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# The Identification and Crystal Structure of 3β-(*p*-Bromobenzoyloxy)-androst-5-eno-(16α,17-*d*)-2′,2′,3′,3′-tetrafluoro-2′,3′-dihydro-6-methylpyran*

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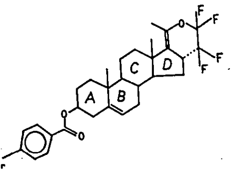
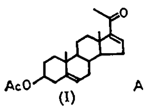
3β-(*p*-Bromobenzoyloxy)-androst-5-eno-(16α,17-*d*)-2′,2′,3′,3′-tetrafluoro-2′,3′-dihydro-6-methylpyran, $C_{30}H_{33}F_4O_3Br$, crystallizes in space group $P2_12_12_1$ with four molecules in a unit cell having dimensions $a=22{\cdot}891$ ($\sigma\sim0{\cdot}01$), $b=10{\cdot}692$ ($\sigma\sim0{\cdot}007$), $c=11{\cdot}313$ ($\sigma\sim0{\cdot}007$) Å. The structure, which was solved by Fourier methods, was refined by block-diagonal least squares to a final $R$ value of 0·059. The refinement was based on 1571 reflections collected with an automatic diffractometer. The structure corresponds to the formula:



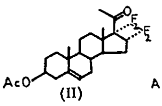
The *A* and *C* rings are distorted slightly from ideal chair geometry; the *B* ring is in the half-chair conformation and the *D* ring is a slightly distorted β-envelope. Bond distances and angles are normal with e.s.d.'s varying from 0·008–0·013 Å and 0·5–0·8° respectively.

## Introduction

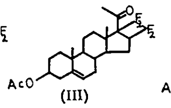
During an investigation of photochemical cyclo-additions of olefins to unsaturated steroidal ketones (Sunder-Plassman, Nelson, Boyle, Cruz, Iriarte, Crabbé, Zderic, Edwards & Fried, 1969), the reaction between tetrafluoroethylene and 3β-acetoxypregna-5,16,-dien-20-one (I) was investigated. The major product was the α,α adduct (II) (36%); the β, β adduct (III) (17%) was also formed.



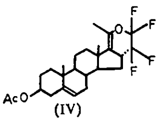
(I)



(II)



(III)



(IV)

In addition, an unknown compound [which the X-ray analysis proved to be (IV)] was produced (14%), the mass spectrum of which showed it to be a mono-adduct of tetrafluoroethylene and (I). The structure of this adduct was not apparent from the usual spectral data, and an X-ray investigation of the 3-*p*-bromobenzoate derivative was therefore undertaken.

## Experimental

The heavy-atom derivative was prepared by Dr Peter Nelson, who also supplied the crystals. The compound crystallizes as prismatic needles, elongated along the *c* axis. Preliminary precession photographs indicated orthorhombic symmetry. The systematic extinctions, *h*00, 0*k*0 and 00*l* with *h*, *k* or *l* odd, are consistent with space group $P2_12_12_1$. Cell dimensions were determined on a Picker diffractometer with full-circle goniostat, using Cu radiation. The cell parameters and direction cosines of the reciprocal axes relative to the instrument coordinate system were refined by least-squares. The refinement which was based on eleven strong reflections gave the following results (estimated standard deviations in parentheses): $a=22{\cdot}891$ (0·020), $b=10{\cdot}692$ (0·007), $c=11{\cdot}313$ (0·007) Å ($\lambda$ Cu $K\alpha=1{\cdot}54051$ Å). These values give a calculated density of 1·41 g.cm$^{-3}$ for $Z=4$. The density observed by flotation in an aqueous solution of KI was 1·41 g.cm$^{-3}$.

The crystal used for determination of cell parameters and collections of intensity data had dimensions of approximately $0{\cdot}40\times0{\cdot}18\times0{\cdot}18$ mm. The calculated linear absorption coefficient for copper radiation is 27 cm$^{-1}$. A set of unique reflections with $\sin\theta/\lambda$ less than 0·59 Å$^{-1}$ was scanned by use of the $2\theta$–$\theta$ technique

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at a scan speed of $2^\circ \text{min}^{-1}$; 1571 reflections had an intensity greater than three times their e.s.d.'s and were recorded as 'observed'. No correction for absorption was applied.

### Determination and refinement of the structure

A sharpened three-dimensional Patterson function clearly revealed the position of the Br atom. In order to minimize errors in the Fourier synthesis based on the Br atom parameters, weights were assigned to the measured $|F|$ values (Sim, 1960). Inspection of the electron density map gave positions of eleven additional atoms. Five more rounds of electron density and structure-factor calculations revealed the remaining atoms (apart from hydrogen) and gave an $R$ index of 0·25.

The next stage of the analysis consisted of two cycles of block-diagonal least-squares refinement of the positional parameters with isotropic temperature factors set at 4·0 Å$^2$. The $R$ index was 0·18. Anisotropic temperature factors were then assigned to all the atoms; and after six more cycles, the refinement was terminated. The last shifts were all well below the corresponding e.s.d.'s, and the final $R$ value was 0·059 for all observed reflections. In the last two cycles the hydrogen atoms, except those on the methyl and hydroxyl groups, were included with isotropic temperature factors of 5·0 Å$^2$. The hydrogen atom positions (Table 1) were calculated from the C atom positions assuming a C–H distance of 1·07 Å.

The positional and thermal parameters for the final structure are given in Tables 2 and 3 respectively, and the observed and calculated structure factors are given in Table 4.

Table 1. *Assumed hydrogen atom positions Hydrogen atom at*

| atom at | $x$ | $y$ | $z$ |
|---|---|---|---|
| C(1) | 0·8331 | 0·2193 | 0·5739 |
|  | 0·8312 | 0·0676 | 0·6306 |
| C(2) | 0·9306 | 0·1359 | 0·6098 |
|  | 0·9192 | 0·1700 | 0·4607 |
| C(3) | 0·9102 | −0·0792 | 0·5763 |
| C(4) | 0·8960 | −0·1647 | 0·3786 |
|  | 0·9013 | −0·0151 | 0·3179 |
| C(6) | 0·8052 | −0·2303 | 0·3687 |
| C(7) | 0·7054 | −0·1845 | 0·4793 |
|  | 0·7001 | −0·1765 | 0·3256 |
| C(8) | 0·7013 | 0·0438 | 0·3257 |
| C(9) | 0·7399 | 0·0320 | 0·5793 |
| C(11) | 0·7162 | 0·2632 | 0·4463 |
|  | 0·7359 | 0·2461 | 0·5944 |
| C(12) | 0·6343 | 0·3016 | 0·5644 |
|  | 0·6444 | 0·1621 | 0·6419 |
| C(14) | 0·6444 | −0·0415 | 0·5354 |
| C(15) | 0·5888 | −0·1625 | 0·4104 |
|  | 0·5952 | −0·0576 | 0·2929 |
| C(16) | 0·5065 | 0·0196 | 0·3432 |
| C(33) | 1·0587 | −0·0656 | 0·3267 |
| C(34) | 1·1609 | −0·0652 | 0·2608 |
| C(35) | 1·2419 | −0·0635 | 0·4064 |
| C(37) | 1·2183 | −0·0490 | 0·6197 |

Table 2. *Final positional parameters and their standard deviations*

The e.s.d. (in parentheses) apply to the least significant digits.

|  | $x$ | $y$ | $z$ |
|---|---|---|---|
| C(1) | 0·84210 (39) | 0·12322 (58) | 0·55510 (59) |
| C(2) | 0·90688 (36) | 0·10999 (61) | 0·53215 (57) |
| C(3) | 0·92103 (34) | −0·02458 (56) | 0·50022 (53) |
| C(4) | 0·88737 (38) | −0·06767 (64) | 0·39335 (63) |
| C(5) | 0·82178 (37) | −0·04921 (52) | 0·41042 (50) |
| C(6) | 0·78649 (38) | −0·14216 (57) | 0·39230 (65) |
| C(7) | 0·71927 (40) | −0·13459 (51) | 0·40229 (68) |
| C(8) | 0·69854 (32) | 0·00246 (47) | 0·41164 (51) |
| C(9) | 0·73795 (35) | 0·07885 (50) | 0·49578 (46) |
| C(10) | 0·80260 (36) | 0·08208 (51) | 0·45147 (51) |
| C(11) | 0·71153 ·35) | 0·20591 (49) | 0·52329 (62) |
| C(12) | 0·64864 (35) | 0·20657 (50) | 0·55765 (54) |
| C(13) | 0·60972 (33) | 0·13954 (52) | 0·47058 (48) |
| C(14) | 0·63603 (30) | 0·00621 (47) | 0·45416 (44) |
| C(15) | 0·58845 (32) | −0·06577 (53) | 0·38622 (50) |
| C(16) | 0·52985 (31) | −0·00466 (54) | 0·42200 (41) |
| C(17) | 0·54895 (32) | 0·10491 (52) | 0·50203 (4)) |
| C(18) | 0·60840 (39) | 0·20992 (58) | 0·34999 (56) |
| C(19) | 0·80912 (42) | 0·17221 (63) | 0·34468 (66) |
| C(20) | 0·51359 (34) | 0·14315 (52) | 0·58827 (44) |
| C(21) | 0·52152 (39) | 0·24545 (56) | 0·67859 (51) |
| O(22) | 0·45839 (24) | 0·08628 (42) | 0·61099 (37) |
| C(23) | 0·43848 (39) | −0·00318 (61) | 0·53516 (54) |
| F(24) | 0·40095 (28) | −0·07295 (48) | 0·59871 (45) |
| F(25) | 0·40936 (23) | 0·04994 (51) | 0·44684 (38) |
| C(26) | 0·48698 (38) | −0·08211 (54) | 0·48285 (52) |
| F(27) | 0·51256 (24) | −0·14866 (38) | 0·57437 (36) |
| F(28) | 0·46287 (25) | −0·16861 (40) | 0·41116 (44) |
| O(29) | 0·98219 (23) | −0·03549 (43) | 0·46646 (36) |
| C(30) | 1·02207 (38) | −0·04774 (59) | 0·55313 (57) |
| O(31) | 1·00809 (30) | −0·04908 (63) | 0·65675 (37) |
| C(32) | 1·08168 (37) | −0·05342 (50) | 0·51049 (51) |
| C(33) | 1·09353 (31) | −0·06100 (59) | 0·38977 (47) |
| C(34) | 1·15126 (39) | −0·06235 (70) | 0·35332 (55) |
| C(35) | 1·19753 (40) | −0·06000 (57) | 0·43548 (64) |
| Br(36) | 1·27568 (5) | −0·05972 (10) | 0·38419 (10) |
| C(37) | 1·18406 (43) | −0·05298 (59) | 0·55551 (65) |
| C(38) | 1·12680 (37) | −0·05115 (57) | 0·59091 (50) |

The absolute configuration of the molecule was not determined directly; rather we considered the configuration of naturally occurring steroids to be well established and used the geometry around C(13) when we assigned the configuration.

### Computing procedures

All calculations were performed on a CDC 6600 computer, using programs referenced in a previous paper (Thom & Cristensen, 1970). The block-diagonal least-squares routine minimizes the weighted sum of $(KF_o - G|F_c|)^2$. The shifts were given by $\Delta' q_n = k_1 \Delta q_n + k_2 \Delta q_{n-1}$, where $\Delta q_n$ is the shift called for in the $n$th cycle (Sparks, 1961, and references cited therein). The values used for $k_1$ and $k_2$ were 0·8 and 0·2 respectively except for the two last cycles where the values 1·0 and 0·0 were used. The weighting scheme used was that of Hughes (1941) with $4F_0(\text{min}) = 13$.

The atomic form factors were those given by Hanson, Herman, Lea & Skillman (1964). No correction was made for anomalous dispersion.

The anisotropic temperature factors are of the form: $\exp[-(h^2\beta_{11}+k^2\beta_{22}+l^2\beta_{33}+hk\beta_{12}+hl\beta_{13}+kl\beta_{23})]$. The $R$ index, defined by $R=\sum||F_o|-|F_c||/\sum|F_o|$, included observed reflections only.

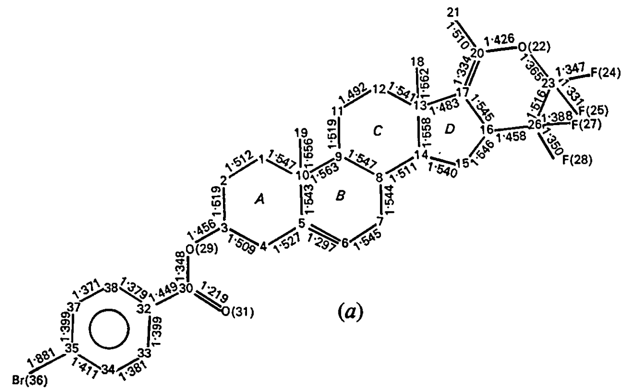

Fig. 1. (*a*) Bond lengths. The e.s.d.'s are in the range 0·008–0·013 Å.

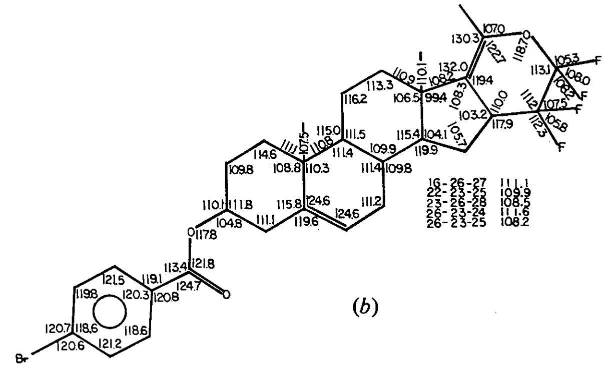

Fig. 1. (*Cont.*) (*b*) Bond angles. The e.s.d.'s are in the range 0·5–0·8°.

## The structure

Interatomic distances and angles caclulated from the final positional parameters are shown in Fig. 1. Torsion angles and fold angles are given in Table 5.

Inspection of Table 3 shows that the majority of the $B_{ii}$ values are in the range commonly encountered. As

Table 3. *Final thermal parameters, with e.s.d.'s in parentheses*

The temperature factor has the form $\exp[-\frac{1}{4}(B_{11}h^2a^{*2}\ldots+2B_{12}hka^*b^*\ldots)]$.

| | $B_{11}$ | $B_{22}$ | $B_{33}$ | $B_{12}$ | $B_{13}$ | $B_{23}$ |
|---|---|---|---|---|---|---|
| C(1) | 5·34 (26) | 4·41 (14) | 5·25 (28) | 0·70 (17) | 0·12 (22) | 0·70 (17) |
| C(2) | 3·24 (23) | 5·11 (15) | 5·29 (32) | −0·05 (17) | 0·94 (25) | 0·08 (20) |
| C(3) | 2·04 (29) | 4·84 (14) | 5·35 (36) | 0·00 (17) | 0·39 (27) | −0·45 (20) |
| C(4) | 3·58 (24) | 5·62 (14) | 5·75 (36) | −0·34 (16) | 0·97 (26) | 1·14 (20) |
| C(5) | 5·60 (27) | 3·92 (12) | 4·31 (32) | −0·42 (16) | 0·56 (25) | 0·18 (18) |
| C(6) | 4·04 (27) | 4·58 (14) | 6·48 (29) | −0·38 (17) | 1·86 (24) | 0·80 (19) |
| C(7) | 6·16 (25) | 3·17 (16) | 7·42 (34) | 0·13 (17) | 0·40 (26) | 0·89 (21) |
| C(8) | 4·62 (23) | 3·18 (14) | 4·92 (30) | −0·44 (16) | 0·94 (23) | 0·04 (19) |
| C(9) | 4·12 (24) | 3·99 (13) | 4·05 (27) | 0·54 (15) | 0·27 (21) | −0·00 (17) |
| C(10) | 5·08 (23) | 3·61 (13) | 4·39 (28) | −0·22 (15) | 1·11 (22) | 0·04 (17) |
| C(11) | 3·01 (23) | 3·47 (14) | 6·83 (31) | −0·25 (15) | 0·27 (23) | 0·74 (19) |
| C(12) | 3·37 (22) | 3·85 (14) | 5·12 (32) | −0·23 (16) | 0·12 (23) | 0·23 (19) |
| C(13) | 3·10 (25) | 4·15 (12) | 4·14 (30) | −0·34 (15) | 0·50 (23) | −0·01 (17) |
| C(14) | 3·60 (25) | 3·41 (15) | 3·44 (30) | −0·08 (17) | −0·05 (25) | −0·27 (18) |
| C(15) | 1·89 (30) | 4·57 (16) | 5·08 (35) | 0·17 (19) | 0·97 (27) | 0·25 (21) |
| C(16) | 2·57 (32) | 5·09 (16) | 3·37 (43) | 0·46 (19) | −0·44 (31) | 0·05 (24) |
| C(17) | 2·74 (28) | 4·71 (12) | 3·59 (36) | 0·12 (16) | −0·48 (25) | −0·52 (19) |
| C(18) | 4·78 (33) | 5·45 (14) | 6·14 (36) | 0·00 (19) | 0·81 (29) | −0·86 (21) |
| C(19) | 5·10 (33) | 4·32 (14) | 5·05 (32) | −0·01 (19) | −0·03 (29) | −0·94 (19) |
| C(20) | 3·62 (29) | 4·75 (15) | 3·49 (48) | −0·45 (19) | −0·14 (31) | 0·18 (24) |
| C(21) | 6·26 (20) | 4·82 (14) | 4·23 (27) | −0·32 (14) | −0·39 (20) | 1·20 (18) |
| O(22) | 3·73 (28) | 6·27 (19) | 4·59 (46) | 0·11 (20) | 0·81 (30) | 0·40 (27) |
| C(23) | 5·06 (18) | 5·12 (11) | 4·81 (29) | 1·28 (12) | 0·47 (19) | −0·30 (17) |
| F(24) | 7·29 (30) | 8·61 (19) | 8·23 (37) | 2·13 (20) | 3·31 (29) | 0·93 (24) |
| F(25) | 4·45 (22) | 9·91 (12) | 8·13 (34) | −0·23 (14) | −0·52 (23) | 0·24 (19) |
| C(26) | 4·81 (27) | 4·60 (16) | 4·82 (31) | 0·49 (19) | 0·33 (24) | −0·02 (21) |
| F(27) | 5·75 (33) | 6·52 (18) | 6·59 (37) | −0·50 (21) | 1·61 (30) | −2·26 (23) |
| F(28) | 7·48 (29) | 6·37 (21) | 8·25 (40) | 2·33 (21) | 1·55 (31) | 1·95 (29) |
| O(29) | 2·48 (29) | 6·35 (24) | 4·68 (40) | −0·61 (24) | 0·59 (33) | −0·08 (31) |
| C(30) | 4·49 (35) | 4·85 (21) | 5·00 (44) | −0·25 (24) | 0·20 (33) | 0·21 (28) |
| O(31) | 6·20 (35) | 10·26 (17) | 3·68 (39) | −0·31 (20) | 0·88 (32) | 0·25 (23) |
| C(32) | 6·25 (20) | 2·77 (10) | 4·76 (28) | −0·37 (12) | 0·17 (21) | 0·27 (16) |
| C(33) | 6·16 (30) | 5·96 (14) | 4·43 (36) | −0·81 (18) | 0·19 (30) | 1·16 (20) |
| C(34) | 3·65 (19) | 6·38 (8) | 4·87 (23) | 0·08 (11) | −0·34 (19) | 0·28 (13) |
| C(35) | 5·68 (19) | 3·99 (9) | 6·19 (29) | 0·43 (11) | −0·14 (21) | −0·00 (15) |
| Br(36) | 3·72 (3) | 10·28 (5) | 10·03 (9) | −0·36 (3) | 0·47 (5) | −0·85 (6) |
| C(37) | 6·43 (19) | 4·51 (9) | 6·15 (27) | −0·12 (12) | −3·00 (20) | −0·00 (14) |
| C(38) | 4·06 (28) | 4·86 (16) | 4·65 (37) | −0·73 (18) | −0·58 (28) | −0·28 (23) |

Table 4. *Observed and calculated structure factors and phase angles*

The columns are $l$, $10F_o$, $10F_c$ and the phase angle.

| | | | |
|---|---|---|---|
| H= 0, K= 0 | | | |
| 2 | 3964 | 4245 | 0 |
| 4 | 1537 | 1546 | 180 |
| 6 | 581 | 585 | 180 |
| 8 | 109 | 123 | 0 |
| 10 | 82 | 87 | 0 |
| H= 0, K= 1 | | | |
| 1 | 100 | 88 | 270 |
| 2 | 1731 | 1859 | 270 |
| 3 | 345 | 437 | 90 |
| 4 | 423 | 469 | 270 |
| 5 | 882 | 901 | 90 |
| 6 | 322 | 365 | 90 |
| 7 | 139 | 136 | 90 |
| 8 | 101 | 106 | 90 |
| 9 | 183 | 198 | 270 |
| 10 | 137 | 136 | 270 |
| 11 | 44 | 41 | 270 |
| 12 | 45 | 48 | 270 |
| H= 0, K= 2 | | | |
| 0 | 3215 | 3438 | 0 |
| 1 | 932 | 968 | 180 |
| 2 | 1725 | 1710 | 0 |
| 3 | 1202 | 1198 | 180 |
| 4 | 425 | 464 | 180 |
| 5 | 247 | 238 | 0 |
| 6 | 327 | 334 | 180 |
| 7 | 581 | 614 | 0 |
| 8 | 165 | 191 | 0 |
| 10 | 54 | 70 | 0 |
| 11 | 159 | 183 | 180 |
| H= 0, K= 3 | | | |
| 1 | 1900 | 1939 | 270 |
| 2 | 490 | 501 | 270 |
| 3 | 1037 | 1073 | 90 |
| 4 | 690 | 723 | 270 |
| 5 | 753 | 777 | 90 |
| 6 | 118 | 121 | 270 |
| 7 | 124 | 134 | 270 |
| 8 | 140 | 155 | 90 |
| 9 | 119 | 122 | 270 |
| H= 0, K= 4 | | | |
| 1 | 559 | 522 | 180 |
| 2 | 98 | 98 | 180 |
| 3 | 240 | 279 | 180 |
| 4 | 141 | 157 | 0 |
| 5 | 574 | 624 | 0 |
| 6 | 156 | 142 | 0 |
| 7 | 357 | 370 | 0 |
| 8 | 151 | 143 | 180 |
| 9 | 117 | 113 | 180 |
| 10 | 115 | 108 | 180 |
| 11 | 111 | 118 | 180 |
| H= 0, K= 5 | | | |
| 1 | 1057 | 1113 | 270 |
| 2 | 246 | 219 | 270 |
| 3 | 122 | 140 | 90 |
| 4 | 69 | 71 | 270 |
| 5 | 215 | 227 | 90 |
| 6 | 51 | 39 | 90 |
| 7 | 153 | 179 | 270 |
| 8 | 88 | 88 | 90 |
| 9 | 113 | 111 | 270 |
| 10 | 109 | 93 | 90 |
| H= 0, K= 6 | | | |
| 0 | 455 | 461 | 180 |
| 1 | 116 | 117 | 180 |
| 3 | 121 | 116 | 180 |
| 4 | 192 | 198 | 0 |
| 5 | 42 | 46 | 0 |
| 6 | 148 | 150 | 180 |
| 7 | 135 | 136 | 0 |
| 8 | 228 | 216 | 180 |
| 10 | 69 | 80 | 180 |
| 11 | 60 | 64 | 180 |
| H= 0, K= 7 | | | |
| 1 | 750 | 746 | 270 |
| 2 | 174 | 178 | 90 |
| 3 | 163 | 148 | 270 |
| 5 | 72 | 73 | 90 |
| 6 | 144 | 137 | 270 |
| 10 | 48 | 42 | 90 |
| 11 | 42 | 48 | 270 |
| H= 0, K= 8 | | | |
| 0 | 502 | 502 | 180 |
| 2 | 98 | 101 | 180 |
| 4 | 245 | 231 | 0 |
| 5 | 96 | 89 | 0 |
| 7 | 123 | 130 | 0 |
| 8 | 91 | 101 | 180 |
| 9 | 42 | 46 | 0 |
| H= 0, K= 9 | | | |
| 1 | 166 | 153 | 270 |
| 2 | 200 | 203 | 90 |
| 3 | 99 | 93 | 270 |
| 4 | 51 | 33 | 90 |
| 6 | 54 | 58 | 270 |
| H= 0, K= 10 | | | |
| 0 | 225 | 216 | 180 |
| 4 | 173 | 166 | 0 |
| 5 | 85 | 72 | 180 |
| 6 | 81 | 75 | 0 |
| 7 | 83 | 80 | 180 |
| H= 0, K= 11 | | | |
| 1 | 200 | 200 | 90 |
| 4 | 63 | 54 | 270 |
| 5 | 94 | 93 | 270 |
| 6 | 83 | 84 | 270 |
| H= 0, K= 12 | | | |
| 1 | 57 | 61 | 0 |
| H= 1, K= 0 | | | |
| 1 | 60 | 46 | 90 |
| 2 | 166 | 111 | 180 |
| 3 | 172 | 175 | 270 |
| 4 | 31 | 11 | 180 |
| 5 | 154 | 155 | 270 |
| 6 | 249 | 228 | 180 |
| 7 | 255 | 244 | 270 |
| 9 | 134 | 125 | 270 |
| 10 | 86 | 71 | 0 |
| 11 | 67 | 75 | 90 |
| 12 | 65 | 45 | 180 |
| 13 | 38 | 34 | 90 |
| H= 1, K= 1 | | | |
| 0 | 198 | 224 | 90 |
| 1 | 500 | 501 | 338 |
| 2 | 514 | 486 | 233 |
| 3 | 314 | 297 | 68 |
| 4 | 854 | 872 | 277 |
| 5 | 679 | 690 | 140 |
| 6 | 230 | 240 | 290 |
| 7 | 265 | 252 | 171 |
| 8 | 162 | 163 | 68 |
| 9 | 153 | 155 | 324 |
| 10 | 55 | 56 | 356 |
| 11 | 54 | 57 | 8 |
| 12 | 56 | 56 | 233 |
| H= 1, K= 2 | | | |
| 0 | 576 | 588 | 90 |
| 1 | 1619 | 1630 | 347 |
| 2 | 345 | 319 | 28 |
| 3 | 240 | 242 | 285 |
| 4 | 510 | 513 | 167 |
| 5 | 147 | 141 | 269 |
| 6 | 490 | 538 | 157 |
| 7 | 227 | 247 | 308 |
| 8 | 86 | 87 | 73 |
| 9 | 86 | 83 | 111 |
| 10 | 83 | 79 | 16 |
| 11 | 114 | 124 | 117 |
| 12 | 40 | 41 | 135 |
| H= 1, K= 3 | | | |
| 0 | 1438 | 1485 | 90 |
| 1 | 773 | 827 | 203 |
| 2 | 426 | 359 | 84 |
| 3 | 172 | 219 | 242 |
| 4 | 391 | 390 | 304 |
| 5 | 185 | 222 | 79 |
| 6 | 256 | 262 | 357 |
| 7 | 74 | 82 | 107 |
| 8 | 51 | 58 | 78 |
| 9 | 135 | 122 | 247 |
| 10 | 71 | 61 | 228 |
| 11 | 76 | 84 | 209 |
| 13 | 43 | 45 | 151 |
| H= 1, K= 4 | | | |
| 0 | 1037 | 1036 | 90 |
| 1 | 838 | 836 | 347 |
| 2 | 501 | 474 | 87 |
| 3 | 389 | 388 | 244 |
| 4 | 112 | 109 | 220 |
| 5 | 343 | 373 | 170 |
| 6 | 85 | 103 | 200 |
| 7 | 262 | 270 | 75 |
| 8 | 65 | 63 | 244 |
| 9 | 175 | 192 | 51 |
| 11 | 77 | 80 | 87 |
| 12 | 45 | 41 | 49 |
| H= 1, K= 5 | | | |
| 0 | 409 | 443 | 270 |
| 1 | 313 | 305 | 291 |
| 2 | 57 | 61 | 159 |
| 3 | 282 | 278 | 280 |
| 4 | 275 | 299 | 72 |
| 5 | 239 | 231 | 109 |
| 6 | 101 | 84 | 158 |
| 7 | 280 | 247 | 140 |
| 8 | 85 | 95 | 185 |
| 9 | 197 | 200 | 196 |
| 11 | 74 | 74 | 210 |
| H= 1, K= 6 | | | |
| 0 | 656 | 672 | 90 |
| 1 | 538 | 534 | 344 |
| 2 | 417 | 462 | 139 |
| 3 | 248 | 255 | 207 |
| 4 | 45 | 53 | 99 |
| 5 | 275 | 290 | 162 |
| 6 | 86 | 89 | 17 |
| 7 | 132 | 141 | 78 |
| 8 | 72 | 83 | 249 |
| 9 | 101 | 98 | 63 |
| 10 | 80 | 76 | 265 |
| H= 1, K= 7 | | | |
| 0 | 539 | 515 | 270 |
| 1 | 267 | 257 | 332 |
| 2 | 113 | 105 | 242 |
| 3 | 91 | 83 | 340 |
| 4 | 328 | 327 | 100 |
| 5 | 165 | 173 | 131 |
| 6 | 178 | 169 | 79 |
| 7 | 155 | 146 | 163 |
| 8 | 48 | 31 | 340 |
| 9 | 57 | 57 | 200 |
| H= 1, K= 8 | | | |
| 0 | 80 | 85 | 90 |
| 1 | 133 | 146 | 166 |
| 2 | 253 | 248 | 147 |
| 3 | 113 | 115 | 195 |
| 4 | 160 | 160 | 125 |
| 5 | 74 | 61 | 222 |
| 6 | 90 | 91 | 40 |
| H= 1, K= 9 | | | |
| 0 | 400 | 379 | 270 |
| 1 | 191 | 195 | 28 |
| 2 | 202 | 199 | 280 |
| 3 | 89 | 100 | 69 |
| 4 | 141 | 136 | 24 |
| 5 | 54 | 56 | 324 |
| 6 | 101 | 101 | 44 |
| 7 | 53 | 43 | 314 |
| 8 | 50 | 49 | 15 |
| H= 1, K= 10 | | | |
| 0 | 123 | 121 | 90 |
| 1 | 96 | 100 | 200 |
| 2 | 80 | 77 | 112 |
| 6 | 62 | 58 | 44 |
| H= 1, K= 11 | | | |
| 0 | 78 | 75 | 270 |
| 1 | 130 | 139 | 17 |
| 2 | 64 | 66 | 313 |
| 3 | 81 | 88 | 38 |
| 5 | 41 | 28 | 81 |
| H= 1, K= 12 | | | |
| 0 | 46 | 47 | 270 |
| 2 | 42 | 40 | 203 |
| 4 | 60 | 55 | 170 |
| H= 2, K= 0 | | | |
| 0 | 437 | 314 | 0 |
| 2 | 466 | 444 | 0 |
| 3 | 72 | 67 | 270 |
| 4 | 751 | 726 | 0 |
| 5 | 408 | 369 | 270 |
| 6 | 249 | 210 | 0 |
| 7 | 101 | 86 | 270 |
| 8 | 233 | 222 | 180 |
| 9 | 90 | 82 | 90 |
| 12 | 94 | 73 | 0 |
| 13 | 51 | 47 | 270 |
| H= 2, K= 1 | | | |
| 0 | 349 | 350 | 0 |
| 1 | 197 | 201 | 250 |
| 2 | 2118 | 1864 | 88 |
| 3 | 674 | 625 | 274 |
| 4 | 290 | 232 | 103 |
| 5 | 280 | 276 | 279 |
| 6 | 579 | 611 | 274 |
| 7 | 90 | 85 | 106 |
| 8 | 168 | 162 | 297 |
| 9 | 139 | 147 | 123 |
| 11 | 48 | 57 | 126 |
| H= 2, K= 2 | | | |
| 0 | 36 | 7 | 0 |
| 1 | 662 | 670 | 37 |
| 2 | 562 | 580 | 331 |
| 3 | 603 | 601 | 12 |
| 4 | 715 | 709 | 341 |
| 5 | 159 | 166 | 170 |
| 6 | 347 | 363 | 355 |
| 7 | 145 | 163 | 169 |
| 10 | 89 | 107 | 214 |
| 11 | 54 | 56 | 202 |
| 12 | 52 | 60 | 254 |
| 13 | 40 | 44 | 212 |
| H= 2, K= 3 | | | |
| 0 | 906 | 819 | 180 |
| 1 | 401 | 369 | 106 |
| 2 | 285 | 300 | 164 |
| 3 | 326 | 388 | 261 |
| 4 | 66 | 73 | 227 |
| 5 | 740 | 739 | 273 |
| 6 | 101 | 98 | 272 |
| 7 | 84 | 72 | 324 |
| 8 | 171 | 182 | 17 |
| 9 | 184 | 181 | 76 |
| 10 | 138 | 153 | 21 |
| H= 2, K= 4 | | | |
| 0 | 54 | 35 | 180 |
| 1 | 661 | 710 | 329 |
| 2 | 221 | 202 | 203 |
| 3 | 413 | 427 | 24 |
| 4 | 142 | 144 | 329 |
| 5 | 389 | 442 | 153 |
| 6 | 230 | 257 | 357 |
| 7 | 269 | 271 | 157 |
| 9 | 106 | 111 | 121 |
| 10 | 92 | 103 | 182 |
| 11 | 80 | 79 | 149 |
| 12 | 52 | 45 | 229 |
| H= 2, K= 5 | | | |
| 0 | 174 | 176 | 180 |
| 1 | 95 | 118 | 48 |
| 2 | 492 | 482 | 249 |
| 3 | 496 | 515 | 283 |
| 4 | 260 | 245 | 248 |
| 5 | 602 | 423 | 273 |
| 6 | 89 | 89 | 68 |
| 7 | 128 | 129 | 256 |
| 8 | 62 | 59 | 68 |
| H= 2, K= 6 | | | |
| 0 | 286 | 294 | 0 |
| 1 | 254 | 257 | 325 |
| 2 | 264 | 258 | 2 |
| 3 | 189 | 205 | 343 |
| 4 | 128 | 131 | 109 |
| 5 | 186 | 198 | 116 |
| 6 | 207 | 215 | 141 |
| 7 | 137 | 138 | 103 |
| 8 | 89 | 92 | 120 |
| 9 | 43 | 36 | 40 |
| 10 | 50 | 46 | 142 |
| H= 2, K= 7 | | | |
| 1 | 169 | 194 | 266 |
| 2 | 126 | 140 | 296 |
| 3 | 195 | 211 | 191 |
| 4 | 91 | 90 | 94 |
| 5 | 343 | 357 | 203 |
| 6 | 133 | 140 | 123 |
| 7 | 164 | 171 | 202 |
| H= 2, K= 8 | | | |
| 0 | 230 | 228 | 0 |
| 1 | 60 | 58 | 9 |
| 2 | 105 | 99 | 308 |
| 3 | 106 | 111 | 36 |
| 4 | 156 | 149 | 254 |
| 5 | 98 | 103 | 61 |
| 6 | 81 | 69 | 294 |
| 7 | 59 | 41 | 107 |
| H= 2, K= 9 | | | |
| 1 | 147 | 146 | 145 |
| 2 | 123 | 133 | 275 |
| 3 | 207 | 205 | 172 |
| 5 | 116 | 106 | 173 |
| H= 2, K= 10 | | | |
| 2 | 91 | 72 | 256 |
| 3 | 68 | 66 | 29 |
| 4 | 62 | 61 | 208 |
| H= 2, K= 11 | | | |
| 0 | 99 | 96 | 0 |
| 2 | 89 | 85 | 309 |
| 3 | 72 | 77 | 163 |
| 4 | 48 | 39 | 308 |
| 5 | 63 | 55 | 151 |
| 6 | 48 | 44 | 39 |
| H= 2, K= 12 | | | |
| 0 | 53 | 41 | 0 |
| 1 | 59 | 62 | 132 |
| 3 | 77 | 70 | 178 |
| H= 3, K= 0 | | | |
| 1 | 203 | 238 | 90 |
| 2 | 1268 | 1159 | 180 |
| 3 | 454 | 419 | 90 |
| 4 | 111 | 121 | 180 |
| 5 | 284 | 247 | 90 |
| 6 | 509 | 498 | 0 |
| 7 | 74 | 92 | 270 |
| 8 | 41 | 54 | 0 |
| 10 | 205 | 175 | 180 |
| 11 | 127 | 127 | 90 |
| 12 | 45 | 60 | 180 |
| H= 3, K= 1 | | | |
| 0 | 205 | 233 | 270 |
| 1 | 624 | 557 | 22 |
| 2 | 360 | 306 | 160 |
| 3 | 181 | 193 | 45 |
| 4 | 235 | 256 | 68 |
| 5 | 327 | 308 | 179 |
| 6 | 115 | 105 | 324 |
| 7 | 257 | 239 | 173 |
| 8 | 185 | 155 | 280 |
| 9 | 45 | 34 | 7 |
| 11 | 112 | 97 | 355 |
| 12 | 72 | 62 | 141 |
| 13 | 54 | 51 | 348 |
| H= 3, K= 2 | | | |
| 0 | 141 | 167 | 90 |
| 1 | 125 | 93 | 222 |
| 2 | 1190 | 1176 | 191 |
| 3 | 537 | 526 | 51 |
| 4 | 365 | 362 | 209 |
| 5 | 376 | 335 | 51 |
| 6 | 310 | 343 | 28 |
| 7 | 101 | 95 | 245 |
| 8 | 175 | 174 | 30 |
| 9 | 68 | 71 | 101 |
| 10 | 48 | 43 | 210 |
| 11 | 126 | 122 | 65 |
| 12 | 44 | 53 | 204 |
| H= 3, K= 3 | | | |
| 0 | 171 | 217 | 270 |
| 1 | 1079 | 1060 | 132 |
| 2 | 235 | 219 | 146 |
| 3 | 949 | 935 | 84 |
| 4 | 433 | 438 | 115 |
| 5 | 213 | 194 | 21 |
| 6 | 111 | 108 | 106 |
| 7 | 101 | 97 | 309 |
| 8 | 109 | 124 | 243 |
| 9 | 82 | 79 | 66 |
| 10 | 61 | 67 | 260 |
| H= 3, K= 4 | | | |
| 0 | 575 | 602 | 90 |
| 1 | 845 | 850 | 180 |
| 2 | 439 | 439 | 141 |
| 3 | 323 | 330 | 324 |
| 4 | 287 | 307 | 212 |
| 5 | 407 | 439 | 347 |
| 6 | 82 | 89 | 206 |
| 7 | 104 | 117 | 88 |
| 8 | 42 | 36 | 140 |
| 9 | 92 | 99 | 133 |
| 10 | 50 | 52 | 252 |
| 11 | 64 | 57 | 50 |
| 12 | 44 | 43 | 269 |
| H= 3, K= 5 | | | |
| 0 | 32 | 44 | 90 |
| 1 | 816 | 819 | 128 |
| 2 | 179 | 136 | 145 |
| 3 | 849 | 862 | 110 |
| 4 | 252 | 244 | 7 |
| 5 | 155 | 124 | 116 |
| 7 | 115 | 137 | 270 |
| 8 | 62 | 74 | 166 |
| 10 | 89 | 90 | 351 |
| 11 | 57 | 63 | 60 |
| 12 | 42 | 44 | 340 |
| H= 3, K= 6 | | | |
| 0 | 161 | 146 | 270 |
| 1 | 549 | 554 | 192 |
| 2 | 447 | 521 | 340 |
| 3 | 162 | 152 | 136 |
| 4 | 68 | 68 | 314 |
| 5 | 277 | 296 | 73 |
| 6 | 373 | 389 | 163 |
| 7 | 127 | 125 | 109 |
| 8 | 218 | 216 | 159 |
| 9 | 76 | 78 | 151 |
| H= 3, K= 7 | | | |
| 1 | 148 | 143 | 54 |
| 2 | 215 | 254 | 291 |
| 3 | 176 | 174 | 121 |
| 4 | 340 | 352 | 272 |
| 5 | 77 | 77 | 199 |
| 6 | 122 | 114 | 302 |
| 7 | 84 | 75 | 257 |
| 8 | 65 | 67 | 26 |
| H= 3, K= 8 | | | |
| 0 | 45 | 45 | 270 |
| 1 | 153 | 165 | 75 |
| 2 | 339 | 301 | 357 |
| 3 | 211 | 219 | 89 |
| 4 | 82 | 76 | 66 |
| 5 | 148 | 144 | 115 |
| 6 | 212 | 209 | 145 |
| 7 | 96 | 103 | 97 |
| 8 | 98 | 87 | 166 |
| 9 | 43 | 36 | 359 |
| 10 | 42 | 38 | 301 |
| H= 3, K= 9 | | | |
| 0 | 63 | 62 | 270 |
| 1 | 118 | 128 | 204 |
| 2 | 89 | 97 | 240 |
| 3 | 107 | 96 | 279 |
| 4 | 117 | 116 | 262 |
| 5 | 86 | 85 | 352 |
| 6 | 77 | 77 | 229 |
| 7 | 61 | 65 | 38 |
| H= 3, K= 10 | | | |
| 1 | 118 | 110 | 357 |
| 2 | 53 | 49 | 66 |
| 3 | 57 | 46 | 220 |
| 4 | 52 | 54 | 58 |
| 5 | 74 | 65 | 239 |
| H= 3, K= 11 | | | |
| 1 | 61 | 56 | 280 |
| 3 | 44 | 46 | 304 |
| 5 | 66 | 67 | 29 |
| H= 3, K= 12 | | | |
| 0 | 48 | 39 | 90 |
| H= 4, K= 0 | | | |
| 0 | 1414 | 1267 | 0 |
| 1 | 296 | 258 | 90 |
| 2 | 261 | 193 | 0 |
| 3 | 1111 | 999 | 90 |
| 4 | 456 | 495 | 180 |
| 5 | 202 | 221 | 90 |
| 7 | 243 | 196 | 270 |
| 8 | 140 | 123 | 0 |
| 9 | 105 | 106 | 270 |
| 10 | 113 | 117 | 0 |
| 12 | 82 | 92 | 0 |
| H= 4, K= 1 | | | |
| 0 | 256 | 221 | 0 |
| 1 | 1121 | 994 | 230 |
| 2 | 421 | 445 | 247 |
| 3 | 756 | 667 | 188 |
| 4 | 388 | 345 | 281 |
| 5 | 358 | 355 | 33 |
| 6 | 195 | 208 | 53 |
| 7 | 370 | 360 | 10 |
| 8 | 171 | 202 | 119 |
| 9 | 127 | 114 | 105 |
| 10 | 91 | 81 | 231 |
| 11 | 165 | 158 | 135 |
| 12 | 69 | 78 | 303 |
| H= 4, K= 2 | | | |
| 0 | 237 | 295 | 0 |
| 1 | 455 | 493 | 162 |
| 2 | 67 | 66 | 54 |
| 3 | 645 | 618 | 163 |
| 4 | 210 | 209 | 174 |
| 5 | 281 | 291 | 88 |
| 6 | 301 | 289 | 247 |
| 7 | 226 | 229 | 354 |
| 8 | 207 | 223 | 304 |
| 9 | 139 | 148 | 265 |
| 10 | 82 | 64 | 179 |
| 11 | 120 | 125 | 197 |
| 13 | 48 | 56 | 188 |
| H= 4, K= 3 | | | |
| 0 | 423 | 439 | 180 |
| 1 | 336 | 359 | 263 |
| 2 | 377 | 359 | 330 |
| 3 | 336 | 315 | 184 |
| 4 | 528 | 686 | 345 |
| 5 | 140 | 118 | 251 |
| 6 | 95 | 108 | 15 |
| 7 | 238 | 257 | 354 |
| 8 | 171 | 189 | 147 |
| 9 | 179 | 184 | 50 |
| 10 | 80 | 100 | 175 |
| 11 | 104 | 94 | 104 |
| 12 | 48 | 52 | 280 |
| H= 4, K= 4 | | | |
| 0 | 174 | 177 | 180 |
| 1 | 378 | 401 | 111 |
| 2 | 804 | 818 | 97 |
| 3 | 604 | 625 | 137 |
| 4 | 265 | 249 | 56 |
| 5 | 293 | 284 | 133 |
| 6 | 254 | 269 | 297 |
| 7 | 102 | 108 | 0 |
| 8 | 143 | 153 | 242 |
| 10 | 63 | 59 | 186 |
| 11 | 46 | 50 | 215 |
| H= 4, K= 5 | | | |
| 0 | 550 | 585 | 180 |
| 1 | 256 | 208 | 54 |
| 2 | 123 | 130 | 146 |
| 3 | 185 | 190 | 25 |
| 4 | 290 | 333 | 354 |
| 5 | 49 | 44 | 228 |
| 6 | 125 | 128 | 36 |
| 7 | 156 | 165 | 204 |
| 8 | 180 | 164 | 129 |
| 9 | 95 | 86 | 112 |
| 10 | 112 | 97 | 140 |
| H= 4, K= 6 | | | |
| 1 | 245 | 243 | 119 |
| 2 | 248 | 229 | 87 |
| 3 | 217 | 211 | 157 |
| 4 | 221 | 217 | 156 |
| 5 | 113 | 118 | 183 |
| 6 | 318 | 337 | 207 |
| 7 | 45 | 25 | 127 |
| 8 | 158 | 164 | 237 |
| 9 | 43 | 47 | 67 |
| H= 4, K= 7 | | | |
| 0 | 116 | 113 | 180 |
| 1 | 288 | 308 | 320 |
| 3 | 321 | 344 | 6 |
| 4 | 200 | 187 | 86 |
| 6 | 113 | 105 | 69 |
| 7 | 154 | 173 | 167 |
| 9 | 72 | 74 | 124 |
| H= 4, K= 8 | | | |
| 2 | 135 | 123 | 150 |
| 3 | 136 | 142 | 218 |
| 4 | 203 | 192 | 146 |
| 5 | 137 | 128 | 206 |
| 6 | 114 | 111 | 166 |
| 7 | 60 | 71 | 83 |
| 9 | 64 | 66 | 74 |
| 10 | 77 | 76 | 12 |
| H= 4, K= 9 | | | |
| 0 | 46 | 58 | 0 |
| 1 | 165 | 159 | 297 |
| 2 | 48 | 41 | 40 |
| 3 | 95 | 89 | 290 |
| 5 | 95 | 109 | 159 |
| 6 | 45 | 42 | 312 |
| 7 | 101 | 100 | 176 |
| 9 | 39 | 43 | 212 |
| H= 4, K= 10 | | | |
| 0 | 86 | 84 | 180 |
| 1 | 125 | 139 | 93 |
| 4 | 66 | 64 | 23 |
| 6 | 56 | 52 | 48 |
| H= 4, K= 11 | | | |
| 1 | 67 | 66 | 257 |
| H= 4, K= 12 | | | |
| 0 | 63 | 68 | 0 |
| 2 | 41 | 44 | 316 |
| H= 5, K= 0 | | | |
| 1 | 89 | 92 | 270 |
| 2 | 650 | 676 | 0 |
| 3 | 173 | 158 | 270 |
| 4 | 89 | 77 | 0 |
| 5 | 672 | 664 | 90 |
| 6 | 281 | 267 | 180 |
| 7 | 565 | 579 | 90 |
| 8 | 184 | 189 | 180 |
| 9 | 67 | 75 | 90 |
| 12 | 44 | 51 | 0 |
| H= 5, K= 1 | | | |
| 0 | 960 | 889 | 90 |
| 1 | 293 | 302 | 327 |
| 2 | 1174 | 1034 | 173 |
| 3 | 667 | 614 | 246 |
| 4 | 658 | 615 | 267 |
| 5 | 427 | 439 | 204 |
| 6 | 223 | 224 | 289 |
| 7 | 283 | 268 | 51 |
| 8 | 151 | 149 | 164 |
| 9 | 445 | 435 | 10 |
| 10 | 93 | 78 | 226 |
| 11 | 216 | 200 | 359 |
| 12 | 129 | 125 | 255 |
| 13 | 42 | 43 | 30 |
| H= 5, K= 2 | | | |
| 0 | 707 | 673 | 270 |
| 1 | 1017 | 956 | 283 |
| 2 | 227 | 233 | 302 |
| 3 | 551 | 523 | 281 |
| 4 | 270 | 284 | 43 |
| 5 | 528 | 513 | 80 |
| 6 | 145 | 148 | 168 |
| 7 | 285 | 278 | 48 |
| 8 | 153 | 159 | 201 |
| 9 | 164 | 177 | 4 |
| 11 | 74 | 86 | 9 |
| 12 | 37 | 17 | 109 |
| 13 | 37 | 42 | 317 |
| H= 5, K= 3 | | | |
| 0 | 131 | 140 | 90 |
| 1 | 555 | 601 | 239 |
| 2 | 788 | 801 | 174 |
| 3 | 621 | 630 | 223 |
| 4 | 463 | 444 | 181 |
| 5 | 227 | 236 | 99 |
| 6 | 125 | 141 | 5 |
| 7 | 357 | 382 | 52 |
| 8 | 73 | 71 | 91 |
| 9 | 177 | 185 | 23 |
| 10 | 148 | 101 | 167 |
| 11 | 86 | 81 | 311 |
| H= 5, K= 4 | | | |
| 1 | 374 | 392 | 335 |
| 2 | 199 | 188 | 292 |
| 3 | 345 | 342 | 260 |
| 4 | 121 | 107 | 175 |
| 5 | 171 | 134 | 273 |
| 6 | 93 | 96 | 151 |
| 7 | 167 | 162 | 23 |
| 8 | 191 | 192 | 262 |
| 9 | 69 | 45 | 32 |
| 10 | 136 | 137 | 272 |
| H= 5, K= 5 | | | |
| 0 | 96 | 93 | 90 |
| 1 | 135 | 145 | 263 |
| 2 | 546 | 557 | 164 |
| 3 | 248 | 244 | 299 |
| 4 | 223 | 212 | 123 |
| 5 | 134 | 156 | 111 |
| 6 | 158 | 162 | 32 |
| 7 | 282 | 302 | 122 |
| 8 | 45 | 41 | 284 |
| 11 | 63 | 64 | 296 |
| 12 | 42 | 36 | 8 |
| H= 5, K= 6 | | | |
| 0 | 57 | 62 | 270 |
| 1 | 177 | 171 | 51 |
| 2 | 51 | 62 | 120 |
| 3 | 137 | 151 | 132 |
| 4 | 178 | 189 | 84 |
| 5 | 152 | 169 | 215 |
| 7 | 51 | 53 | 262 |
| 8 | 129 | 143 | 271 |
| 9 | 64 | 79 | 49 |
| 10 | 62 | 63 | 278 |
| H= 5, K= 7 | | | |
| 0 | 221 | 228 | 270 |
| 1 | 108 | 90 | 312 |
| 2 | 99 | 101 | 175 |
| 3 | 96 | 89 | 238 |
| 4 | 248 | 263 | 79 |
| 5 | 184 | 187 | 168 |
| 6 | 168 | 167 | 52 |
| 7 | 216 | 225 | 155 |
| 9 | 129 | 127 | 148 |
| 10 | 43 | 51 | 282 |
| H= 5, K= 8 | | | |
| 0 | 81 | 87 | 270 |
| 1 | 55 | 89 | 119 |
| 2 | 161 | 171 | 199 |
| 3 | 142 | 138 | 158 |
| 4 | 124 | 117 | 203 |
| 5 | 145 | 159 | 205 |
| 6 | 66 | 70 | 330 |
| 7 | 68 | 72 | 204 |
| 8 | 86 | 86 | 337 |
| 9 | 38 | 31 | 131 |
| 10 | 43 | 37 | 296 |
| H= 5, K= 9 | | | |
| 0 | 69 | 67 | 270 |
| 1 | 83 | 103 | 45 |
| 2 | 95 | 89 | 1 |
| 3 | 111 | 104 | 66 |
| 4 | 75 | 80 | 33 |
| 7 | 63 | 62 | 168 |
| 8 | 63 | 66 | 278 |
| 9 | 47 | 55 | 174 |
| H= 5, K= 10 | | | |
| 0 | 66 | 69 | 90 |
| 1 | 130 | 126 | 191 |
| 2 | 112 | 111 | 172 |
| 3 | 84 | 79 | 221 |
| 4 | 51 | 58 | 181 |
| 5 | 57 | 48 | 279 |
| H= 5, K= 11 | | | |
| 3 | 45 | 52 | 36 |
| 4 | 51 | 47 | 245 |
| 6 | 35 | 40 | 235 |
| H= 5, K= 12 | | | |
| 1 | 37 | 14 | 194 |
| H= 6, K= 0 | | | |
| 0 | 316 | 307 | 180 |
| 1 | 803 | 794 | 90 |
| 2 | 332 | 311 | 180 |
| 3 | 694 | 678 | 270 |
| 4 | 101 | 97 | 0 |
| 5 | 575 | 564 | 270 |
| 6 | 119 | 121 | 180 |
| 7 | 250 | 239 | 90 |
| 8 | 528 | 534 | 180 |
| 9 | 154 | 144 | 90 |
| 10 | 240 | 236 | 180 |
| 11 | 168 | 148 | 270 |
| 12 | 73 | 70 | 0 |
| 13 | 117 | 112 | 270 |
| H= 6, K= 1 | | | |
| 0 | 298 | 334 | 0 |
| 1 | 685 | 666 | 2 |
| 2 | 912 | 809 | 80 |
| 3 | 834 | 823 | 327 |
| 4 | 98 | 89 | 68 |
| 5 | 328 | 297 | 268 |
| 6 | 329 | 324 | 277 |
| 7 | 63 | 66 | 358 |
| 8 | 181 | 167 | 310 |
| 9 | 212 | 199 | 23 |
| 10 | 113 | 125 | 347 |
| 11 | 51 | 57 | 33 |
| 12 | 51 | 54 | 311 |
| 13 | 48 | 34 | 241 |
| H= 6, K= 2 | | | |
| 0 | 748 | 686 | 180 |
| 1 | 448 | 447 | 52 |
| 2 | 846 | 826 | 249 |
| 3 | 183 | 188 | 336 |
| 4 | 232 | 234 | 309 |
| 5 | 347 | 347 | 182 |
| 6 | 413 | 397 | 82 |
| 7 | 268 | 248 | 135 |
| 9 | 120 | 119 | 84 |
| 10 | 148 | 150 | 196 |
| 11 | 48 | 35 | 282 |
| H= 6, K= 3 | | | |
| 0 | 371 | 423 | 0 |
| 1 | 245 | 222 | 199 |
| 2 | 188 | 174 | 297 |
| 3 | 551 | 553 | 244 |
| 4 | 481 | 479 | 242 |
| 5 | 549 | 551 | 255 |
| 6 | 259 | 269 | 293 |
| 7 | 78 | 76 | 90 |
| 8 | 264 | 245 | 8 |
| 9 | 256 | 263 | 72 |
| 10 | 74 | 78 | 29 |
| H= 6, K= 4 | | | |
| 1 | 313 | 289 | 6 |
| 2 | 681 | 703 | 265 |
| 3 | 302 | 303 | 52 |
| 4 | 46 | 51 | 127 |
| 5 | 255 | 248 | 162 |
| 6 | 339 | 259 | 80 |
| 7 | 159 | 179 | 171 |
| 8 | 94 | 91 | 269 |
| 10 | 135 | 125 | 265 |
| 12 | 41 | 41 | 248 |
| H= 6, K= 5 | | | |
| 0 | 411 | 422 | 0 |
| 1 | 61 | 51 | 100 |
| 2 | 191 | 198 | 272 |
| 3 | 182 | 177 | 238 |
| 4 | 151 | 172 | 213 |
| 5 | 127 | 152 | 238 |
| 6 | 131 | 132 | 35 |
| 7 | 77 | 85 | 86 |
| 8 | 129 | 125 | 25 |
| 10 | 45 | 51 | 359 |
| H= 6, K= 6 | | | |
| 0 | 389 | 391 | 0 |
| 1 | 65 | 65 | 3 |
| 2 | 310 | 323 | 298 |
| 3 | 221 | 208 | 85 |
| 4 | 283 | 288 | 218 |
| 5 | 284 | 313 | 120 |
| 6 | 160 | 159 | 188 |
| 7 | 77 | 99 | 159 |
| 8 | 56 | 62 | 344 |
| 9 | 57 | 64 | 280 |
| 10 | 72 | 62 | 337 |
| H= 6, K= 7 | | | |
| 0 | 128 | 124 | 0 |
| 1 | 144 | 125 | 195 |
| 2 | 130 | 131 | 290 |
| 3 | 105 | 101 | 151 |
| 4 | 177 | 181 | 169 |
| 5 | 87 | 94 | 49 |
| 6 | 178 | 184 | 158 |
| 7 | 156 | 150 | 83 |
| 8 | 42 | 46 | 343 |
| 9 | 130 | 132 | 98 |
| 10 | 55 | 57 | 341 |
| H= 6, K= 8 | | | |
| 0 | 148 | 148 | 0 |
| 1 | 199 | 201 | 288 |
| 2 | 72 | 69 | 277 |
| 3 | 199 | 210 | 81 |
| 4 | 132 | 148 | 204 |
| 5 | 181 | 195 | 104 |
| 6 | 68 | 70 | 203 |
| 8 | 55 | 54 | 356 |
| 9 | 45 | 50 | 263 |
| H= 6, K= 9 | | | |
| 1 | 126 | 135 | 183 |
| 2 | 118 | 115 | 251 |
| 3 | 168 | 178 | 166 |
| 4 | 139 | 134 | 225 |
| 5 | 104 | 105 | 85 |
| 6 | 48 | 48 | 173 |
| 7 | 92 | 88 | 44 |
| H= 6, K= 10 | | | |
| 1 | 51 | 67 | 224 |
| 2 | 77 | 73 | 75 |
| 3 | 43 | 49 | 172 |
| H= 6, K= 11 | | | |
| 2 | 130 | 129 | 296 |
| 3 | 86 | 87 | 126 |
| 4 | 117 | 109 | 316 |
| H= 7, K= 0 | | | |
| 1 | 722 | 694 | 90 |
| 2 | 191 | 203 | 180 |
| 3 | 759 | 690 | 90 |
| 4 | 228 | 212 | 180 |
| 5 | 101 | 129 | 270 |
| 7 | 351 | 331 | 270 |
| 8 | 75 | 82 | 180 |
| 9 | 47 | 61 | 270 |
| H= 7, K= 1 | | | |
| 0 | 469 | 453 | 270 |
| 1 | 871 | 829 | 181 |
| 2 | 309 | 325 | 330 |
| 3 | 844 | 640 | 341 |
| 4 | 395 | 407 | 74 |
| 5 | 584 | 545 | 351 |
| 6 | 319 | 343 | 110 |
| 7 | 224 | 224 | 139 |
| 9 | 119 | 115 | 153 |
| 10 | 96 | 99 | 312 |
| 12 | 43 | 57 | 262 |
| H= 7, K= 2 | | | |
| 0 | 661 | 636 | 90 |
| 1 | 195 | 219 | 108 |
| 2 | 974 | 926 | 202 |
| 3 | 244 | 273 | 60 |
| 4 | 921 | 931 | 241 |
| 5 | 245 | 272 | 303 |
| 6 | 168 | 156 | 220 |
| 7 | 263 | 265 | 247 |
| 8 | 98 | 91 | 104 |
| 9 | 156 | 179 | 156 |
| 10 | 65 | 62 | 311 |
| 11 | 94 | 101 | 103 |
| 12 | 42 | 40 | 283 |
| H= 7, K= 3 | | | |
| 0 | 426 | 385 | 270 |
| 1 | 668 | 665 | 202 |
| 2 | 660 | 638 | 342 |
| 3 | 362 | 407 | 342 |
| 4 | 260 | 221 | 66 |
| 5 | 407 | 421 | 3 |
| 6 | 284 | 297 | 142 |
| 7 | 99 | 93 | 14 |
| 8 | 68 | 71 | 214 |
| 9 | 49 | 43 | 41 |
| 10 | 89 | 87 | 310 |
| H= 7, K= 4 | | | |
| 0 | 605 | 633 | 90 |
| 1 | 304 | 312 | 181 |
| 2 | 352 | 341 | 203 |
| 3 | 221 | 252 | 338 |
| 4 | 766 | 777 | 236 |
| 5 | 350 | 352 | 350 |
| 6 | 118 | 148 | 235 |
| 6 | 159 | 148 | 235 |
| 8 | 118 | 126 | 46 |
| 9 | 188 | 190 | 181 |
| 10 | 57 | 50 | 291 |
| 11 | 83 | 87 | 171 |
| 12 | 63 | 57 | 262 |
| H= 7, K= 5 | | | |
| 0 | 86 | 92 | 270 |
| 1 | 223 | 236 | 54 |
| 2 | 201 | 214 | 341 |
| 3 | 235 | 240 | 148 |
| 5 | 151 | 160 | 222 |
| 6 | 243 | 255 | 173 |
| 7 | 54 | 48 | 353 |
| 10 | 132 | 131 | 344 |
| 11 | 45 | 40 | 259 |
| H= 7, K= 6 | | | |
| 0 | 330 | 365 | 90 |
| 1 | 98 | 126 | 261 |
| 2 | 108 | 104 | 325 |
| 3 | 136 | 129 | 357 |
| 4 | 324 | 372 | 292 |
| 5 | 157 | 181 | 55 |
| 6 | 84 | 88 | 271 |
| 7 | 77 | 70 | 212 |
| 9 | 136 | 141 | 227 |
| 10 | 61 | 61 | 312 |
| 11 | 69 | 64 | 214 |
| H= 7, K= 7 | | | |
| 1 | 237 | 240 | 0 |
| 2 | 67 | 75 | 9 |
| 3 | 185 | 217 | 159 |
| 4 | 42 | 44 | 111 |
| 5 | 157 | 165 | 158 |
| 7 | 77 | 78 | 353 |
| 8 | 63 | 65 | 20 |
| 9 | 71 | 67 | 25 |
| 10 | 44 | 54 | 351 |
| H= 7, K= 8 | | | |
| 0 | 57 | 58 | 90 |
| 1 | 66 | 63 | 289 |
| 2 | 59 | 61 | 31 |
| 3 | 134 | 132 | 211 |
| 5 | 56 | 52 | 166 |
| 6 | 48 | 40 | 58 |
| 7 | 43 | 34 | 340 |
| 8 | 60 | 65 | 34 |
| 9 | 74 | 79 | 266 |
| H= 7, K= 9 | | | |
| 1 | 77 | 80 | 65 |
| 3 | 154 | 173 | 134 |
| 4 | 88 | 72 | 334 |
| 5 | 92 | 113 | 137 |
| 6 | 63 | 73 | 33 |
| H= 7, K= 10 | | | |
| 1 | 71 | 70 | 240 |
| 2 | 53 | 54 | 147 |
| 3 | 80 | 81 | 274 |
| 4 | 64 | 68 | 116 |
| 5 | 45 | 34 | 293 |
| H= 7, K= 11 | | | |
| 1 | 49 | 45 | 62 |
| 3 | 53 | 62 | 102 |
| H= 8, K= 0 | | | |
| 0 | 474 | 492 | 0 |
| 1 | 849 | 859 | 270 |
| 2 | 60 | 63 | 180 |
| 3 | 556 | 580 | 90 |
| 4 | 256 | 244 | 180 |
| 5 | 459 | 490 | 90 |
| 6 | 42 | 38 | 0 |
| 7 | 89 | 73 | 90 |
| 9 | 88 | 82 | 90 |
| H= 8, K= 1 | | | |
| 0 | 221 | 221 | 180 |
| 1 | 405 | 430 | 209 |
| 2 | 239 | 179 | 71 |
| 3 | 252 | 274 | 163 |
| 4 | 328 | 315 | 4 |
| 5 | 297 | 310 | 9 |
| 6 | 92 | 95 | 264 |
| 7 | 183 | 197 | 348 |
| 8 | 265 | 256 | 232 |
| 9 | 76 | 62 | 171 |
| 10 | 196 | 221 | 271 |
| 12 | 40 | 63 | 246 |
| H= 8, K= 2 | | | |
| 1 | 783 | 760 | 273 |
| 2 | 263 | 208 | 221 |
| 3 | 191 | 225 | 51 |
| 4 | 483 | 456 | 244 |
| 5 | 330 | 325 | 77 |
| 6 | 265 | 249 | 298 |
| 8 | 142 | 125 | 43 |
| 9 | 64 | 68 | 174 |
| 10 | 98 | 97 | 108 |
| 11 | 48 | 45 | 114 |
| H= 8, K= 3 | | | |
| 0 | 668 | 705 | 180 |
| 1 | 591 | 585 | 226 |
| 2 | 310 | 338 | 323 |
| 3 | 577 | 593 | 147 |
| 4 | 766 | 800 | 348 |
| 5 | 188 | 178 | 128 |
| 6 | 192 | 190 | 326 |
| 7 | 91 | 104 | 331 |
| 8 | 107 | 106 | 212 |
| 9 | 51 | 58 | 14 |
| H= 8, K= 4 | | | |
| 0 | 40 | 41 | 180 |
| 1 | 146 | 151 | 274 |
| 2 | 201 | 189 | 151 |
| 3 | 74 | 76 | 164 |
| 4 | 203 | 212 | 248 |
| 5 | 122 | 117 | 169 |
| 6 | 250 | 276 | 288 |
| 7 | 110 | 113 | 138 |
| 9 | 112 | 123 | 150 |
| 10 | 77 | 80 | 142 |
| 11 | 49 | 64 | 178 |
| H= 8, K= 5 | | | |
| 0 | 345 | 357 | 180 |
| 1 | 180 | 200 | 320 |
| 2 | 118 | 129 | 37 |
| 3 | 151 | 171 | 62 |
| 4 | 439 | 477 | 350 |
| 6 | 149 | 174 | 302 |
| 7 | 60 | 60 | 201 |
| 8 | 154 | 166 | 207 |
| 10 | 49 | 58 | 186 |
| H= 8, K= 6 | | | |
| 0 | 77 | 93 | 180 |
| 1 | 115 | 115 | 84 |
| 2 | 132 | 168 | 53 |
| 3 | 151 | 168 | 263 |
| 4 | 148 | 151 | 306 |
| 5 | 78 | 88 | 223 |
| 6 | 200 | 228 | 242 |
| 7 | 49 | 47 | 166 |
| 8 | 103 | 120 | 226 |
| 9 | 73 | 65 | 220 |
| 10 | 59 | 58 | 207 |
| 11 | 46 | 47 | 213 |
| H= 8, K= 7 | | | |
| 0 | 40 | 46 | 180 |
| 1 | 109 | 110 | 18 |
| 2 | 118 | 123 | 59 |
| 3 | 173 | 200 | 53 |
| 5 | 76 | 79 | 160 |
| 6 | 151 | 176 | 245 |
| 7 | 64 | 72 | 192 |
| 8 | 83 | 68 | 259 |
| 9 | 48 | 53 | 50 |
| H= 8, K= 8 | | | |
| 3 | 120 | 134 | 304 |
| 5 | 141 | 153 | 302 |
| 6 | 63 | 73 | 255 |
| 7 | 45 | 33 | 289 |
| 8 | 74 | 75 | 211 |
| 9 | 54 | 43 | 247 |
| H= 8, K= 9 | | | |
| 1 | 95 | 106 | 76 |
| 2 | 104 | 106 | 237 |
| 3 | 54 | 43 | 147 |
| 4 | 86 | 87 | 224 |
| 5 | 77 | 87 | 179 |
| 6 | 55 | 55 | 313 |
| H= 8, K= 10 | | | |
| 0 | 64 | 67 | 180 |
| 3 | 105 | 108 | 283 |
| 5 | 56 | 51 | 254 |
| H= 8, K= 11 | | | |
| 3 | 50 | 57 | 221 |
| H= 9, K= 0 | | | |
| 1 | 798 | 772 | 270 |
| 2 | 662 | 567 | 0 |
| 3 | 514 | 519 | 270 |
| 4 | 98 | 112 | 180 |
| 5 | 435 | 418 | 90 |
| 6 | 260 | 268 | 180 |
| 7 | 60 | 73 | 90 |
| 8 | 103 | 109 | 180 |
| 9 | 242 | 220 | 270 |
| 11 | 51 | 59 | 270 |
| H= 9, K= 1 | | | |
| 1 | 816 | 750 | 1 |
| 2 | 510 | 421 | 266 |
| 3 | 294 | 312 | 231 |
| 4 | 475 | 446 | 285 |
| 5 | 423 | 429 | 185 |
| 6 | 130 | 143 | 44 |
| 7 | 155 | 170 | 103 |
| 8 | 143 | 155 | 81 |
| 9 | 65 | 73 | 345 |
| 11 | 72 | 74 | 281 |
| H= 9, K= 2 | | | |
| 0 | 435 | 447 | 270 |
| 1 | 603 | 577 | 281 |
| 2 | 522 | 503 | 192 |
| 3 | 525 | 541 | 268 |
| 4 | 465 | 450 | 135 |
| 5 | 121 | 122 | 115 |
| 6 | 260 | 276 | 150 |
| 7 | 98 | 120 | 93 |
| 8 | 133 | 146 | 246 |
| 10 | 120 | 125 | 322 |
| 11 | 68 | 70 | 330 |
| H= 9, K= 3 | | | |
| 0 | 325 | 313 | 278 |
| 1 | 315 | 331 | 254 |
| 2 | 608 | 572 | 206 |
| 3 | 297 | 276 | 228 |
| 4 | 173 | 169 | 310 |
| 5 | 240 | 277 | 143 |
| 6 | 286 | 303 | 351 |
| 7 | 74 | 79 | 77 |
| 9 | 118 | 129 | 338 |
| 10 | 70 | 86 | 87 |
| 12 | 74 | 73 | 45 |
| H= 9, K= 4 | | | |
| 0 | 767 | 773 | 270 |
| 1 | 164 | 167 | 272 |
| 2 | 255 | 272 | 203 |
| 3 | 262 | 271 | 247 |
| 4 | 510 | 537 | 124 |
| 5 | 132 | 132 | 339 |
| 6 | 120 | 112 | 135 |
| 7 | 148 | 166 | 32 |
| 8 | 189 | 192 | 273 |
| 9 | 68 | 80 | 94 |
| 10 | 61 | 85 | 282 |
| 11 | 67 | 66 | 74 |
| H= 9, K= 5 | | | |
| 0 | 80 | 84 | 270 |
| 1 | 112 | 114 | 166 |
| 2 | 458 | 478 | 187 |
| 3 | 65 | 59 | 98 |
| 5 | 119 | 138 | 57 |
| 6 | 161 | 186 | 18 |
| 7 | 43 | 53 | 50 |
| 8 | 83 | 85 | 98 |
| 9 | 65 | 77 | 281 |
| 10 | 91 | 93 | 109 |
| 11 | 39 | 38 | 308 |
| H= 9, K= 6 | | | |
| 0 | 104 | 120 | 270 |
| 1 | 210 | 214 | 63 |
| 2 | 70 | 60 | 353 |
| 3 | 209 | 210 | 106 |
| 4 | 180 | 201 | 73 |
| 5 | 95 | 112 | 235 |
| 6 | 156 | 165 | 115 |
| 7 | 101 | 110 | 246 |
| 8 | 85 | 93 | 184 |
| H= 9, K= 7 | | | |
| 0 | 83 | 95 | 270 |
| 1 | 137 | 138 | 172 |
| 2 | 68 | 78 | 188 |
| 3 | 101 | 99 | 9 |
| 4 | 78 | 89 | 89 |
| 6 | 84 | 100 | 25 |
| 7 | 138 | 133 | 187 |
| 9 | 60 | 64 | 155 |
| 10 | 47 | 49 | 117 |
| H= 9, K= 8 | | | |
| 0 | 98 | 107 | 90 |
| 1 | 151 | 109 | 68 |
| 2 | 74 | 74 | 107 |
| 3 | 95 | 95 | 101 |
| 5 | 127 | 151 | 235 |
| 7 | 63 | 76 | 248 |
| 8 | 51 | 59 | 154 |
| H= 9, K= 9 | | | |
| 1 | 103 | 109 | 157 |
| 2 | 56 | 59 | 116 |
| 4 | 72 | 90 | 86 |
| 8 | 57 | 60 | 32 |
| H= 9, K= 10 | | | |
| 0 | 80 | 91 | 90 |
| H= 9, K= 11 | | | |
| 0 | 44 | 55 | 90 |
| 1 | 78 | 81 | 173 |
| 4 | 37 | 31 | 166 |
| H= 10, K= 0 | | | |
| 0 | 1511 | 1357 | 0 |
| 1 | 209 | 148 | 270 |
| 2 | 501 | 446 | 0 |
| 3 | 563 | 570 | 270 |
| 4 | 265 | 247 | 180 |
| 5 | 435 | 483 | 270 |
| 6 | 109 | 110 | 180 |
| 7 | 251 | 245 | 90 |
| 8 | 46 | 55 | 180 |
| 9 | 296 | 292 | 90 |
| 11 | 66 | 64 | 270 |
| H= 10, K= 1 | | | |
| 0 | 1087 | 947 | 0 |
| 1 | 866 | 800 | 340 |
| 2 | 541 | 463 | 309 |
| 3 | 731 | 724 | 353 |
| 4 | 442 | 397 | 251 |
| 5 | 283 | 283 | 143 |
| 6 | 107 | 108 | 315 |
| 7 | 239 | 262 | 162 |
| 8 | 104 | 97 | 44 |
| 9 | 116 | 114 | 318 |
| 10 | 64 | 54 | 273 |
| 11 | 111 | 113 | 338 |
| 12 | 64 | 60 | 256 |
| H= 10, K= 2 | | | |
| 0 | 515 | 449 | 0 |
| 1 | 455 | 426 | 48 |
| 2 | 1042 | 975 | 284 |
| 3 | 493 | 476 | 306 |
| 4 | 308 | 231 | 240 |
| 6 | 382 | 364 | 125 |
| 7 | 227 | 224 | 60 |
| 9 | 121 | 128 | 71 |
| 10 | 118 | 106 | 281 |
| 11 | 91 | 98 | 194 |
| H= 10, K= 3 | | | |
| 0 | 723 | 697 | 0 |
| 1 | 638 | 591 | 281 |
| 2 | 385 | 372 | 349 |
| 3 | 89 | 86 | 117 |
| 4 | 325 | 301 | 236 |
| 5 | 298 | 293 | 152 |
| 6 | 50 | 55 | 234 |
| 7 | 116 | 117 | 206 |
| 9 | 234 | 236 | 307 |
| 11 | 113 | 121 | 302 |
| 12 | 79 | 78 | 216 |
| H= 10, K= 4 | | | |
| 1 | 73 | 67 | 274 |
| 2 | 698 | 693 | 263 |
| 3 | 75 | 77 | 129 |
| 4 | 168 | 178 | 260 |
| 5 | 68 | 79 | 227 |
| 6 | 210 | 242 | 65 |
| 7 | 53 | 45 | 320 |
| 7 | 53 | 45 | 320 |
| 8 | 97 | 98 | 10 |
| 10 | 118 | 128 | 243 |
| H= 10, K= 5 | | | |
| 0 | 527 | 517 | 0 |
| 1 | 343 | 337 | 245 |
| 2 | 148 | 130 | 348 |
| 3 | 127 | 135 | 174 |
| 4 | 145 | 184 | 154 |
| 5 | 130 | 124 | 32 |
| 7 | 82 | 91 | 318 |
| 8 | 88 | 96 | 339 |
| 9 | 89 | 86 | 273 |
| 11 | 47 | 42 | 307 |
| H= 10, K= 6 | | | |
| 0 | 100 | 90 | 180 |
| 1 | 315 | 353 | 278 |
| 2 | 385 | 394 | 258 |
| 4 | 129 | 118 | 269 |
| 5 | 156 | 161 | 115 |
| 6 | 117 | 131 | 48 |
| 7 | 46 | 39 | 315 |
| 8 | 54 | 65 | 2 |
| 10 | 38 | 43 | 320 |
| H= 10, K= 7 | | | |
| 0 | 154 | 145 | 0 |
| 1 | 153 | 154 | 180 |
| 2 | 113 | 120 | 71 |
| 3 | 139 | 149 | 193 |
| 4 | 159 | 161 | 135 |
| 5 | 54 | 55 | 343 |
| 6 | 62 | 59 | 194 |
| 7 | 45 | 47 | 31 |
| 8 | 80 | 82 | 302 |
| 9 | 41 | 38 | 125 |
| H= 10, K= 8 | | | |
| 0 | 149 | 163 | 180 |
| 1 | 298 | 313 | 266 |
| 2 | 101 | 103 | 206 |
| 3 | 51 | 45 | 156 |
| 4 | 45 | 53 | 255 |
| 5 | 87 | 98 | 84 |
| 6 | 60 | 62 | 269 |
| 7 | 45 | 48 | 354 |
| 8 | 39 | 40 | 244 |
| 9 | 33 | 34 | 298 |
| H= 10, K= 9 | | | |
| 0 | 73 | 93 | 180 |
| 1 | 124 | 121 | 159 |
| 2 | 66 | 66 | 199 |
| 3 | 144 | 147 | 174 |
| 5 | 42 | 39 | 326 |
| 7 | 79 | 84 | 358 |
| H= 10, K= 10 | | | |
| 0 | 136 | 142 | 180 |
| 1 | 77 | 79 | 251 |
| 2 | 140 | 141 | 129 |
| 6 | 51 | 49 | 310 |
| H= 10, K= 11 | | | |
| 0 | 77 | 84 | 180 |
| 1 | 42 | 48 | 138 |
| 4 | 37 | 36 | 20 |
| H= 11, K= 0 | | | |
| 1 | 508 | 514 | 90 |
| 2 | 647 | 517 | 180 |
| 4 | 183 | 185 | 180 |
| 5 | 133 | 146 | 270 |
| 8 | 89 | 97 | 180 |
| 9 | 151 | 170 | 270 |
| 12 | 63 | 60 | 0 |
| H= 11, K= 1 | | | |
| 0 | 113 | 121 | 270 |
| 2 | 606 | 604 | 356 |
| 3 | 202 | 192 | 289 |
| 4 | 390 | 359 | 0 |
| 6 | 63 | 66 | 149 |
| 7 | 219 | 214 | 188 |
| 8 | 106 | 106 | 155 |
| 9 | 130 | 126 | 197 |
| H= 11, K= 2 | | | |
| 0 | 254 | 262 | 90 |
| 1 | 293 | 311 | 68 |
| 2 | 361 | 305 | 200 |
| 3 | 376 | 348 | 85 |
| 5 | 56 | 47 | 318 |
| 6 | 195 | 197 | 238 |
| 9 | 60 | 61 | 214 |
| 10 | 87 | 79 | 349 |
| 11 | 43 | 48 | 92 |
| H= 11, K= 3 | | | |
| 0 | 245 | 235 | 90 |
| 1 | 344 | 312 | 171 |
| 2 | 750 | 744 | 0 |
| 3 | 56 | 55 | 88 |
| 4 | 333 | 319 | 338 |
| 5 | 70 | 80 | 313 |
| 6 | 291 | 300 | 172 |
| 8 | 213 | 225 | 162 |
| 10 | 62 | 55 | 45 |
| H= 11, K= 4 | | | |
| 0 | 583 | 591 | 90 |
| 1 | 122 | 131 | 342 |
| 2 | 179 | 154 | 109 |
| 3 | 51 | 40 | 297 |
| 4 | 228 | 248 | 246 |
| 5 | 171 | 168 | 167 |
| 6 | 62 | 57 | 295 |
| 7 | 171 | 177 | 173 |
| 8 | 65 | 79 | 346 |
| 9 | 65 | 70 | 139 |
| 10 | 74 | 87 | 307 |
| 11 | 41 | 52 | 97 |
| H= 11, K= 5 | | | |
| 0 | 195 | 236 | 270 |
| 1 | 115 | 108 | 84 |
| 2 | 421 | 428 | 345 |
| 3 | 98 | 94 | 150 |
| 4 | 133 | 118 | 336 |
| 5 | 44 | 49 | 103 |
| 6 | 227 | 235 | 190 |
| 7 | 164 | 175 | 62 |
| 8 | 132 | 139 | 181 |
| 9 | 81 | 90 | 27 |
| 11 | 33 | 36 | 332 |
| H= 11, K= 6 | | | |
| 0 | 463 | 450 | 90 |
| 1 | 215 | 202 | 357 |
| 2 | 201 | 182 | 86 |
| 3 | 80 | 89 | 157 |
| 4 | 93 | 86 | 324 |
| 5 | 165 | 160 | 142 |
| 7 | 98 | 94 | 116 |
| 8 | 55 | 59 | 112 |
| H= 11, K= 7 | | | |
| 0 | 262 | 294 | 270 |
| 2 | 202 | 217 | 301 |
| 4 | 122 | 130 | 30 |
| 7 | 51 | 56 | 70 |
| 9 | 63 | 67 | 43 |
| H= 11, K= 8 | | | |
| 0 | 289 | 302 | 90 |
| 1 | 72 | 72 | 275 |
| 2 | 212 | 216 | 90 |
| 3 | 77 | 72 | 253 |
| 4 | 111 | 117 | 150 |
| 5 | 65 | 71 | 117 |
| 7 | 76 | 75 | 89 |
| 8 | 55 | 65 | 56 |
| H= 11, K= 9 | | | |
| 0 | 117 | 113 | 270 |
| 1 | 72 | 62 | 68 |
| 2 | 58 | 53 | 242 |
| 3 | 106 | 122 | 157 |
| 4 | 46 | 42 | 66 |
| 5 | 68 | 69 | 181 |
| 6 | 60 | 59 | 66 |
| H= 11, K= 10 | | | |
| 0 | 50 | 50 | 90 |
| 1 | 68 | 78 | 242 |
| 2 | 54 | 47 | 154 |
| 3 | 92 | 93 | 270 |
| 5 | 42 | 45 | 0 |
| H= 12, K= 0 | | | |
| 0 | 209 | 241 | 180 |
| 1 | 300 | 330 | 270 |
| 3 | 623 | 629 | 90 |
| 4 | 394 | 383 | 0 |
| 5 | 479 | 466 | 90 |
| 6 | 277 | 259 | 0 |
| 10 | 67 | 79 | 180 |
| H= 12, K= 1 | | | |
| 0 | 262 | 257 | 180 |
| 1 | 233 | 249 | 176 |
| 2 | 432 | 435 | 113 |
| 3 | 215 | 189 | 208 |
| 4 | 218 | 188 | 64 |
| 5 | 636 | 643 | 332 |
| 6 | 45 | 35 | 338 |
| 7 | 476 | 474 | 342 |
| 8 | 48 | 50 | 193 |
| 9 | 71 | 82 | 351 |
| 10 | 43 | 57 | 301 |
| 11 | 58 | 59 | 173 |
| H= 12, K= 2 | | | |
| 0 | 137 | 129 | 0 |
| 1 | 379 | 357 | 315 |
| 2 | 311 | 303 | 68 |
| 3 | 351 | 368 | 37 |
| 4 | 226 | 236 | 351 |
| 5 | 348 | 348 | 102 |
| 6 | 413 | 406 | 313 |
| 7 | 165 | 166 | 167 |
| 8 | 177 | 172 | 307 |
| 9 | 57 | 54 | 232 |
| H= 12, K= 3 | | | |
| 0 | 604 | 624 | 180 |
| 1 | 197 | 184 | 176 |
| 2 | 219 | 204 | 260 |
| 3 | 180 | 191 | 168 |
| 4 | 295 | 309 | 329 |
| 5 | 208 | 205 | 334 |
| 6 | 49 | 51 | 167 |
| 8 | 82 | 84 | 154 |
| 9 | 185 | 202 | 344 |
| 11 | 41 | 43 | 332 |
| H= 12, K= 4 | | | |
| 1 | 79 | 103 | 330 |
| 2 | 438 | 453 | 95 |
| 3 | 72 | 83 | 60 |
| 4 | 235 | 217 | 90 |
| 5 | 127 | 146 | 207 |
| 6 | 202 | 195 | 303 |
| 7 | 92 | 87 | 247 |
| 10 | 54 | 54 | 21 |
| H= 12, K= 5 | | | |
| 0 | 386 | 386 | 180 |
| 1 | 127 | 119 | 292 |
| 2 | 221 | 203 | 158 |
| 3 | 47 | 38 | 77 |
| 4 | 102 | 120 | 1 |
| 6 | 129 | 132 | 332 |
| 7 | 86 | 84 | 289 |
| 8 | 63 | 56 | 245 |
| 9 | 79 | 92 | 321 |
| H= 12, K= 6 | | | |
| 0 | 119 | 115 | 180 |
| 1 | 98 | 113 | 269 |
| 2 | 104 | 103 | 125 |
| 3 | 238 | 260 | 274 |
| 5 | 102 | 93 | 317 |
| 4 | 103 | 123 | 279 |
| 7 | 88 | 98 | 14 |
| 8 | 80 | 84 | 280 |
| 9 | 55 | 58 | 314 |
| 10 | 35 | 34 | 91 |
| H= 12, K= 7 | | | |
| 0 | 153 | 159 | 180 |
| 1 | 136 | 147 | 8 |
| 2 | 155 | 178 | 89 |
| 3 | 162 | 175 | 346 |
| 4 | 161 | 187 | 58 |
| 5 | 101 | 107 | 245 |
| 7 | 92 | 88 | 214 |
| 8 | 78 | 70 | 309 |
| H= 12, K= 8 | | | |
| 0 | 58 | 38 | 180 |
| 1 | 60 | 74 | 285 |
| 5 | 50 | 43 | 298 |
| 6 | 61 | 63 | 242 |
| 8 | 39 | 35 | 195 |
| H= 12, K= 9 | | | |
| 0 | 85 | 97 | 0 |
| 1 | 80 | 76 | 96 |
| 2 | 63 | 58 | 32 |
| 4 | 46 | 42 | 68 |
| 5 | 74 | 83 | 250 |
| 7 | 43 | 45 | 203 |
| H= 12, K= 10 | | | |
| 0 | 68 | 77 | 180 |
| 1 | 115 | 111 | 97 |
| 2 | 85 | 90 | 229 |
| 3 | 54 | 53 | 130 |
| 4 | 41 | 41 | 216 |
| H= 13, K= 0 | | | |
| 1 | 464 | 475 | 270 |
| 2 | 187 | 229 | 180 |
| 3 | 461 | 422 | 270 |
| 4 | 108 | 100 | 0 |
| 5 | 226 | 263 | 90 |
| 7 | 174 | 183 | 90 |
| 9 | 82 | 90 | 270 |
| 11 | 72 | 72 | 270 |
| H= 13, K= 1 | | | |
| 0 | 268 | 316 | 270 |
| 1 | 342 | 343 | 19 |
| 2 | 109 | 123 | 219 |
| 3 | 204 | 218 | 159 |
| 4 | 197 | 224 | 90 |
| 5 | 337 | 345 | 183 |
| 6 | 126 | 145 | 55 |
| 7 | 61 | 65 | 191 |
| 8 | 66 | 76 | 286 |
| 10 | 74 | 81 | 248 |
| 11 | 58 | 49 | 186 |
| H= 13, K= 2 | | | |
| 0 | 516 | 496 | 270 |
| 1 | 386 | 378 | 260 |
| 2 | 378 | 385 | 201 |
| 3 | 473 | 459 | 270 |
| 4 | 265 | 288 | 93 |
| 5 | 63 | 87 | 33 |
| 6 | 203 | 222 | 42 |
| 7 | 106 | 116 | 78 |
| 8 | 124 | 145 | 316 |
| 9 | 54 | 51 | 272 |
| 10 | 63 | 70 | 311 |
| 11 | 45 | 45 | 288 |
| H= 13, K= 3 | | | |
| 0 | 75 | 94 | 270 |
| 1 | 354 | 361 | 71 |
| 2 | 292 | 309 | 192 |
| 3 | 507 | 525 | 94 |
| 4 | 49 | 65 | 62 |
| 5 | 179 | 170 | 130 |
| 6 | 209 | 240 | 359 |
| 8 | 108 | 137 | 306 |
| 10 | 80 | 79 | 246 |
| 11 | 54 | 49 | 186 |
| H= 13, K= 4 | | | |
| 0 | 493 | 488 | 270 |
| 1 | 186 | 219 | 164 |
| 2 | 165 | 191 | 188 |
| 3 | 172 | 180 | 39 |
| 4 | 491 | 511 | 108 |
| 5 | 187 | 207 | 17 |
| 6 | 252 | 256 | 82 |
| 7 | 49 | 45 | 16 |
| 8 | 92 | 99 | 308 |
| 10 | 53 | 63 | 279 |
| H= 13, K= 5 | | | |
| 1 | 341 | 375 | 114 |
| 2 | 350 | 378 | 172 |
| 3 | 377 | 420 | 85 |
| 4 | 67 | 62 | 191 |
| 5 | 127 | 116 | 45 |
| 6 | 163 | 179 | 349 |
| 8 | 51 | 52 | 344 |
| 9 | 51 | 54 | 188 |
| 10 | 37 | 27 | 240 |
| H= 13, K= 6 | | | |
| 1 | 365 | 386 | 142 |
| 2 | 198 | 231 | 41 |
| 3 | 369 | 380 | 101 |
| 4 | 250 | 281 | 64 |
| 5 | 138 | 145 | 39 |
| 6 | 106 | 123 | 120 |
| 7 | 91 | 89 | 300 |
| 8 | 48 | 69 | 215 |
| H= 13, K= 7 | | | |
| 0 | 65 | 69 | 270 |
| 1 | 279 | 301 | 173 |
| 2 | 149 | 149 | 239 |
| 3 | 105 | 115 | 124 |
| 4 | 121 | 142 | 258 |
| 5 | 106 | 103 | 21 |
| 8 | 52 | 56 | 77 |
| 9 | 35 | 33 | 148 |
| H= 13, K= 8 | | | |
| 0 | 52 | 67 | 90 |
| 1 | 128 | 134 | 115 |
| 2 | 203 | 229 | 356 |
| 3 | 154 | 151 | 92 |
| 4 | 94 | 113 | 339 |
| 6 | 47 | 53 | 83 |
| 7 | 67 | 69 | 280 |
| 8 | 66 | 62 | 85 |
| H= 13, K= 9 | | | |
| 0 | 57 | 71 | 90 |
| 1 | 137 | 142 | 179 |
| 5 | 95 | 99 | 25 |
| H= 13, K= 10 | | | |
| 1 | 48 | 47 | 111 |
| 3 | 63 | 71 | 141 |
| 4 | 53 | 51 | 330 |
| 5 | 41 | 45 | 202 |
| H= 13, K= 11 | | | |
| 0 | 51 | 47 | 90 |
| 1 | 37 | 40 | 242 |
| H= 14, K= 0 | | | |
| 0 | 298 | 315 | 0 |
| 1 | 445 | 444 | 90 |
| 3 | 241 | 257 | 90 |
| 4 | 51 | 69 | 180 |
| 5 | 60 | 4 | 270 |
| 6 | 98 | 82 | 0 |
| 9 | 44 | 74 | 90 |
| 11 | 51 | 51 | 270 |
| H= 14, K= 1 | | | |
| 1 | 337 | 348 | 332 |
| 2 | 277 | 314 | 253 |
| 3 | 444 | 455 | 23 |
| 4 | 163 | 167 | 195 |
| 5 | 129 | 129 | 354 |
| 6 | 171 | 199 | 87 |
| 7 | 198 | 184 | 286 |
| 8 | 54 | 60 | 73 |
| 9 | 54 | 59 | 309 |
| 10 | 63 | 66 | 278 |
| H= 14, K= 2 | | | |
| 0 | 177 | 234 | 0 |
| 1 | 490 | 510 | 111 |
| 2 | 159 | 177 | 248 |
| 3 | 181 | 196 | 183 |
| 4 | 143 | 149 | 211 |
| 5 | 147 | 136 | 283 |
| 6 | 195 | 211 | 326 |
| 7 | 48 | 53 | 272 |
| 8 | 190 | 193 | 301 |
| 9 | 60 | 55 | 180 |
| H= 14, K= 3 | | | |
| 0 | 181 | 202 | 0 |
| 2 | 239 | 251 | 290 |
| 3 | 188 | 191 | 359 |
| 4 | 205 | 209 | 220 |
| 5 | 92 | 85 | 352 |
| 6 | 99 | 94 | 217 |
| 7 | 215 | 233 | 301 |
| 9 | 119 | 143 | 311 |
| H= 14, K= 4 | | | |
| 0 | 122 | 123 | 0 |
| 1 | 107 | 122 | 116 |
| 2 | 231 | 225 | 322 |
| 4 | 190 | 198 | 333 |
| 5 | 159 | 178 | 273 |
| 7 | 100 | 110 | 310 |
| 8 | 95 | 94 | 303 |
| H= 14, K= 5 | | | |
| 0 | 343 | 377 | 0 |
| 1 | 92 | 70 | 306 |
| 2 | 301 | 327 | 55 |
| 3 | 194 | 194 | 47 |
| 3 | 191 | 194 | 47 |
| 4 | 87 | 91 | 117 |
| 6 | 77 | 72 | 223 |
| 9 | 45 | 57 | 287 |
| H= 14, K= 6 | | | |
| 0 | 66 | 58 | 0 |
| 1 | 83 | 107 | 233 |
| 2 | 118 | 124 | 323 |
| 3 | 55 | 69 | 155 |
| 4 | 68 | 69 | 352 |
| 5 | 62 | 75 | 80 |
| H= 14, K= 7 | | | |
| 1 | 63 | 65 | 110 |
| 2 | 93 | 109 | 51 |
| H= 14, K= 8 | | | |
| 2 | 43 | 42 | 304 |
| 5 | 63 | 73 | 74 |
| 6 | 66 | 68 | 167 |
| 7 | 46 | 55 | 59 |
| H= 14, K= 9 | | | |
| 0 | 73 | 86 | 180 |
| 2 | 72 | 72 | 151 |
| 3 | 51 | 57 | 236 |
| 5 | 54 | 54 | 183 |
| H= 14, K= 10 | | | |
| 4 | 55 | 61 | 351 |
| H= 15, K= 1 | | | |
| 0 | 315 | 302 | 90 |
| H= 15, K= 2 | | | |
| 3 | 223 | 225 | 170 |
| 5 | 148 | 170 | 175 |
| 6 | 211 | 254 | 207 |
| H= 15, K= 3 | | | |
| 0 | 380 | 353 | 90 |
| 2 | 127 | 165 | 16 |
| 4 | 269 | 290 | 255 |
| 5 | 153 | 162 | 79 |
| 6 | 289 | 297 | 225 |
| 7 | 106 | 118 | 97 |
| 8 | 48 | 65 | 195 |
| 10 | 48 | 51 | 54 |
| H= 15, K= 4 | | | |
| 0 | 190 | 225 | 90 |
| 1 | 200 | 210 | 341 |
| 2 | 101 | 91 | 269 |
| H= 15, K= 5 | | | |
| 3 | 270 | 252 | 276 |
| 8 | 45 | 37 | 299 |
| H= 15, K= 6 | | | |
| 0 | 106 | 124 | 90 |
| 3 | 79 | 92 | 177 |
| 4 | 61 | 76 | 231 |
| 9 | 61 | 65 | 330 |
| H= 15, K= 7 | | | |
| 1 | 223 | 224 | 342 |
| 2 | 91 | 92 | 286 |
| 3 | 83 | 77 | 244 |
| 5 | 71 | 78 | 154 |
| 6 | 56 | 55 | 42 |
| 8 | 56 | 51 | 264 |
| H= 15, K= 8 | | | |
| 0 | 57 | 60 | 90 |
| 4 | 50 | 49 | 197 |
| H= 15, K= 9 | | | |
| 0 | 122 | 139 | 270 |
| 3 | 42 | 32 | 52 |
| H= 15, K= 10 | | | |
| 2 | 42 | 46 | 118 |

the structure was refined by block-diagonal least-squares approximation, the large values of $B_{22}$ and $B_{33}$ for the Br atom could in part be due to the correlation with the scale factor; however, one would expect this to have manifested itself in $B_{11}$ as well. Analysis of the vibration parameters for the Br atom shows that this atom has its two largest principal motions in directions perpendicular to the C–Br bond at angles of approximately 45° with the plane of the benzene ring.

The conformation of the *A*-ring clearly deviates slightly from ideal chair geometry: 1,4-related atoms are displaced from the least-squares plane through the other four atoms of the ring (Table 6) by amounts which differ significantly from 0·728 Å (Sim, 1965).

Ring *B* has a normal half-chair conformation; atoms C(8) and C(9) are displaced from the least-squares plane through atoms C(4), C(5), C(6), C(7) and C(10) by −0·37 and 0·38 Å respectively (Norton, Kartha & Lu, 1964; Christensen, 1970).

The *C* ring shows a slight deviation from ideal chair geometry. The conformations of the *A* and *C* rings are in agreement with earlier observations of overall flattering both in simple six-membered rings (Davis & Hassel, 1963) and in steroids (Norton, 1965; High & Kraut, 1966). The average C–C–C angle in the *C* ring is 111·8°.

The torsion angle C(14)–C(15)–C(16)–C(17) is 3·8°, indicating that the *D* ring is a slightly distorted *β*-envelope (Brutcher & Leopold, 1966); C(13) is displaced 0·65 Å from the least-squares plane through C(14), C(15), C(16) and C(17). The fold angle about C(14)–C(17) is near 41°.

The least-squares plane through atoms C(16), C(17), C(20), O(22) and C(23) in the six-membered ring attached to the *D* ring shows that atom C(26) is displaced by 0·61 Å from the plane. The ring thus approximates closely to an envelope form.

The four fluorine atoms have a staggered configuration as shown by the torsion angles in Table 5 and also by the intramolecular distances between the atoms, where we find six pairs of atoms at about van der Waals contact and three others that are well clear.

Inspection of Fig. 1(*a*) shows that one of the C–F distances [C(26)–F(27)] is 0·045 Å longer than the

Table 5. *Torsion and fold angles*

*A*
Torsion angle (*T*), *B–D* view along *B–D*, angle is rotation of *A–B* to cover *D–E*, positive clockwise.
*E*

*E*
Fold angle (*F*), *D–B* fold along *D–B*, angle is positive for *B* below *ADE* when viewed as in diagram.
*A*

| *A* | *B* | *D* | *E* | Angle |
|---|---|---|---|---|
| 1 | 2 | 3 | 4 | 58·12 (*T*) |
| 2 | 3 | 4 | 5 | −54·94 (*T*) |
| 3 | 4 | 5 | 10 | 50·62 (*T*) |
| 4 | 5 | 10 | 1 | −46·87 (*T*) |
| 5 | 6 | 7 | 8 | 11·49 (*T*) |
| 5 | 10 | 1 | 2 | 50·29 (*T*) |
| 6 | 7 | 8 | 9 | −42·50 (*T*) |
| 7 | 8 | 9 | 10 | 60·56 (*T*) |
| 8 | 9 | 10 | 5 | −44·05 (*T*) |
| 8 | 9 | 11 | 12 | 47·63 (*T*) |
| 9 | 10 | 5 | 6 | 13·08 (*T*) |
| 9 | 11 | 12 | 13 | −52·68 (*T*) |
| 10 | 1 | 2 | 3 | −56·91 (*T*) |
| 11 | 12 | 13 | 14 | 53·66 (*T*) |
| 12 | 13 | 14 | 8 | −57·89 (*T*) |
| 13 | 14 | 8 | 9 | 55·70 (*T*) |
| 13 | 14 | 15 | 16 | −28·64 (*T*) |
| 14 | 8 | 9 | 11 | −47·37 (*T*) |
| 14 | 15 | 16 | 17 | 3·81 (*T*) |
| 15 | 16 | 17 | 13 | 24·17 (*T*) |
| 16 | 17 | 13 | 14 | −41·11 (*T*) |
| 16 | 26 | 23 | 22 | −129·95 (*T*) |
| 17 | 13 | 14 | 15 | 42·24 (*T*) |
| 17 | 16 | 26 | 23 | 49·45 (*T*) |
| 20 | 17 | 16 | 26 | −23·52 (*T*) |
| 22 | 20 | 17 | 16 | 0·48 (*T*) |
| 23 | 22 | 20 | 17 | −6·11 (*T*) |
| 26 | 23 | 22 | 20 | 33·62 (*T*) |
| 27 | 26 | 23 | 24 | −53·60 (*T*) |
| 27 | 26 | 23 | 25 | −172·97 (*T*) |
| 28 | 26 | 23 | 24 | 60·32 (*T*) |
| 28 | 26 | 23 | 25 | −59·05 (*T*) |
| 9 | 8 | 11 | 12 | −41·52 (*F*) |
| 9 | 8 | 11 | 14 | −43·86 (*F*) |
| 13 | 12 | 14 | 8 | 50·08 (*F*) |
| 13 | 12 | 14 | 11 | 47·67 (*F*) |
| 15 | 17 | 14 | 13 | 42·53 (*F*) |
| 16 | 17 | 14 | 13 | 40·00 (*F*) |

Table 6. *Least-squares planes*

The normal equations are given. Deviations are in Å. Planes are defined by atoms listed before slash (/).

(1) $1·8229x-3·0617y+10·8017z=6·0839$
Deviations: 4, −0·010; 5, −0·002; 6, 0·023; 7, −0·015; 10, 0·005/8, −0·371; 9, 0·375.

(2) $-2·1068x-6·4968y+8·9244z=2·6573$
Deviations: 14, 0·015; 15, −0·023; 16, 0·023; 17, −0·015/13, −0·649.

(3) $9·2689x-7·1626y+7·040z=7·8901$
Deviations: 16, 0·025; 17, −0·019; 20, −0·014; 22, 0·042; 23, −0·035/26, 0·611.

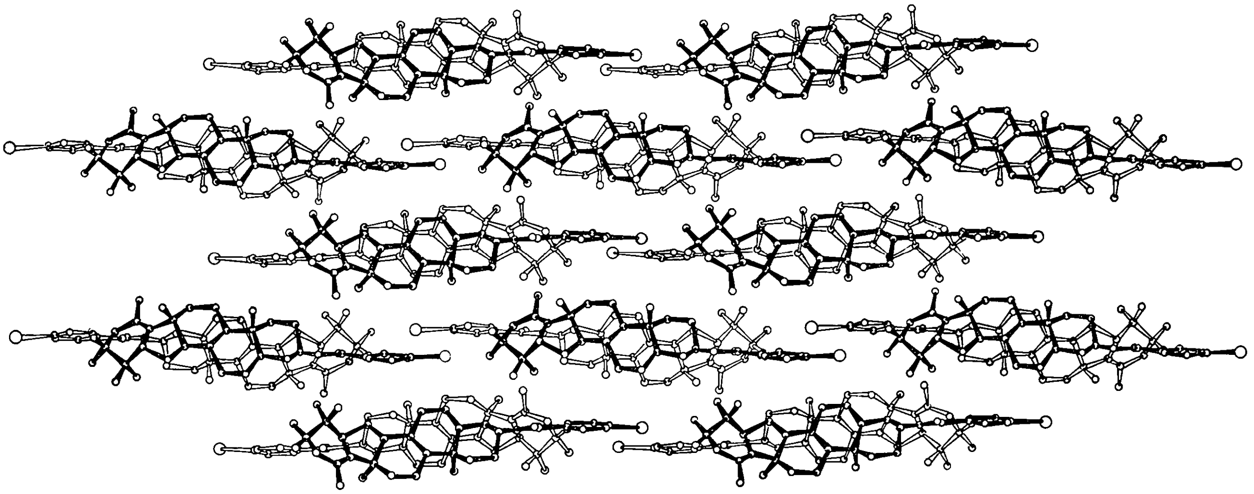

Fig. 2. Projection of the structure along [001]. The *a* axis runs horizontally.

average of the three others, which are not significantly different. (Accepted values are 1·38 Å for C–mono F and 1·33 Å for C–poly F bond lengths.) It is tempting to link this lengthening with the short intermolecular distance between the methyl carbon C(21) and F(27) which is 3·12 Å, and thus 0·23 Å shorter than the sum of van der Waals radii ($CH_3$ 2·0 Å and F 1·35 Å. All other intermolecular distances are normal.

The packing is illustrated in Fig. 2.

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# Structure Cristalline et Moléculaire de l'α-*p*-Chlorophenyl-α-methyl-α′-cyanosuccinimide

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Crystals of α-*p*-chlorophenyl-α-methyl-α′-cyanosuccinimide are monoclinic, space group $P2_1/c$ with $a = 15.53$, $b = 8.59$, $c = 8.86$ Å, $\beta = 111.25°$, $Z = 4$, formula $C_{12}H_9O_2N_2Cl$. The structure has been determined from three-dimensional X-ray diffraction data and refined by the least-squares method to $R = 0.066$. The phenyl group is planar but the two *para* substituents (chlorine and carbon) seem significantly displaced from the ring plane. In the five-membered ring considerable distortion occurs as a result of steric hindrance between the methyl group and the neighbouring cyano group.

## Introduction

L'étude de cette succinimide a été entreprise afin de définir à quel isomère géométrique aboutissait la synthèse chimique, les substituants méthyl et nitrile de l'hétérocycle pouvant se placer en position *cis* ou *trans*. Cette détermination de la configuration moléculaire du groupement succinimide doit permettre une étude quantitative du couplage des vibrations des deux carbonyles en infrarouge (Fayat, 1969).