46 | | | 5 | 130 | 121 |
| | | 9 | 48 | 53 | | | 10 | 77 | 69 | | | 7 | 123 | 115 | | | 6 | 112 | 117 | | | 6 | 170 | 162 |
| | | 10 | 94 | 99 | 3 | 9 | 0 | 142 | 151 | | | 8 | 48 | 55 | 4 | 11 | 0 | 160 | 138 | | | 7 | 83 | 60 |
| 3 | 1 | 0 | 96 | 94 | | | 1 | 177 | 182 | | | 9 | 133 | 116 | | | 1 | 127 | 108 | | | 8 | 126 | 139 |
| | | 1 | 227 | 250 | | | 2 | 115 | 109 | | | 10 | 74 | 64 | | | 2 | 153 | 154 | | | 10 | 110 | 104 |
| | | 2 | 95 | 94 | | | 3 | 163 | 151 | | | 11 | 71 | 60 | | | 3 | 52 | 39 | | | 11 | 52 | 45 |
| | | 3 | 149 | 157 | | | 4 | 160 | 153 | | | 12 | 72 | 72 | | | 4 | 119 | 103 | 5 | 4 | 0 | 154 | 139 |
| | | 4 | 178 | 186 | | | 5 | 147 | 150 | 4 | 1 | 0 | 44 | 37 | | | 5 | 134 | 153 | | | 1 | 217 | 236 |
| | | 5 | 110 | 111 | | | 6 | 109 | 96 | | | 1 | 165 | 179 | | | 6 | 116 | 116 | | | 2 | 78 | 74 |
| | | 6 | 96 | 92 | | | 7 | 76 | 68 | | | 2 | 167 | 159 | 4 | 12 | 0 | 57 | 36 | | | 3 | 188 | 182 |
| | | 7 | 91 | 87 | | | 8 | 102 | 109 | | | 3 | 46 | 39 | | | 1 | 156 | 145 | | | 4 | 126 | 111 |
| | | 8 | 139 | 150 | | | 9 | 91 | 96 | | | 4 | 113 | 122 | | | 2 | 180 | 214 | | | 5 | 140 | 126 |
| | | 9 | 50 | 35 | | | 10 | 78 | 77 | | | 5 | 209 | 247 | | | 3 | 121 | 132 | | | 6 | 144 | 138 |
| | | 10 | 90 | 75 | 3 | 10 | 0 | 59 | 33 | | | 6 | 113 | 120 | | | 4 | 47 | 27 | | | 7 | 131 | 114 |
| | | 11 | 45 | 35 | | | 1 | 148 | 143 | | | 7 | 76 | 65 | | | 5 | 105 | 110 | | | 8 | 81 | 80 |
| | | 12 | 109 | 81 | | | 2 | 170 | 175 | | | 8 | 93 | 89 | | | 6 | 124 | 132 | | | 9 | 52 | 62 |
| 3 | 2 | 1 | 244 | 276 | | | 3 | 136 | 132 | | | 9 | 183 | 187 | 4 | 13 | 0 | 57 | 47 | | | 10 | 102 | 106 |
| | | 2 | 153 | 152 | | | 4 | 88 | 68 | | | 10 | 98 | 86 | | | 1 | 80 | 77 | | | 11 | 68 | 74 |
| | | 3 | 180 | 159 | | | 5 | 87 | 89 | | | 11 | 54 | 48 | | | 2 | 109 | 99 | 5 | 5 | 0 | 151 | 149 |
| | | 4 | 180 | 189 | | | 6 | 111 | 118 | | | 12 | 85 | 56 | | | 3 | 47 | 35 | | | 1 | 141 | 155 |
| | | 5 | 174 | 175 | | | 7 | 88 | 90 | 4 | 2 | 0 | 93 | 91 | | | 4 | 53 | 54 | | | 2 | 93 | 86 |
| | | 6 | 162 | 167 | | | 8 | 69 | 64 | | | 1 | 79 | 70 | | | 5 | 95 | 115 | | | 3 | 161 | 166 |
| | | 7 | 77 | 73 | | | 10 | 71 | 75 | | | 2 | 271 | 273 | | | 6 | 88 | 98 | | | 4 | 112 | 115 |
| | | 8 | 105 | 105 | 3 | 11 | 0 | 83 | 81 | | | 3 | 93 | 80 | 4 | 14 | 0 | 127 | 104 | | | 5 | 71 | 56 |
| | | 9 | 81 | 78 | | | 1 | 106 | 104 | | | 4 | 114 | 103 | | | 1 | 50 | 52 | | | 6 | 91 | 88 |
| | | 10 | 114 | 108 | | | 2 | 47 | 37 | | | 5 | 75 | 70 | | | 2 | 89 | 105 | | | 7 | 86 | 84 |
| | | 11 | 47 | 44 | | | 3 | 88 | 82 | | | 6 | 145 | 145 | | | 3 | 65 | 67 | | | 8 | 60 | 61 |
| | | 12 | 51 | 61 | | | 4 | 86 | 78 | | | 7 | 49 | 40 | | | 4 | 57 | 80 | | | 10 | 64 | 76 |
| 3 | 3 | 0 | 210 | 246 | | | 5 | 71 | 71 | | | 8 | 36 | 31 | | | 6 | 63 | 63 | | | 11 | 37 | 24 |
| | | 1 | 197 | 211 | | | 6 | 52 | 42 | | | 9 | 74 | 67 | 4 | 15 | 0 | 78 | 59 | 5 | 6 | 1 | 75 | 92 |
| | | 2 | 151 | 149 | | | 7 | 56 | 51 | | | 10 | 39 | 29 | | | 1 | 64 | 34 | | | 2 | 99 | 91 |
| | | 3 | 227 | 201 | | | 8 | 97 | 89 | | | 11 | 37 | 31 | | | 2 | 51 | 49 | | | 3 | 121 | 110 |
| | | 4 | 192 | 176 | | | 9 | 65 | 53 | 4 | 3 | 0 | 114 | 106 | | | 3 | 88 | 78 | | | 4 | 85 | 69 |
| | | 5 | 163 | 148 | | | 10 | 37 | 32 | | | 1 | 115 | 101 | | | 4 | 80 | 65 | | | 5 | 81 | 71 |

TABLE 2 (*Continued*)

| h | k | l | $F_o$ | $F_c$ | h | k | l | $F_o$ | $F_c$ | h | k | l | $F_o$ | $F_c$ | h | k | l | $F_o$ | $F_c$ | h | k | l | $F_o$ | $F_c$ |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | 6 | 146 | 135 | | | 2 | 27 | 19 | | | 3 | 99 | 108 | | | 2 | 170 | 173 | | | 6 | 66 | 60 |
| 5 | 7 | 1 | 155 | 186 | | | 3 | 35 | 25 | | | 6 | 54 | 54 | | | 3 | 84 | 76 | | | 7 | 101 | 113 |
| | | 2 | 148 | 161 | | | 4 | 79 | 72 | 6 | 17 | 0 | 129 | 156 | | | 4 | 141 | 134 | | | 9 | 88 | 93 |
| | | 3 | 142 | 143 | | | 5 | 183 | 191 | | | 1 | 75 | 73 | | | 5 | 53 | 61 | | | 11 | 74 | 77 |
| | | 4 | 101 | 82 | | | 6 | 58 | 45 | | | 3 | 54 | 60 | | | 6 | 147 | 143 | 8 | 4 | 0 | 194 | 201 |
| | | 5 | 109 | 106 | | | 7 | 50 | 48 | | | 4 | 119 | 135 | 7 | 10 | 0 | 56 | 49 | | | 1 | 127 | 108 |
| | | 6 | 134 | 127 | | | 8 | 35 | 34 | 6 | 18 | 1 | 78 | 63 | | | 1 | 157 | 140 | | | 2 | 145 | 141 |
| 5 | 8 | 1 | 177 | 195 | | | 9 | 154 | 159 | | | 2 | 46 | 35 | | | 2 | 48 | 45 | | | 3 | 81 | 82 |
| | | 2 | 132 | 118 | | | 10 | 51 | 43 | | | 3 | 85 | 96 | | | 3 | 114 | 115 | | | 4 | 155 | 149 |
| | | 3 | 155 | 146 | | | 11 | 50 | 48 | | | 4 | 43 | 49 | | | 4 | 66 | 61 | | | 5 | 103 | 108 |
| | | 4 | 74 | 63 | 6 | 3 | 0 | 238 | 252 | 6 | 19 | 0 | 90 | 93 | | | 5 | 129 | 129 | | | 6 | 58 | 48 |
| | | 5 | 166 | 158 | | | 1 | 48 | 45 | | | 1 | 69 | 67 | 7 | 11 | 1 | 71 | 70 | | | 7 | 36 | 39 |
| | | 6 | 93 | 86 | | | 2 | 194 | 176 | 7 | 0 | 1 | 192 | 212 | | | 2 | 91 | 85 | | | 8 | 59 | 56 |
| 5 | 9 | 0 | 116 | 112 | | | 3 | 59 | 47 | | | 3 | 140 | 159 | | | 3 | 58 | 50 | | | 9 | 64 | 67 |
| | | 1 | 162 | 171 | | | 4 | 157 | 166 | | | 4 | 60 | 57 | | | 4 | 76 | 68 | | | 10 | 29 | 34 |
| | | 2 | 198 | 204 | | | 6 | 94 | 88 | | | 5 | 113 | 95 | | | 5 | 73 | 77 | 8 | 5 | 0 | 108 | 110 |
| | | 3 | 145 | 123 | | | 7 | 50 | 43 | | | 6 | 46 | 32 | | | 6 | 103 | 85 | | | 1 | 52 | 40 |
| | | 4 | 121 | 102 | | | 11 | 40 | 33 | | | 8 | 100 | 109 | 7 | 12 | 0 | 40 | 52 | | | 2 | 201 | 203 |
| | | 5 | 115 | 101 | 6 | 4 | 0 | 37 | 28 | 7 | 1 | 0 | 139 | 136 | | | 1 | 113 | 84 | | | 3 | 115 | 122 |
| | | 6 | 153 | 145 | | | 1 | 125 | 116 | | | 1 | 127 | 137 | | | 2 | 48 | 44 | | | 4 | 103 | 105 |
| 5 | 10 | 1 | 148 | 141 | | | 2 | 65 | 61 | | | 2 | 96 | 93 | | | 3 | 105 | 99 | | | 5 | 70 | 73 |
| | | 2 | 104 | 95 | | | 3 | 206 | 212 | | | 3 | 102 | 110 | | | 4 | 79 | 65 | | | 6 | 136 | 131 |
| | | 3 | 131 | 117 | | | 4 | 41 | 31 | | | 4 | 124 | 123 | | | 5 | 70 | 64 | | | 7 | 111 | 133 |
| | | 4 | 92 | 80 | | | 6 | 71 | 63 | | | 5 | 73 | 70 | | | 6 | 38 | 26 | | | 8 | 65 | 86 |
| | | 5 | 129 | 131 | | | 7 | 159 | 175 | | | 6 | 118 | 117 | 7 | 13 | 0 | 138 | 148 | | | 9 | 53 | 61 |
| | | 6 | 74 | 62 | | | 9 | 33 | 39 | | | 8 | 123 | 122 | | | 1 | 70 | 50 | | | 10 | 71 | 70 |
| 5 | 11 | 0 | 56 | 29 | | | 10 | 33 | 38 | | | 10 | 81 | 81 | | | 2 | 67 | 70 | 8 | 6 | 0 | 183 | 195 |
| | | 1 | 131 | 119 | | | 11 | 100 | 114 | | | 11 | 44 | 48 | | | 3 | 46 | 37 | | | 1 | 147 | 163 |
| | | 2 | 107 | 78 | 6 | 5 | 2 | 40 | 24 | 7 | 2 | 0 | 47 | 36 | | | 4 | 133 | 126 | | | 2 | 80 | 86 |
| | | 3 | 74 | 70 | | | 3 | 59 | 58 | | | 1 | 231 | 263 | | | 6 | 79 | 83 | | | 3 | 130 | 146 |
| | | 4 | 46 | 38 | | | 4 | 276 | 298 | | | 2 | 82 | 71 | 7 | 14 | 0 | 86 | 69 | | | 4 | 141 | 142 |
| | | 5 | 112 | 99 | | | 5 | 36 | 30 | | | 3 | 204 | 208 | | | 2 | 68 | 58 | | | 5 | 150 | 145 |
| | | 6 | 59 | 56 | | | 6 | 46 | 45 | | | 4 | 57 | 59 | | | 3 | 139 | 145 | | | 6 | 52 | 44 |
| 5 | 12 | 0 | 80 | 73 | | | 7 | 33 | 30 | | | 5 | 149 | 164 | | | 4 | 57 | 47 | 8 | 7 | 0 | 100 | 82 |
| | | 1 | 80 | 64 | | | 8 | 118 | 128 | | | 6 | 71 | 72 | | | 5 | 81 | 95 | | | 1 | 41 | 34 |
| | | 3 | 95 | 94 | | | 9 | 43 | 42 | | | 8 | 61 | 67 | 7 | 15 | 0 | 152 | 146 | | | 2 | 162 | 151 |
| | | 4 | 104 | 99 | | | 10 | 70 | 77 | | | 9 | 80 | 79 | | | 1 | 71 | 45 | | | 3 | 102 | 108 |
| | | 6 | 50 | 43 | 6 | 6 | 1 | 136 | 165 | | | 10 | 34 | 27 | | | 2 | 76 | 80 | | | 4 | 87 | 89 |
| 5 | 13 | 0 | 128 | 143 | | | 2 | 58 | 63 | | | 11 | 68 | 72 | | | 3 | 49 | 51 | | | 5 | 74 | 64 |
| | | 1 | 119 | 102 | | | 3 | 239 | 253 | 7 | 3 | 0 | 249 | 254 | | | 4 | 128 | 129 | | | 6 | 134 | 118 |
| | | 3 | 88 | 88 | | | 5 | 59 | 50 | | | 1 | 66 | 63 | | | 6 | 72 | 80 | 8 | 8 | 0 | 160 | 156 |
| | | 4 | 129 | 126 | | | 6 | 86 | 61 | | | 2 | 180 | 168 | 7 | 16 | 0 | 65 | 66 | | | 1 | 54 | 54 |
| | | 5 | 71 | 75 | 6 | 7 | 1 | 69 | 74 | | | 3 | 96 | 101 | | | 1 | 116 | 91 | | | 2 | 100 | 99 |
| | | 6 | 77 | 68 | | | 3 | 37 | 36 | | | 4 | 189 | 187 | | | 3 | 83 | 99 | | | 3 | 47 | 48 |
| 5 | 14 | 0 | 89 | 91 | | | 4 | 227 | 239 | | | 5 | 60 | 47 | | | 4 | 46 | 41 | | | 4 | 110 | 112 |
| | | 1 | 129 | 104 | | | 5 | 86 | 74 | | | 6 | 179 | 178 | | | 6 | 34 | 43 | | | 5 | 83 | 71 |
| | | 2 | 47 | 29 | | | 6 | 50 | 46 | | | 7 | 57 | 62 | 7 | 17 | 0 | 40 | 43 | | | 6 | 60 | 54 |
| | | 3 | 127 | 142 | 6 | 8 | 1 | 40 | 33 | | | 8 | 126 | 130 | | | 1 | 43 | 28 | 8 | 9 | 0 | 88 | 76 |
| | | 4 | 104 | 88 | | | 2 | 44 | 26 | | | 10 | 109 | 111 | | | 3 | 37 | 43 | | | 3 | 58 | 45 |
| | | 5 | 66 | 60 | | | 3 | 123 | 118 | 7 | 4 | 0 | 35 | 26 | | | 4 | 377 | 44 | | | 4 | 76 | 72 |
| | | 6 | 66 | 57 | | | 4 | 63 | 56 | | | 1 | 194 | 209 | 7 | 18 | 2 | 41 | 61 | | | 5 | 83 | 85 |
| 5 | 15 | 0 | 148 | 162 | | | 5 | 51 | 53 | | | 2 | 68 | 78 | | | 3 | 54 | 55 | | | 6 | 42 | 37 |
| | | 1 | 101 | 80 | | | 6 | 60 | 42 | | | 3 | 195 | 198 | 7 | 19 | 0 | 44 | 24 | 8 | 10 | 0 | 90 | 84 |
| | | 2 | 50 | 34 | 6 | 9 | 0 | 113 | 126 | | | 4 | 66 | 48 | | | 1 | 55 | 32 | | | 1 | 110 | 105 |
| | | 3 | 91 | 93 | | | 1 | 82 | 78 | | | 5 | 141 | 136 | 8 | 0 | 0 | 108 | 116 | | | 2 | 114 | 118 |
| | | 4 | 130 | 128 | | | 3 | 79 | 63 | | | 6 | 83 | 81 | | | 1 | 168 | 172 | | | 3 | 112 | 98 |
| | | 5 | 43 | 46 | | | 4 | 64 | 60 | | | 7 | 126 | 121 | | | 2 | 204 | 211 | | | 4 | 66 | 60 |
| | | 6 | 67 | 61 | | | 5 | 74 | 65 | | | 8 | 35 | 31 | | | 3 | 223 | 244 | | | 5 | 63 | 68 |
| 5 | 16 | 0 | 94 | 67 | | | 6 | 95 | 87 | | | 9 | 59 | 53 | | | 4 | 81 | 85 | | | 6 | 81 | 81 |
| | | 1 | 96 | 79 | 6 | 10 | 0 | 78 | 57 | | | 10 | 59 | 63 | | | 5 | 124 | 120 | 8 | 11 | 0 | 140 | 151 |
| | | 3 | 90 | 95 | | | 1 | 132 | 128 | | | 11 | 61 | 66 | | | 6 | 126 | 120 | | | 1 | 67 | 51 |
| | | 4 | 59 | 60 | | | 3 | 40 | 41 | 7 | 5 | 0 | 119 | 102 | | | 7 | 136 | 141 | | | 2 | 91 | 82 |
| | | 5 | 37 | 29 | | | 4 | 46 | 37 | | | 1 | 106 | 113 | | | 9 | 95 | 69 | | | 3 | 41 | 28 |
| | | 6 | 56 | 51 | | | 5 | 139 | 172 | | | 2 | 96 | 79 | | | 11 | 100 | 92 | | | 4 | 142 | 136 |
| 5 | 17 | 0 | 84 | 75 | | | 6 | 52 | 32 | | | 3 | 103 | 104 | 8 | 1 | 0 | 190 | 189 | | | 5 | 87 | 103 |
| | | 1 | 88 | 65 | 6 | 11 | 1 | 75 | 72 | | | 4 | 111 | 102 | | | 1 | 99 | 89 | | | 6 | 82 | 88 |
| | | 3 | 49 | 57 | | | 2 | 224 | 264 | | | 5 | 26 | 25 | | | 2 | 130 | 136 | 8 | 12 | 0 | 80 | 61 |
| 5 | 18 | 1 | 83 | 64 | | | 3 | 75 | 83 | | | 6 | 128 | 122 | | | 4 | 155 | 168 | | | 1 | 123 | 126 |
| | | 2 | 49 | 45 | | | 4 | 54 | 43 | | | 7 | 66 | 67 | | | 5 | 149 | 155 | | | 2 | 101 | 123 |
| | | 3 | 43 | 38 | | | 6 | 155 | 159 | | | 8 | 81 | 98 | | | 6 | 81 | 85 | | | 3 | 111 | 115 |
| | | 4 | 35 | 28 | 6 | 12 | 0 | 57 | 52 | | | 10 | 77 | 85 | | | 7 | 72 | 79 | | | 4 | 57 | 43 |
| | | 5 | 54 | 67 | | | 1 | 177 | 155 | | | 11 | 32 | 32 | | | 8 | 114 | 104 | | | 5 | 83 | 89 |
| 5 | 19 | 0 | 44 | 23 | | | 3 | 79 | 83 | 7 | 6 | 1 | 130 | 149 | | | 9 | 101 | 113 | | | 6 | 68 | 76 |
| | | 1 | 60 | 52 | | | 4 | 53 | 38 | | | 2 | 48 | 50 | | | 10 | 66 | 63 | 8 | 13 | 0 | 103 | 123 |
| | | 3 | 36 | 40 | | | 5 | 153 | 174 | | | 3 | 115 | 118 | | | 11 | 46 | 52 | | | 1 | 59 | 41 |
| 6 | 0 | 0 | 73 | 74 | | | 6 | 56 | 64 | | | 5 | 100 | 100 | 8 | 2 | 0 | 174 | 167 | | | 2 | 69 | 55 |
| | | 1 | 188 | 218 | 6 | 13 | 0 | 40 | 26 | | | 6 | 93 | 86 | | | 1 | 96 | 84 | | | 4 | 105 | 102 |
| | | 3 | 95 | 87 | | | 1 | 79 | 66 | 7 | 7 | 0 | 115 | 94 | | | 2 | 223 | 237 | | | 5 | 77 | 82 |
| | | 4 | 70 | 61 | | | 2 | 166 | 192 | | | 1 | 94 | 96 | | | 3 | 117 | 118 | | | 6 | 78 | 64 |
| | | 5 | 242 | 270 | | | 3 | 70 | 73 | | | 2 | 133 | 134 | | | 4 | 102 | 101 | 8 | 14 | 0 | 91 | 72 |
| | | 9 | 228 | 228 | | | 6 | 95 | 107 | | | 3 | 99 | 99 | | | 5 | 54 | 39 | | | 1 | 73 | 62 |
| 6 | 1 | 0 | 59 | 48 | 6 | 14 | 1 | 49 | 41 | | | 4 | 130 | 126 | | | 6 | 85 | 83 | | | 2 | 75 | 72 |
| | | 1 | 74 | 66 | | | 2 | 46 | 40 | | | 5 | 51 | 48 | | | 7 | 75 | 74 | | | 3 | 65 | 62 |
| | | 2 | 314 | 361 | | | 3 | 44 | 31 | | | 6 | 126 | 114 | | | 8 | 42 | 35 | | | 4 | 74 | 68 |
| | | 3 | 74 | 72 | | | 4 | 42 | 38 | 7 | 8 | 1 | 183 | 209 | | | 10 | 31 | 35 | | | 6 | 50 | 45 |
| | | 6 | 185 | 211 | | | 6 | 72 | 73 | | | 2 | 56 | 46 | | | 11 | 56 | 54 | 8 | 15 | 2 | 49 | 49 |
| | | 7 | 51 | 51 | 6 | 15 | 0 | 158 | 132 | | | 3 | 151 | 157 | 8 | 3 | 0 | 62 | 41 | | | 3 | 99 | 57 |
| | | 8 | 83 | 84 | | | 1 | 80 | 62 | | | 4 | 45 | 34 | | | 1 | 61 | 47 | | | 4 | 40 | 37 |
| | | 10 | 82 | 75 | | | 2 | 44 | 31 | | | 5 | 202 | 185 | | | 2 | 91 | 78 | | | 6 | 57 | 65 |
| | | 11 | 39 | 38 | | | 3 | 62 | 73 | | | 6 | 79 | 80 | | | 3 | 81 | 76 | 8 | 16 | 0 | 97 | 93 |
| 6 | 2 | 0 | 105 | 91 | | | 4 | 105 | 102 | 7 | 9 | 0 | 86 | 89 | | | 4 | 44 | 37 | | | 1 | 109 | 97 |
| | | 1 | 130 | 127 | 6 | 16 | 1 | 100 | 72 | | | 1 | 88 | 81 | | | 5 | 104 | 97 | | | 3 | 65 | 74 |

TABLE 2 (*Continued*)

| h | k | l | $F_o$ | $F_c$ | h | k | l | $F_o$ | $F_c$ | h | k | l | $F_o$ | $F_c$ | h | k | l | $F_o$ | $F_c$ | h | k | l | $F_o$ | $F_c$ |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | 4 | 64 | 70 | | | 4 | 132 | 131 | | | 9 | 66 | 76 | | | 5 | 112 | 109 | 12 | 2 | 0 | 180 | 179 |
| 8 | 17 | 0 | 83 | 74 | | | 5 | 90 | 93 | | | 10 | 34 | 41 | | | 6 | 103 | 103 | | | 1 | 43 | 28 |
| | | 2 | 84 | 96 | | | 6 | 86 | 93 | 10 | 6 | 0 | 68 | 50 | | | 7 | 80 | 79 | | | 2 | 65 | 67 |
| | | 3 | 45 | 46 | 9 | 10 | 1 | 107 | 91 | | | 1 | 131 | 133 | | | 8 | 92 | 86 | | | 4 | 120 | 124 |
| | | 4 | 68 | 69 | | | 2 | 97 | 86 | | | 2 | 133 | 129 | | | 9 | 74 | 72 | | | 5 | 59 | 54 |
| 8 | 18 | 0 | 55 | 69 | | | 3 | 88 | 95 | | | 3 | 58 | 52 | | | 10 | 73 | 75 | | | 8 | 56 | 54 |
| | | 1 | 97 | 97 | | | 4 | 53 | 40 | | | 4 | 60 | 52 | 11 | 4 | 0 | 92 | 71 | | | 9 | 45 | 48 |
| | | 3 | 61 | 65 | | | 6 | 87 | 95 | | | 5 | 139 | 157 | | | 1 | 141 | 138 | 12 | 3 | 0 | 59 | 56 |
| 9 | 0 | 1 | 84 | 77 | 9 | 11 | 0 | 70 | 70 | | | 6 | 98 | 103 | | | 2 | 151 | 153 | | | 1 | 53 | 30 |
| | | 2 | 69 | 46 | | | 1 | 100 | 82 | 10 | 7 | 0 | 89 | 62 | | | 3 | 128 | 120 | | | 2 | 60 | 40 |
| | | 3 | 59 | 58 | | | 3 | 87 | 95 | | | 1 | 90 | 82 | | | 4 | 88 | 93 | | | 3 | 46 | 43 |
| | | 4 | 77 | 68 | | | 4 | 77 | 72 | | | 2 | 187 | 202 | | | 5 | 88 | 90 | | | 4 | 46 | 32 |
| | | 5 | 69 | 72 | 9 | 12 | 0 | 55 | 50 | | | 3 | 53 | 55 | | | 6 | 80 | 70 | | | 5 | 76 | 77 |
| | | 6 | 119 | 115 | | | 3 | 45 | 31 | | | 4 | 47 | 40 | | | 7 | 50 | 56 | | | 7 | 83 | 74 |
| | | 8 | 78 | 60 | | | 4 | 69 | 52 | | | 5 | 98 | 88 | | | 8 | 64 | 70 | | | 8 | 26 | 29 |
| | | 10 | 98 | 104 | | | 6 | 76 | 76 | | | 6 | 102 | 104 | | | 9 | 49 | 51 | | | 9 | 67 | 81 |
| 9 | 1 | 0 | 94 | 85 | 9 | 13 | 1 | 108 | 88 | 10 | 8 | 0 | 57 | 35 | 11 | 5 | 0 | 40 | 31 | 12 | 4 | 1 | 40 | 35 |
| | | 1 | 170 | 176 | | | 2 | 140 | 133 | | | 1 | 62 | 53 | | | 1 | 79 | 76 | | | 2 | 178 | 184 |
| | | 2 | 82 | 74 | | | 3 | 95 | 104 | | | 2 | 91 | 64 | | | 2 | 47 | 42 | | | 3 | 55 | 50 |
| | | 3 | 127 | 133 | | | 4 | 69 | 49 | | | 3 | 47 | 36 | | | 3 | 67 | 65 | | | 5 | 40 | 37 |
| | | 4 | 72 | 76 | | | 6 | 68 | 75 | | | 5 | 89 | 92 | | | 4 | 59 | 59 | | | 6 | 81 | 97 |
| | | 5 | 82 | 78 | 9 | 14 | 0 | 100 | 81 | | | 6 | 57 | 52 | | | 5 | 57 | 54 | | | 7 | 43 | 51 |
| | | 6 | 74 | 69 | | | 1 | 137 | 111 | 10 | 9 | 0 | 140 | 129 | | | 6 | 79 | 78 | | | 9 | 23 | 26 |
| | | 7 | 65 | 62 | | | 2 | 65 | 45 | | | 1 | 62 | 48 | | | 8 | 80 | 93 | 12 | 5 | 0 | 96 | 80 |
| | | 8 | 78 | 81 | | | 3 | 82 | 84 | | | 2 | 84 | 92 | | | 9 | 45 | 46 | | | 1 | 138 | 141 |
| | | 10 | 40 | 39 | | | 4 | 83 | 79 | | | 3 | 58 | 59 | 11 | 6 | 0 | 57 | 50 | | | 3 | 58 | 54 |
| 9 | 2 | 1 | 162 | 165 | | | 5 | 78 | 103 | | | 4 | 118 | 99 | | | 1 | 113 | 122 | | | 4 | 68 | 77 |
| | | 2 | 77 | 63 | | | 6 | 55 | 57 | | | 6 | 39 | 33 | | | 2 | 42 | 29 | | | 5 | 131 | 166 |
| | | 3 | 140 | 141 | 9 | 15 | 0 | 55 | 30 | 10 | 10 | 0 | 106 | 113 | | | 3 | 86 | 90 | | | 8 | 40 | 40 |
| | | 4 | 107 | 110 | | | 2 | 107 | 133 | | | 1 | 66 | 37 | | | 4 | 46 | 41 | | | 9 | 95 | 126 |
| | | 5 | 113 | 119 | | | 3 | 81 | 91 | | | 3 | 106 | 114 | | | 5 | 73 | 79 | 12 | 6 | 1 | 62 | 50 |
| | | 6 | 97 | 104 | | | 4 | 51 | 41 | | | 4 | 100 | 86 | 11 | 7 | 0 | 70 | 43 | | | 2 | 181 | 211 |
| | | 7 | 79 | 81 | | | 6 | 65 | 82 | | | 6 | 69 | 61 | | | 1 | 95 | 92 | | | 3 | 74 | 76 |
| | | 8 | 88 | 103 | 9 | 16 | 1 | 67 | 58 | 10 | 11 | 0 | 162 | 163 | | | 2 | 48 | 38 | | | 6 | 133 | 138 |
| | | 9 | 69 | 77 | | | 3 | 33 | 34 | | | 1 | 101 | 89 | | | 3 | 89 | 94 | 12 | 7 | 0 | 90 | 86 |
| | | 10 | 78 | 84 | | | 4 | 62 | 65 | | | 3 | 71 | 80 | | | 4 | 100 | 92 | | | 1 | 112 | 100 |
| 9 | 3 | 0 | 142 | 138 | 9 | 17 | 0 | 62 | 46 | | | 4 | 146 | 149 | | | 6 | 56 | 47 | | | 3 | 40 | 23 |
| | | 1 | 200 | 177 | | | 1 | 80 | 65 | | | 6 | 42 | 27 | 11 | 8 | 0 | 156 | 148 | | | 4 | 63 | 64 |
| | | 2 | 200 | 193 | | | 2 | 37 | 46 | 10 | 12 | 0 | 107 | 114 | | | 1 | 141 | 134 | | | 5 | 119 | 132 |
| | | 3 | 144 | 128 | | | 3 | 34 | 35 | | | 1 | 91 | 67 | | | 2 | 84 | 62 | | | 6 | 45 | 38 |
| | | 4 | 117 | 127 | 9 | 18 | 1 | 35 | 28 | | | 3 | 111 | 113 | | | 3 | 88 | 98 | 12 | 8 | 0 | 97 | 72 |
| | | 5 | 115 | 125 | 10 | 0 | 0 | 160 | 158 | | | 4 | 98 | 94 | | | 4 | 111 | 120 | | | 1 | 43 | 37 |
| | | 6 | 134 | 132 | | | 1 | 97 | 92 | | | 6 | 54 | 50 | | | 5 | 86 | 91 | | | 2 | 106 | 115 |
| | | 7 | 70 | 67 | | | 2 | 87 | 90 | 10 | 13 | 0 | 129 | 153 | | | 6 | 66 | 69 | | | 3 | 60 | 68 |
| | | 8 | 93 | 95 | | | 3 | 160 | 175 | | | 1 | 97 | 81 | 11 | 9 | 0 | 98 | 94 | | | 4 | 56 | 58 |
| | | 9 | 46 | 37 | | | 4 | 122 | 133 | | | 3 | 56 | 57 | | | 1 | 128 | 112 | | | 6 | 75 | 77 |
| | | 10 | 64 | 70 | | | 6 | 59 | 43 | | | 4 | 106 | 106 | | | 3 | 103 | 117 | 12 | 9 | 0 | 39 | 34 |
| 9 | 4 | 0 | 110 | 87 | | | 7 | 180 | 180 | 10 | 14 | 0 | 47 | 42 | | | 4 | 95 | 85 | | | 1 | 34 | 20 |
| | | 1 | 162 | 160 | | | 8 | 86 | 81 | | | 3 | 54 | 59 | | | 5 | 67 | 66 | | | 3 | 62 | 62 |
| | | 2 | 73 | 65 | 10 | 1 | 0 | 206 | 240 | | | 4 | 54 | 50 | | | 6 | 68 | 82 | | | 4 | 34 | 37 |
| | | 3 | 124 | 117 | | | 1 | 106 | 94 | 10 | 15 | 0 | 72 | 48 | 11 | 10 | 0 | 104 | 124 | | | 6 | 62 | 59 |
| | | 4 | 115 | 114 | | | 2 | 79 | 58 | | | 1 | 87 | 63 | | | 1 | 127 | 103 | 12 | 10 | 0 | 160 | 158 |
| | | 5 | 120 | 126 | | | 3 | 137 | 142 | | | 2 | 51 | 75 | | | 2 | 52 | 29 | | | 1 | 66 | 54 |
| | | 6 | 91 | 84 | | | 4 | 169 | 185 | | | 3 | 44 | 44 | | | 3 | 98 | 105 | | | 3 | 36 | 37 |
| | | 7 | 71 | 80 | | | 5 | 59 | 44 | | | 4 | 32 | 32 | | | 4 | 98 | 100 | | | 4 | 129 | 133 |
| | | 8 | 99 | 114 | | | 7 | 81 | 91 | 10 | 16 | 0 | 44 | 30 | | | 6 | 64 | 55 | 12 | 11 | 1 | 102 | 79 |
| | | 9 | 64 | 64 | | | 8 | 74 | 80 | | | 1 | 88 | 61 | 11 | 11 | 0 | 54 | 49 | | | 2 | 78 | 63 |
| | | 10 | 58 | 60 | | | 10 | 57 | 51 | | | 2 | 70 | 73 | | | 1 | 41 | 39 | | | 3 | 128 | 127 |
| 9 | 5 | 0 | 52 | 40 | 10 | 2 | 0 | 127 | 104 | | | 3 | 26 | 23 | | | 2 | 45 | 39 | | | 4 | 42 | 30 |
| | | 1 | 144 | 141 | | | 1 | 44 | 26 | | | 4 | 43 | 44 | | | 3 | 64 | 61 | | | 6 | 50 | 49 |
| | | 2 | 108 | 87 | | | 3 | 86 | 91 | 10 | 17 | 1 | 76 | 81 | | | 4 | 46 | 34 | 12 | 12 | 0 | 156 | 167 |
| | | 3 | 113 | 107 | | | 4 | 92 | 93 | 11 | 0 | 1 | 109 | 97 | | | 6 | 76 | 77 | | | 1 | 80 | 67 |
| | | 4 | 51 | 48 | | | 5 | 60 | 57 | | | 3 | 121 | 122 | 11 | 12 | 1 | 119 | 89 | | | 3 | 36 | 35 |
| | | 5 | 87 | 87 | | | 7 | 114 | 132 | | | 5 | 56 | 54 | | | 2 | 67 | 68 | | | 4 | 96 | 132 |
| | | 6 | 86 | 95 | | | 8 | 63 | 58 | | | 6 | 60 | 46 | | | 3 | 77 | 85 | | | 6 | 36 | 37 |
| | | 7 | 53 | 52 | | | 9 | 54 | 57 | | | 7 | 89 | 60 | | | 6 | 39 | 58 | 12 | 13 | 1 | 53 | 38 |
| | | 8 | 45 | 45 | 10 | 3 | 0 | 134 | 118 | 11 | 1 | 0 | 56 | 37 | 11 | 13 | 1 | 114 | 80 | | | 2 | 55 | 55 |
| | | 9 | 36 | 30 | | | 1 | 49 | 34 | | | 1 | 78 | 72 | | | 2 | 64 | 62 | | | 3 | 72 | 81 |
| | | 10 | 45 | 54 | | | 2 | 155 | 152 | | | 2 | 86 | 80 | | | 3 | 54 | 50 | | | 4 | 33 | 35 |
| 9 | 6 | 0 | 54 | 33 | | | 4 | 90 | 88 | | | 3 | 67 | 69 | | | 4 | 47 | 39 | 12 | 14 | 1 | 64 | 57 |
| | | 1 | 68 | 62 | | | 5 | 51 | 39 | | | 4 | 71 | 70 | 11 | 14 | 1 | 120 | 96 | | | 3 | 41 | 37 |
| | | 2 | 46 | 43 | | | 6 | 80 | 81 | | | 5 | 70 | 67 | | | 2 | 95 | 120 | | | 4 | 54 | 56 |
| | | 3 | 86 | 83 | | | 7 | 34 | 32 | | | 6 | 95 | 106 | | | 3 | 62 | 61 | 12 | 15 | 0 | 63 | 34 |
| | | 4 | 95 | 88 | | | 8 | 31 | 33 | | | 7 | 47 | 56 | | | 4 | 41 | 39 | | | 1 | 58 | 47 |
| | | 6 | 80 | 66 | | | 9 | 50 | 46 | | | 8 | 69 | 70 | 11 | 15 | 0 | 45 | 35 | | | 3 | 24 | 20 |
| 9 | 7 | 0 | 110 | 109 | | | 10 | 36 | 29 | | | 9 | 50 | 48 | | | 2 | 56 | 69 | 12 | 16 | 1 | 50 | 47 |
| | | 1 | 120 | 137 | 10 | 4 | 1 | 113 | 107 | 11 | 2 | 0 | 89 | 83 | | | 3 | 38 | 34 | 13 | 0 | 1 | 44 | 26 |
| | | 2 | 47 | 50 | | | 2 | 128 | 111 | | | 1 | 148 | 143 | | | 4 | 40 | 40 | | | 2 | 48 | 45 |
| | | 3 | 96 | 99 | | | 4 | 50 | 42 | | | 2 | 105 | 99 | 11 | 16 | 1 | 80 | 70 | | | 3 | 60 | 53 |
| | | 4 | 100 | 98 | | | 5 | 133 | 141 | | | 3 | 145 | 139 | | | 2 | 58 | 66 | | | 4 | 68 | 67 |
| | | 5 | 129 | 139 | | | 6 | 76 | 70 | | | 4 | 91 | 84 | | | 3 | 45 | 42 | | | 8 | 91 | 73 |
| | | 6 | 73 | 78 | | | 7 | 48 | 43 | | | 5 | 93 | 96 | 12 | 0 | 0 | 200 | 217 | 13 | 1 | 1 | 123 | 110 |
| 9 | 8 | 0 | 56 | 51 | | | 8 | 36 | 44 | | | 6 | 96 | 110 | | | 1 | 69 | 54 | | | 2 | 42 | 30 |
| | | 1 | 99 | 103 | | | 9 | 89 | 105 | | | 7 | 65 | 73 | | | 4 | 177 | 191 | | | 3 | 105 | 111 |
| | | 2 | 96 | 88 | | | 10 | 37 | 36 | | | 8 | 78 | 75 | | | 5 | 70 | 63 | | | 5 | 81 | 84 |
| | | 3 | 132 | 132 | 10 | 5 | 1 | 102 | 94 | | | 9 | 42 | 44 | | | 6 | 50 | 42 | | | 6 | 63 | 63 |
| | | 5 | 83 | 80 | | | 2 | 202 | 230 | | | 10 | 64 | 72 | | | 8 | 109 | 104 | | | 7 | 66 | 60 |
| | | 6 | 93 | 87 | | | 3 | 79 | 76 | 11 | 3 | 0 | 69 | 54 | | | 9 | 65 | 55 | 13 | 2 | 0 | 101 | 87 |
| 9 | 9 | 0 | 156 | 161 | | | 5 | 111 | 108 | | | 1 | 137 | 131 | 12 | 1 | 1 | 93 | 89 | | | 1 | 47 | 38 |
| | | 1 | 115 | 115 | | | 6 | 117 | 124 | | | 2 | 119 | 108 | | | 2 | 90 | 89 | | | 2 | 115 | 125 |
| | | 2 | 59 | 42 | | | 7 | 36 | 36 | | | 3 | 131 | 126 | | | 3 | 141 | 145 | | | 3 | 54 | 58 |
| | | 3 | 112 | 116 | | | 8 | 32 | 32 | | | 4 | 99 | 104 | | | 6 | 64 | 57 | | | 4 | 116 | 122 |

TABLE 2 (*Continued*)

| *h* | *k* | *l* | $F_o$ | $F_c$ | *h* | *k* | | $F_o$ | $F_c$ | *h* | *k* | *l* | $F_o$ | $F_c$ | *h* | *k* | *l* | $F_o$ | $F_c$ | *h* | *k* | | $F_o$ | $F_c$ |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | 6 | 93 | 96 | | | 6 | 123 | 128 | 14 | 11 | 0 | 92 | 65 | 15 | 11 | 4 | 29 | 36 | | | 1 | 55 | 55 |
| | | 8 | 87 | 99 | | | 7 | 82 | 88 | | | 1 | 119 | 102 | 15 | 12 | 1 | 71 | 60 | | | 2 | 44 | 55 |
| 13 | 3 | 0 | 40 | 33 | | | 8 | 54 | 54 | | | 3 | 60 | 66 | 15 | 13 | 1 | 72 | 39 | | | 3 | 65 | 71 |
| | | 1 | 165 | 155 | 14 | 1 | 0 | 111 | 101 | | | 4 | 52 | 56 | 16 | 0 | 1 | 83 | 63 | | | 4 | 68 | 61 |
| | | 2 | 44 | 41 | | | 1 | 100 | 93 | 14 | 12 | 2 | 80 | 101 | | | 2 | 125 | 152 | | | 5 | 37 | 39 |
| | | 3 | 157 | 149 | | | 2 | 74 | 82 | | | 3 | 44 | 41 | | | 3 | 44 | 39 | | | 6 | 68 | 63 |
| | | 5 | 108 | 115 | | | 3 | 76 | 80 | | | 4 | 55 | 54 | | | 5 | 66 | 66 | 17 | 3 | 0 | 78 | 62 |
| | | 6 | 45 | 45 | | | 4 | 83 | 75 | 14 | 13 | 1 | 77 | 65 | | | 6 | 90 | 86 | | | 1 | 92 | 92 |
| | | 7 | 87 | 89 | | | 5 | 89 | 102 | | | 3 | 39 | 37 | 16 | 1 | 1 | 84 | 84 | | | 2 | 47 | 51 |
| | | 9 | 73 | 72 | | | 7 | 54 | 49 | 15 | 0 | 1 | 109 | 96 | | | 2 | 93 | 94 | | | 3 | 79 | 93 |
| 13 | 4 | 0 | 84 | 71 | 14 | 2 | 2 | 102 | 103 | | | 3 | 67 | 69 | | | 3 | 43 | 30 | | | 4 | 56 | 60 |
| | | 1 | 44 | 27 | | | 3 | 57 | 52 | | | 5 | 78 | 79 | | | 5 | 78 | 101 | | | 5 | 47 | 50 |
| | | 2 | 132 | 114 | | | 4 | 36 | 26 | | | 6 | 49 | 39 | | | 6 | 64 | 52 | 17 | 4 | 0 | 60 | 44 |
| | | 4 | 81 | 83 | | | 5 | 58 | 63 | 15 | 1 | 1 | 72 | 62 | 16 | 2 | 0 | 46 | 37 | | | 1 | 45 | 39 |
| | | 6 | 95 | 100 | | | 6 | 71 | 66 | | | 3 | 65 | 63 | | | 1 | 51 | 37 | | | 2 | 42 | 51 |
| | | 8 | 71 | 84 | | | 7 | 64 | 68 | | | 4 | 73 | 64 | | | 2 | 90 | 109 | | | 3 | 51 | 54 |
| 13 | 5 | 1 | 120 | 112 | 14 | 3 | 0 | 91 | 94 | | | 6 | 45 | 35 | | | 4 | 35 | 30 | | | 4 | 47 | 54 |
| | | 3 | 87 | 97 | | | 2 | 79 | 86 | 15 | 2 | 0 | 112 | 87 | | | 5 | 48 | 46 | 17 | 5 | 0 | 56 | 37 |
| | | 4 | 48 | 49 | | | 4 | 68 | 64 | | | 1 | 112 | 104 | | | 6 | 61 | 65 | | | 1 | 71 | 70 |
| | | 5 | 67 | 61 | | | 6 | 47 | 50 | | | 2 | 88 | 93 | 16 | 3 | 0 | 56 | 50 | | | 3 | 62 | 74 |
| | | 7 | 44 | 47 | | | 7 | 51 | 41 | | | 3 | 78 | 75 | | | 2 | 46 | 40 | | | 4 | 30 | 30 |
| | | 8 | 40 | 52 | 14 | 4 | 0 | 116 | 104 | | | 4 | 77 | 77 | | | 3 | 50 | 42 | 17 | 6 | 2 | 30 | 27 |
| 13 | 6 | 0 | 56 | 38 | | | 1 | 42 | 28 | | | 5 | 68 | 82 | | | 4 | 40 | 28 | | | 3 | 24 | 18 |
| | | 1 | 43 | 46 | | | 3 | 39 | 38 | | | 6 | 53 | 59 | 16 | 4 | 0 | 113 | 123 | | | 4 | 30 | 34 |
| | | 4 | 71 | 54 | | | 4 | 80 | 78 | 15 | 3 | 0 | 53 | 25 | | | 1 | 36 | 30 | 17 | 7 | 1 | 87 | 76 |
| | | 6 | 66 | 73 | | | 5 | 63 | 64 | | | 1 | 88 | 90 | | | 2 | 45 | 43 | | | 2 | 34 | 59 |
| 13 | 7 | 1 | 117 | 121 | | | 6 | 48 | 36 | | | 2 | 50 | 40 | | | 3 | 45 | 41 | | | 3 | 57 | 57 |
| | | 3 | 105 | 103 | | | 7 | 47 | 57 | | | 3 | 100 | 106 | | | 4 | 77 | 87 | 17 | 8 | 1 | 67 | 51 |
| | | 5 | 55 | 74 | | | 8 | 46 | 56 | | | 4 | 58 | 54 | 16 | 5 | 0 | 71 | 91 | | | 3 | 37 | 38 |
| 13 | 8 | 0 | 115 | 131 | 14 | 5 | 0 | 82 | 66 | | | 5 | 56 | 65 | | | 1 | 49 | 42 | 17 | 9 | 1 | 81 | 74 |
| | | 1 | 47 | 48 | | | 1 | 94 | 89 | | | 6 | 61 | 57 | | | 3 | 73 | 87 | | | 2 | 50 | 63 |
| | | 2 | 84 | 94 | | | 2 | 87 | 97 | | | 7 | 64 | 71 | | | 4 | 64 | 75 | 17 | 10 | 1 | 66 | 38 |
| | | 3 | 37 | 32 | | | 3 | 94 | 112 | 15 | 4 | 0 | 77 | 81 | | | 6 | 23 | 28 | 18 | 0 | 0 | 86 | 82 |
| | | 4 | 128 | 127 | | | 4 | 45 | 43 | | | 1 | 102 | 102 | 16 | 6 | 1 | 47 | 40 | | | 1 | 78 | 81 |
| | | 6 | 83 | 96 | | | 5 | 55 | 58 | | | 2 | 64 | 58 | | | 3 | 63 | 57 | | | 3 | 38 | 38 |
| 13 | 9 | 1 | 143 | 133 | | | 6 | 42 | 45 | | | 3 | 91 | 83 | | | 4 | 96 | 105 | | | 4 | 57 | 67 |
| | | 2 | 48 | 50 | | | 7 | 79 | 95 | | | 4 | 68 | 77 | 16 | 7 | 0 | 73 | 70 | 18 | 1 | 1 | 42 | 36 |
| | | 3 | 118 | 131 | 14 | 6 | 0 | 161 | 148 | | | 5 | 50 | 42 | | | 1 | 58 | 49 | | | 2 | 97 | 109 |
| | | 5 | 75 | 90 | | | 1 | 47 | 32 | | | 6 | 51 | 56 | | | 3 | 74 | 77 | | | 3 | 59 | 52 |
| | | 6 | 41 | 34 | | | 2 | 50 | 63 | | | 7 | 36 | 41 | | | 4 | 59 | 67 | 18 | 2 | 1 | 39 | 38 |
| 13 | 10 | 0 | 93 | 100 | | | 4 | 127 | 131 | 15 | 5 | 1 | 37 | 33 | | | 6 | 25 | 12 | | | 4 | 42 | 43 |
| | | 1 | 38 | 26 | | | 6 | 54 | 56 | | | 2 | 42 | 44 | 16 | 8 | 0 | 107 | 81 | 18 | 3 | 0 | 67 | 71 |
| | | 2 | 58 | 53 | 14 | 7 | 0 | 98 | 79 | | | 3 | 42 | 34 | | | 1 | 45 | 35 | | | 1 | 34 | 19 |
| | | 3 | 39 | 36 | | | 1 | 83 | 76 | | | 4 | 32 | 29 | | | 3 | 35 | 30 | | | 2 | 38 | 39 |
| | | 4 | 80 | 76 | | | 2 | 92 | 79 | | | 6 | 64 | 72 | | | 4 | 55 | 63 | | | 3 | 25 | 25 |
| | | 6 | 63 | 77 | | | 3 | 88 | 92 | | | 7 | 32 | 46 | 16 | 9 | 0 | 44 | 25 | | | 4 | 40 | 49 |
| 13 | 11 | 1 | 104 | 85 | | | 4 | 67 | 60 | 15 | 6 | 1 | 90 | 78 | | | 1 | 44 | 29 | 18 | 4 | 0 | 17 | 15 |
| | | 3 | 67 | 69 | | | 6 | 46 | 42 | | | 3 | 85 | 88 | | | 3 | 26 | 9 | | | 1 | 31 | 33 |
| | | 4 | 37 | 25 | 14 | 8 | 0 | 94 | 73 | | | 6 | 32 | 31 | | | 4 | 35 | 36 | | | 2 | 44 | 60 |
| | | 6 | 49 | 44 | | | 3 | 48 | 43 | 15 | 7 | 1 | 81 | 62 | 16 | 10 | 1 | 44 | 38 | | | 3 | 57 | 61 |
| 13 | 12 | 1 | 37 | 27 | | | 4 | 67 | 68 | | | 3 | 58 | 54 | 16 | 11 | 0 | 26 | 6 | 18 | 5 | 0 | 97 | 106 |
| | | 3 | 48 | 43 | | | 6 | 27 | 27 | | | 4 | 52 | 45 | | | 1 | 86 | 67 | | | 1 | 42 | 40 |
| | | 4 | 49 | 39 | 14 | 9 | 0 | 76 | 66 | | | 6 | 67 | 64 | | | 2 | 50 | 66 | 18 | 6 | 1 | 53 | 45 |
| 13 | 13 | 1 | 125 | 92 | | | 1 | 51 | 45 | 15 | 8 | 1 | 91 | 74 | 17 | 0 | 1 | 55 | 38 | | | 2 | 47 | 61 |
| | | 3 | 55 | 66 | | | 2 | 48 | 65 | | | 2 | 83 | 102 | | | 4 | 58 | 52 | 18 | 7 | 1 | 43 | 33 |
| | | 4 | 39 | 36 | | | 3 | 37 | 35 | | | 3 | 74 | 74 | | | 6 | 73 | 49 | 19 | 0 | 1 | 44 | 49 |
| 13 | 14 | 1 | 28 | 24 | | | 4 | 65 | 71 | | | 4 | 66 | 58 | 17 | 1 | 0 | 62 | 43 | 19 | 1 | 0 | 51 | 36 |
| | | 2 | 73 | 88 | | | 6 | 24 | 34 | | | 6 | 71 | 74 | | | 1 | 88 | 82 | | | 2 | 25 | 37 |
| | | 3 | 27 | 32 | 14 | 10 | 0 | 63 | 34 | 15 | 9 | 1 | 105 | 92 | | | 2 | 31 | 30 | 19 | 2 | 1 | 64 | 77 |
| 13 | 15 | 1 | 87 | 83 | | | 1 | 34 | 13 | | | 4 | 55 | 57 | | | 3 | 79 | 72 | 19 | 3 | 0 | 57 | 60 |
| 14 | 0 | 0 | 68 | 51 | | | 2 | 78 | 97 | 15 | 10 | 1 | 88 | 62 | | | 4 | 35 | 31 | | | 1 | 33 | 23 |
| | | 2 | 142 | 149 | | | 3 | 34 | 37 | | | 2 | 97 | 78 | | | 5 | 47 | 58 | | | 2 | 40 | 60 |
| | | 3 | 63 | 52 | | | 4 | 40 | 32 | | | 3 | 56 | 58 | | | 6 | 26 | 28 | 19 | 4 | 1 | 60 | 79 |
| | | 4 | 56 | 58 | | | 5 | 48 | 47 | | | 4 | 32 | 31 | 17 | 2 | 0 | 56 | 44 | 19 | 5 | 0 | 21 | 29 |
| | | 5 | 47 | 55 | | | 6 | 68 | 69 | | | | | | | | | | | | | | | |

TABLE 3

Bond lengths and their standard deviations (in parentheses) in Å

| | | | |
|---|---|---|---|
| Pt(1)–O(1) | 2·22(0·03) | Pt(2)–O(2) | 2·22(0·04) |
| Pt(1)–O(2) | 2·29(0·04) | Pt(2)–O(1) | 2·23(0·03) |
| Pt(1)–N(1) | 2·19(0·03) | Pt(2)–N(2) | 2·08(0·04) |
| Pt(1)–C(12) | 2·07(0·06) | Pt(2)–C(14) | 2·17(0·09) |
| Pt(2)–C(10) | 2·03(0·03) | Pt(2)–C(13) | 2·01(0·06) |
| Pt(1)–C(11) | 2·00(0·04) | Pt(2)–C(15) | 2·12(0·04) |
| O(1)–C(1) | 1·22(0·05) | O(2)–C(17) | 1·27(0·06) |
| C(1)–C(2) | 1·51(0·07) | C(17)–C(18) | 1·36(0·06) |
| C(2)–C(3) | 1·45(0·07) | C(18)–C(19) | 1·43(0·06) |
| C(3)–C(4) | 1·36(0·07) | C(19)–C(20) | 1·30(0·06) |
| C(4)–C(5) | 1·48(0·08) | C(20)–C(21) | 1·44(0·06) |
| C(5)–C(9) | 1·43(0·07) | C(21)–C(16) | 1·40(0·05) |
| C(9)–C(1) | 1·50(0·06) | C(16)–C(17) | 1·52(0·05) |
| C(5)–C(6) | 1·43(0·08) | C(21)–C(22) | 1·34(0·07) |
| C(6)–C(7) | 1·25(0·07) | C(22)–C(23) | 1·41(0·07) |
| C(7)–C(8) | 1·59(0·07) | C(23)–C(24) | 1·55(0·06) |
| C(8)–N(1) | 1·25(0·06) | C(24)–N(2) | 1·37(0·06) |
| C(9)–N(1) | 1·33(0·05) | C(16)–N(2) | 1·41(0·05) |

TABLE 4

Bond angles and their standard deviations

| | | | |
|---|---|---|---|
| At platinum (all ±1°) | | | |
| O(1)–Pt(1)–O(2) | 80° | O(2)–Pt(2)–O(1) | 81° |
| O(1)–Pt(1)–N(1) | 76 | O(2)–Pt(2)–N(2) | 75 |
| O(2)–Pt(1)–N(1) | 90 | O(1)–Pt(2)–N(2) | 90 |
| (all ±2°) | | | |
| C(10)–Pt(1)–C(12) | 85 | C(14)–Pt(2)–C(13) | 94 |
| C(11)–Pt(1)–C(12) | 85 | C(14)–Pt(2)–C(15) | 84 |
| C(10)–Pt(1)–C(11) | 90 | C(13)–Pt(2)–C(15) | 89 |
| O(1)–Pt(1)–C(10) | 96 | O(2)–Pt(2)–C(13) | 93 |
| O(1)–Pt(1)–C(11) | 98 | O(2)–Pt(2)–C(15) | 101 |
| O(2)–Pt(1)–C(12) | 99 | O(1)–Pt(2)–C(14) | 92 |
| O(2)–Pt(1)–C(11) | 91 | O(1)–Pt(2)–C(15) | 91 |
| N(1)–Pt(1)–C(12) | 102 | N(2)–Pt(2)–C(14) | 102 |
| N(1)–Pt(1)–C(10) | 89 | N(2)–Pt(2)–C(13) | 89 |
| At oxygen | | | |
| Pt(1)–O(1)–Pt(2) | 99 ± 1° | Pt(2)–O(2)–Pt(1) | 97 ± 1·5° |
| Pt(1)–O(1)–C(1) | 113 ± 3 | Pt(2)–O(2)–C(17) | 113 ± 3 |
| Pt(2)–O(1)–C(1) | 111 ± 3 | Pt(1)–O(2)–C(17) | 119 ± 3 |
| In the 8-quinolinolate groups (all ±4°) | | | |
| O(1)–C(1)–C(2) | 128° | O(2)–C(17)–C(18) | 122° |
| O(1)–C(1)–C(9) | 120 | O(2)–C(17)–C(16) | 119 |
| C(9)–C(1)–C(2) | 113 | C(16)–C(17)–C(18) | 118 |
| C(1)–C(2)–C(3) | 121 | C(17)–C(18)–C(19) | 120 |
| C(2)–C(3)–C(4) | 124 | C(18)–C(19)–C(20) | 121 |
| C(3)–C(4)–C(5) | 119 | C(19)–C(20)–C(21) | 124 |
| C(4)–C(5)–C(6) | 119 | C(20)–C(21)–C(22) | 130 |
| C(4)–C(5)–C(9) | 119 | C(20)–C(21)–C(16) | 117 |
| C(6)–C(5)–C(9) | 122 | C(22)–C(21)–C(16) | 114 |
| C(5)–C(6)–C(7) | 114 | C(21)–C(22)–C(23) | 128 |
| C(6)–C(7)–C(8) | 124 | C(22)–C(23)–C(24) | 109 |
| C(7)–C(8)–N(1) | 115 | C(23)–C(24)–N(2) | 127 |
| C(8)–N(1)–C(9) | 120 | C(24)–N(2)–C(16) | 109 |
| Pt(1)–N(1)–C(8) | 124 | Pt(2)–N(2)–C(24) | 129 |
| Pt(1)–N(1)–C(9) | 111 | Pt(2)–N(2)–C(16) | 119 |
| N(1)–C(9)–C(5) | 119 | N(2)–C(16)–C(21) | 131 |
| N(1)–C(9)–C(1) | 117 | N(2)–C(16)–C(17) | 109 |
| C(1)–C(9)–C(5) | 124 | C(17)–C(16)–C(21) | 120 |

TABLE 5

Deviations of the atoms from planes (Å)

Atoms included in calculating the plane:

| I | | II | | III | | IV | |
|---|---|---|---|---|---|---|---|
| O(1) | −0·08 | O(2) | +0·10 | C(10) | −0·20 | C(13) | −0·05 |
| N(1) | +0·10 | N(2) | −0·01 | C(12) | +0·02 | C(14) | +0·05 |
| C(1) | −0·01 | C(17) | −0·07 | O(1) | +0·01 | O(1) | −0·04 |
| C(2) | 0·00 | C(18) | −0·02 | O(2) | −0·01 | O(2) | +0·04 |
| C(3) | −0·03 | C(19) | −0·05 | | | | |
| C(4) | +0·03 | C(20) | +0·05 | | | | |
| C(5) | +0·02 | C(21) | 0·00 | | | | |
| C(6) | −0·01 | C(22) | −0·01 | | | | |
| C(7) | −0·12 | C(23) | +0·12 | | | | |
| C(8) | 0·00 | C(24) | −0·13 | | | | |
| C(9) | +0·10 | C(16) | +0·01 | | | | |

Atoms not included in calculating the plane:

| I | | II | | III | | IV | |
|---|---|---|---|---|---|---|---|
| Pt(1) | +0·41 | Pt(2) | −0·40 | Pt(1) | −0·03 | Pt(2) | −0·04 |
| Pt(2) | −2·19 | Pt(1) | +2·22 | | | | |

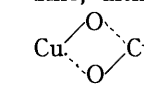
Equations of the planes

| | | | | |
|---|---|---|---|---|
| I | −0·749$X$ | −0·626$Y$ | −0·218$Z$ | +2·460 = 0 |
| II | −0·898$X$ | −0·178$Y$ | −0·403$Z$ | +3·169 = 0 |
| III | −0·392$X$ | +0·827$Y$ | −0·403$Z$ | −1·992 = 0 |
| IV | −0·275$X$ | +0·929$Y$ | −0·247$Z$ | −2·692 = 0 |

equivalent but crystallographically independent bonds; the average difference both in the light-atom–light-atom and the platinum–light-atom bond lengths is, as shown in Table 3, 0·07 Å, which is the same as the average standard deviation for the bonds involving only light atoms, but twice that for the platinum–light-atom bonds. This suggests, quite reasonably, that it is for the atoms directly attached to platinum that the parameter interaction is largest and for which the standard deviations have been underestimated by the block diagonal refinement.

The weighted mean Pt–C(methyl) bond length is 2·06 Å, in agreement with values found in other determinations;[1,2] the Pt–N bond length, 2·13 Å, is also the same as that found in $Me_3$ acac bipy Pt.[2] In several compounds (*e.g.*, dimolybdenum decachloride[8]) the bond length metal–X(bridging) has been found to be greater than metal–X(non-bridging). The Pt–O bond lengths in this complex appear to follow this trend, being 0·07 Å longer than those in the β-diketone complexes,[1] but the difference is not statistically significant. The ready fission of the Pt-O′ bond shown by the experiments of Kite and Truter[4] is not reflected in any significant difference between the Pt–O and the Pt–O′ bond lengths.

Other 8-hydroxyquinoline complexes have been studied in detail by Palenik.[9] He found the bond lengths in the chelated 8-quinolinolato-ligand to be the same in the β-form of anhydrous bis-(8-quinolinolato)copper(II) and in bis-(8-quinolinolato)diaquozinc, although in the former compound one 8-quinolinolate forms an unsymmetrical



Cu bridge while in the latter compound there is no bridging. Within our larger experimental error, the bond lengths in the 8-quinolinolate ligand, with a symmetrical bridge, are the same as those in the copper and zinc compounds. Palenik found that the oxygen taking part in bridging was displaced from the plane of the quinoline ring towards the second copper atom. From Table 5 it can be seen that there is apparently a similar effect but the displacements of the oxygen atoms are only three times their minimum standard deviations and the displacements of the other atoms do not follow a logical pattern in the halves of the dimer. The platinum atoms are undoubtedly not coplanar with the 8-quinolinolate ligands.

The strain in the formation of a four-membered ring is shared by the platinum and oxygen atoms; all have bond angles 10° less than the ideal values (90° at Pt and 109·5° at O). The angle at the platinum atom in the chelate ring, 75°, is also significantly less than 90°; comparison with other 8-quinolinolates[9] suggests that this results from the larger covalent radius of platinum, the N · · · O distance being similar in all the compounds. The angles involving the methyl groups are all 90°. As in the other trimethylplatinum complexes, the atom forms three short Pt–C bonds mutually at right angles, and three relatively longer bonds the angles among which are 90° or less.

## Experimental

The colourless crystals were prepared by Kite and Truter.[4] Microscopic investigation, particularly the appearance of etch pits indicated that they belonged to a polar crystal class. Preliminary examination by *X*-rays at room temperature gave the space group and approximate unit-cell dimensions from which the number of formula units was deduced.

For intensity measurements the crystal was cooled in a stream of gaseous nitrogen with an apparatus adapted from that described by Robertson.[10] No phase transformation took place on cooling. The temperature was measured from time to time and found to be 120° ± 5°K. Accurate values of the cell dimensions were obtained from Al-calibrated Weissenberg photographs. Equant crystals of side 0·17—0·19 mm. were used. Equi-inclination Weissenberg

[8] D. E. Sands and A. Zalkin, *Acta Cryst.*, 1959, **12**, 723.
[9] G. J. Palenik, *Acta Cryst.*, 1964, **17**, 687, 696.
[10] J. H. Robertson, *J. Sci. Instr.*, 1960, **37**, 41.

photographs were taken about the three principal axes up to 3*kl*, *h*5*l*, and *hk*6; 2152 of a possible 2624 reflections gave measurable intensities. Intensities were estimated visually with the aid of a calibration strip. Lorentz, polarisation, and absorption (as for a sphere of radius 0·09 mm.) corrections were applied, and then the individual layers were correlated to give a set of relative structure amplitudes; these calculations were carried out on the Leeds University Pegasus Computer with programmes written by J. G. F. Smith. The scale factor was one of the parameters in the refinement.

Structure factors and least-squares refinement calculations were carried out on the Pegasus computer with programmes written by Cruickshank and Pilling.[11] The function minimised was $R = \Sigma w(|F_o| - |F_c|)^2$ where the weighting factor, $w$, was $1/|F_o|$. For platinum we used the scattering factor of Thomas and Umeda,[12] corrected for the real part of the anomalous dispersion; [13] for the other atoms we used the Berghuis *et al.*[14] scattering factors, all for neutral atoms. Three dimensional Fourier difference syntheses were carried out on the computer.[11]

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[11] D. W. J. Cruickshank, D. E. Pilling, and (in part) A. Bujosa, F. M. Lovell, and M. R. Truter, in "Computing Methods and the Phase Problem in X-ray Crystal Analysis," Pergamon Press, London, 1961, p. 32.
[12] L. H. Thomas and K. Umeda, *J. Chem. Phys.*, 1957, **26**, 293.
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[14] J. Berghuis, I. M. Haanappel, M. Potters, B. O. Loopstra, C. H. MacGillavry, and A. L. Veenendaal, *Acta Cryst.*, 1955, **8**, 478.