and must await a more accurate determination of these compounds.

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# The Crystal Structure of Phenylcyclobutenedione*

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The crystal structure of phenylcyclobutenedione, $C_{10}H_6O_2$, has been determined by three-dimensional analysis of X-ray diffraction data. The crystals are monoclinic, space group $P2_1/c$, with

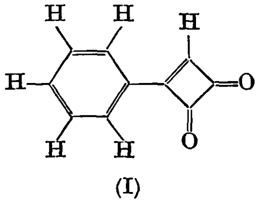
$$a = 6{\cdot}998 \pm 0{\cdot}005,\ b = 9{\cdot}287 \pm 0{\cdot}020,\ c = 12{\cdot}338 \pm 0{\cdot}005\ \text{Å};\ \beta = 103{\cdot}31 \pm 0{\cdot}30°.$$

The unit cell contains four molecules. The three-dimensional Patterson function led to a trial structure which was refined by difference maps and least-squares calculations.

The molecule is very nearly planar and lies close to the $(20\bar{1})$ plane. The bond distances suggest a considerable degree of conjugation between the benzene ring and the cyclobutenedione group, which is no doubt responsible for the stability of the compound.

## Introduction

Phenylcyclobutenedione, $C_{10}H_6O_2$ (I) was synthesized in these laboratories by Smutny & Roberts (1955). In view of the bond-angle strain associated with a four-membered ring, the phenylcyclobutenedione molecule is surprisingly stable; whereas cyclobutene itself decomposes at room temperature, phenylcyclobutenedione is stable up to 150 °C. This surprising stability and our general interest in the geometry of small-ring compounds have prompted this investigation.



(I)

## Experimental

Phenylcyclobutenedione crystallizes from acetone solution in the form of yellow monoclinic needles with the needle axis parallel to *a*. Rotation and multiple-film equi-inclination Weissenberg photographs were prepared for layer lines 0 through 6 about *a* and 0 through 8 about *b*, copper X-radiation being used. For the *a*-axis photographs, a needle-shaped crystal about 0·2 mm in diameter was selected; for the *b*-axis photographs a larger crystal was cleaved and shaped into roughly cylindrical form by means of acetone-soaked filter paper, the resulting specimen again being about 0·2 mm in diameter. The diffraction spots on the *b*-axis photographs were streaked, suggesting that the crystal had been damaged when cleaved. However, a careful comparison of intensities of equivalent reflections measured about the two axes showed no serious dis-

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crepancies; and, other than giving reduced weight to many of the intensities observed only about $b$, we did not worry further about the crystal damage.

All reflections within the copper sphere were recorded.* Of a total of about 1620 permitted by the space group, about 420 were too weak to be observed. Intensities were measured by visual comparison with a standard strip and were corrected for Lorentz and polarization effects. $F^2$ values from the various photographs were put on the same arbitrary scale by an averaging method.

At a late stage in the refinement, intensities from the $a$-axis photographs were re-estimated by a second, disinterested observer. Agreement with the original values was in general excellent, although a few discrepancies — obviously due to indexing errors — were noted on the fifth layer line. As a result of this re-estimation of intensities about 15 values of $F_o$ were changed and the weights of a few more were reduced.

The unit-cell dimensions $a$, $c$, and $\beta$ were determined from a Straumanis-type rotation photograph about $b$ taken with chromium radiation; the value for $b$ was obtained from an $0kl$ Weissenberg photograph for which the effective camera radius was obtained from the previously determined value of $c^*$. The resulting cell constants and estimated limits of error are:

$$a = 6{\cdot}998 \pm 0{\cdot}005,\ b = 9{\cdot}287 \pm 0{\cdot}020,$$
$$c = 12{\cdot}338 \pm 0{\cdot}005\ \text{Å};\ \beta = 103{\cdot}31 \pm 0{\cdot}30^\circ$$
$$(\lambda\ \text{Cr}\ K\alpha = 2{\cdot}2896\ \text{Å})\ .$$

The absence of reflections $0k0$ with $k$ odd and $h0l$ with $l$ odd indicates the space group $P2_1/c$. The density determined by flotation in mixed solvents is 1·348 g.cm$^{-3}$; the density calculated on the basis of four molecules in the unit cell is 1·346 g.cm$^{-3}$.

## Determination and refinement of the structure

Preliminary values for the scale factor and isotropic temperature factor were obtained from a Wilson plot, and a sharpened three-dimensional Patterson map, with the origin peak removed, was calculated. This map indicated that the molecules lie nearly parallel to the $20\bar{1}$ plane — that is, nearly perpendicular to the $a$ axis. With the help of some low-order structure factors the approximate position of the molecule projected onto (010) was soon found; because of serious overlap, however, no refinement of this projection was attempted.

After several fruitless attempts to determine the $y$ parameters from the $0kl$ reflections, the three-dimensional Patterson map was inspected more closely. For this purpose it was re-plotted in sections parallel to $(20\bar{1})$, so that all intramolecular vectors lay approximately in the zero section. Four tentative structures were found to be in general agreement with the Patterson map. Two of these were immediately discarded on the basis of packing considerations and the earlier $h0l$ calculations, and the remaining two differed only in the relative $y$ parameters of neighboring molecules. Structure factors for the $0kl$ reflections were calculated for both structures, leading to $R$ indices of 0·59 and 0·46; the structure with the higher $R$ index, however, showed better agreement for most of the low-order reflections and was selected as being probably correct. Three-dimensional refinement by Fourier and least-squares methods was then undertaken.

The initial refinement calculations were carried out in 1956 on an IBM 604 calculating punch and associated equipment. Positions of the 12 heavy atoms were adjusted by two structure-factor least-squares

Table 1. *The final parameters and their estimated standard deviations*

All values have been multiplied by $10^4$ except for the hydrogen atoms, whose values have been multiplied by $10^3$. The temperature factors are expressed in the form $T = \exp(-\alpha h^2 - \beta k^2 - \gamma l^2 - \delta hk - \varepsilon hl - \eta kl)$. The hydrogen atoms were assigned isotropic temperature factors with $B = 5$

| | $x$ | $y$ | $z$ | $\alpha$ | $\beta$ | $\gamma$ | $\delta$ | $\varepsilon$ | $\eta$ |
|---|---|---|---|---|---|---|---|---|---|
| C(1) | 1781(4) | 5352(3) | 3733(2) | 228(7) | 138(4) | 71(2) | −30(8) | 28(5) | 2(4) |
| C(2) | 1409(4) | 6664(4) | 3198(2) | 272(8) | 173(5) | 81(2) | 9(9) | 14(6) | 59(5) |
| C(3) | 1711(4) | 7936(3) | 3799(3) | 258(8) | 136(5) | 119(3) | 56(8) | 70(7) | 77(6) |
| C(4) | 2397(5) | 7886(3) | 4940(3) | 339(10) | 114(5) | 126(4) | 10(9) | 120(8) | −6(6) |
| C(5) | 2759(4) | 6584(3) | 5486(2) | 311(8) | 125(4) | 78(2) | −20(8) | 79(6) | −13(4) |
| C(6) | 2454(3) | 5295(3) | 4878(2) | 203(6) | 111(4) | 68(2) | −7(6) | 53(5) | 4(4) |
| C(7) | 2860(3) | 3909(3) | 5433(2) | 209(6) | 116(4) | 64(2) | −19(6) | 58(5) | −8(4) |
| C(8) | 3514(4) | 3468(3) | 6504(2) | 332(9) | 129(4) | 64(2) | −16(8) | 56(6) | 4(4) |
| C(9) | 3450(4) | 1932(3) | 6234(2) | 289(8) | 127(4) | 75(2) | −25(8) | 58(6) | 33(4) |
| C(10) | 2700(4) | 2384(3) | 5006(2) | 243(7) | 110(4) | 70(2) | −23(7) | 30(5) | −1(4) |
| O(1) | 3820(4) | 0805(2) | 6743(2) | 474(8) | 127(3) | 99(2) | 13(7) | 73(6) | 64(4) |
| O(2) | 2233(3) | 1791(2) | 4127(2) | 397(7) | 139(3) | 78(2) | −20(7) | −8(5) | −47(3) |
| H(1) | 160(5) | 439(5) | 334(3) | | | | | | |
| H(2) | 096(5) | 665(4) | 233(3) | | | | | | |
| H(3) | 144(5) | 889(4) | 344(3) | | | | | | |
| H(4) | 246(5) | 871(4) | 535(3) | | | | | | |
| H(5) | 323(5) | 656(4) | 627(3) | | | | | | |
| H(6) | 384(5) | 405(4) | 723(3) | | | | | | |

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* The copper X-ray tube was badly contaminated with iron. As a result, the intensities of many reflections on the fifth layer lines about the two axes — and in particular of all the $55l$ reflections — could be estimated only with extreme difficulty because of interference with 4th-order reflections involving the iron contaminant. Most of these reflections were given low weight in the least-squares refinements.

Table 2. *Observed and calculated structure factors*

The three columns within each group contain the values of $l$, $10F_o$ and $10F_c$.
Reflections indicated by an asterisk (*) were given zero weight in the least-squares calculations

| 0,0,l | | |
|---|---|---|
| 0 | --- | 3284 |
| 2 | 545* | 686 |
| 4 | 204 | -229 |
| 6 | 325 | 358 |
| 8 | 114 | 107 |
| 10 | 30 | 22 |
| 12 | <25 | 14 |
| 14 | <19 | 0 |

| 1,0,l | | |
|---|---|---|
| $\overline{14}$ | 45 | -43 |
| $\overline{12}$ | 80 | -78 |
| $\overline{10}$ | 53 | 48 |
| $\bar{8}$ | 197 | 208 |
| $\bar{6}$ | 80 | 76 |
| $\bar{4}$ | 34 | -35 |
| $\bar{2}$ | 53 | -58 |
| 0 | 145* | -141 |
| 2 | 83 | 80 |
| 4 | 49 | 52 |
| 6 | 216 | -246 |
| 8 | 144 | -143 |
| 10 | 34 | 37 |
| 12 | 71 | 64 |
| 14 | 20 | 27 |

| 2,0,l | | |
|---|---|---|
| $\overline{14}$ | <13 | 7 |
| $\overline{12}$ | <16 | -9 |
| $\overline{10}$ | 53 | -50 |
| $\bar{8}$ | 261 | -256 |
| $\bar{6}$ | 27 | 0 |
| $\bar{4}$ | 95 | 96 |
| $\bar{2}$ | 1362* | -1797 |
| 0 | 1090* | -1316 |
| 2 | 186 | 185 |
| 4 | 231 | -248 |
| 6 | 174 | -168 |
| 8 | <12 | -3 |
| 10 | 27 | -28 |
| 12 | <14 | -1 |

| 3,0,l | | |
|---|---|---|
| $\overline{14}$ | 57 | 56 |
| $\overline{12}$ | 27 | 23 |
| $\overline{10}$ | 83 | -85 |
| $\bar{8}$ | 72 | -78 |
| $\bar{6}$ | 38 | -37 |
| $\bar{4}$ | <10 | 5 |
| $\bar{2}$ | 231 | 231 |
| 0 | 30* | 20 |
| 2 | 102 | -99 |
| 4 | 121 | 131 |
| 6 | 140 | 143 |
| 8 | 30 | 26 |
| 10 | 53 | -51 |
| 12 | 24 | -27 |

| 4,0,l | | |
|---|---|---|
| $\overline{14}$ | 10 | -9 |
| $\overline{12}$ | 15 | 13 |
| $\overline{10}$ | 117 | 118 |
| $\bar{8}$ | 98 | 91 |
| $\bar{6}$ | 95 | -100 |
| $\bar{4}$ | 360 | 437 |
| $\bar{2}$ | 628* | 785 |
| 0 | 68 | 60 |
| 2 | 72 | 70 |
| 4 | 167 | 159 |
| 6 | 19 | 11 |
| 8 | <11 | 7 |

| 5,0,l | | |
|---|---|---|
| $\overline{14}$ | 35 | -28 |
| $\overline{12}$ | 11 | 15 |
| $\overline{10}$ | 34 | 28 |
| $\bar{8}$ | 38 | 38 |
| $\bar{6}$ | 34 | 33 |
| $\bar{4}$ | 117 | -111 |
| $\bar{2}$ | 83 | -75 |
| 0 | 34 | 35 |
| 2 | 64 | -50 |
| 4 | 91 | -85 |
| 6 | 38 | -38 |
| 8 | 19 | 22 |
| 10 | 19 | 23 |

| 6,0,l | | |
|---|---|---|
| $\overline{12}$ | 38 | -37 |
| $\overline{10}$ | 72 | -63 |
| $\bar{8}$ | <14 | 11 |
| $\bar{6}$ | 80 | -77 |
| $\bar{4}$ | 288 | -302 |
| $\bar{2}$ | 128 | -128 |
| 0 | <10 | -2 |
| 2 | 91 | -88 |
| 4 | 40 | -38 |
| 6 | <14 | 5 |
| 8 | <11 | 5 |

| 7,0,l | | |
|---|---|---|
| $\overline{10}$ | <24 | -13 |
| $\bar{8}$ | 23 | -26 |
| $\bar{6}$ | 28 | 33 |
| $\bar{4}$ | 47 | 54 |
| $\bar{2}$ | <19 | -1 |
| 0 | 16 | 24 |
| 2 | 47 | 47 |
| 4 | 26 | 26 |

| 8,0,l | | |
|---|---|---|
| $\bar{8}$ | 17 | 14 |
| $\bar{6}$ | 95 | 92 |
| $\bar{4}$ | 95 | 86 |
| $\bar{2}$ | <19 | 4 |
| 0 | 19 | 24 |
| 2 | 24 | 33 |

| 0,1,l | | |
|---|---|---|
| 1 | 261* | 354 |
| 2 | 493 | -553 |
| 3 | 197 | 210 |
| 4 | 360 | 429 |
| 5 | 98 | 91 |
| 6 | 125 | 128 |
| 7 | 98 | 91 |
| 8 | 163 | -167 |
| 9 | <24 | -4 |
| 10 | 68 | -64 |
| 11 | 72 | -76 |
| 12 | <25 | -14 |
| 13 | 19 | -17 |
| 14 | 24 | 19 |
| 15 | <19 | 10 |

| 1,1,l | | |
|---|---|---|
| $\overline{15}$ | <19 | 3 |
| $\overline{14}$ | 27 | -29 |
| $\overline{13}$ | 42 | -42 |
| $\overline{12}$ | 23 | -21 |
| $\overline{11}$ | <23 | -21 |
| $\overline{10}$ | 22 | -21 |
| $\bar{9}$ | 30 | -26 |
| $\bar{8}$ | 30 | -33 |
| $\bar{7}$ | 34 | 22 |
| $\bar{6}$ | 87 | 84 |
| $\bar{5}$ | 284 | 321 |
| $\bar{4}$ | 170 | 183 |
| $\bar{3}$ | 42 | -36 |
| $\bar{2}$ | 114 | -125 |
| $\bar{1}$ | 87 | -80 |
| 0 | 174 | -152 |
| 1 | 182 | 203 |
| 2 | 72 | 67 |
| 3 | 318 | -356 |
| 4 | 121 | 116 |
| 5 | 167 | -160 |
| 6 | 34 | 32 |
| 7 | 45 | 43 |
| 8 | <27 | -4 |
| 9 | <28 | 10 |
| 10 | <29 | -15 |
| 11 | 68 | 67 |
| 12 | 53 | -49 |
| 13 | <24 | 7 |
| 14 | <19 | -16 |

| 2,1,l | | |
|---|---|---|
| $\overline{15}$ | <10 | -3 |
| $\overline{14}$ | <13 | 4 |
| $\overline{13}$ | 49 | 46 |
| $\overline{12}$ | 15 | -20 |
| $\overline{11}$ | 38 | 41 |
| $\overline{10}$ | 83 | -86 |
| $\bar{9}$ | 30 | -36 |
| $\bar{8}$ | 19 | -21 |
| $\bar{7}$ | 80 | -73 |
| $\bar{6}$ | 238 | 269 |
| $\bar{5}$ | 159 | -166 |
| $\bar{4}$ | 87 | -79 |
| $\bar{3}$ | 151 | -150 |
| $\bar{2}$ | 144 | -171 |
| $\bar{1}$ | 265 | -311 |
| 0 | 537 | 642 |
| 1 | 212 | -204 |
| 2 | 140 | -136 |
| 3 | 49 | -41 |
| 4 | 269 | -290 |
| 5 | 87 | -82 |
| 6 | 117 | 124 |
| 7 | 64 | -57 |
| 8 | 117 | 114 |
| 9 | 64 | 63 |
| 10 | 38 | 43 |
| 11 | 38 | 38 |
| 12 | <14 | -5 |
| 13 | <28 | -3 |

| 3,1,l | | |
|---|---|---|
| $\overline{14}$ | 11 | 12 |
| $\overline{13}$ | 23 | 24 |
| $\overline{12}$ | <16 | 5 |
| $\overline{11}$ | <16 | 4 |
| $\overline{10}$ | 49 | 46 |
| $\bar{9}$ | <15 | 12 |
| $\bar{8}$ | <13 | 1 |
| $\bar{7}$ | 129 | -125 |
| $\bar{6}$ | 125 | -113 |
| $\bar{5}$ | 61 | -59 |
| $\bar{4}$ | 11 | 8 |
| $\bar{3}$ | 95 | 91 |
| $\bar{2}$ | 83 | 76 |
| $\bar{1}$ | 136 | -130 |
| 0 | 11 | 6 |
| 1 | 121 | 122 |
| 2 | 27 | -24 |
| 3 | 189 | 196 |
| 4 | 34 | -36 |
| 5 | <13 | 5 |
| 6 | 34 | -30 |
| 7 | <15 | -2 |
| 8 | <16 | -11 |
| 9 | 59 | -60 |
| 10 | 30 | 32 |
| 11 | 30 | -32 |
| 12 | 47 | 40 |
| 13 | <14 | 9 |

| 4,1,l | | |
|---|---|---|
| $\overline{15}$ | 13 | -15 |
| $\overline{14}$ | <10 | 5 |
| $\overline{13}$ | 34 | -32 |
| $\overline{12}$ | 30 | 26 |
| $\overline{11}$ | <12 | -1 |
| $\overline{10}$ | 30 | 27 |
| $\bar{9}$ | 42 | 39 |
| $\bar{8}$ | 98 | -91 |
| $\bar{7}$ | 83 | 81 |
| $\bar{6}$ | 38 | -36 |
| $\bar{5}$ | 72 | 67 |
| $\bar{4}$ | 106 | 102 |
| $\bar{3}$ | 129 | 133 |
| $\bar{2}$ | 265 | -272 |
| $\bar{1}$ | 178 | 166 |
| 0 | 148 | -152 |
| 1 | 19 | 15 |
| 2 | 174 | 187 |
| 3 | 30 | 25 |
| 4 | 11 | -3 |
| 5 | 68 | 63 |
| 6 | 106 | -101 |
| 7 | 19 | -19 |
| 8 | 53 | -53 |
| 9 | 34 | -33 |
| 10 | 15 | -18 |
| 11 | <9 | -9 |

| 5,1,l | | |
|---|---|---|
| $\overline{14}$ | <8 | 4 |
| $\overline{13}$ | <10 | -5 |
| $\overline{12}$ | 15 | -17 |
| $\overline{11}$ | <11 | -1 |
| $\overline{10}$ | 29 | -23 |
| $\bar{9}$ | 27 | 34 |
| $\bar{8}$ | 34 | 31 |
| $\bar{7}$ | 34 | 43 |
| $\bar{6}$ | 17 | 11 |
| $\bar{5}$ | 41 | -34 |
| $\bar{4}$ | 25 | -22 |
| $\bar{3}$ | 27 | 19 |
| $\bar{2}$ | 19 | 17 |
| $\bar{1}$ | <11 | 3 |
| 0 | 8 | -12 |
| 1 | 102 | -96 |
| 2 | <10 | -0 |
| 3 | 45 | -42 |
| 4 | 27 | 24 |
| 5 | <12 | -8 |
| 6 | 27 | 22 |
| 7 | 34 | 31 |
| 8 | 12 | 3 |
| 9 | 38 | 41 |
| 10 | 30 | -35 |

| 6,1,l | | |
|---|---|---|
| $\overline{13}$ | <10 | 9 |
| $\overline{12}$ | <13 | -10 |
| $\overline{11}$ | 15 | -16 |
| $\overline{10}$ | 19 | 26 |
| $\bar{9}$ | 38 | -39 |
| $\bar{8}$ | 30 | 31 |
| $\bar{7}$ | 34 | -30 |
| $\bar{6}$ | 45 | -38 |
| $\bar{5}$ | 57 | -52 |
| $\bar{4}$ | 75 | 60 |
| $\bar{3}$ | 114 | -103 |
| $\bar{2}$ | 148 | 144 |
| $\bar{1}$ | 38 | -29 |
| 0 | 34 | -30 |
| 1 | <12 | -0 |
| 2 | 34 | -35 |
| 3 | 34 | -32 |
| 4 | 49 | 50 |
| 5 | <15 | -5 |
| 6 | 38 | 39 |
| 7 | 13 | 13 |
| 8 | 14 | 22 |

| 7,1,l | | |
|---|---|---|
| $\overline{10}$ | <17 | -4 |
| $\bar{9}$ | <18 | -19 |
| $\bar{8}$ | <19 | -2 |
| $\bar{7}$ | <19 | 5 |
| $\bar{6}$ | <19 | 12 |
| $\bar{5}$ | <19 | 13 |
| $\bar{4}$ | <19 | -18 |
| $\bar{3}$ | <19 | -6 |
| $\bar{2}$ | <19 | -4 |
| $\bar{1}$ | 24 | 23 |
| 0 | <19 | 10 |
| 1 | 33 | 32 |
| 2 | <18 | -8 |
| 3 | <18 | 13 |
| 4 | <17 | -14 |

| 8,1,l | | |
|---|---|---|
| $\bar{9}$ | 23 | 15 |
| $\bar{8}$ | <19 | 6 |
| $\bar{7}$ | 19 | 17 |
| $\bar{6}$ | <19 | -4 |
| $\bar{5}$ | 43 | 47 |
| $\bar{4}$ | 47 | -61 |
| $\bar{3}$ | 28 | 32 |
| $\bar{2}$ | 24 | -25 |
| $\bar{1}$ | <19 | 1 |
| 0 | 19 | 17 |
| 1 | 19 | 10 |
| 2 | 19 | -15 |

| 0,2,l | | |
|---|---|---|
| 0 | 352* | -534 |
| 1 | 98 | -96 |
| 2 | 235 | -275 |
| 3 | 91 | -87 |
| 4 | 42 | 42 |
| 5 | 106 | -98 |
| 6 | 45 | 43 |
| 7 | <21 | -5 |
| 8 | 61 | -61 |
| 9 | <24 | 4 |
| 10 | 42 | -48 |
| 11 | 23 | 24 |
| 12 | 19 | -24 |
| 13 | 11 | -11 |
| 14 | 14 | -12 |

| 1,2,l | | |
|---|---|---|
| $\overline{14}$ | 34 | 32 |
| $\overline{13}$ | <27 | 7 |
| $\overline{12}$ | <28 | -10 |
| $\overline{11}$ | 80 | 83 |
| $\overline{10}$ | 106 | -105 |
| $\bar{9}$ | 49 | -43 |
| $\bar{8}$ | <11 | -2 |
| $\bar{7}$ | 30 | -33 |
| $\bar{6}$ | 27 | 25 |
| $\bar{5}$ | 114 | -112 |
| $\bar{4}$ | 53 | -49 |
| $\bar{3}$ | 159 | -181 |
| $\bar{2}$ | 110 | 116 |
| $\bar{1}$ | 310* | 398 |
| 0 | 61 | -51 |
| 1 | 30 | 29 |
| 2 | 38 | 38 |
| 3 | 140 | -140 |
| 4 | <15 | -6 |
| 5 | <15 | -2 |
| 6 | 57 | -58 |
| 7 | 102 | -103 |
| 8 | 132 | 124 |
| 9 | 49 | 54 |
| 10 | 80 | 78 |
| 11 | 53 | 53 |
| 12 | 34 | -35 |
| 13 | 23 | -19 |

| 2,2,l | | |
|---|---|---|
| $\overline{15}$ | 14 | -16 |
| $\overline{14}$ | <13 | 7 |
| $\overline{13}$ | <15 | 2 |
| $\overline{12}$ | 27 | 32 |
| $\overline{11}$ | <16 | -7 |
| $\overline{10}$ | 57 | 56 |
| $\bar{9}$ | 15 | -15 |
| $\bar{8}$ | <14 | 2 |
| $\bar{7}$ | 34 | -32 |
| $\bar{6}$ | 57 | -64 |
| $\bar{5}$ | 23 | -24 |
| $\bar{4}$ | 64 | 69 |
| $\bar{3}$ | 80 | -79 |
| $\bar{2}$ | 269 | 299 |
| $\bar{1}$ | 87 | -91 |
| 0 | 261 | 305 |
| 1 | 95 | 92 |
| 2 | 45 | 41 |
| 3 | 121 | 118 |
| 4 | 45 | -44 |
| 5 | 38 | 36 |
| 6 | 42 | 37 |
| 7 | <13 | 7 |
| 8 | 27 | 26 |
| 9 | 45 | -47 |
| 10 | 30 | 29 |
| 11 | <15 | -11 |
| 12 | 27 | 25 |
| 13 | 25 | 27 |

| 3,2,l | | |
|---|---|---|
| $\overline{14}$ | 19 | -15 |
| $\overline{13}$ | 42 | -43 |
| $\overline{12}$ | 42 | 45 |
| $\overline{11}$ | 19 | -16 |
| $\overline{10}$ | 28 | 25 |
| $\bar{9}$ | 27 | 26 |
| $\bar{8}$ | 27 | -19 |
| $\bar{7}$ | 38 | 35 |
| $\bar{6}$ | 30 | 31 |
| $\bar{5}$ | 148 | 146 |
| $\bar{4}$ | 34 | -38 |
| $\bar{3}$ | 83 | -87 |
| $\bar{2}$ | 42 | -39 |
| $\bar{1}$ | 125 | -132 |
| 0 | 19 | -20 |
| 1 | 72 | 66 |
| 2 | 38 | -38 |
| 3 | 38 | -39 |
| 4 | 72 | 72 |
| 5 | 64 | 61 |
| 6 | 61 | -56 |
| 7 | 23 | 17 |
| 8 | 117 | -115 |
| 9 | 64 | -66 |
| 10 | <15 | -1 |
| 11 | <13 | 8 |
| 12 | 16 | 13 |

| 4,2,l | | |
|---|---|---|
| $\overline{14}$ | 9 | -10 |
| $\overline{13}$ | 10 | 9 |
| $\overline{12}$ | 30 | -29 |
| $\overline{11}$ | 30 | 27 |
| $\overline{10}$ | 16 | -14 |
| $\bar{9}$ | 30 | 26 |
| $\bar{8}$ | 30 | 26 |
| $\bar{7}$ | 15 | -9 |
| $\bar{6}$ | 13 | 10 |
| $\bar{5}$ | 8 | -2 |
| $\bar{4}$ | 83 | -74 |
| $\bar{3}$ | 109 | 98 |
| $\bar{2}$ | 159 | -141 |
| $\bar{1}$ | 27 | -22 |
| 0 | 38 | -43 |
| 1 | 64 | -62 |
| 2 | 11 | 11 |
| 3 | 36 | -37 |
| 4 | 30 | -28 |
| 5 | 34 | -34 |
| 6 | <11 | -1 |
| 7 | 30 | 32 |
| 8 | <11 | -5 |
| 9 | 28 | 31 |
| 10 | 27 | -26 |
| 11 | 15 | -13 |

| 5,2,l | | |
|---|---|---|
| $\overline{14}$ | 8 | -9 |
| $\overline{13}$ | 21 | 23 |
| $\overline{12}$ | 19 | -19 |
| $\overline{11}$ | <11 | -10 |
| $\overline{10}$ | 11 | 11 |
| $\bar{9}$ | <11 | -11 |
| $\bar{8}$ | <11 | -4 |
| $\bar{7}$ | 49 | -49 |
| $\bar{6}$ | 15 | -9 |
| $\bar{5}$ | 28 | -25 |
| $\bar{4}$ | 28 | 22 |
| $\bar{3}$ | 59 | 53 |
| $\bar{2}$ | 27 | 20 |
| $\bar{1}$ | 15 | -9 |
| 0 | 42 | 41 |
| 1 | 29 | 28 |
| 2 | 27 | -22 |
| 3 | <10 | 9 |
| 4 | <11 | -2 |
| 5 | 28 | -26 |
| 6 | 86 | 76 |
| 7 | 35 | 32 |
| 8 | 36 | 34 |
| 9 | 10 | 8 |

| 6,2,l | | |
|---|---|---|
| $\overline{13}$ | 21 | -18 |
| $\overline{12}$ | <12 | 7 |
| $\overline{11}$ | 28 | -27 |
| $\overline{10}$ | 15 | -9 |
| $\bar{9}$ | <15 | 0 |
| $\bar{8}$ | 14 | -14 |
| $\bar{7}$ | 20 | 19 |
| $\bar{6}$ | <13 | 9 |
| $\bar{5}$ | 32 | -36 |
| $\bar{4}$ | 45 | 43 |
| $\bar{3}$ | 10 | -8 |
| $\bar{2}$ | 10 | 11 |
| $\bar{1}$ | 27 | 29 |
| 0 | 13 | -11 |
| 1 | 9 | 10 |
| 2 | 25 | 23 |
| 3 | 34 | 30 |
| 4 | <15 | 2 |
| 5 | <15 | -2 |
| 6 | 13 | -15 |
| 7 | 24 | -28 |
| 8 | 10 | 12 |

| 7,2,l | | |
|---|---|---|
| $\overline{10}$ | <16 | -5 |
| $\bar{9}$ | <18 | 11 |
| $\bar{8}$ | <19 | 7 |
| $\bar{7}$ | 24 | 20 |
| $\bar{6}$ | <19 | 0 |
| $\bar{5}$ | <19 | -3 |
| $\bar{4}$ | <19 | -10 |
| $\bar{3}$ | <19 | -3 |
| $\bar{2}$ | 24 | -21 |
| $\bar{1}$ | <19 | -6 |
| 0 | <19 | -9 |
| 1 | 22 | -22 |
| 2 | <19 | 7 |
| 3 | <19 | 1 |
| 4 | 26 | -27 |
| 5 | 8 | -8 |
| 6 | 33 | -32 |

| 8,2,l | | |
|---|---|---|
| $\bar{5}$ | <14 | 8 |
| $\bar{4}$ | <14 | 1 |
| $\bar{3}$ | 12 | -15 |
| $\bar{2}$ | 14 | 15 |
| $\bar{1}$ | <14 | -4 |
| 0 | <14 | -7 |
| 1 | 10 | -11 |
| 2 | <14 | -6 |

| 0,3,l | | |
|---|---|---|
| 1 | 272 | 341 |
| 2 | 201 | -217 |
| 3 | 131 | 128 |
| 4 | 87 | 84 |
| 5 | 182 | -191 |
| 6 | 110 | -106 |
| 7 | 76 | 71 |
| 8 | 61 | -63 |
| 9 | 220 | 227 |
| 10 | 25 | 27 |
| 11 | 62 | 60 |
| 12 | 21 | -16 |
| 13 | 13 | 9 |
| 14 | <17 | -8 |

| 1,3,l | | |
|---|---|---|
| $\overline{15}$ | 31 | -25 |
| $\overline{14}$ | 26 | 22 |
| $\overline{13}$ | 24 | 21 |
| $\overline{12}$ | 14 | 12 |
| $\overline{11}$ | 29 | -24 |
| $\overline{10}$ | 114 | 109 |
| $\bar{9}$ | 73 | -70 |
| $\bar{8}$ | 74 | 74 |
| $\bar{7}$ | 23 | 22 |
| $\bar{6}$ | 100 | -90 |
| $\bar{5}$ | 167 | -181 |
| $\bar{4}$ | 130 | 135 |
| $\bar{3}$ | 363 | -455 |
| $\bar{2}$ | 29 | 22 |
| $\bar{1}$ | 129 | -126 |
| 0 | 68 | -62 |
| 1 | 310 | 342 |
| 2 | 227 | 232 |
| 3 | 337 | 397 |
| 4 | 76 | -68 |
| 5 | 53 | 46 |
| 6 | 19 | 15 |
| 7 | 34 | 25 |
| 8 | 144 | 144 |
| 9 | 45 | 48 |
| 10 | 45 | 38 |
| 11 | 38 | -31 |
| 12 | 19 | 19 |
| 13 | 22 | 14 |
| 14 | 45 | 34 |

| 2,3,l | | |
|---|---|---|
| $\overline{15}$ | <9 | -7 |
| $\overline{14}$ | 19 | -16 |
| $\overline{13}$ | 15 | -17 |
| $\overline{12}$ | <16 | 2 |
| $\overline{11}$ | 136 | -142 |
| $\overline{10}$ | 42 | -39 |
| $\bar{9}$ | 151 | -150 |
| $\bar{8}$ | 98 | -105 |
| $\bar{7}$ | 80 | 87 |
| $\bar{6}$ | 27 | 26 |
| $\bar{5}$ | 57 | 59 |
| $\bar{4}$ | 91 | -98 |
| $\bar{3}$ | 201 | -198 |
| $\bar{2}$ | 155 | -149 |
| $\bar{1}$ | 227 | -223 |
| 0 | 151 | 155 |
| 1 | 254 | -263 |
| 2 | 61 | -55 |
| 3 | 87 | 91 |
| 4 | 49 | 46 |
| 5 | 53 | 54 |
| 6 | 80 | 80 |
| 7 | 201 | -200 |
| 8 | 45 | -43 |
| 9 | 98 | -105 |
| 10 | <16 | -2 |
| 11 | <15 | -9 |
| 12 | <13 | 9 |
| 13 | 38 | -33 |

| 3,3,l | | |
|---|---|---|
| $\overline{14}$ | <11 | -4 |
| $\overline{13}$ | <13 | -3 |
| $\overline{12}$ | 45 | -48 |
| $\overline{11}$ | 72 | 73 |
| $\overline{10}$ | 72 | -72 |
| $\bar{9}$ | 23 | 15 |
| $\bar{8}$ | 30 | 29 |
| $\bar{7}$ | 15 | 11 |
| $\bar{6}$ | 30 | -22 |
| $\bar{5}$ | 220 | 217 |
| $\bar{4}$ | 34 | -36 |
| $\bar{3}$ | 193 | 187 |
| $\bar{2}$ | 64 | 70 |
| $\bar{1}$ | 53 | -48 |
| 0 | 140 | -135 |
| 1 | 265 | -278 |
| 2 | 23 | -24 |
| 3 | 140 | -140 |
| 4 | 27 | 24 |
| 5 | 14 | -11 |
| 6 | 106 | -108 |
| 7 | 45 | -43 |
| 8 | 61 | -59 |
| 9 | <15 | 10 |
| 10 | 19 | -18 |
| 11 | 13 | 13 |
| 12 | 34 | -31 |

| 4,3,l | | |
|---|---|---|
| $\overline{14}$ | 8 | 6 |
| $\overline{13}$ | 53 | 52 |
| $\overline{12}$ | 27 | 23 |
| $\overline{11}$ | 117 | 111 |
| $\overline{10}$ | 72 | 68 |
| $\bar{9}$ | 30 | 16 |
| $\bar{8}$ | 27 | 25 |
| $\bar{7}$ | 53 | -55 |
| $\bar{6}$ | 27 | 23 |
| $\bar{5}$ | 45 | 45 |
| $\bar{4}$ | 102 | 97 |
| $\bar{3}$ | 95 | 83 |
| $\bar{2}$ | 19 | -20 |
| $\bar{1}$ | 136 | 140 |
| 0 | 8 | 9 |
| 1 | 42 | 41 |
| 2 | <9 | 0 |
| 3 | 64 | -61 |
| 4 | 61 | -59 |
| 5 | 106 | 102 |
| 6 | 30 | 27 |
| 7 | 114 | 110 |
| 8 | 19 | 20 |
| 9 | <10 | 5 |
| 10 | <9 | -4 |
| 11 | 31 | 25 |

| 5,3,l | | |
|---|---|---|
| $\overline{14}$ | 11 | 15 |
| $\overline{13}$ | 34 | -35 |
| $\overline{12}$ | 34 | 38 |
| $\overline{11}$ | 34 | -41 |
| $\overline{10}$ | <11 | 6 |
| $\bar{9}$ | <11 | 6 |
| $\bar{8}$ | <11 | -4 |
| $\bar{7}$ | 53 | -56 |
| $\bar{6}$ | 15 | 11 |
| $\bar{5}$ | 110 | -102 |
| $\bar{4}$ | 30 | -30 |
| $\bar{3}$ | 34 | -33 |
| $\bar{2}$ | 34 | 32 |
| $\bar{1}$ | 87 | 82 |
| 0 | 42 | 39 |
| 1 | 132 | 114 |
| 2 | <10 | -8 |
| 3 | 23 | 21 |
| 4 | 53 | 51 |
| 5 | 27 | 20 |
| 6 | 57 | 51 |
| 7 | 23 | 19 |
| 8 | 19 | 19 |
| 9 | 17 | -18 |
| 10 | 19 | 20 |

| 6,3,l | | |
|---|---|---|
| $\overline{13}$ | 49 | -46 |
| $\overline{12}$ | 38 | -34 |
| $\overline{11}$ | 34 | -35 |
| $\overline{10}$ | 30 | -31 |
| $\bar{9}$ | 15 | 15 |
| $\bar{8}$ | 15 | -14 |
| $\bar{7}$ | <15 | -3 |
| $\bar{6}$ | 34 | -35 |
| $\bar{5}$ | 27 | -30 |
| $\bar{4}$ | 23 | -20 |
| $\bar{3}$ | 38 | -39 |
| $\bar{2}$ | <12 | -4 |
| $\bar{1}$ | 45 | -46 |
| 0 | <13 | -4 |
| 1 | 19 | 18 |
| 2 | 27 | 25 |
| 3 | 38 | -32 |
| 4 | <15 | -7 |
| 5 | 83 | -80 |
| 6 | 19 | -19 |
| 7 | 15 | -11 |
| 8 | <9 | -3 |

| 7,3,l | | |
|---|---|---|
| $\overline{11}$ | 11 | 7 |
| $\overline{10}$ | <15 | 2 |
| $\bar{9}$ | <15 | 9 |
| $\bar{8}$ | <15 | 1 |
| $\bar{7}$ | 34 | 39 |
| $\bar{6}$ | 15 | 10 |
| $\bar{5}$ | 30 | 27 |
| $\bar{4}$ | <15 | -2 |
| $\bar{3}$ | 15 | -12 |
| $\bar{2}$ | 23 | -18 |
| $\bar{1}$ | 42 | -52 |
| 0 | <15 | -5 |
| 1 | 27 | -23 |
| 2 | 23 | -20 |
| 3 | <15 | -1 |
| 4 | 34 | -30 |
| 5 | 19 | -20 |
| 6 | 13 | -17 |

| 8,3,l | | |
|---|---|---|
| $\bar{8}$ | 13 | 11 |
| $\bar{7}$ | 11 | 11 |
| $\bar{6}$ | 15 | 13 |
| $\bar{5}$ | 12 | 11 |
| $\bar{4}$ | <11 | 6 |
| $\bar{3}$ | 19 | 19 |
| $\bar{2}$ | <11 | 0 |
| $\bar{1}$ | <11 | 2 |
| 0 | <11 | -8 |
| 1 | <11 | 5 |

| 0,4,l | | |
|---|---|---|
| 0 | 106 | -89 |
| 1 | 125 | 127 |
| 2 | 185 | 183 |
| 3 | 170 | -155 |
| 4 | 98 | 94 |
| 5 | 125 | -109 |
| 6 | 87 | 78 |
| 7 | 83 | 80 |
| 8 | 204 | 217 |
| 9 | 140 | -144 |
| 10 | 102 | 99 |
| 11 | 95 | -96 |
| 12 | 27 | 26 |
| 13 | 49 | 49 |
| 14 | 30 | 33 |

| 1,4,l | | |
|---|---|---|
| $\overline{14}$ | <19 | 8 |
| $\overline{13}$ | 23 | 23 |
| $\overline{12}$ | <27 | -4 |
| $\overline{11}$ | <28 | -11 |
| $\overline{10}$ | 83 | -87 |
| $\bar{9}$ | 57 | 59 |
| $\bar{8}$ | 110 | -107 |
| $\bar{7}$ | 193 | 194 |
| $\bar{6}$ | 27 | -23 |
| $\bar{5}$ | 72 | 55 |
| $\bar{4}$ | 151 | -139 |
| $\bar{3}$ | 45 | -44 |
| $\bar{2}$ | 235 | -235 |
| $\bar{1}$ | 19 | 20 |
| 0 | 114 | 132 |
| 1 | 76 | -76 |
| 2 | 208 | 204 |
| 3 | 34 | -34 |
| 4 | 27 | 18 |
| 5 | 182 | 194 |
| 6 | 64 | 64 |
| 7 | 140 | 132 |
| 8 | 102 | 102 |
| 9 | 27 | 20 |
| 10 | 34 | 33 |
| 11 | <27 | 5 |
| 12 | 17 | -15 |
| 13 | 19 | 17 |

| 2,4,l | | |
|---|---|---|
| $\overline{14}$ | 23 | -23 |
| $\overline{13}$ | 19 | -19 |
| $\overline{12}$ | 42 | -44 |
| $\overline{11}$ | 98 | -111 |
| $\overline{10}$ | 140 | -145 |
| $\bar{9}$ | 15 | 18 |
| $\bar{8}$ | 114 | -108 |
| $\bar{7}$ | 34 | -28 |
| $\bar{6}$ | 38 | -39 |
| $\bar{5}$ | 182 | -174 |
| $\bar{4}$ | 151 | -148 |
| $\bar{3}$ | 83 | 82 |
| $\bar{2}$ | 27 | 22 |
| $\bar{1}$ | 11 | 7 |
| 0 | 72 | -68 |
| 1 | 72 | 69 |
| 2 | 136 | -135 |
| 3 | 155 | 151 |
| 4 | 23 | -21 |
| 5 | 95 | -101 |
| 6 | 174 | -187 |
| 7 | 68 | 73 |
| 8 | 140 | -155 |
| 9 | 155 | 167 |
| 10 | 34 | -34 |
| 11 | 15 | -15 |
| 12 | 30 | -31 |
| 13 | 47 | -41 |

| 3,4,l | | |
|---|---|---|
| $\overline{14}$ | <16 | -5 |
| $\overline{13}$ | <19 | 1 |
| $\overline{12}$ | 38 | 40 |
| $\overline{11}$ | <15 | -8 |
| $\overline{10}$ | 95 | 94 |
| $\bar{9}$ | 106 | -106 |
| $\bar{8}$ | 49 | 42 |
| $\bar{7}$ | 72 | -70 |
| $\bar{6}$ | 61 | 57 |
| $\bar{5}$ | 19 | 16 |
| $\bar{4}$ | 182 | 171 |
| $\bar{3}$ | 53 | -54 |
| $\bar{2}$ | <15 | 6 |
| $\bar{1}$ | 38 | 33 |
| 0 | 148 | -139 |
| 1 | 57 | 65 |
| 2 | 53 | -44 |
| 3 | 76 | -67 |
| 4 | <14 | -13 |
| 5 | 117 | -122 |
| 6 | 61 | -59 |
| 7 | 72 | -74 |
| 8 | 49 | -51 |
| 9 | 19 | -10 |
| 10 | 15 | 10 |
| 11 | <11 | -3 |
| 12 | <9 | 14 |

| 4,4,l | | |
|---|---|---|
| $\overline{14}$ | 23 | 19 |
| $\overline{13}$ | 45 | 49 |
| $\overline{12}$ | 61 | 64 |
| $\overline{11}$ | 27 | 16 |
| $\overline{10}$ | 83 | 82 |
| $\bar{9}$ | 15 | -13 |
| $\bar{8}$ | 30 | 26 |
| $\bar{7}$ | 98 | 95 |
| $\bar{6}$ | 57 | 54 |
| $\bar{5}$ | 28 | 29 |
| $\bar{4}$ | 42 | 29 |
| $\bar{3}$ | 49 | -44 |
| $\bar{2}$ | <19 | 6 |
| $\bar{1}$ | 49 | -43 |
| 0 | 102 | 90 |
| 1 | 129 | -120 |
| 2 | 14 | 11 |
| 3 | 42 | 41 |
| 4 | 87 | 86 |
| 5 | 23 | 19 |
| 6 | 144 | 144 |
| 7 | 144 | -136 |
| 8 | 53 | 51 |
| 9 | 38 | -41 |
| 10 | 23 | 21 |
| 11 | 33 | 35 |

| 5,4,l | | |
|---|---|---|
| $\overline{13}$ | <19 | -2 |
| $\overline{12}$ | 66 | -53 |
| $\overline{11}$ | 42 | 43 |
| $\overline{10}$ | 57 | -42 |
| $\bar{9}$ | 49 | 46 |
| $\bar{8}$ | 27 | -26 |
| $\bar{7}$ | 11 | -8 |
| $\bar{6}$ | 83 | -83 |
| $\bar{5}$ | 30 | 29 |
| $\bar{4}$ | 42 | -47 |
| $\bar{3}$ | 19 | 18 |
| $\bar{2}$ | 63 | 51 |
| $\bar{1}$ | 19 | -21 |
| 0 | 49 | 48 |
| 1 | <10 | -4 |
| 2 | <11 | 6 |
| 3 | 49 | 43 |
| 4 | <11 | 12 |
| 5 | 80 | 74 |
| 6 | 30 | 36 |
| 7 | 30 | 33 |
| 8 | <10 | 4 |
| 9 | <8 | -2 |

| 6,4,l | | |
|---|---|---|
| $\overline{12}$ | 45 | -40 |
| $\overline{11}$ | <12 | 9 |
| $\overline{10}$ | 19 | -22 |
| $\bar{9}$ | 27 | -25 |
| $\bar{8}$ | 15 | -11 |
| $\bar{7}$ | 42 | -43 |
| $\bar{6}$ | 15 | -17 |
| $\bar{5}$ | <14 | 5 |
| $\bar{4}$ | <14 | -4 |
| $\bar{3}$ | 30 | 29 |
| $\bar{2}$ | 38 | -36 |
| $\bar{1}$ | 68 | 68 |
| 0 | 19 | -18 |
| 1 | 15 | 14 |
| 2 | 27 | -22 |
| 3 | 34 | -34 |
| 4 | 83 | -81 |
| 5 | 53 | 55 |
| 6 | 49 | -53 |
| 7 | 52 | 55 |

| 7,4,l | | |
|---|---|---|
| $\bar{8}$ | 36 | 32 |
| $\bar{7}$ | <12 | -3 |
| $\bar{6}$ | 38 | 35 |
| $\bar{5}$ | 11 | -18 |
| $\bar{4}$ | <13 | -7 |
| $\bar{3}$ | <13 | -8 |
| $\bar{2}$ | 19 | -26 |
| $\bar{1}$ | <13 | 2 |
| 0 | <13 | -12 |
| 1 | <13 | 1 |
| 2 | <13 | 3 |
| 3 | 34 | -35 |
| 4 | <11 | -12 |
| 5 | 34 | -36 |

| 8,4,l | | |
|---|---|---|
| $\bar{8}$ | <11 | 2 |
| $\bar{7}$ | <12 | 10 |
| $\bar{6}$ | <13 | 3 |
| $\bar{5}$ | <13 | -10 |
| $\bar{4}$ | 10 | 11 |
| $\bar{3}$ | 28 | -28 |
| $\bar{2}$ | <19 | 13 |
| $\bar{1}$ | 24 | -22 |
| 0 | <13 | 5 |

| 0,5,l | | |
|---|---|---|
| 1 | 212 | -209 |
| 2 | 114 | -118 |
| 3 | 132 | -130 |
| 4 | 155 | -139 |
| 5 | 148 | 147 |
| 6 | 27 | -20 |
| 7 | <23 | 6 |
| 8 | <23 | -0 |
| 9 | 87 | -80 |
| 10 | 23 | -24 |
| 11 | 24 | 21 |
| 12 | <21 | -5 |
| 13 | <17 | 10 |

| 1,5,l | | |
|---|---|---|
| $\overline{14}$ | 19 | 17 |
| $\overline{13}$ | 19 | 15 |
| $\overline{12}$ | 27 | -25 |
| $\overline{11}$ | 42 | -40 |
| $\overline{10}$ | 35 | 33 |
| $\bar{9}$ | 64 | -62 |
| $\bar{8}$ | 80 | 73 |
| $\bar{7}$ | 27 | -22 |
| $\bar{6}$ | 106 | -104 |
| $\bar{5}$ | 43 | -42 |
| $\bar{4}$ | 72 | -65 |
| $\bar{3}$ | 68 | 68 |
| $\bar{2}$ | 68 | 61 |
| $\bar{1}$ | 42 | 38 |
| 0 | 72 | 63 |
| 1 | 49 | -53 |
| 2 | 27 | 26 |
| 3 | <24 | 10 |
| 4 | 148 | -150 |
| 5 | <27 | -3 |
| 6 | <27 | 10 |
| 7 | 53 | 54 |
| 8 | 83 | 72 |
| 9 | 83 | 76 |
| 10 | 45 | -35 |
| 11 | <26 | -3 |
| 12 | <22 | 8 |
| 13 | 28 | -22 |

| 2,5,l | | |
|---|---|---|
| $\overline{13}$ | 30 | -26 |
| $\overline{12}$ | 15 | -12 |
| $\overline{11}$ | 38 | 41 |
| $\overline{10}$ | 15 | -14 |
| $\bar{9}$ | 49 | 54 |
| $\bar{8}$ | 19 | 19 |
| $\bar{7}$ | 102 | -98 |
| $\bar{6}$ | 49 | -42 |
| $\bar{5}$ | 15 | 15 |
| $\bar{4}$ | 121 | -115 |
| $\bar{3}$ | 151 | 150 |
| $\bar{2}$ | 23 | -28 |
| $\bar{1}$ | 159 | 150 |
| 0 | 34 | 35 |
| 1 | 167 | 180 |
| 2 | 140 | 142 |
| 3 | 72 | -73 |
| 4 | 91 | 91 |
| 5 | 83 | -76 |
| 6 | <16 | 4 |
| 7 | 57 | 64 |
| 8 | 23 | 26 |
| 9 | <16 | -7 |
| 10 | 19 | 20 |
| 11 | 15 | -16 |

| 3,5,l | | |
|---|---|---|
| $\overline{13}$ | 13 | 14 |
| $\overline{12}$ | <13 | 2 |
| $\overline{11}$ | 38 | 36 |
| $\overline{10}$ | 64 | -65 |
| $\bar{9}$ | 23 | 26 |
| $\bar{8}$ | <16 | 5 |
| $\bar{7}$ | 49 | 45 |
| $\bar{6}$ | 80 | 72 |
| $\bar{5}$ | <14 | -9 |
| $\bar{4}$ | 15 | -24 |
| $\bar{3}$ | 45 | -51 |
| $\bar{2}$ | 42 | -39 |
| $\bar{1}$ | 13 | -9 |
| 0 | 61 | -57 |
| 1 | 19 | -16 |
| 2 | 80 | 77 |
| 3 | 15 | 14 |
| 4 | 45 | 44 |
| 5 | <15 | -15 |
| 6 | 72 | -69 |
| 7 | 80 | -74 |
| 8 | 19 | 17 |
| 9 | 23 | -19 |
| 10 | 15 | 17 |
| 11 | 15 | 15 |

| 4,5,l | | |
|---|---|---|
| $\overline{12}$ | 15 | 15 |
| $\overline{11}$ | 42 | -43 |
| $\overline{10}$ | <11 | -9 |
| $\bar{9}$ | 27 | 24 |
| $\bar{8}$ | <11 | -9 |
| $\bar{7}$ | 30 | 23 |
| $\bar{6}$ | 53 | 47 |
| $\bar{5}$ | 68 | -66 |
| $\bar{4}$ | 30 | 26 |
| $\bar{3}$ | 80 | -73 |
| $\bar{2}$ | <10 | 2 |
| $\bar{1}$ | 114 | -101 |
| 0 | 64 | -65 |
| 1 | <10 | -6 |
| 2 | 106 | -99 |
| 3 | 68 | 63 |
| 4 | 27 | -22 |
| 5 | 19 | -18 |
| 6 | 19 | -17 |
| 7 | <10 | 1 |
| 8 | 38 | -36 |
| 9 | 27 | 24 |

| 5,5,l | | |
|---|---|---|
| $\overline{12}$ | 24 | 25 |
| $\overline{11}$ | 10 | -17 |
| $\overline{10}$ | 33 | 31 |
| $\bar{9}$ | 24 | -25 |
| $\bar{8}$ | 25 | -25 |
| $\bar{7}$ | 20 | -16 |
| $\bar{6}$ | 13 | -12 |
| $\bar{5}$ | 11 | 15 |
| $\bar{4}$ | 24 | 25 |
| $\bar{3}$ | 19 | 19 |
| $\bar{2}$ | 34 | 31 |
| $\bar{1}$ | 34 | 30 |
| 0 | 38 | -14 |
| 1 | <19 | 3 |
| 2 | 37 | -39 |
| 3 | <11 | -2 |
| 4 | 35 | 36 |
| 5 | 38 | 40 |
| 6 | <10 | 11 |
| 7 | 25 | 24 |
| 8 | 25 | -26 |

| 6,5,l | | |
|---|---|---|
| $\overline{11}$ | <10 | 3 |
| $\overline{10}$ | 15 | 12 |
| $\bar{9}$ | 15 | -16 |
| $\bar{8}$ | <24 | -8 |
| $\bar{7}$ | 15 | 21 |
| $\bar{6}$ | 15 | -13 |
| $\bar{5}$ | 34 | 37 |
| $\bar{4}$ | <15 | -3 |
| $\bar{3}$ | 34 | 36 |
| $\bar{2}$ | <15 | 8 |
| $\bar{1}$ | 11 | 13 |
| 0 | 61 | 55 |
| 1 | 27 | -26 |
| 2 | 30 | 28 |
| 3 | <14 | -3 |
| 4 | <13 | 6 |
| 5 | <12 | -1 |
| 6 | 38 | 34 |
| 7 | 24 | -23 |

| 0,6,l | | |
|---|---|---|
| 0 | 125 | 125 |
| 1 | 57 | 51 |
| 2 | 42 | 34 |
| 3 | 34 | 24 |
| 4 | 129 | -120 |
| 5 | 30 | -31 |
| 6 | 102 | -93 |
| 7 | 23 | 20 |
| 8 | <26 | -7 |
| 9 | 34 | 34 |
| 10 | 10 | -12 |
| 11 | <21 | -7 |
| 12 | <18 | -8 |
| 13 | 24 | -19 |

| 1,6,l | | |
|---|---|---|
| $\overline{13}$ | <17 | -1 |
| $\overline{12}$ | 23 | -21 |
| $\overline{11}$ | 28 | -20 |
| $\overline{10}$ | 68 | 58 |
| $\bar{9}$ | 45 | 37 |
| $\bar{8}$ | 23 | -19 |
| $\bar{7}$ | 49 | 51 |
| $\bar{6}$ | 23 | -11 |
| $\bar{5}$ | 64 | -57 |
| $\bar{4}$ | 34 | 27 |
| $\bar{3}$ | 27 | 17 |
| $\bar{2}$ | 125 | -117 |
| $\bar{1}$ | 178 | 173 |
| 0 | 76 | 74 |
| 1 | 98 | 89 |
| 2 | 42 | 38 |
| 3 | 49 | -53 |
| 4 | 19 | 9 |
| 5 | <28 | 11 |
| 6 | 80 | 67 |
| 7 | 53 | 53 |
| 8 | 64 | -64 |
| 9 | 11 | -12 |
| 10 | 11 | -17 |
| 11 | <14 | -4 |
| 12 | 47 | 47 |

| 2,6,l | | |
|---|---|---|
| $\overline{13}$ | 15 | -13 |
| $\overline{12}$ | 10 | 7 |
| $\overline{11}$ | <15 | 11 |
| $\overline{10}$ | <15 | -3 |
| $\bar{9}$ | 15 | 14 |
| $\bar{8}$ | 38 | 40 |
| $\bar{7}$ | 15 | -16 |
| $\bar{6}$ | 98 | 102 |
| $\bar{5}$ | <15 | 7 |
| $\bar{4}$ | 49 | 47 |
| $\bar{3}$ | 27 | 28 |
| $\bar{2}$ | 68 | -66 |
| $\bar{1}$ | 61 | -58 |
| 0 | 87 | -97 |
| 1 | 57 | -60 |
| 2 | 53 | 55 |
| 3 | 30 | 30 |
| 4 | 98 | 98 |
| 5 | <16 | -3 |
| 6 | 19 | 17 |
| 7 | 42 | -47 |
| 8 | 23 | 23 |
| 9 | <15 | -10 |
| 10 | 13 | 9 |
| 11 | 24 | 17 |
| 12 | <7 | -3 |

| 3,6,l | | |
|---|---|---|
| $\overline{13}$ | 16 | 15 |
| $\overline{12}$ | 16 | -19 |
| $\overline{11}$ | <13 | -8 |
| $\overline{10}$ | <15 | -7 |
| $\bar{9}$ | 53 | -53 |
| $\bar{8}$ | 15 | 14 |
| $\bar{7}$ | <16 | 9 |
| $\bar{6}$ | 49 | -47 |
| $\bar{5}$ | 23 | 23 |
| $\bar{4}$ | 47 | 39 |
| $\bar{3}$ | 102 | -89 |
| $\bar{2}$ | 19 | 14 |
| $\bar{1}$ | 102 | -98 |
| 0 | 49 | -51 |
| 1 | <15 | 4 |
| 2 | <15 | -10 |
| 3 | 19 | 11 |
| 4 | 80 | -79 |
| 5 | 34 | -38 |
| 6 | 15 | 15 |
| 7 | <15 | -2 |
| 8 | 45 | 45 |
| 9 | 15 | 11 |
| 10 | 40 | -38 |

| 4,6,l | | |
|---|---|---|
| $\overline{12}$ | <8 | 2 |
| $\overline{11}$ | <10 | -3 |
| $\overline{10}$ | <10 | -9 |
| $\bar{9}$ | 11 | 11 |
| $\bar{8}$ | 42 | -41 |
| $\bar{7}$ | <15 | -2 |
| $\bar{6}$ | 57 | -62 |
| $\bar{5}$ | 15 | -16 |
| $\bar{4}$ | <15 | -4 |
| $\bar{3}$ | 34 | 35 |
| $\bar{2}$ | 72 | 70 |
| $\bar{1}$ | 68 | 69 |
| 0 | <11 | -1 |
| 1 | <11 | 2 |
| 2 | 57 | -54 |
| 3 | 11 | -12 |
| 4 | 11 | -7 |
| 5 | 30 | 32 |
| 6 | 19 | -20 |
| 7 | 19 | 21 |
| 8 | 15 | -15 |
| 9 | <7 | -7 |

| 5,6,l | | |
|---|---|---|
| $\overline{12}$ | <6 | 6 |
| $\overline{11}$ | 23 | 26 |
| $\overline{10}$ | 10 | -11 |
| $\bar{9}$ | 19 | 17 |
| $\bar{8}$ | 19 | 20 |
| $\bar{7}$ | <15 | -12 |
| $\bar{6}$ | 19 | 16 |
| $\bar{5}$ | 30 | 30 |
| $\bar{4}$ | 19 | -19 |
| $\bar{3}$ | 61 | 60 |
| $\bar{2}$ | 19 | 29 |
| $\bar{1}$ | 19 | 21 |
| 0 | 15 | 13 |
| 1 | <11 | -5 |
| 2 | 42 | 46 |
| 3 | 19 | 17 |
| 4 | 23 | 22 |
| 5 | 10 | 10 |
| 6 | 33 | -29 |
| 7 | 10 | -11 |
| 8 | 17 | 14 |

| 6,6,l | | |
|---|---|---|
| $\overline{10}$ | 10 | 10 |
| $\bar{9}$ | <12 | -2 |
| $\bar{8}$ | 15 | 22 |
| $\bar{7}$ | <14 | 8 |
| $\bar{6}$ | 15 | 19 |
| $\bar{5}$ | 11 | -12 |
| $\bar{4}$ | 23 | -25 |
| $\bar{3}$ | 42 | -44 |
| $\bar{2}$ | 15 | -13 |
| $\bar{1}$ | 23 | -21 |
| 0 | 23 | 22 |
| 1 | <14 | 7 |
| 2 | <14 | -4 |
| 3 | 11 | -13 |
| 4 | <12 | 4 |
| 5 | 22 | -17 |
| 6 | 14 | 13 |

| 7,6,l | | |
|---|---|---|
| $\bar{8}$ | 11 | -15 |
| $\bar{7}$ | <11 | -9 |
| $\bar{6}$ | <12 | 0 |
| $\bar{5}$ | 22 | -28 |
| $\bar{4}$ | <14 | -1 |
| $\bar{3}$ | 17 | -19 |
| $\bar{2}$ | <14 | -12 |
| $\bar{1}$ | <14 | -2 |
| 0 | 19 | -19 |
| 1 | <13 | -5 |
| 2 | 23 | -20 |

| 0,7,l | | |
|---|---|---|
| 1 | 238 | 221 |
| 2 | 19 | -19 |
| 3 | 57 | -59 |
| 4 | 76 | 82 |
| 5 | 53 | 57 |
| 6 | 114 | 104 |
| 7 | 91 | 87 |
| 8 | 19 | -20 |
| 9 | <24 | 2 |
| 10 | 53 | -44 |
| 11 | <19 | 4 |
| 12 | <13 | -10 |

| 1,7,l | | |
|---|---|---|
| $\overline{12}$ | <18 | -1 |
| $\overline{11}$ | 38 | -32 |
| $\overline{10}$ | <26 | -4 |
| $\bar{9}$ | 42 | 37 |
| $\bar{8}$ | 24 | 25 |
| $\bar{7}$ | <28 | 16 |
| $\bar{6}$ | 129 | 133 |
| $\bar{5}$ | 49 | -37 |
| $\bar{4}$ | 117 | 102 |
| $\bar{3}$ | 64 | 67 |
| $\bar{2}$ | 125 | 114 |
| $\bar{1}$ | 10 | 12 |
| 0 | 155 | 145 |
| 1 | 83 | -78 |
| 2 | 87 | 76 |
| 3 | <28 | 21 |
| 4 | 121 | 133 |
| 5 | <29 | 3 |
| 6 | 64 | 69 |
| 7 | 53 | -57 |
| 8 | <27 | 8 |
| 9 | <26 | 12 |
| 10 | <23 | 9 |
| 11 | 33 | 36 |

| 2,7,l | | |
|---|---|---|
| $\overline{12}$ | 27 | -24 |
| $\overline{11}$ | <12 | 6 |
| $\overline{10}$ | 30 | -30 |
| $\bar{9}$ | 49 | -46 |
| $\bar{8}$ | 42 | 41 |
| $\bar{7}$ | 80 | -76 |
| $\bar{6}$ | 64 | 67 |
| $\bar{5}$ | 42 | 44 |
| $\bar{4}$ | <16 | -8 |
| $\bar{3}$ | 95 | -92 |
| $\bar{2}$ | 19 | -16 |
| $\bar{1}$ | 235 | -243 |
| 0 | 34 | 34 |
| 1 | <14 | 1 |
| 2 | 45 | -47 |
| 3 | <16 | -2 |
| 4 | 125 | -139 |
| 5 | 87 | -92 |
| 6 | 27 | -30 |
| 7 | 19 | -18 |
| 8 | 45 | 47 |
| 9 | <13 | -6 |
| 10 | 23 | 23 |
| 11 | <8 | -3 |

| 3,7,l | | |
|---|---|---|
| $\overline{12}$ | <10 | 3 |
| $\overline{11}$ | <11 | -9 |
| $\overline{10}$ | <13 | 5 |
| $\bar{9}$ | 23 | -18 |
| $\bar{8}$ | 72 | -70 |
| $\bar{7}$ | 30 | 27 |
| $\bar{6}$ | 98 | -93 |
| $\bar{5}$ | 30 | -31 |
| $\bar{4}$ | 83 | -74 |
| $\bar{3}$ | 27 | -24 |
| $\bar{2}$ | 132 | -130 |
| $\bar{1}$ | 61 | 55 |
| 0 | 76 | -75 |
| 1 | <16 | 4 |
| 2 | 72 | -72 |
| 3 | <16 | -12 |
| 4 | 64 | -69 |
| 5 | 45 | 44 |
| 6 | 27 | -25 |
| 7 | 11 | 15 |
| 8 | 23 | -21 |
| 9 | 25 | -29 |

| 4,7,l | | |
|---|---|---|
| $\overline{12}$ | 15 | 18 |
| $\overline{11}$ | 14 | 14 |
| $\overline{10}$ | <9 | -8 |
| $\bar{9}$ | 53 | 49 |
| $\bar{8}$ | 38 | -36 |
| $\bar{7}$ | <10 | -5 |
| $\bar{6}$ | <11 | 2 |
| $\bar{5}$ | 11 | 11 |
| $\bar{4}$ | 30 | 30 |
| $\bar{3}$ | 151 | 144 |
| $\bar{2}$ | 15 | -17 |
| $\bar{1}$ | 64 | 56 |
| 0 | <11 | -3 |
| 1 | 19 | -20 |
| 2 | 98 | 98 |
| 3 | 53 | 52 |
| 4 | 64 | 69 |
| 5 | 30 | 29 |
| 6 | 19 | -19 |
| 7 | <9 | 4 |
| 8 | 23 | -25 |

| 5,7,l | | |
|---|---|---|
| $\overline{10}$ | 19 | 23 |
| $\bar{9}$ | 9 | -13 |
| $\bar{8}$ | 45 | 54 |
| $\bar{7}$ | <10 | 6 |
| $\bar{6}$ | 34 | 41 |
| $\bar{5}$ | 15 | 19 |
| $\bar{4}$ | 76 | 74 |
| $\bar{3}$ | 27 | -26 |
| $\bar{2}$ | 76 | 76 |
| $\bar{1}$ | 15 | -12 |
| 0 | 38 | 37 |
| 1 | <11 | 6 |
| 2 | 34 | 33 |
| 3 | 18 | -20 |
| 4 | 20 | 22 |
| 5 | 20 | -20 |
| 6 | 21 | 22 |

| 6,7,l | | |
|---|---|---|
| $\bar{9}$ | <9 | -8 |
| $\bar{8}$ | <10 | 5 |
| $\bar{7}$ | <12 | 5 |
| $\bar{6}$ | 23 | -23 |
| $\bar{5}$ | 49 | -51 |
| $\bar{4}$ | <13 | -9 |
| $\bar{3}$ | 53 | -53 |
| $\bar{2}$ | <14 | 14 |
| $\bar{1}$ | <13 | 7 |
| 0 | 41 | -38 |
| 1 | <13 | -13 |
| 2 | 58 | -58 |
| 3 | 23 | -24 |
| 4 | <10 | -9 |

| 7,7,l | | |
|---|---|---|
| $\bar{5}$ | <15 | 9 |
| $\bar{4}$ | 47 | -49 |
| $\bar{3}$ | <17 | 9 |
| $\bar{2}$ | 22 | -29 |
| $\bar{1}$ | <15 | -1 |

| 0,8,l | | |
|---|---|---|
| 0 | 95 | -92 |
| 1 | 110 | -122 |
| 2 | 42 | 36 |
| 3 | 27 | -19 |
| 4 | 114 | 110 |
| 5 | 114 | 108 |
| 6 | 27 | 24 |
| 7 | <24 | 1 |
| 8 | <23 | -7 |
| 9 | <20 | -10 |
| 10 | <17 | -12 |
| 11 | <13 | -8 |

| 1,8,l | | |
|---|---|---|
| $\overline{11}$ | <17 | 1 |
| $\overline{10}$ | <22 | -13 |
| $\bar{9}$ | <24 | 14 |
| $\bar{8}$ | <27 | -11 |
| $\bar{7}$ | 19 | -18 |
| $\bar{6}$ | 28 | 28 |
| $\bar{5}$ | 21 | 26 |
| $\bar{4}$ | 38 | 38 |
| $\bar{3}$ | 106 | 101 |
| $\bar{2}$ | 21 | 19 |
| $\bar{1}$ | 132 | 123 |
| 0 | <29 | 1 |
| 1 | 136 | 131 |
| 2 | 57 | -52 |
| 3 | 64 | 57 |
| 4 | 64 | -62 |
| 5 | 21 | -19 |
| 6 | <28 | -3 |
| 7 | <27 | 8 |
| 8 | <25 | 18 |
| 9 | <22 | 8 |
| 10 | <18 | 6 |

| 2,8,l | | |
|---|---|---|
| $\overline{11}$ | <10 | -5 |
| $\overline{10}$ | 15 | 13 |
| $\bar{9}$ | 13 | -10 |
| $\bar{8}$ | <11 | 1 |
| $\bar{7}$ | 72 | 75 |
| $\bar{6}$ | 72 | -79 |
| $\bar{5}$ | 53 | 57 |
| $\bar{4}$ | 72 | -76 |
| $\bar{3}$ | 102 | -112 |
| $\bar{2}$ | 53 | 55 |
| $\bar{1}$ | 34 | 39 |
| 0 | 19 | 17 |
| 1 | 87 | 88 |
| 2 | 80 | -86 |
| 3 | 80 | -81 |
| 4 | 38 | -40 |
| 5 | 23 | -27 |
| 6 | <19 | -3 |
| 7 | 15 | 19 |
| 8 | <12 | 3 |
| 9 | 11 | 8 |

| 3,8,l | | |
|---|---|---|
| $\overline{10}$ | <10 | 6 |
| $\bar{9}$ | <12 | 5 |
| $\bar{8}$ | <14 | -7 |
| $\bar{7}$ | <14 | -8 |
| $\bar{6}$ | <15 | -7 |
| $\bar{5}$ | 51 | -57 |
| $\bar{4}$ | <16 | -8 |
| $\bar{3}$ | 83 | -78 |
| $\bar{2}$ | 15 | -17 |
| $\bar{1}$ | 110 | -113 |
| 0 | 34 | 31 |
| 1 | 72 | -71 |
| 2 | 64 | 65 |
| 3 | <15 | 1 |
| 4 | 30 | 26 |
| 5 | <14 | -4 |
| 6 | <13 | -6 |
| 7 | <12 | -10 |

| 4,8,l | | |
|---|---|---|
| $\overline{10}$ | 11 | -9 |
| $\bar{9}$ | 34 | -31 |
| $\bar{8}$ | 34 | 32 |
| $\bar{7}$ | 68 | -65 |
| $\bar{6}$ | 57 | 61 |
| $\bar{5}$ | 38 | 38 |
| $\bar{4}$ | <10 | -4 |
| $\bar{3}$ | 27 | 25 |
| $\bar{2}$ | 27 | -23 |
| $\bar{1}$ | 80 | -75 |
| 0 | 38 | 40 |
| 1 | 19 | 19 |
| 2 | 30 | 33 |
| 3 | 42 | 41 |
| 4 | <10 | 3 |
| 5 | 11 | -13 |
| 6 | <8 | 2 |
| 7 | 14 | -13 |

| 5,8,l | | |
|---|---|---|
| $\bar{9}$ | <7 | 4 |
| $\bar{8}$ | <8 | -3 |
| $\bar{7}$ | 28 | 28 |
| $\bar{6}$ | <10 | -6 |
| $\bar{5}$ | 30 | 37 |
| $\bar{4}$ | <10 | 9 |
| $\bar{3}$ | 64 | 68 |
| $\bar{2}$ | <10 | -10 |
| $\bar{1}$ | 64 | 60 |
| 0 | 34 | -41 |
| 1 | 6 | 11 |
| 2 | 24 | -29 |
| 3 | <19 | 5 |
| 4 | <19 | -7 |

| 6,8,l | | |
|---|---|---|
| $\bar{7}$ | <9 | 4 |
| $\bar{5}$ | 27 | -26 |
| $\bar{4}$ | <8 | 9 |
| $\bar{3}$ | 27 | 28 |
| $\bar{2}$ | 11 | -14 |
| $\bar{1}$ | 15 | 15 |
| 0 | 19 | -20 |
| 1 | 30 | -27 |
| 2 | <9 | -0 |

| 0,9,l | | |
|---|---|---|
| 1 | 53 | -46 |
| 2 | <25 | 20 |
| 3 | <25 | 11 |
| 4 | <25 | -16 |
| 5 | 53 | -49 |
| 6 | <23 | 7 |
| 7 | 53 | -55 |
| 8 | <19 | 5 |
| 9 | <16 | -15 |

| 1,9,l | | |
|---|---|---|
| $\overline{10}$ | <14 | 3 |
| $\bar{9}$ | <19 | 18 |
| $\bar{8}$ | <23 | -7 |
| $\bar{7}$ | <25 | 6 |
| $\bar{6}$ | <27 | -11 |
| $\bar{5}$ | <27 | -16 |
| $\bar{4}$ | 49 | -44 |
| $\bar{3}$ | <28 | 4 |
| $\bar{2}$ | 28 | 25 |
| $\bar{1}$ | <29 | 0 |
| 0 | 57 | 56 |
| 1 | <29 | -19 |
| 2 | 20 | -31 |
| 3 | 19 | 21 |
| 4 | <27 | -16 |
| 5 | <27 | 15 |
| 6 | <25 | -13 |
| 7 | <23 | -16 |
| 8 | <20 | -6 |
| 9 | <16 | -15 |

| 2,9,l | | |
|---|---|---|
| $\bar{9}$ | 31 | 26 |
| $\bar{8}$ | <12 | 8 |
| $\bar{7}$ | 53 | 49 |
| $\bar{6}$ | <14 | 0 |
| $\bar{5}$ | <14 | 3 |
| $\bar{4}$ | 23 | 19 |
| $\bar{3}$ | 15 | 13 |
| $\bar{2}$ | <16 | 1 |
| $\bar{1}$ | 64 | 61 |
| 0 | 27 | -26 |
| 1 | <16 | -5 |
| 2 | 19 | 20 |
| 3 | 19 | 15 |
| 4 | 11 | 10 |
| 5 | 57 | 63 |
| 6 | <15 | -8 |
| 7 | 30 | 31 |

| 3,9,l | | |
|---|---|---|
| $\bar{8}$ | <11 | 3 |
| $\bar{7}$ | <12 | -2 |
| $\bar{6}$ | 31 | 26 |
| $\bar{5}$ | <14 | -0 |
| $\bar{4}$ | <14 | 6 |
| $\bar{3}$ | <15 | -2 |
| $\bar{2}$ | 45 | -44 |
| $\bar{1}$ | 27 | 24 |
| 0 | <15 | 0 |
| 1 | <14 | -0 |
| 2 | 15 | 11 |
| 3 | 27 | -24 |
| 4 | <13 | 7 |
| 5 | <12 | 1 |

| 4,9,l | | |
|---|---|---|
| $\bar{9}$ | 19 | -26 |
| $\bar{8}$ | <10 | -4 |
| $\bar{7}$ | 15 | -9 |
| $\bar{6}$ | 19 | -19 |
| $\bar{5}$ | <10 | 6 |
| $\bar{4}$ | <10 | -7 |
| $\bar{3}$ | 38 | -40 |
| $\bar{2}$ | 25 | 22 |
| $\bar{1}$ | 19 | -16 |
| 0 | <10 | -7 |
| 1 | 20 | 11 |
| 2 | 15 | -17 |
| 3 | 42 | -37 |
| 4 | <8 | -0 |
| 5 | 34 | -37 |

| 5,9,l | | |
|---|---|---|
| $\bar{7}$ | <12 | 4 |
| $\bar{6}$ | <13 | -2 |
| $\bar{5}$ | <14 | 3 |
| $\bar{4}$ | 17 | 12 |
| $\bar{3}$ | <14 | -12 |
| $\bar{2}$ | <14 | 12 |
| $\bar{1}$ | <14 | -15 |
| 0 | <13 | -1 |

| 0,10,l | | |
|---|---|---|
| 0 | <23 | 7 |
| 1 | <27 | -13 |
| 2 | <23 | 1 |
| 3 | <22 | -10 |
| 4 | <21 | -14 |
| 5 | <28 | -4 |
| 6 | 22 | -21 |
| 7 | 19 | -21 |

| 1,10,l | | |
|---|---|---|
| $\bar{8}$ | <15 | 6 |
| $\bar{7}$ | <19 | 15 |
| $\bar{6}$ | <23 | 12 |
| $\bar{5}$ | 27 | 26 |
| $\bar{4}$ | <25 | -12 |
| $\bar{3}$ | <26 | 21 |
| $\bar{2}$ | <26 | 3 |
| $\bar{1}$ | 45 | -45 |
| 0 | <27 | -4 |
| 1 | <26 | -1 |
| 2 | <26 | 13 |
| 3 | 35 | 31 |
| 4 | <24 | 4 |
| 5 | <22 | 9 |
| 6 | <20 | -12 |

| 2,10,l | | |
|---|---|---|
| $\bar{7}$ | 15 | -15 |
| $\bar{6}$ | 19 | 15 |
| $\bar{5}$ | 23 | -17 |
| $\bar{4}$ | <11 | 2 |
| $\bar{3}$ | 19 | -18 |
| $\bar{2}$ | <14 | -7 |
| $\bar{1}$ | <14 | 9 |
| 0 | <14 | -1 |
| 1 | <14 | 7 |
| 2 | <13 | 7 |
| 3 | <13 | -4 |
| 4 | 27 | 23 |
| 5 | <10 | 7 |

| 3,10,l | | |
|---|---|---|
| $\bar{6}$ | <10 | -0 |
| $\bar{5}$ | 32 | -24 |
| $\bar{4}$ | <11 | -0 |
| $\bar{3}$ | 19 | 19 |
| $\bar{2}$ | <12 | 1 |
| $\bar{1}$ | 15 | 13 |
| 0 | <12 | -2 |
| 1 | 26 | -23 |
| 2 | 11 | -13 |

| 4,10,l | | |
|---|---|---|
| $\bar{6}$ | <6 | -3 |
| $\bar{5}$ | 25 | 20 |
| $\bar{4}$ | 10 | 6 |
| $\bar{3}$ | <8 | -0 |
| $\bar{2}$ | <8 | 0 |
| $\bar{1}$ | 9 | -5 |
| 0 | <8 | -3 |
| 1 | <7 | 1 |
| 2 | 15 | -13 |

| 0,11,l | | |
|---|---|---|
| 1 | 18 | -15 |
| 2 | 27 | -23 |
| 3 | 47 | 36 |
| 4 | 48 | -52 |

| 1,11,l | | |
|---|---|---|
| $\bar{4}$ | <18 | -3 |
| $\bar{3}$ | <19 | 0 |
| $\bar{2}$ | 28 | 27 |
| $\bar{1}$ | <21 | -1 |
| 0 | 32 | 35 |
| 1 | <20 | 10 |
| 2 | <20 | 5 |
| 3 | 36 | -33 |

| 2,11,l | | |
|---|---|---|
| $\bar{4}$ | 38 | -33 |
| $\bar{3}$ | 8 | -5 |
| $\bar{2}$ | 11 | -8 |
| $\bar{1}$ | 23 | 22 |
| 0 | 11 | 7 |
| 1 | 15 | -18 |
| 2 | 45 | 42 |
| 3 | 27 | -27 |

cycles using the weighting function suggested by Hughes (1941), and approximate coordinates for the hydrogen atoms were obtained from a difference map. In 1957 calculations were transferred to a Datatron 205 computer. The heavy-atom coordinates were further adjusted through five least-squares cycles and individual anisotropic temperature factors were estimated and adjusted from two difference maps. At this stage the molecular dimensions were quite satisfactory (indeed, no interatomic distance differed by as much as 0·03 Å from the final value), but the $R$ index of 0·13 suggested that there were significant residual errors in the model.

Refinement was continued in 1961, when a Burroughs 220 computer became available to us. A total of 16 structure-factor least-squares calculations were carried out in which the coordinates of all eighteen atoms, anisotropic temperature factors of the twelve heavy atoms, and a scale factor were included as parameters. The quantity minimized in the least-squares process was $\Sigma w(F_o^2 - F_c^2)^2$. Atomic form factors were those of Berghuis, Haanappel, Potters, Loopstra, MacGillavry & Veenendaal (1955) for oxygen and carbon and those of McWeeny (1951) for hydrogen. For the first seven cycles, during which the $R$ index dropped to 0·09, the weighting function was that suggested by Hughes (1941).* For the final nine cycles we chose a function which we believe more truly represents the pattern of observational uncertainties in $F^2$; that is,

$$\begin{aligned}\sigma(F^2) = 1/\sqrt{w} &= KF_o^2, \quad \text{for } F_o \geq 5\cdot0\\ &= 5KF_o, \quad \text{for } F_o \leq 5\cdot0\,.\end{aligned}$$

The change in weights led to a sharp drop in the estimated standard deviations of all parameters except the coordinates of the hydrogen atoms, whose e.s.d.'s remained about constant.

Refinement was stopped when the maximum indicated shift in a heavy-atom coordinate was 12% of its e.s.d., in a hydrogen-atom coordinate 21% of its e.s.d., and in a temperature parameter 17% of its e.s.d. The final $R$ index for 1188 observed reflections of non-zero weight was 0·079.

The final parameters and their estimated standard deviations are listed in Table 1. Observed and calculated structure factors are listed in Table 2. At the conclusion of the refinement an electron density map in the plane of the molecule, based on all observed structure factors and the signs listed in Table 2, was calculated. This map is shown in Fig. 1. A difference map in the plane of the molecule was also calculated, using as coefficients the differences between the observed structure factors with the signs of the final $F_c$'s (Table 1) and the structure factors calculated for only the heavy atoms. This map is shown in Fig. 2.

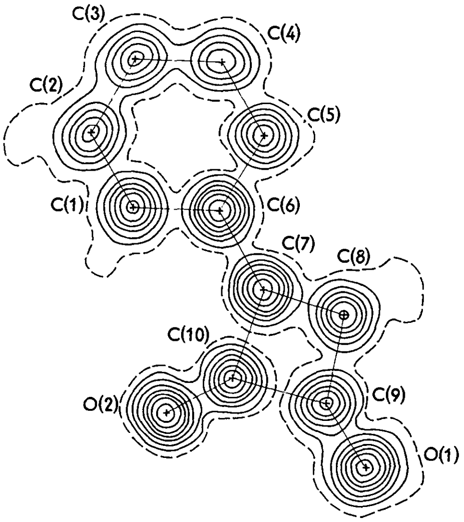

Fig. 1. The electron density in the plane of the molecule, calculated at the conclusion of the refinement. Contours are at intervals of 1·0 e.Å$^{-3}$ beginning with the 0·6 e.Å$^{-3}$ level, which is dashed.

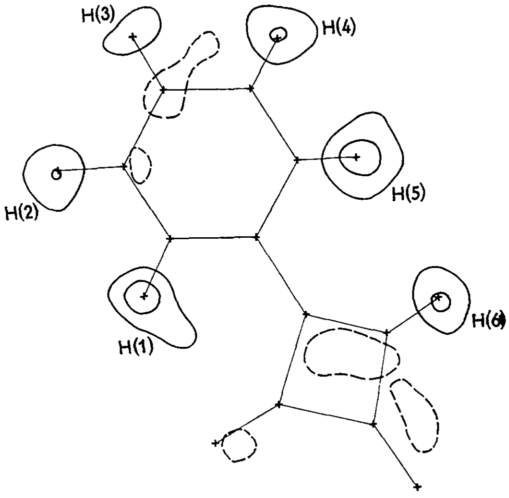

Fig. 2. A difference map in the plane of the molecule. The coefficients were the differences between the observed structure factors with the signs of the final $F_c$'s and the structure factors calculated for only the heavy atoms. The contours are at 0·2 and 0·4 e.Å$^{-3}$ and at $-0·2$ e.Å$^{-3}$ (dashed). The crosses are the final least-squares positions of the atoms.

## Discussion

### *Accuracy*

The estimated standard deviations in the positional parameters (Table 1) are approximately 0·003 Å for the heavy atoms and 0·04 Å for the hydrogen atoms. The corresponding standard deviations in bond dis-

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* At intermediate stages of refinement we have found convergence to be more rapid when the weighting function places less emphasis on the weak reflections than would be demanded merely from a consideration of observational uncertainties.

tances would be about 0·004 Å for distances between pairs of heavy atoms and 0·04 Å for C–H bonds. Additional uncertainties are undoubtedly introduced by systematic errors in the data and, more important, by the effects of thermal libration. We consider that realistic values for the estimated standard deviations are approximately 0·006 Å for distances between pairs of heavy atoms (except for the C–O distances, which are discussed in the following paragraph) and 0·06 Å for the apparent C–H distances. These values are compatible with the spread of observed distances presumed to be essentially equal (the C–C distances within the benzene ring and the C–H distances).

### *The temperature factors*

In Table 3 are listed the magnitudes and direction cosines relative to *a*, *b*, and *c** of the principal axes of the vibration ellipsoids implied by the temperature parameters of Table 1. Although the temperature factors are large for all atoms (as would be expected for a structure containing no strong intermolecular forces), most of the anisotropies are not very great, and it appears that most of the thermal motion is associated with a general lattice vibration involving translation of the molecules. This type of vibration would not affect the intramolecular distances. There are two other motions, however, which seem to be important and would cause an apparent shortening of the bond distances: (1) a rigid-body libration of the molecules about an axis normal to the plane of the molecule and passing through its center of gravity in the vicinity of C(7); (2) an out-of-plane motion which is particularly pronounced for the two oxygen atoms, and does not seem to be a rigid-body motion. The rigid-body libration can be seen quite clearly in the electron-density map (Fig. 1); its r.m.s. amplitude is about 3½°. If this motion is truly a rigid-body oscillation, the effect on the bond distances is small — less than 0·003 Å. The effects of the out-of-plane motions of the oxygen atoms on the C–O distances, on the other hand, are potentially much more important. Thus, if it is assumed that the large motions of the oxygen atoms represent a pivoting about the attached carbon atoms the C–O distances should be increased by about 0·02 Å.

Table 3. *Magnitudes B and direction cosines relative to a, b, and c* of the principal axes of the thermal ellipsoids*

| Atom | Axis *i* | $B_i$ | $q_{ia}$ | $q_{ib}$ | $q_{ic^*}$ |
|---|---|---|---|---|---|
| C(1) | 1 | 5·17 | −0·652 | 0·678 | 0·338 |
| | 2 | 4·46 | −0·450 | −0·706 | 0·547 |
| | 3 | 3·71 | 0·610 | 0·205 | 0·766 |
| C(2) | 1 | 7·05 | −0·393 | 0·739 | 0·547 |
| | 2 | 5·43 | 0·856 | 0·512 | −0·076 |
| | 3 | 3·61 | 0·336 | −0·439 | 0·834 |
| C(3) | 1 | 7·82 | −0·083 | 0·472 | 0·878 |
| | 2 | 5·06 | 0·932 | 0·349 | −0·100 |
| | 3 | 3·56 | −0·353 | 0·810 | −0·469 |
| C(4) | 1 | 7·35 | 0·230 | −0·024 | 0·973 |
| | 2 | 6·04 | 0·970 | 0·089 | −0·227 |
| | 3 | 3·92 | −0·081 | 0·996 | 0·044 |
| C(5) | 1 | 5·81 | 0·960 | −0·165 | 0·225 |
| | 2 | 4·63 | −0·279 | −0·565 | 0·777 |
| | 3 | 4·12 | 0·001 | 0·809 | 0·588 |
| C(6) | 1 | 4·00 | −0·405 | 0·624 | 0·668 |
| | 2 | 3·82 | 0·593 | −0·376 | 0·711 |
| | 3 | 3·67 | 0·696 | 0·684 | −0·218 |
| C(7) | 1 | 4·22 | −0·518 | 0·773 | −0·366 |
| | 2 | 3·70 | 0·851 | 0·509 | −0·131 |
| | 3 | 3·60 | −0·085 | 0·379 | 0·921 |
| C(8) | 1 | 6·29 | 0·992 | −0·123 | 0·025 |
| | 2 | 4·44 | 0·120 | 0·986 | 0·113 |
| | 3 | 3·65 | −0·039 | −0·109 | 0·993 |
| C(9) | 1 | 5·74 | 0·850 | −0·458 | −0·262 |
| | 2 | 4·85 | 0·499 | 0·535 | 0·682 |
| | 3 | 3·55 | −0·172 | −0·710 | 0·683 |
| C(10) | 1 | 5·01 | −0·895 | 0·207 | 0·395 |
| | 2 | 3·93 | 0·199 | −0·607 | 0·769 |
| | 3 | 3·62 | 0·399 | 0·767 | 0·503 |
| O(1) | 1 | 9·04 | 0·997 | −0·054 | −0·058 |
| | 2 | 6·60 | 0·078 | 0·534 | 0·842 |
| | 3 | 3·46 | 0·015 | 0·844 | −0·536 |
| O(2) | 1 | 8·48 | 0·948 | 0·087 | −0·307 |
| | 2 | 5·51 | −0·247 | 0·807 | −0·536 |
| | 3 | 3·39 | 0·201 | 0·584 | 0·787 |

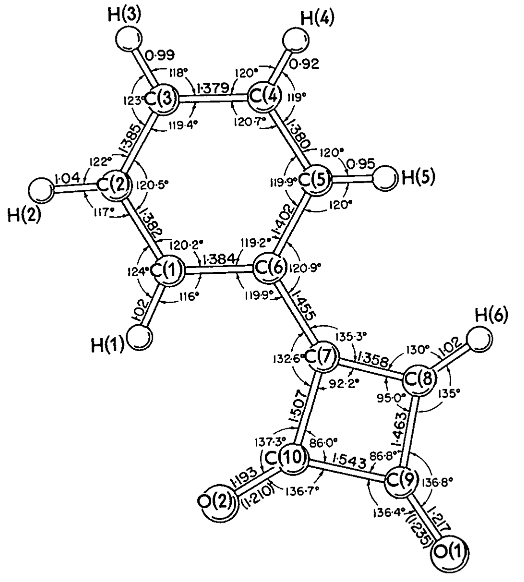


Fig. 3. The bond distances and angles. The values in parentheses have been corrected for the out-of-plane libration of the oxygen atoms (see text).

In arriving at our best estimates of the C–O bond distances (Fig. 3), we have somewhat arbitrarily increased the apparent C(9)–O(1) distance by 0·017 Å and the apparent C(10)–O(2) distance by 0·018 Å. We estimate the standard deviations in these corrected values to be about 0·01 Å.

### *The geometry of the molecule*

The phenylcyclobutenedione molecule is slightly but significantly non-planar. The equation for the best plane of the molecule calculated with all twelve heavy atoms weighted equally is

$$0{\cdot}9936X+0{\cdot}0395Y-0{\cdot}1056Z=0{\cdot}0813\ ,$$

where the direction cosines are relative to $a$, $b$, and $c^*$ and the origin-to-plane distance is in Å. The largest deviations from this plane are 0·017 Å for C(4), 0·012 Å for O(2), 0·010 Å for O(1), −0·014 Å for C(6), and −0·011 Å for C(1). On the other hand, the atoms C(1)–C(7) all lie within 0·006 Å of the plane

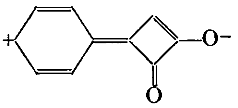
$$0{\cdot}9936X+0{\cdot}0320Y-0{\cdot}1081Z=0{\cdot}1401$$

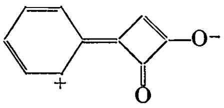
and the atoms C(6)–C(10), O(1) and O(2) all lie within 0·004 Å of the plane

$$0{\cdot}9936X+0{\cdot}0464Y-0{\cdot}1031Z=0{\cdot}0477\ .$$

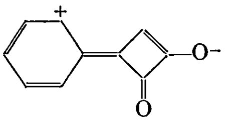
The relation between the two planes is not a simple twist around the C(6)–C(7) bond but involves a buckling of the molecule approximately about the C(1) · · · C(8) line.

The interatomic distances and bond angles are in Fig. 3. The average C–C distance within the benzene ring is 1·385 Å, which should probably be increased by about 0·002 Å to take account of libration effects. This is close to the value 1·394 Å usually chosen as the normal distance within a benzene ring. Within the four-membered ring, the observed values for the C(6)–C(7), C(7)–C(8), C(8)–C(9) and C(9)–O(1) distances suggest an appreciable contribution — about 20% in all — of the structures



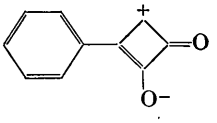


and



The contribution of these structures would be expected to cause small variations (a maximum of about 0·025 Å) in the individual C–C distances within the benzene ring. A small trend in the right direction is actually observed, although it is of doubtful significance.

The C(9)–C(10) distance of 1·543 Å is close to the value 1·54 Å found for the single-bond distances in cyclobutene (Goldish, Hedberg & Schomaker, 1956) and in 1-methylcyclobutene (Shand, Schomaker & Fischer, 1944), and also to the values 1·56 and 1·53 Å in oxalic acid (Cox, Dougill & Jeffrey, 1952) and oxalic acid dihydrate (Ahmed & Cruickshank, 1953). The C(7)–C(10) distance of 1·507 Å is significantly shorter, suggesting a small contribution (perhaps 10%) of the structure



These various resonating structures are doubtless responsible for the stability of the molecule.

The average apparent C–H distance, 0·99 Å, is representative of values found in many other recent X-ray diffraction investigations. It is significantly shorter than the standard internuclear separation of 1·09 Å. Some of the shortening may be due to thermal motion of the hydrogen atoms, but the main part is unexplained.

### *Packing of the molecules*

A drawing of the structure of phenylcyclobutenedione viewed down the $b$ axis is shown in Fig. 4, and the shortest intermolecular distances are listed in Table 4.

Table 4. *Closest intermolecular approaches*

Distances less than 3·65 Å between heavy atoms and less than 3·00 Å between a hydrogen atom and a heavy atom are included. The atoms in the first column belong to the reference molecule at $(x, y, z)$. Values in parentheses are distances from the protons attached to the carbon atoms

| From atom | To atom | In molecule at | Distance |
|---|---|---|---|
| C(1) | C(8) | $(1-x, 1-y, 1-z)$ | 3·55 Å |
| C(2) | C(8) | $(1-x, 1-y, 1-z)$ | 3·49 |
| C(3) | C(9) | $(1-x, 1-y, 1-z)$ | 3·40 |
| C(3) | O(1) | $(1-x, 1-y, 1-z)$ | 3·54 |
| C(4) | C(9) | $(1-x, 1-y, 1-z)$ | 3·54 |
| C(4) | C(10) | $(1-x, 1-y, 1-z)$ | 3·43 |
| C(5) | C(7) | $(1-x, 1-y, 1-z)$ | 3·54 |
| C(5) | C(10) | $(1-x, 1-y, 1-z)$ | 3·50 |
| C(6) | C(6) | $(1-x, 1-y, 1-z)$ | 3·55 |
| C(6) | C(7) | $(1-x, 1-y, 1-z)$ | 3·47 |
| C(2) | C(8) | $(\bar{x}, 1-y, 1-z)$ | 3·55 |
| C(3) | C(9) | $(\bar{x}, 1-y, 1-z)$ | 3·61 |
| C(4) | C(10) | $(\bar{x}, 1-y, 1-z)$ | 3·59 |
| C(6) | C(6) | $(\bar{x}, 1-y, 1-z)$ | 3·56 |
| C(3) | O(2) | $(x, 1+y, z)$ | 3·61 (2·84) |
| C(4) | O(1) | $(x, 1+y, z)$ | 3·50 (2·62) |
| C(8) | O(2) | $(x, \frac{1}{2}-y, \frac{1}{2}+z)$ | 3·56 (2·93) |
| C(1) | O(1) | $(x, \frac{1}{2}-y, -\frac{1}{2}+z)$ | 3·29 (2·78) |
| C(2) | O(1) | $(x, \frac{1}{2}-y, -\frac{1}{2}+z)$ | 3·57 (3·23) |
| C(8) | O(1) | $(1-x, \frac{1}{2}+y, \frac{3}{2}-z)$ | 3·32 (2·45) |
| C(2) | O(2) | $(\bar{x}, \frac{1}{2}+y, \frac{1}{2}-z)$ | 3·37 (2·53) |

The molecule lies very nearly in the $(20\bar{1})$ plane, which has an interplanar spacing of 3·49 Å. The actual interplanar spacing between the two molecules related by the symmetry center at $(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$ (Fig. 4) is 3·39 Å ,while the spacing between molecules related

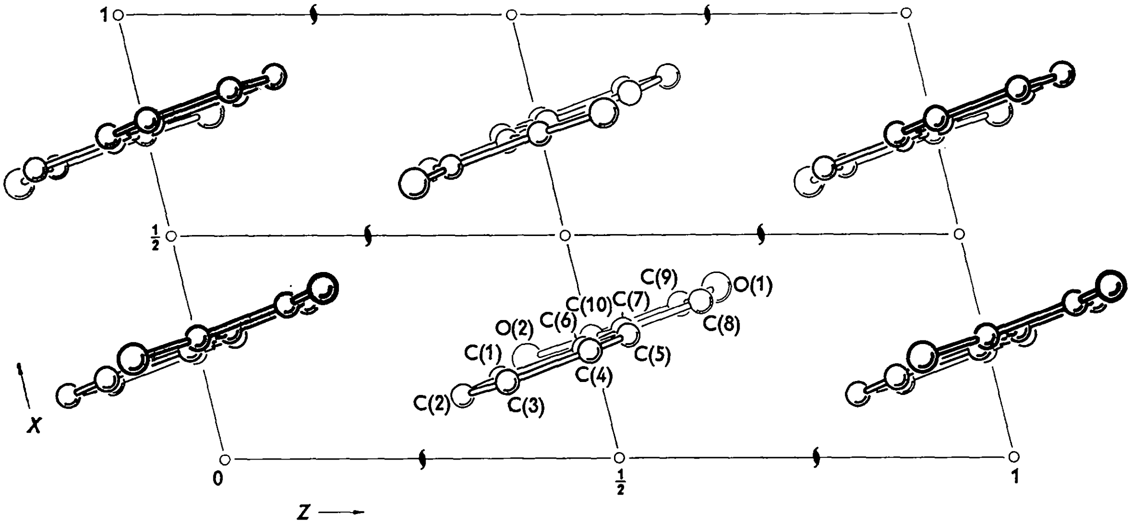


Fig. 4. The structure viewed down the *b* axis.

by the center at $(0, \frac{1}{2}, \frac{1}{2})$ is 3·56 Å. Aside from the contacts across these symmetry centers, all of the short intermolecular distances involve one of the two oxygen atoms. The C(8) · · · O(1) distance (3·32 Å) across the screw axis at $x=\frac{1}{2}$, $z=\frac{3}{4}$ and theC(2)· · ·O(2) (3·37 Å) across the screw axis at $x=0$, $z=\frac{1}{4}$ are particularly noteworthy. The protons on C(8) and C(2) are pointed more or less towards the oxygen atoms, the C(8)–H(6) · · · O(1) angle being 142·6° and the C(2)–H(2) · · · O(2) angle being 137·5°; moreover, the H · · · O distances of about 2·5 Å are slightly shorter than the sum of the van der Waals radii of hydrogen and oxygen, 2·6 Å (Pauling, 1960). We hesitate, however, to go so far as to call the interactions 'hydrogen bonds'.

We wish to thank Mr W. Mendell for re-estimating the intensities of the *a*-axis photographs. One of us (C.-H. W.) is grateful to E. I. du Pont de Nemours and Co. for financial support during part of the time in which this investigation was being carried out.

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