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# The Crystal and Molecular Structures of Some Molecules Showing S···O Interaction. II. 3-Phenyl-1-propene-1,3-dione-1-(dimethyl mercaptole)

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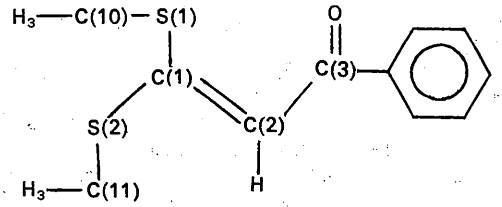
Crystals of 3-phenyl-1-propene-1,3-dione-1-(dimethyl mercaptole), $C_{11}H_{12}OS_2$, belong to the monoclinic system, $a=5{\cdot}972$ (7), $b=10{\cdot}382$ (25), $c=19{\cdot}536$ (11), $\beta=109{\cdot}42$ (2)°, space group $P2_1/c$, $Z=4$ molecules per cell. The structure was solved by direct methods using Cu $K\alpha$ diffractometric intensity data. The molecule shows an S···O distance of 2·727 (10) Å.

3-Phenyl-1-propene-1,3-dione-1-(dimethyl mercaptole) PDM, (I), was the second compound whose crystal structure was examined in order to add more to our understanding of the S···O interaction. Enough is known of this type of interaction to expect that the central part of a molecule such as (I) will almost certainly be flat with sulphur quite close to oxygen. Crystal structure analysis confirms this.



(I)

## Experimental

Crystals of PDM prepared by Kelber's (1910) method were kindly supplied by Professor P. Yates. They were obtained as somewhat poorly formed yellow needles, elongated along the monoclinic *y* axis, on crystallization from an ethyl acetate, pentane mixture.

Initial photographic examination of the crystals showed them to be monoclinic, space group $P2_1/c$. Subsequently they were studied with a Picker automated four-circle diffractometer using Ni-filtered Cu $K\alpha$ radiation. A least-squares refinement based on $2\theta$ of 42 reflexions gave the following cell dimensions: $a=5{\cdot}972$ (7), $b=10{\cdot}382$ (25), $c=19{\cdot}536$ (11) Å, $\beta=109{\cdot}42$ (0·02)° whence $V=1142{\cdot}3$ Å$^3$. The crystal density, by flotation in n-hexane/carbon tetrachloride was $1{\cdot}26_5$ g.cm$^{-3}$ which, using a molecular weight of 224·3, calculates to $1{\cdot}30_4$ g.cm$^{-3}$ for four molecules of PDM per cell.

Intensity data were collected in $\theta$–$2\theta$ scanning mode with Al foil attenuators for counting rates in excess of $10^4$ sec$^{-1}$. The scanning range $\Delta(2\theta)$ used was $1{\cdot}80+0{\cdot}86\tan\theta_m$ degrees where $\theta_m$ was the computed position of the diffraction maximum for a mean weighted wavelength (Alexander & Smith, 1964). The maximum usable $2\theta$ was 130°. Only the independent reflexions were measured.

The crystal used for data collection measured $0{\cdot}1\times0{\cdot}1\times0{\cdot}3$ mm (along *y*) and, with $\mu=36{\cdot}01$ cm$^{-1}$, no absorption corrections were made. Standard deviations in $F_o$ were calculated by the statistical treatment given by Cetlin & Abrahams (1963); Abrahams (1964) and Abrahams & Bernstein (1965). Reflexions were regarded as unobserved if the background-corrected intensity was zero or negative and with a maximum possible intensity of 20 counts. If $0\le|F_o|<\sigma(|F_o|)$, the reflexion was retained with structure amplitude $|F_o|$ but still regarded as unobserved. Of the 1882 independent intensity measurements made, 322 were classified as unobserved.

The structure was solved by the symbolic addition procedure, Karle & Karle (1966). Conversion of $F_o$ to normalized structure factors, $E$, was carried out by the method described by Norment (1961). There were 91 independent reflexions with $|E|\ge2{\cdot}0$ and 242 with $|E|\ge1{\cdot}5$ and reasonably uniform distribution between the eighty parity groups. Using only one symbol it was possible to generate phases for 198 reflexions from $\sum_2$

relations with a strong indication that this symbol was of negative phase. With this assignment the $E$ map showed clearly all the non-hydrogen atoms (except the carbon atoms of the methyl groups). These atoms were then used to phase all the reflexions allowing the two missing carbon atoms to be located. A check on the

Table 1. *Final atomic coordinates, anisotropic thermal parameters* (Å$^2$) *and their standard deviations*

The temperature factor $T$ is of form $\exp\left[-\frac{1}{4}(h^2a^{*2}B_{11}+k^2b^{*2}B_{22}+l^2c^{*2}B_{33}+2hka^*b^*B_{12}+2hla^*c^*B_{13}+2klb^*c^*B_{23})\right]$.

| | $10^4x$ | $10^4y$ | $10^4z$ | $10^2B_{11}$ | $10^2B_{22}$ | $10^2B_{33}$ | $10^2B_{12}$ | $10^2B_{13}$ | $10^2B_{23}$ |
|---|---|---|---|---|---|---|---|---|---|
| S(1) | 5264 (5) | 1585 (3) | 4812 (15) | 334 (15) | 303 (12) | 403 (14) | 6 (11) | 15 (11) | 96 (11) |
| S(2) | 7300 (5) | 4107 (3) | 4649 (15) | 353 (15) | 328 (13) | 436 (15) | −56 (12) | 7 (11) | 64 (11) |
| O | 684 (13) | 1511 (7) | 3895 (38) | 356 (39) | 284 (33) | 524 (39) | 15 (30) | −13 (32) | 204 (31) |
| C(1) | 4843 (17) | 3079 (9) | 4378 (55) | 249 (47) | 267 (46) | 297 (49) | −62 (38) | 24 (40) | −51 (39) |
| C(2) | 2739 (18) | 3433 (10) | 3857 (58) | 329 (51) | 260 (44) | 437 (57) | 32 (42) | 115 (45) | 44 (45) |
| C(3) | 729 (18) | 2580 (9) | 3610 (56) | 374 (55) | 210 (44) | 348 (50) | 19 (40) | 72 (42) | −49 (41) |
| C(4) | −1386 (19) | 3024 (10) | 2982 (55) | 365 (56) | 239 (47) | 301 (49) | 76 (42) | 97 (43) | 0 (40) |
| C(5) | −1223 (20) | 3986 (11) | 2509 (59) | 393 (62) | 496 (59) | 361 (53) | 138 (53) | 90 (49) | 145 (50) |
| C(6) | −3262 (21) | 4356 (11) | 1934 (60) | 371 (62) | 428 (64) | 425 (57) | 30 (54) | 9 (48) | −86 (50) |
| C(7) | −5435 (22) | 3732 (13) | 1840 (62) | 403 (67) | 563 (79) | 413 (60) | 132 (58) | 39 (51) | −92 (54) |
| C(8) | −5569 (21) | 2729 (11) | 2312 (63) | 386 (66) | 370 (57) | 410 (60) | −5 (49) | −25 (52) | −94 (49) |
| C(9) | −3546 (19) | 2363 (11) | 2874 (61) | 286 (54) | 403 (59) | 450 (57) | −148 (47) | 111 (47) | −279 (50) |
| C(10) | 8446 (19) | 1558 (12) | 5355 (64) | 275 (53) | 310 (60) | 602 (72) | 44 (49) | −166 (50) | 44 (57) |
| C(11) | 6406 (20) | 5491 (10) | 4045 (60) | 499 (65) | 288 (48) | 564 (62) | 68 (48) | 97 (51) | 299 (47) |

Table 2. *Hydrogen positions*

($a$) as observed from a difference synthesis and used in $F_c$; ($b$) as calculated making normal angle assumptions and assuming a C–H length of 1·075 Å

| | | ($a$) | | | ($b$) | | |
|---|---|---|---|---|---|---|---|
| Atom | Attached to carbon atom | $10^4x$ | $10^4y$ | $10^4z$ | $10^4x$ | $10^4y$ | $10^4z$ |
| H(1) | C(2) | 2450 | 4220 | 3510 | 2593 | 4382 | 3636 |
| H(2) | C(5) | 240 | 4750 | 2610 | 451 | 4447 | 2581 |
| H(3) | C(6) | −3900 | 4830 | 1490 | −3159 | 5111 | 1569 |
| H(4) | C(7) | −6850 | 4160 | 1440 | −7001 | 4021 | 1406 |
| H(5) | C(8) | −7200 | 2190 | 2300 | −7130 | 2250 | 2237 |
| H(6) | C(9) | −3550 | 1780 | 3400 | −3622 | 1580 | 3226 |
| H(7) | C(10) | 8520 | 680 | 5330 | 8706 | 639 | 5619 |
| H(8) | C(10) | 9720 | 1580 | 4950 | 9520 | 1645 | 5011 |
| H(9) | C(10) | 8850 | 2170 | 5700 | 8874 | 2325 | 5747 |
| H(10) | C(11) | 8050 | 6000 | 4160 | 7918 | 6121 | 4211 |
| H(11) | C(11) | 6000 | 4900 | 3540 | 6012 | 5203 | 3489 |
| H(12) | C(11) | 5300 | 6180 | 4210 | 4878 | 5954 | 4109 |

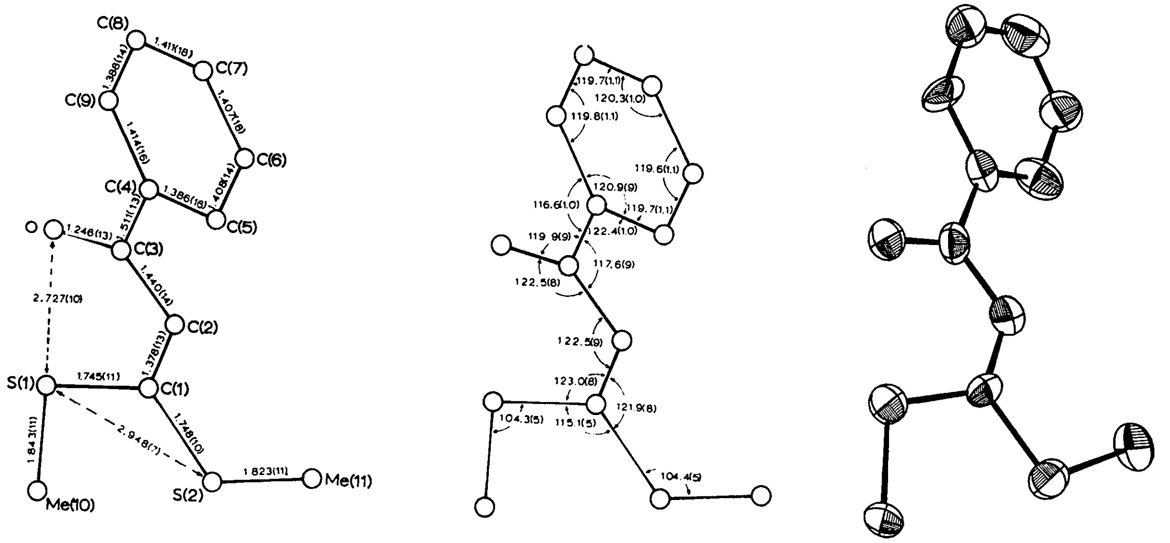


Fig. 1. Atomic numbering scheme, bond lengths, bond angles and perspective view of a molecule of PDM seen from about 80 Å, showing 50% probability thermal ellipsoids (Johnson, 1965).

original 198 phases showed that only one reflexion, $hkl=254$ with $|E|=1{\cdot}58$, had been given the wrong sign.

Refinement was by minimization of $\sum(w|F_o|-|F_c|)^2$ using a local version of *ORFLS* (Busing, Martin & Levy, 1962) with scattering factors of neutral atoms taken from *International Tables for X-ray Crystallography* (1962). The inclusion of unobserved reflexions had no significant effect on final non-hydrogen parameters. The atomic numbering scheme is given in Fig. 1 and the atomic parameters listed in Table 1. A difference synthesis revealed the positions of all the hydrogen atoms. A comparison between the observed coordinates and those expected, using a C–H length of 1·075 Å is given in Table 2 assuming that one C–H bond of each methyl group is parallel to S(2)–C(1).

Hydrogen atoms at their observed positions and with the anisotropic thermal motion parameters of the atoms to which they are attached were included in the final $F_c$ calculation given in Table 4. The scattering factor curve used was that given in *International Tables for X-ray Crystallography* (1962). The conventional $R$ values are 0·119 for all reflexions and 0·10 when unobserved reflexions are omitted.

## Discussion

Bond lengths and angles for non-hydrogen atoms derived from the parameters listed in Table 1 are given together with the thermal ellipsoids in Fig. 1.

The molecule has an *s-cis* conformation of the bonds C(1)–C(2) and C(3)–O about the single bond C(2)–C(3) just as in the analogous part of the desaurin molecule (see Lynch, Mellor & Nyburg, 1971). The C(1)–S bond distances in PDM, 1·745 (11) and 1·748 (10) Å are about $3\sigma/2$ shorter than those in desaurin and hence the difference is of marginal significance. The S–C bond lengths to the methyl groups are, at 1·823 (11) and 1·843 (11) Å, virtually identical and in accord with the accepted 1·82 Å for a C($sp^3$)–S bond (Abrahams, 1956).

Table 3. *Deviations of atoms from least-squares planes*

Starred deviations refer to atoms omitted from the least-squares analysis. All planes of form $Px+Qy+Rz=S$ with $x$, $y$, $z$ fractional coordinates.

| | Plane *A* $\Delta$(Å) | Plane *B* $\Delta$(Å) | Plane *C* $\Delta$(Å) | Plane *D* $\Delta$(Å) |
|---|---|---|---|---|
| S(1) | | 0·0004 | 0·0136 | 0·0149 |
| S(2) | | 0·0004 | −0·0127* | −0·0043 |
| O | | −0·0308* | −0·0275 | −0·0305 |
| C(1) | | −0·0013 | −0·0076 | −0·0035 |
| C(2) | | 0·0005 | −0·0152 | −0·0123 |
| C(3) | | 0·0468* | 0·0366 | 0·0358 |
| C(4) | −0·0194 | | | |
| C(5) | 0·0095 | | | |
| C(6) | 0·0050 | | | |
| C(7) | −0·0094 | | | |
| C(8) | −0·0006 | | | |
| C(9) | 0·0148 | | | |
| Me(10) | | 0·2125* | 0·2325* | 0·2366* |
| Me(11) | | 0·1635* | 0·1302* | 0·1407* |
| *P* | −2·6616 | −3·5265 | −3·5295 | −3·5396 |
| *Q* | 6·9544 | 3·9428 | 4·0432 | 4·0231 |
| *R* | 13·836 | 16·955 | 16·854 | 16·858 |
| *S* | 6·5785 | 6·9277 | 6·9067 | 6·9016 |

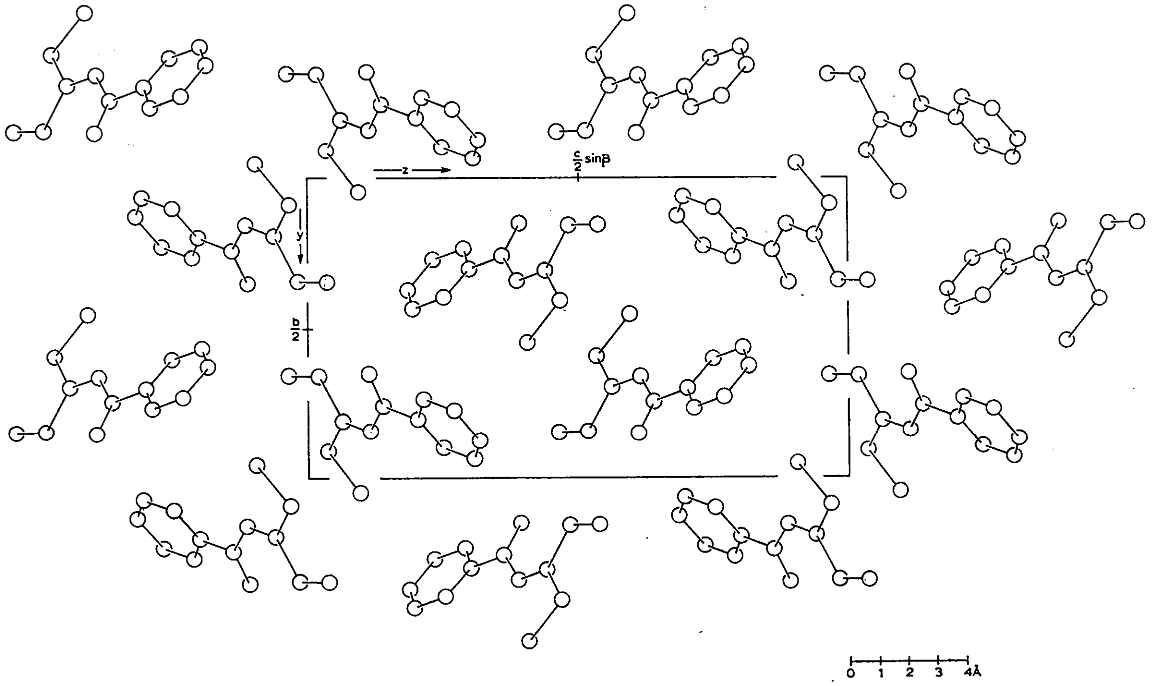


Fig. 2. Molecular packing viewed along [100].

Table 4. *Calculated and observed structure factors*

Unobserved reflexions are marked *.

| H | L | 10Fo | 10Fc |
|---|---|---|---|
| K = 0 | | | |
| 0 | 2 | 497 | 506 |
| 0 | 4 | 724 | 708 |
| 0 | 6 | 97 | 120 |
| 0 | 8 | 174 | 191 |
| 0 | 10 | 116 | 87 |
| 0 | 12 | 383 | -317 |
| 0 | 14 | 296 | -269 |
| 0 | 16 | 109 | -92 |
| 0 | 18 | 177 | -164 |
| 0 | 20 | 49 | -51 |
| 1 | -22 | 21 | -32 |
| 1 | -20 | 52 | 53 |
| 1 | -18 | 110 | -104 |
| 1 | -16 | 64 | 74 |
| 1 | -14 | 98 | 101 |
| 1 | -12 | 15 | -18 |
| 1 | -10 | 17 | 42 |
| 1 | -8 | 359 | 369 |
| 1 | -6 | 446 | 430 |
| 1 | -4 | 552 | -484 |
| 1 | -2 | 386 | -348 |
| 1 | 0 | 677 | -783 |
| 1 | 2 | 361 | -423 |
| 1 | 4 | 609 | -712 |
| 1 | 6 | 788 | -899 |
| 1 | 8 | 57 | 27 |
| 1 | 10 | 278 | -294 |
| 1 | 12 | 116 | -133 |
| 1 | 14 | 106 | -128 |
| 1 | 16 | 67 | 29 |
| 1 | 18 | 88 | 87 |
| 1 | 20 | 132 | 152 |
| 2 | -22 | 16 | -7 |
| 2 | -20 | 27 | -41 |
| 2 | -18 | 45 | 25 |
| 2 | -16 | 160 | 162 |
| 2 | -14 | 17 | 9 |
| 2 | -12 | 236 | 225 |
| 2 | -10 | 203 | -207 |
| 2 | -8 | 107 | 90 |
| 2 | -6 | 54 | 51 |
| 2 | -4 | 240 | -222 |
| 2 | -2 | 538 | -502 |
| 2 | 0 | 216 | 224 |
| 2 | 2 | 471 | 459 |
| 2 | 4 | 367 | 340 |
| 2 | 6 | 167 | 137 |
| 2 | 8 | 309 | 308 |
| 2 | 10 | 377 | 379 |
| 2 | 12 | 288 | 290 |
| 2 | 14 | 293 | 286 |
| 2 | 16 | 96 | 85 |
| 2 | 18 | 21 | 34 |
| 3 | -22 | 120 | 119 |
| 3 | -20 | 150 | 118 |
| 3 | -18 | 154 | 149 |
| 3 | -16 | 42 | -21 |
| 3 | -14 | 94 | 59 |
| 3 | -12 | 54 | -51 |
| 3 | -10 | 38 | -6 |
| 3 | -8 | 298 | 291 |
| 3 | -6 | 49 | -81 |
| 3 | -4 | 816 | -774 |
| 3 | -2 | 344 | -358 |
| 3 | 0 | 226 | -219 |
| 3 | 2 | 135 | -128 |
| 3 | 4 | 67 | -50 |
| 3 | 6 | 122 | -124 |
| 3 | 8 | 175 | 157 |
| 3 | 10 | 88 | 113 |
| 3 | 12 | 133 | -110 |
| 3 | 14 | 91 | -84 |
| 3 | 16 | 106 | -92 |
| 4 | -20 | 120 | -119 |
| 4 | -18 | 95 | -94 |
| 4 | -16 | 99 | -100 |
| 4 | -14 | 120 | -131 |
| 4 | -12 | 172 | -183 |
| 4 | -10 | 184 | -178 |
| 4 | -8 | 111 | 98 |
| 4 | -6 | 317 | 291 |
| 4 | -4 | 346 | 335 |
| 4 | -2 | 294 | 290 |
| 4 | 0 | 242 | 216 |
| 4 | 2 | 618 | 603 |
| 4 | 4 | 18 | 11 |
| 4 | 6 | 45 | 63 |
| 4 | 8 | 47 | -40 |
| 4 | 10 | 14 | 0 |
| 4 | 12 | 14 | 38 |
| 5 | -20 | 46 | -51 |
| 5 | -18 | 97 | 108 |
| 5 | -16 | 94 | -28 |
| 5 | -14 | 163 | 180 |
| 5 | -12 | 176 | 190 |
| 5 | -10 | 100 | 114 |
| 5 | -8 | 232 | 242 |
| 5 | -6 | 217 | 222 |
| 5 | -4 | 36 | 25 |
| 5 | -2 | 194 | -206 |
| 5 | 0 | 355 | -356 |
| 5 | 2 | 127 | -139 |
| 5 | 4 | 197 | -214 |
| 5 | 6 | 298 | -322 |
| 5 | 8 | 234 | -267 |
| 6 | -16 | 23 | -23 |
| 6 | -14 | 31 | 10 |
| 6 | -12 | 53 | -53 |
| 6 | -10 | 63 | -31 |
| 6 | -8 | 184 | -213 |
| 6 | -6 | 115 | -94 |
| 6 | -4 | 83 | 59 |
| 6 | -2 | 56 | -46 |
| 6 | 0 | 17 | 19 |
| 6 | 2 | 51 | 53 |
| 6 | 4 | 83 | 103 |
| K = 1 | | | |
| 0 | 1 | 159 | 133 |
| 0 | 2 | 811 | 837 |
| 0 | 3 | 267 | 227 |
| 0 | 4 | 421 | 392 |
| 0 | 5 | 425 | 456 |
| 0 | 6 | 146 | 128 |
| 0 | 7 | 197 | -199 |
| 0 | 8 | 266 | 266 |
| 0 | 9 | 135 | -124 |
| 0 | 10 | 517 | 461 |
| 0 | 11 | 244 | -214 |
| 0 | 12 | 216 | 212 |
| 0 | 13 | 67 | -45 |
| 0 | 14 | 37 | -3 |
| 0 | 15 | 136 | -113 |
| 0 | 16 | 160 | 158 |
| 0 | 17 | 58 | -61 |
| 0 | 18 | 41 | -4 |
| 0 | 19 | 48 | 31 |
| 0 | 20 | 116 | 110 |
| 0 | 21 | 33 | 17 |
| 1 | -22 | 35 | -29 |
| 1 | -21 | 50 | -55 |
| 1 | -20 | 106 | 137 |
| 1 | -19 | 190 | -197 |
| 1 | -18 | 23 | -29 |
| 1 | -17 | 65 | -71 |
| 1 | -16 | 29 | 20 |
| 1 | -15 | 17 | -19 |
| 1 | -14 | 82 | 67 |
| 1 | -13 | 83 | 110 |
| 1 | -12 | 15 | -50 |
| 1 | -11 | 215 | 230 |
| 1 | -10 | 48 | 63 |
| 1 | -9 | 160 | 161 |
| 1 | -8 | 110 | 136 |
| 1 | -7 | 399 | 403 |
| 1 | -6 | 681 | 712 |
| 1 | -5 | 1126 | 1169 |
| 1 | -4 | 1359 | 1441 |
| 1 | -3 | 241 | 219 |
| 1 | -2 | 149 | -110 |
| 1 | -1 | 400 | 380 |
| 1 | 0 | 383 | 425 |
| 1 | 1 | 415 | -433 |
| 1 | 2 | 349 | 386 |
| 1 | 3 | 215 | -265 |
| 1 | 4 | 97 | 111 |
| 1 | 5 | 88 | 66 |
| 1 | 6 | 226 | -234 |
| 1 | 7 | 210 | -178 |
| 1 | 8 | 497 | -567 |
| 1 | 9 | 182 | -142 |
| 1 | 10 | 155 | -171 |
| 1 | 11 | 65 | -69 |
| 1 | 12 | 222 | -246 |
| 1 | 13 | 58 | -57 |
| 1 | 14 | 180 | -186 |
| 1 | 15 | 80 | 80 |
| 1 | 16 | 184 | -197 |
| 1 | 17 | 21 | 14 * |
| 1 | 18 | 119 | -144 |
| 1 | 19 | 61 | 58 |
| 1 | 20 | 79 | -88 |
| 2 | -22 | 87 | -82 |
| 2 | -21 | 79 | 84 |
| 2 | -20 | 61 | -56 |
| 2 | -19 | 104 | 98 |
| 2 | -18 | 105 | 113 |
| 2 | -17 | 127 | 128 |
| 2 | -16 | 120 | -108 |
| 2 | -15 | 143 | 145 |
| 2 | -14 | 190 | -159 |
| 2 | -13 | 227 | 230 |
| 2 | -12 | 98 | 53 |
| 2 | -11 | 65 | 66 |
| 2 | -10 | 92 | -105 |
| 2 | -9 | 53 | 44 |
| 2 | -8 | 315 | -294 |
| 2 | -7 | 264 | -267 |
| 2 | -6 | 141 | -152 |
| 2 | -5 | 50 | -67 |
| 2 | -4 | 79 | -50 |
| 2 | -3 | 463 | -447 |
| 2 | -2 | 272 | -252 |
| 2 | -1 | 523 | -522 |
| 2 | 0 | 25 | -16 * |
| 2 | 1 | 773 | -723 |
| 2 | 2 | 77 | -62 |
| 2 | 3 | 229 | -234 |
| 2 | 4 | 390 | 378 |
| 2 | 5 | 240 | -245 |
| 2 | 6 | 203 | -184 |
| 2 | 7 | 91 | -109 |
| 2 | 8 | 27 | 9 * |
| 2 | 9 | 186 | -169 |
| 2 | 10 | 17 | -20 * |
| 2 | 11 | 74 | 52 |
| 2 | 12 | 100 | 115 |
| 2 | 13 | 133 | 120 |
| 2 | 14 | 46 | 32 |
| 2 | 15 | 167 | 172 |
| 2 | 16 | 198 | 182 |
| 2 | 17 | 45 | 35 |
| 2 | 18 | 99 | 81 |
| 3 | -22 | 15 | -11 * |
| 3 | -21 | 47 | 39 |
| 3 | -20 | 80 | 71 |
| 3 | -19 | 18 | -25 * |
| 3 | -18 | 103 | 86 |
| 3 | -17 | 44 | -38 |
| 3 | -16 | 180 | 171 |
| 3 | -15 | 175 | -187 |
| 3 | -14 | 101 | 98 |
| 3 | -13 | 75 | -83 |
| 3 | -12 | 177 | 169 |
| 3 | -11 | 115 | -115 |
| 3 | -10 | 125 | 115 |
| 3 | -9 | 118 | -99 |
| 3 | -8 | 139 | 145 |
| 3 | -7 | 320 | -312 |
| 3 | -6 | 173 | 166 |
| 3 | -5 | 187 | -176 |
| 3 | -4 | 273 | 263 |
| 3 | -3 | 250 | 234 |
| 3 | -2 | 79 | -55 |
| 3 | -1 | 350 | 342 |
| 3 | 0 | 158 | -153 |
| 3 | 1 | 256 | 224 |
| 3 | 2 | [illegible] | 16 * |
| 3 | 3 | 338 | 323 |
| 3 | 4 | 44 | 51 |
| 3 | 5 | 295 | 281 |
| 3 | 6 | 40 | -17 |
| 3 | 7 | 446 | 451 |
| 3 | 8 | 51 | -32 |
| 3 | 9 | 160 | 163 |
| 3 | 10 | 123 | 119 |
| 3 | 11 | 88 | 62 |
| 3 | 12 | 18 | -9 * |
| 3 | 13 | 23 | -4 * |
| 3 | 14 | 31 | 2 * |
| 3 | 15 | 81 | -73 |
| 3 | 16 | 94 | -95 |
| 4 | -21 | 18 | -12 * |
| 4 | -20 | 35 | -19 * |
| 4 | -19 | 17 | -4 * |
| 4 | -18 | 55 | -36 |
| 4 | -17 | 18 | 19 * |
| 4 | -16 | 18 | 19 * |
| 4 | -15 | 58 | -52 |
| 4 | -14 | 69 | -85 |
| 4 | -13 | 57 | -16 |
| 4 | -12 | 95 | -98 |
| 4 | -11 | 35 | -28 * |
| 4 | -10 | 170 | 182 |
| 4 | -9 | 87 | -63 |
| 4 | -8 | 459 | -458 |
| 4 | -7 | 97 | 97 |
| 4 | -6 | 186 | -196 |
| 4 | -5 | 78 | 79 |
| 4 | -4 | 232 | -241 |
| 4 | -3 | 153 | 138 |
| 4 | -2 | 272 | -281 |
| 4 | -1 | 208 | 216 |
| 4 | 0 | 117 | -113 |
| 4 | 1 | 35 | -19 * |
| 4 | 2 | 62 | -77 |
| 4 | 3 | 37 | -7 * |
| 4 | 4 | 382 | 386 |
| 4 | 5 | 82 | -82 |
| 4 | 6 | 33 | 63 * |
| 4 | 7 | 144 | -137 |
| 4 | 8 | 64 | 71 |
| 4 | 9 | 119 | -124 |
| 4 | 10 | 85 | 67 |
| 4 | 11 | 198 | -199 |
| 4 | 12 | 106 | 102 |
| 4 | 13 | 138 | -145 |
| 5 | -20 | 45 | -18 |
| 5 | -19 | 55 | -30 |
| 5 | -18 | 31 | 0 * |
| 5 | -17 | 73 | -64 |
| 5 | -16 | 33 | -32 * |
| 5 | -15 | 18 | 12 * |
| 5 | -14 | 28 | -35 * |
| 5 | -13 | 31 | -19 * |
| 5 | -12 | 102 | 112 |
| 5 | -11 | 80 | 73 |
| 5 | -10 | 94 | 79 |
| 5 | -9 | 126 | 109 |
| 5 | -8 | 122 | 125 |
| 5 | -7 | 90 | 54 |
| 5 | -6 | 188 | 173 |
| 5 | -5 | 65 | 47 |
| 5 | -4 | 224 | 238 |
| 5 | -3 | 34 | 9 |
| 5 | -2 | 395 | 388 |
| 5 | -1 | 110 | -91 |
| 5 | 0 | 134 | -120 |
| 5 | 1 | 69 | 51 |
| 5 | 2 | 117 | 103 |
| 5 | 3 | 86 | -80 |
| 5 | 4 | 43 | -19 |
| 5 | 5 | 18 | 10 * |
| 5 | 6 | 39 | 31 |
| 5 | 7 | 32 | 21 * |
| 5 | 8 | 55 | -46 |
| 5 | 9 | 25 | 13 * |
| 6 | -11 | 85 | 57 |
| 6 | -10 | 47 | 19 |
| 6 | -9 | 25 | -22 * |
| 6 | -8 | 19 | -17 * |
| 6 | -7 | 68 | -60 |
| 6 | -6 | 160 | -158 |
| 6 | -5 | 144 | 148 |
| 6 | -4 | 40 | -50 |
| 6 | -3 | 45 | -38 |
| 6 | -2 | 72 | -76 |
| 6 | -1 | 96 | -96 |
| 6 | 0 | 110 | -97 |
| 6 | 1 | 90 | -98 |
| 6 | 2 | 143 | -162 |
| 6 | 3 | 45 | -97 |
| 6 | 4 | 97 | -103 |
| K = 2 | | | |
| 0 | 0 | 708 | -711 |
| 0 | 1 | 696 | 690 |
| 0 | 2 | 213 | 183 |
| 0 | 3 | 245 | -234 |
| 0 | 4 | 192 | -173 |
| 0 | 5 | 445 | 373 |
| 0 | 6 | 18 | 11 * |
| 0 | 7 | 429 | 407 |
| 0 | 8 | 149 | -125 |
| 0 | 9 | 49 | 62 |
| 0 | 10 | 103 | -81 |
| 0 | 11 | 123 | -127 |
| 0 | 12 | 91 | 71 |
| 0 | 13 | 187 | -161 |
| 0 | 14 | 218 | -204 |
| 0 | 15 | 309 | -268 |
| 0 | 16 | 53 | -44 |
| 0 | 17 | 100 | -77 |
| 0 | 18 | 59 | -52 |
| 0 | 19 | 184 | -163 |
| 0 | 20 | 32 | 14 * |
| 0 | 21 | 81 | -74 |
| 1 | -22 | 61 | -57 |
| 1 | -21 | 26 | -44 * |
| 1 | -20 | 91 | -101 |
| 1 | -19 | 18 | -21 * |
| 1 | -18 | 52 | 39 |
| 1 | -17 | 173 | -184 |
| 1 | -16 | 62 | -54 |
| 1 | -15 | 311 | -328 |
| 1 | -14 | 69 | 75 |
| 1 | -13 | 308 | -320 |
| 1 | -12 | 124 | 132 |
| 1 | -11 | 295 | -302 |
| 1 | -10 | 12 | 23 * |
| 1 | -9 | 491 | -490 |
| 1 | -8 | 289 | 276 |
| 1 | -7 | 194 | -215 |
| 1 | -6 | 386 | -371 |
| 1 | -5 | 226 | -212 |
| 1 | -4 | 1166 | 1220 |
| 1 | -3 | 337 | 331 |
| 1 | -2 | 194 | 188 |
| 1 | -1 | 179 | 172 |
| 1 | 0 | 99 | 90 |
| 1 | 1 | 58 | -70 |
| 1 | 2 | 144 | -159 |
| 1 | 3 | 98 | 129 |
| 1 | 4 | 53 | 22 |
| 1 | 5 | 450 | 494 |
| 1 | 6 | 219 | 107 |
| 1 | 7 | 359 | 379 |
| 1 | 8 | 149 | 156 |
| 1 | 9 | 257 | 203 |
| 1 | 10 | 124 | -117 |
| 1 | 11 | 32 | -26 * |
| 1 | 12 | 27 | 31 |
| 1 | 13 | 52 | 70 |
| 1 | 14 | 40 | 6 |
| 1 | 15 | 85 | 95 |
| 1 | 16 | 90 | 83 |
| 1 | 17 | 42 | 51 |
| 1 | 18 | 59 | 78 |
| 1 | 19 | 15 | -22 * |
| 2 | -22 | 15 | 5 * |
| 2 | -21 | 24 | -21 * |
| 2 | -20 | 49 | 17 |
| 2 | -19 | 38 | 26 * |
| 2 | -18 | 86 | 93 |
| 2 | -17 | 18 | -12 * |
| 2 | -16 | 63 | 47 |
| 2 | -15 | 127 | 137 |
| 2 | -14 | 26 | 53 * |
| 2 | -13 | 194 | 187 |
| 2 | -12 | 57 | -54 |
| 2 | -11 | 615 | 625 |
| 2 | -10 | 229 | 204 |
| 2 | -9 | 724 | 735 |
| 2 | -8 | 15 | -23 * |
| 2 | -7 | 230 | 251 |
| 2 | -6 | 23 | -21 * |
| 2 | -5 | 253 | 248 |
| 2 | -4 | 396 | -375 |
| 2 | -3 | 327 | 308 |
| 2 | -2 | 207 | -200 |
| 2 | -1 | 319 | 292 |
| 2 | 0 | 612 | -551 |
| 2 | 1 | 49 | -35 |
| 2 | 2 | 392 | -404 |
| 2 | 3 | 702 | -641 |
| 2 | 4 | 29 | -30 * |
| 2 | 5 | 388 | -394 |
| 2 | 6 | 148 | -136 |
| 2 | 7 | 298 | -304 |
| 2 | 8 | 55 | -35 |
| 2 | 9 | 262 | -236 |
| 2 | 10 | 66 | 48 |
| 2 | 11 | 299 | -281 |
| 2 | 12 | 103 | 82 |
| 2 | 13 | 192 | -199 |
| 2 | 14 | 18 | -7 * |
| 2 | 15 | 18 | -5 * |
| 2 | 16 | 17 | 10 * |
| 2 | 17 | 18 | 0 * |
| 2 | 18 | 27 | 3 * |
| 3 | -22 | 32 | 4 * |
| 3 | -21 | 39 | 25 * |
| 3 | -20 | 15 | -7 * |
| 3 | -19 | 36 | 9 * |
| 3 | -18 | 44 | -42 |
| 3 | -17 | 80 | 95 |
| 3 | -16 | 34 | 29 * |
| 3 | -15 | 47 | -28 |
| 3 | -14 | 76 | -80 |
| 3 | -13 | 92 | 108 |
| 3 | -12 | 84 | -82 |
| 3 | -11 | 102 | -80 |
| 3 | -10 | 104 | -101 |
| 3 | -9 | 40 | -41 |
| 3 | -8 | 118 | -106 |
| 3 | -7 | 274 | -264 |
| 3 | -6 | 263 | -241 |
| 3 | -5 | 291 | -296 |
| 3 | -4 | 167 | 138 |
| 3 | -3 | 637 | -622 |
| 3 | -2 | 254 | 230 |
| 3 | -1 | 95 | -132 |
| 3 | 0 | 345 | 320 |
| 3 | 1 | 368 | -355 |
| 3 | 2 | 148 | 168 |
| 3 | 3 | 346 | -375 |
| 3 | 4 | 157 | 138 |
| 3 | 5 | 164 | -181 |
| 3 | 6 | 283 | 268 |
| 3 | 7 | 109 | 88 |
| 3 | 8 | 33 | -3 * |
| 3 | 9 | 303 | 289 |
| 3 | 10 | 132 | 190 |
| 3 | 11 | 266 | 273 |
| 3 | 12 | 54 | 60 |
| 3 | 13 | 144 | 135 |
| 3 | 14 | 40 | 14 |
| 3 | 15 | 180 | 174 |
| 4 | -19 | 17 | 2 * |
| 4 | -18 | 45 | -19 |
| 4 | -17 | 72 | 82 |
| 4 | -16 | 73 | -52 |
| 4 | -15 | 18 | 20 * |
| 4 | -14 | 84 | 69 |
| 4 | -13 | 32 | 58 * |
| 4 | -12 | 108 | -104 |
| 4 | -11 | 70 | -58 |
| 4 | -10 | 137 | 132 |
| 4 | -9 | 55 | 77 |
| 4 | -8 | 17 | -16 * |
| 4 | -7 | 101 | 103 |
| 4 | -6 | 44 | 15 |
| 4 | -5 | 29 | 25 * |
| 4 | -4 | 80 | 103 |
| 4 | -3 | 106 | 101 |
| 4 | -2 | 44 | 23 |
| 4 | -1 | 244 | 243 |
| 4 | 0 | 19 | 8 * |
| 4 | 1 | 250 | 257 |
| 4 | 2 | 175 | -164 |
| 4 | 3 | 406 | 422 |
| 4 | 4 | 19 | -17 * |
| 4 | 5 | 40 | 8 * |
| 4 | 6 | 43 | 47 |
| 4 | 7 | 117 | 100 |
| 4 | 8 | 99 | -94 |
| 4 | 9 | 18 | -35 * |
| 4 | 10 | 130 | -124 |
| 4 | 11 | 98 | -95 |
| 4 | 12 | 101 | 101 |
| 5 | -20 | 98 | 3 |
| 5 | -19 | 72 | -62 |
| 5 | -18 | 64 | -39 |
| 5 | -17 | 32 | -40 * |
| 5 | -16 | 66 | 56 |
| 5 | -15 | 167 | -159 |
| 5 | -14 | 59 | -63 |
| 5 | -13 | 146 | -141 |
| 5 | -12 | 15 | -4 * |
| 5 | -11 | 99 | -94 |
| 5 | -10 | 45 | 31 |
| 5 | -9 | 98 | -100 |
| 5 | -8 | 49 | 24 |
| 5 | -7 | 78 | -71 |
| 5 | -6 | 44 | 44 |
| 5 | -5 | 18 | 33 * |
| 5 | -4 | 97 | -110 |
| 5 | -3 | 62 | -32 |
| 5 | -2 | 124 | 134 |
| 5 | -1 | 133 | 127 |
| 5 | 0 | 55 | 48 |
| 5 | 1 | 33 | 6 * |
| 5 | 2 | 53 | -26 |
| 5 | 3 | 55 | -29 |
| 5 | 4 | 56 | -4 |
| 5 | 5 | 25 | -35 * |
| 5 | 6 | 40 | -19 |
| 5 | 7 | 70 | -71 |
| 5 | 8 | 67 | 31 |
| 5 | 9 | 42 | -36 |
| 6 | -16 | 44 | 50 |
| 6 | -15 | 62 | 45 |
| 6 | -14 | 44 | 17 |
| 6 | -13 | 71 | 81 |
| 6 | -12 | 41 | 50 |
| 6 | -11 | 106 | 86 |
| 6 | -10 | 19 | 10 * |
| 6 | -9 | 177 | 167 |
| 6 | -8 | 20 | 27 * |
| 6 | -7 | 141 | 132 |
| 6 | -6 | 62 | -34 |
| 6 | -5 | 43 | 42 |
| 6 | -4 | 141 | -124 |
| 6 | -3 | 89 | 90 |
| 6 | -2 | 51 | -58 |
| 6 | -1 | 64 | 53 |
| 6 | 0 | 69 | -60 |
| 6 | 1 | 50 | 50 |
| 6 | 2 | 91 | -69 |
| 6 | 3 | 50 | 27 |
| K = 3 | | | |
| 0 | 1 | 687 | 606 |
| 0 | 2 | 330 | -295 |
| 0 | 3 | 428 | 404 |
| 0 | 4 | 618 | 569 |
| 0 | 5 | 321 | 303 |
| 0 | 6 | 202 | 182 |
| 0 | 7 | 369 | 316 |
| 0 | 8 | 808 | 862 |
| 0 | 9 | 281 | 280 |
| 0 | 10 | 368 | 347 |
| 0 | 11 | 136 | 125 |
| 0 | 12 | 78 | 67 |
| 0 | 13 | 20 | -5 * |
| 0 | 14 | 129 | 132 |
| 0 | 15 | 166 | 160 |
| 0 | 16 | 174 | -157 |
| 0 | 17 | 81 | -48 |
| 0 | 18 | 43 | -12 |
| 0 | 19 | 106 | -76 |
| 0 | 20 | 60 | -52 |
| 1 | -21 | 56 | 39 |
| 1 | -20 | 51 | -59 |
| 1 | -19 | 131 | 131 |
| 1 | -18 | 118 | -123 |
| 1 | -17 | 115 | 136 |
| 1 | -16 | 18 | -18 * |
| 1 | -15 | 26 | 32 * |
| 1 | -14 | 129 | -139 |
| 1 | -13 | 17 | 18 * |
| 1 | -12 | 161 | -190 |
| 1 | -11 | 89 | -75 |
| 1 | -10 | 104 | -99 |
| 1 | -9 | 184 | -179 |
| 1 | -8 | 198 | 201 |
| 1 | -7 | 297 | -293 |
| 1 | -6 | 118 | 127 |
| 1 | -5 | 798 | -829 |
| 1 | -4 | 485 | 485 |
| 1 | -3 | 116 | -92 |
| 1 | -2 | 219 | 213 |
| 1 | -1 | 106 | -102 |
| 1 | 0 | 373 | 431 |
| 1 | 1 | 239 | -230 |
| 1 | 2 | 363 | 397 |
| 1 | 3 | 203 | -222 |
| 1 | 4 | 322 | 367 |
| 1 | 5 | 350 | -369 |
| 1 | 6 | 164 | 122 |
| 1 | 7 | 148 | -117 |
| 1 | 8 | 157 | -144 |
| 1 | 9 | 98 | -88 |
| 1 | 10 | 393 | -439 |
| 1 | 11 | 110 | -135 |
| 1 | 12 | 115 | -84 |
| 1 | 13 | 60 | -65 |
| 1 | 14 | 219 | -252 |
| 1 | 15 | 77 | -11 |
| 1 | 16 | 109 | -83 |
| 1 | 17 | 93 | 66 |
| 1 | 18 | 89 | -98 |
| 1 | 19 | 15 | 20 * |
| 2 | -22 | 43 | -22 |
| 2 | -21 | 85 | -96 |
| 2 | -20 | 53 | -42 |
| 2 | -19 | 27 | -50 * |
| 2 | -18 | 64 | -61 |
| 2 | -17 | 39 | -45 * |
| 2 | -16 | 32 | -39 * |
| 2 | -15 | 88 | -74 |
| 2 | -14 | 23 | 1 * |
| 2 | -13 | 188 | -200 |
| 2 | -12 | 121 | 124 |
| 2 | -11 | 116 | -127 |
| 2 | -10 | 29 | 15 * |
| 2 | -9 | 313 | 312 |
| 2 | -8 | 496 | 461 |
| 2 | -7 | 201 | 198 |
| 2 | -6 | 56 | 48 |
| 2 | -5 | 91 | 111 |
| 2 | -4 | 191 | 186 |
| 2 | -3 | 91 | -56 |
| 2 | -2 | 82 | 73 |
| 2 | -1 | 31 | -2 |
| 2 | 0 | 85 | 71 |
| 2 | 1 | 910 | 855 |
| 2 | 2 | 311 | 253 |
| 2 | 3 | 212 | 251 |
| 2 | 4 | 352 | -323 |
| 2 | 5 | 345 | 315 |
| 2 | 6 | 241 | -250 |
| 2 | 7 | 257 | 254 |
| 2 | 8 | 173 | -180 |
| 2 | 9 | 258 | 261 |
| 2 | 10 | 108 | -84 |
| 2 | 11 | 257 | 264 |
| 2 | 12 | 83 | 31 |
| 2 | 13 | 18 | -3 * |
| 2 | 14 | 82 | 77 |
| 2 | 15 | 53 | -79 * |
| 2 | 16 | 68 | 41 |
| 2 | 17 | 15 | 6 * |
| 3 | -21 | 15 | 7 * |
| 3 | -20 | 17 | 24 * |
| 3 | -19 | 107 | 100 |
| 3 | -18 | 32 | 10 * |
| 3 | -17 | 88 | 61 |
| 3 | -16 | 144 | 143 |
| 3 | -15 | 177 | 183 |
| 3 | -14 | 187 | 184 |
| 3 | -13 | 66 | 69 |
| 3 | -12 | 129 | 141 |
| 3 | -11 | 71 | -65 |
| 3 | -10 | 42 | -40 |
| 3 | -9 | 46 | 19 |
| 3 | -8 | 45 | 44 |
| 3 | -7 | 15 | 18 * |
| 3 | -6 | 133 | -127 |
| 3 | -5 | 122 | -125 |
| 3 | -4 | 273 | -258 |
| 3 | -3 | 313 | -307 |
| 3 | -2 | 255 | -248 |
| 3 | -1 | 255 | -248 |
| 3 | 0 | 174 | -168 |
| 3 | 1 | 166 | -167 |
| 3 | 2 | 238 | -250 |
| 3 | 3 | 206 | -199 |
| 3 | 4 | 54 | 36 |
| 3 | 5 | 364 | -339 |
| 3 | 6 | 49 | -41 |
| 3 | 7 | 377 | -380 |
| 3 | 8 | 260 | 259 |
| 3 | 9 | 132 | -132 |
| 3 | 10 | 45 | -32 |
| 3 | 11 | 17 | 3 * |
| 3 | 12 | 143 | 141 |
| 3 | 13 | 31 | -14 * |
| 3 | 14 | 87 | 69 |
| 3 | 15 | 27 | 3 * |
| 4 | -21 | 47 | -29 |
| 4 | -20 | 53 | 59 |
| 4 | -19 | 105 | -104 |
| 4 | -18 | 23 | 12 * |
| 4 | -17 | 108 | -106 |
| 4 | -16 | 18 | -9 * |
| 4 | -15 | 38 | -15 * |
| 4 | -14 | 55 | -52 |
| 4 | -13 | 65 | -55 |
| 4 | -12 | 150 | 140 |
| 4 | -11 | 19 | 17 * |
| 4 | -10 | 221 | -223 |
| 4 | -9 | 29 | 4 * |
| 4 | -8 | 159 | -156 |
| 4 | -7 | 90 | 74 |
| 4 | -6 | 76 | -83 |
| 4 | -5 | 196 | 190 |
| 4 | -4 | 97 | -82 |
| 4 | -3 | 59 | 37 |
| 4 | -2 | 99 | -111 |
| 4 | -1 | 39 | -26 |
| 4 | 0 | 85 | 85 |
| 4 | 1 | 78 | 51 |
| 4 | 2 | 191 | 173 |
| 4 | 3 | 124 | 136 |
| 4 | 4 | 80 | 76 |
| 4 | 5 | 235 | 240 |
| 4 | 6 | 262 | 280 |
| 4 | 7 | 112 | 114 |
| 4 | 8 | 18 | 28 * |
| 4 | 9 | 116 | 117 |
| 4 | 10 | 113 | 120 |
| 4 | 11 | 92 | 115 |
| 4 | 12 | 31 | 31 * |
| 5 | -19 | 70 | 68 |
| 5 | -18 | 66 | -55 |
| 5 | -17 | 98 | 105 |
| 5 | -16 | 143 | -136 |
| 5 | -15 | 62 | 75 |
| 5 | -14 | 75 | 56 |
| 5 | -13 | 52 | 30 |
| 5 | -12 | 56 | -54 |
| 5 | -11 | 39 | 33 * |
| 5 | -10 | 54 | 43 |
| 5 | -9 | 41 | 20 |
| 5 | -8 | 69 | 52 |
| 5 | -7 | 45 | 17 |
| 5 | -6 | 79 | 67 |
| 5 | -5 | 15 | 10 * |
| 5 | -4 | 172 | 189 |
| 5 | -3 | 123 | -93 |
| 5 | -2 | 107 | 94 |
| 5 | -1 | 32 | 5 * |
| 5 | 0 | 173 | 180 |
| 5 | 1 | 102 | -106 |
| 5 | 2 | 85 | 78 |
| 5 | 3 | 84 | -96 |
| 5 | 4 | 59 | -7 |
| 5 | 5 | 146 | -162 |
| 5 | 6 | 87 | -63 |
| 5 | 7 | 166 | -188 |
| 5 | 8 | 81 | -59 |
| 6 | -12 | 66 | 61 |
| 6 | -11 | 75 | -69 |
| 6 | -10 | 84 | 75 |
| 6 | -9 | 28 | -28 * |
| 6 | -8 | 26 | -21 * |
| 6 | -7 | 47 | 28 * |
| 6 | -6 | 172 | 165 |
| 6 | -5 | 18 | 25 * |
| 6 | -4 | 92 | -67 |
| 6 | -3 | 33 | 15 * |
| 6 | -2 | 23 | 19 * |
| 6 | -1 | 64 | 39 |
| 6 | 0 | 127 | 121 |
| 6 | 1 | 95 | 91 |
| 6 | 2 | 98 | -100 |
| 6 | 3 | 133 | 131 |
| K = 4 | | | |
| 0 | 0 | 693 | -658 |
| 0 | 1 | 29 | 45 |
| 0 | 2 | 731 | -708 |
| 0 | 3 | 51 | 1 |
| 0 | 4 | 283 | -254 |
| 0 | 5 | 241 | 187 |
| 0 | 6 | 209 | -177 |
| 0 | 7 | 381 | 373 |
| 0 | 8 | 106 | -68 |
| 0 | 9 | 426 | 379 |
| 0 | 10 | 30 | -8 * |
| 0 | 11 | 270 | 263 |
| 0 | 12 | 73 | 59 |
| 0 | 13 | 263 | 258 |
| 0 | 14 | 356 | 314 |
| 0 | 15 | 65 | 63 |
| 0 | 16 | 37 | 28 * |
| 0 | 17 | 74 | 63 |
| 0 | 18 | 93 | 82 |
| 0 | 19 | 45 | -18 |
| 0 | 20 | 66 | 49 |
| 1 | -21 | 17 | -23 * |
| 1 | -20 | 30 | 27 * |
| 1 | -19 | 18 | -42 * |
| 1 | -18 | 78 | -93 |
| 1 | -17 | 48 | 69 |
| 1 | -16 | 32 | -36 * |
| 1 | -15 | 18 | 17 * |
| 1 | -14 | 21 | 4 * |
| 1 | -13 | 17 | -17 * |
| 1 | -12 | 19 | -4 * |
| 1 | -11 | 52 | 31 |
| 1 | -10 | 25 | 42 * |
| 1 | -9 | 57 | 68 |
| 1 | -8 | 383 | -410 |
| 1 | -7 | 602 | 624 |
| 1 | -6 | 270 | 251 |
| 1 | -5 | 60 | 67 |
| 1 | -4 | 117 | -112 |
| 1 | -3 | 346 | 338 |
| 1 | -2 | 360 | 348 |
| 1 | -1 | 263 | 271 |
| 1 | 0 | 92 | 76 |
| 1 | 1 | 340 | 357 |
| 1 | 2 | 208 | 229 |
| 1 | 3 | 445 | 485 |
| 1 | 4 | 188 | 225 |
| 1 | 5 | 191 | 94 |
| 1 | 6 | 524 | 505 |
| 1 | 7 | 213 | -238 |
| 1 | 8 | 209 | 232 |
| 1 | 9 | 213 | -245 |
| 1 | 10 | 49 | 18 |
| 1 | 11 | 366 | -431 |
| 1 | 12 | 31 | 27 * |
| 1 | 13 | 176 | -181 |
| 1 | 14 | 18 | 36 * |
| 1 | 15 | 232 | 247 |
| 1 | 16 | 33 | 4 |
| 1 | 17 | 104 | -130 |
| 1 | 18 | 95 | -110 |
| 2 | -21 | 15 | -17 * |
| 2 | -20 | 42 | 34 |
| 2 | -19 | 119 | -124 |
| 2 | -18 | 46 | 32 |
| 2 | -17 | 66 | -37 |
| 2 | -16 | 64 | -50 |
| 2 | -15 | 103 | -117 |
| 2 | -14 | 40 | -25 * |
| 2 | -13 | 103 | -87 |
| 2 | -12 | 54 | 44 |
| 2 | -11 | 127 | -122 |
| 2 | -10 | 230 | -246 |
| 2 | -9 | 80 | -72 |
| 2 | -8 | 145 | 149 |
| 2 | -7 | 164 | 163 |
| 2 | -6 | 55 | -62 |
| 2 | -5 | 94 | 81 |
| 2 | -4 | 111 | 100 |
| 2 | -3 | 61 | -65 |
| 2 | -2 | 57 | 14 |
| 2 | -1 | 70 | -45 |
| 2 | 0 | 41 | 56 |
| 2 | 1 | 180 | -169 |
| 2 | 2 | 26 | -22 * |
| 2 | 3 | 61 | -39 |
| 2 | 4 | 163 | -173 |
| 2 | 5 | 239 | -217 |
| 2 | 6 | 210 | -206 |
| 2 | 7 | 196 | -213 |
| 2 | 8 | 176 | -174 |
| 2 | 9 | 19 | -26 * |
| 2 | 10 | 211 | -202 |
| 2 | 11 | 132 | 103 |
| 2 | 12 | 242 | -236 |
| 2 | 13 | 169 | 187 |
| 2 | 14 | 45 | -28 |
| 2 | 15 | 52 | 49 |
| 2 | 16 | 46 | -23 |
| 2 | 17 | 101 | 88 |
| 3 | -21 | 32 | 1 * |
| 3 | -20 | 54 | -45 |
| 3 | -19 | 67 | 62 |
| 3 | -18 | 134 | -119 |
| 3 | -17 | 101 | 75 |
| 3 | -16 | 125 | -122 |
| 3 | -15 | 201 | 193 |
| 3 | -14 | 37 | -18 * |
| 3 | -13 | 333 | 341 |
| 3 | -12 | 33 | 28 * |
| 3 | -11 | 96 | 85 |
| 3 | -10 | 98 | 105 |
| 3 | -9 | 102 | 85 |
| 3 | -8 | 27 | -2 * |
| 3 | -7 | 49 | -51 |
| 3 | -6 | 237 | 235 |
| 3 | -5 | 15 | -2 * |
| 3 | -4 | 298 | 292 |
| 3 | -3 | 75 | 80 |
| 3 | -2 | 78 | 75 |
| 3 | -1 | 325 | 298 |
| 3 | 0 | 237 | 218 |
| 3 | 1 | 36 | -4 |
| 3 | 2 | 32 | 29 * |
| 3 | 3 | 32 | -1 * |
| 3 | 4 | 80 | 54 |
| 3 | 5 | 86 | 108 |
| 3 | 6 | 18 | -12 * |
| 3 | 7 | 166 | 182 |
| 3 | 8 | 58 | 77 |
| 3 | 9 | 120 | -126 |
| 3 | 10 | 22 | -44 * |
| 3 | 11 | 66 | 49 |
| 3 | 12 | 25 | 28 * |
| 3 | 13 | 51 | -28 |
| 3 | 14 | 25 | -10 * |
| 4 | -20 | 92 | 99 |
| 4 | -19 | 62 | 38 |
| 4 | -18 | 58 | 53 |
| 4 | -17 | 18 | -29 * |
| 4 | -16 | 88 | 86 |
| 4 | -15 | 121 | -128 |
| 4 | -14 | 67 | 48 |
| 4 | -13 | 117 | -129 |
| 4 | -12 | 244 | 258 |
| 4 | -11 | 287 | -291 |
| 4 | -10 | 72 | -56 |
| 4 | -9 | 154 | -160 |
| 4 | -8 | 55 | -68 |
| 4 | -7 | 246 | -244 |
| 4 | -6 | 137 | -142 |
| 4 | -5 | 111 | -123 |
| 4 | -4 | 66 | -75 |
| 4 | -3 | 138 | -137 |
| 4 | -2 | 129 | -119 |
| 4 | -1 | 88 | -94 |
| 4 | 0 | 250 | -253 |
| 4 | 1 | 32 | -48 * |
| 4 | 2 | 215 | -186 |
| 4 | 3 | 73 | 46 |
| 4 | 4 | 76 | -65 |
| 4 | 5 | 117 | 129 |
| 4 | 6 | 88 | -74 |
| 4 | 7 | 139 | 155 |
| 4 | 8 | 40 | 37 |
| 4 | 9 | 104 | 107 |
| 4 | 10 | 20 | -36 * |
| 4 | 11 | 64 | 69 |
| 5 | -18 | 34 | 17 * |
| 5 | -17 | 63 | -28 |
| 5 | -16 | 89 | -82 |
| 5 | -15 | 75 | 29 |
| 5 | -14 | 89 | -90 |
| 5 | -13 | 50 | 47 |
| 5 | -12 | 77 | -79 |
| 5 | -11 | 109 | 105 |
| 5 | -10 | 69 | -60 |
| 5 | -9 | 108 | 107 |
| 5 | -8 | 81 | -85 |
| 5 | -7 | 121 | 110 |
| 5 | -6 | 172 | 177 |
| 5 | -5 | 195 | 177 |
| 5 | -4 | 22 | 48 * |
| 5 | -3 | 125 | 108 |
| 5 | -2 | 43 | -14 |
| 5 | -1 | 201 | 219 |
| 5 | 0 | 134 | 144 |
| 5 | 1 | 129 | 124 |
| 5 | 2 | 142 | 137 |
| 5 | 3 | 73 | 80 |
| 5 | 4 | 115 | 115 |
| 5 | 5 | 64 | 4 |
| 5 | 6 | 157 | 173 |
| 5 | 7 | 65 | -46 |
| 6 | -10 | 71 | 60 |
| 6 | -9 | 23 | 2 * |
| 6 | -8 | 22 | 15 * |
| 6 | -7 | 51 | -41 |
| 6 | -6 | 48 | 49 |
| 6 | -5 | 63 | 58 |
| 6 | -4 | 16 | 13 * |
| 6 | -3 | 60 | -56 |
| 6 | -2 | 39 | 32 |
| 6 | -1 | 136 | -154 |
| 6 | 0 | 21 | 14 * |
| 6 | 1 | 122 | -145 |
| K = 5 | | | |
| 0 | 1 | 291 | -285 |
| 0 | 2 | 297 | -266 |
| 0 | 3 | 515 | -463 |
| 0 | 4 | 254 | -212 |
| 0 | 5 | 169 | -136 |
| 0 | 6 | 112 | 113 |
| 0 | 7 | 111 | -87 |
| 0 | 8 | 151 | 135 |
| 0 | 9 | 43 | -22 |
| 0 | 10 | 134 | -120 |
| 0 | 11 | 163 | 106 |
| 0 | 12 | 271 | -265 |
| 0 | 13 | 52 | 53 |
| 0 | 14 | 124 | -126 |
| 0 | 15 | 219 | 192 |
| 0 | 16 | 49 | -25 |
| 0 | 17 | 97 | 87 |
| 0 | 18 | 118 | -101 |
| 0 | 19 | 52 | 42 |
| 1 | -20 | 15 | -11 * |
| 1 | -19 | 23 | 52 * |
| 1 | -18 | 43 | -62 * |
| 1 | -17 | 31 | -39 * |
| 1 | -16 | 108 | -116 |
| 1 | -15 | 18 | 41 * |
| 1 | -14 | 219 | -236 |
| 1 | -13 | 41 | -31 * |
| 1 | -12 | 173 | -175 |
| 1 | -11 | 109 | -97 |
| 1 | -10 | 100 | -107 |
| 1 | -9 | 86 | -80 |
| 1 | -8 | 280 | 298 |
| 1 | -7 | 71 | -95 |
| 1 | -6 | 205 | -176 |
| 1 | -5 | 147 | -139 |
| 1 | -4 | 201 | -209 |
| 1 | -3 | 108 | -118 |
| 1 | -2 | 206 | -180 |
| 1 | -1 | 108 | -99 |
| 1 | 0 | 120 | 136 |
| 1 | 1 | 130 | 157 |
| 1 | 2 | 27 | 5 |
| 1 | 3 | 148 | 163 |
| 1 | 4 | 108 | 115 |
| 1 | 5 | 396 | 456 |
| 1 | 6 | 237 | 189 |
| 1 | 7 | 201 | 249 |
| 1 | 8 | 176 | 190 |
| 1 | 9 | 332 | 361 |
| 1 | 10 | 255 | 274 |
| 1 | 11 | 59 | 49 |
| 1 | 12 | 131 | -34 |
| 1 | 13 | 85 | 73 |
| 1 | 14 | 120 | 119 |
| 1 | 15 | 62 | -24 |
| 1 | 16 | 130 | 135 |
| 1 | 17 | 85 | -72 |
| 1 | 18 | 89 | 105 |
| 2 | -20 | 45 | -44 |
| 2 | -19 | 27 | -42 * |
| 2 | -18 | 70 | 79 |
| 2 | -17 | 62 | -60 |
| 2 | -16 | 67 | 45 |
| 2 | -15 | 18 | -14 * |
| 2 | -14 | 131 | 133 |
| 2 | -13 | 198 | -208 |
| 2 | -12 | 259 | 257 |
| 2 | -11 | 27 | -4 * |
| 2 | -10 | 325 | 332 |
| 2 | -9 | 339 | -358 |
| 2 | -8 | 330 | 346 |
| 2 | -7 | 87 | 101 |
| 2 | -6 | 170 | 151 |
| 2 | -5 | 123 | 117 |
| 2 | -4 | 213 | 204 |
| 2 | -3 | 180 | 167 |
| 2 | -2 | 184 | 161 |
| 2 | -1 | 327 | 323 |
| 2 | 0 | 61 | -95 |
| 2 | 1 | 176 | 177 |
| 2 | 2 | 82 | 89 |
| 2 | 3 | 109 | 100 |
| 2 | 4 | 323 | -305 |
| 2 | 5 | 42 | -68 |
| 2 | 6 | 345 | -357 |
| 2 | 7 | 209 | -210 |
| 2 | 8 | 96 | -60 |
| 2 | 9 | 145 | -121 |
| 2 | 10 | 178 | -159 |
| 2 | 11 | 257 | -252 |
| 2 | 12 | 65 | -29 |
| 2 | 13 | 73 | -85 |
| 2 | 14 | 177 | 191 |
| 2 | 15 | 91 | -110 |
| 2 | 16 | 58 | -66 |
| 3 | -20 | 46 | -25 |
| 3 | -19 | 86 | -71 |
| 3 | -18 | 17 | 20 * |
| 3 | -17 | 59 | -34 * |
| 3 | -16 | 61 | -58 |
| 3 | -15 | 65 | -62 |
| 3 | -14 | 121 | -109 |
| 3 | -13 | 105 | 87 |
| 3 | -12 | 30 | 20 * |
| 3 | -11 | 178 | 180 |
| 3 | -10 | 135 | -141 |
| 3 | -9 | 142 | 143 |
| 3 | -8 | 272 | -278 |
| 3 | -7 | 337 | 344 |
| 3 | -6 | 283 | -273 |
| 3 | -5 | 64 | 51 |
| 3 | -4 | 186 | -183 |
| 3 | -3 | 192 | 189 |
| 3 | -2 | 105 | -97 |
| 3 | -1 | 53 | -68 |
| 3 | 0 | 213 | -195 |
| 3 | 1 | 75 | -88 |
| 3 | 2 | 201 | -204 |
| 3 | 3 | 131 | -132 |
| 3 | 4 | 30 | -58 * |
| 3 | 5 | 109 | -111 |
| 3 | 6 | 84 | 50 |
| 3 | 7 | 102 | -75 |
| 3 | 8 | 48 | 28 |
| 3 | 9 | 45 | 51 |
| 3 | 10 | 173 | 181 |
| 3 | 11 | 78 | -78 |
| 3 | 12 | 61 | 36 |
| 3 | 13 | 61 | 42 |
| 3 | 14 | 118 | 115 |
| 4 | -19 | 75 | 67 |
| 4 | -18 | 49 | 65 |
| 4 | -17 | 86 | 86 |
| 4 | -16 | 21 | 5 |
| 4 | -15 | 87 | 89 |
| 4 | -14 | 51 | -40 |
| 4 | -13 | 112 | 109 |
| 4 | -12 | 33 | -21 * |
| 4 | -11 | 18 | -8 * |
| 4 | -10 | 217 | 212 |
| 4 | -9 | 49 | -62 |
| 4 | -8 | 136 | 150 |
| 4 | -7 | 140 | -145 |
| 4 | -6 | 92 | 88 |
| 4 | -5 | 129 | -129 |
| 4 | -4 | 170 | 180 |
| 4 | -3 | 131 | -121 |
| 4 | -2 | 169 | 160 |
| 4 | -1 | 169 | -186 |
| 4 | 0 | 240 | 239 |
| 4 | 1 | 131 | -73 |
| 4 | 2 | 102 | 80 |
| 4 | 3 | 84 | -88 |
| 4 | 4 | 100 | 105 |
| 4 | 5 | 109 | 112 |
| 4 | 6 | 50 | -59 |
| 4 | 7 | 53 | 55 |
| 4 | 8 | 17 | 10 * |
| 4 | 9 | 16 | -15 * |
| 4 | 10 | 62 | -70 |
| 5 | -17 | 15 | -8 * |
| 5 | -16 | 35 | -1 * |
| 5 | -15 | 70 | -74 |
| 5 | -14 | 122 | -103 |
| 5 | -13 | 33 | -8 * |
| 5 | -12 | 97 | -87 |
| 5 | -11 | 90 | -89 |
| 5 | -10 | 36 | -39 * |
| 5 | -9 | 49 | -67 |
| 5 | -8 | 46 | -28 |
| 5 | -7 | 38 | -52 * |
| 5 | -6 | 117 | -125 |
| 5 | -5 | 61 | -63 |
| 5 | -4 | 133 | -137 |
| 5 | -3 | 18 | -4 * |
| 5 | -2 | 25 | -23 * |
| 5 | -1 | 30 | 11 * |
| 5 | 0 | 54 | -15 |
| 5 | 1 | 84 | 77 |
| 5 | 2 | 36 | 70 * |
| 5 | 3 | 174 | 163 |
| 5 | 4 | 102 | -91 |
| 5 | 5 | 123 | 130 |
| 5 | 6 | 44 | -37 |
| 6 | -11 | 54 | -41 |
| 6 | -10 | 28 | 28 * |
| 6 | -9 | 40 | 41 |
| 6 | -8 | 131 | 116 |
| 6 | -7 | 54 | -34 |
| 6 | -6 | 70 | 62 |
| 6 | -5 | 132 | 112 |
| 6 | -4 | 96 | 97 |
| 6 | -3 | 65 | 79 |
| 6 | -2 | 33 | 37 * |
| 6 | -1 | 26 | 25 |
| K = 6 | | | |
| 0 | 0 | 29 | 16 * |
| 0 | 1 | 83 | 75 |
| 0 | 2 | 356 | 308 |
| 0 | 3 | 27 | -0 * |
| 0 | 4 | 110 | -92 |
| 0 | 5 | 33 | 14 |
| 0 | 6 | 133 | 111 |
| 0 | 7 | 46 | 50 |
| 0 | 8 | 162 | 149 |
| 0 | 9 | 34 | 37 |
| 0 | 10 | 280 | 265 |
| 0 | 11 | 84 | 41 |
| 0 | 12 | 103 | 93 |
| 0 | 13 | 97 | -77 |
| 0 | 14 | 48 | 24 |
| 0 | 15 | 69 | 59 |
| 0 | 16 | 68 | 78 |
| 0 | 17 | 70 | 58 |
| 0 | 18 | 91 | 85 |
| 1 | -19 | 25 | 27 * |
| 1 | -18 | 113 | 123 |
| 1 | -17 | 30 | 26 * |
| 1 | -16 | 65 | 59 |
| 1 | -15 | 61 | 46 |
| 1 | -14 | 66 | -89 |
| 1 | -13 | 59 | 74 |
| 1 | -12 | 132 | 137 |
| 1 | -11 | 89 | -88 |
| 1 | -10 | 151 | -141 |
| 1 | -9 | 149 | 187 |
| 1 | -8 | 235 | -241 |
| 1 | -7 | 93 | 89 |
| 1 | -6 | 371 | -401 |
| 1 | -5 | 285 | 276 |
| 1 | -4 | 494 | -447 |
| 1 | -3 | 21 | 20 * |
| 1 | -2 | 458 | -451 |
| 1 | -1 | 192 | -163 |
| 1 | 0 | 135 | -126 |
| 1 | 1 | 27 | -22 * |
| 1 | 2 | 59 | -52 |
| 1 | 3 | 49 | 56 |
| 1 | 4 | 259 | 159 |
| 1 | 5 | 150 | -186 |
| 1 | 6 | 157 | -27 |
| 1 | 7 | 107 | -59 |
| 1 | 8 | 106 | -46 |
| 1 | 9 | 93 | -97 |
| 1 | 10 | 222 | 223 |
| 1 | 11 | 63 | 45 |
| 1 | 12 | 53 | -25 |
| 1 | 13 | 46 | 15 |
| 1 | 14 | 56 | -24 |
| 1 | 15 | 47 | -28 |
| 1 | 16 | 135 | -150 |
| 1 | 17 | 27 | -12 * |
| 2 | -19 | 37 | 9 |
| 2 | -18 | 106 | -112 |
| 2 | -17 | 35 | -10 * |
| 2 | -16 | 78 | -83 |
| 2 | -15 | 47 | 31 |
| 2 | -14 | 115 | -117 |
| 2 | -13 | 66 | -67 |
| 2 | -12 | 191 | -195 |
| 2 | -11 | 32 | 46 * |
| 2 | -10 | 31 | 39 * |
| 2 | -9 | 144 | -165 |
| 2 | -8 | 45 | -66 |
| 2 | -7 | 126 | -135 |
| 2 | -6 | 198 | 195 |
| 2 | -5 | 96 | -79 |
| 2 | -4 | 305 | 282 |
| 2 | -3 | 261 | -259 |
| 2 | -2 | 471 | 470 |
| 2 | -1 | 44 | -49 |
| 2 | 0 | 444 | 443 |
| 2 | 1 | 122 | 136 |
| 2 | 2 | 407 | 415 |
| 2 | 3 | 67 | 83 |
| 2 | 4 | 378 | 371 |
| 2 | 5 | 249 | 256 |
| 2 | 6 | 167 | 158 |
| 2 | 7 | 91 | -99 |
| 2 | 8 | 65 | 33 |
| 2 | 9 | 124 | 116 |
| 2 | 10 | 18 | 32 * |
| 2 | 11 | 117 | 121 |
| 2 | 12 | 38 | 57 * |
| 2 | 13 | 18 | -54 * |
| 2 | 14 | 75 | -60 |
| 2 | 15 | 60 | 41 |
| 3 | -19 | 38 | -14 |
| 3 | -18 | 54 | 51 |
| 3 | -17 | 59 | -54 |
| 3 | -16 | 111 | 120 |
| 3 | -15 | 30 | 26 * |
| 3 | -14 | 18 | -30 * |
| 3 | -13 | 33 | -32 * |
| 3 | -12 | 182 | 186 |
| 3 | -11 | 25 | 1 * |
| 3 | -10 | 136 | 134 |
| 3 | -9 | 55 | -57 |
| 3 | -8 | 298 | 311 |
| 3 | -7 | 18 | -30 * |
| 3 | -6 | 21 | -27 * |
| 3 | -5 | 215 | 218 |
| 3 | -4 | 110 | 113 |
| 3 | -3 | 177 | 185 |
| 3 | -2 | 136 | -134 |
| 3 | -1 | 45 | 45 |
| 3 | 0 | 317 | -336 |
| 3 | 1 | 55 | -52 |
| 3 | 2 | 355 | -346 |
| 3 | 3 | 27 | 18 * |
| 3 | 4 | 340 | -347 |
| 3 | 5 | 39 | 31 * |
| 3 | 6 | 311 | -272 |
| 3 | 7 | 60 | -58 |
| 3 | 8 | 199 | -205 |
| 3 | 9 | 54 | 10 * |
| 3 | 10 | 165 | -170 |
| 3 | 11 | 60 | -103 |
| 3 | 12 | 15 | -28 * |
| 4 | -18 | 34 | 20 * |
| 4 | -17 | 22 | 21 * |
| 4 | -16 | 61 | 62 |
| 4 | -15 | 17 | -20 * |
| 4 | -14 | 32 | 18 * |
| 4 | -13 | 41 | -24 |
| 4 | -12 | 64 | -55 |
| 4 | -11 | 80 | 73 |
| 4 | -10 | 69 | -74 |
| 4 | -9 | 112 | -90 |
| 4 | -8 | 69 | 56 |
| 4 | -7 | 53 | 57 |
| 4 | -6 | 82 | -77 |
| 4 | -5 | 102 | -106 |
| 4 | -4 | 85 | -101 |
| 4 | -3 | 15 | -13 * |
| 4 | -2 | 87 | -92 |
| 4 | -1 | 67 | -70 |
| 4 | 0 | 73 | 57 |
| 4 | 1 | 67 | -69 |
| 4 | 2 | 56 | 11 |
| 4 | 3 | 68 | 54 |
| 4 | 4 | 114 | 124 |
| 4 | 5 | 18 | 24 * |
| 4 | 6 | 77 | 45 |
| 4 | 7 | 37 | -10 * |
| 4 | 8 | 140 | 134 |
| 4 | 9 | 31 | -24 * |
| 5 | -15 | 34 | -14 * |
| 5 | -14 | 34 | 29 * |
| 5 | -13 | 30 | 23 * |
| 5 | -12 | 62 | -39 |
| 5 | -11 | 63 | 40 |
| 5 | -10 | 83 | -76 |
| 5 | -9 | 55 | 57 |
| 5 | -8 | 24 | -10 * |
| 5 | -7 | 18 | 46 * |
| 5 | -6 | 18 | -6 * |
| 5 | -5 | 29 | 8 * |
| 5 | -4 | 20 | -40 * |
| 5 | -3 | 54 | 63 |
| 5 | -2 | 74 | -76 |
| 5 | -1 | 30 | -6 * |
| 5 | 0 | 34 | -17 * |
| 5 | 1 | 34 | -61 * |
| 5 | 2 | 16 | -4 |
| 5 | 3 | 44 | -48 |
| 5 | 4 | 38 | 22 * |
| 5 | 5 | 27 | -24 |
| K = 7 | | | |
| 0 | 1 | 336 | -312 |
| 0 | 2 | 31 | -27 * |
| 0 | 3 | 335 | -324 |
| 0 | 4 | 32 | -49 |
| 0 | 5 | 170 | -158 |
| 0 | 6 | 43 | -13 |
| 0 | 7 | 133 | -120 |
| 0 | 8 | 92 | -95 |
| 0 | 9 | 22 | 22 * |
| 0 | 10 | 81 | -67 |
| 0 | 11 | 52 | 46 |
| 0 | 12 | 86 | 71 |
| 0 | 13 | 130 | 107 |
| 0 | 14 | 63 | 62 |
| 0 | 15 | 103 | 110 |
| 0 | 16 | 61 | 68 |
| 0 | 17 | 116 | 101 |
| 1 | -18 | 91 | 102 |
| 1 | -17 | 58 | -54 |
| 1 | -16 | 125 | 141 |
| 1 | -15 | 19 | -24 * |
| 1 | -14 | 159 | 164 |
| 1 | -13 | 37 | -57 * |
| 1 | -12 | 73 | 57 |
| 1 | -11 | 57 | -59 |
| 1 | -10 | 80 | 116 |
| 1 | -9 | 107 | -124 |
| 1 | -8 | 162 | 170 |
| 1 | -7 | 45 | -59 |
| 1 | -6 | 157 | 181 |
| 1 | -5 | 17 | -9 * |
| 1 | -4 | 36 | 17 |
| 1 | -3 | 215 | 203 |
| 1 | -2 | 55 | -45 |
| 1 | -1 | 65 | 37 |
| 1 | 0 | 169 | -169 |
| 1 | 1 | 204 | 218 |
| 1 | 2 | 143 | -172 |
| 1 | 3 | 298 | 364 |
| 1 | 4 | 154 | -113 |
| 1 | 5 | 202 | 236 |
| 1 | 6 | 112 | 48 |
| 1 | 7 | 210 | 212 |
| 1 | 8 | 186 | -204 |
| 1 | 9 | 55 | -48 |
| 1 | 10 | 38 | -19 |
| 1 | 11 | 143 | 158 |
| 1 | 12 | 114 | 74 |
| 1 | 13 | 70 | 81 |
| 1 | 14 | 81 | 55 |
| 1 | 15 | 53 | -27 |
| 1 | 16 | 41 | -5 |
| 2 | -18 | 58 | -14 |
| 2 | -17 | 16 | -33 * |
| 2 | -16 | 59 | -51 |
| 2 | -15 | 52 | -75 * |
| 2 | -14 | 18 | -18 * |
| 2 | -13 | 96 | 112 |
| 2 | -12 | 201 | 239 |
| 2 | -11 | 18 | -19 * |
| 2 | -10 | 90 | -65 |
| 2 | -9 | 30 | -17 * |
| 2 | -8 | 220 | -211 |
| 2 | -7 | 18 | -24 * |
| 2 | -6 | 299 | -298 |
| 2 | -5 | 39 | 31 * |
| 2 | -4 | 281 | -269 |
| 2 | -3 | 245 | 254 |
| 2 | -2 | 109 | -96 |
| 2 | -1 | 93 | -73 |
| 2 | 0 | [illegible] | 83 |
| 2 | 1 | 141 | -151 |
| 2 | 2 | 132 | 126 |
| 2 | 3 | 151 | -144 |
| 2 | 4 | 97 | 106 |
| 2 | 5 | 18 | -21 * |
| 2 | 6 | 278 | 266 |
| 2 | 7 | 136 | -154 |
| 2 | 8 | 97 | 84 |
| 2 | 9 | 177 | -162 |
| 2 | 10 | 94 | 98 |
| 2 | 11 | 202 | -171 |
| 2 | 12 | 17 | -23 * |
| 2 | 13 | 83 | -71 |
| 2 | 14 | 99 | 108 |
| 3 | -18 | 14 | -20 * |
| 3 | -17 | 44 | -88 |
| 3 | -16 | 90 | 93 |
| 3 | -15 | 18 | 13 * |
| 3 | -14 | 28 | 10 * |
| 3 | -13 | 64 | -90 |
| 3 | -12 | 49 | -52 |
| 3 | -11 | 88 | 94 |
| 3 | -10 | 38 | 1 * |
| 3 | -9 | 115 | 116 |
| 3 | -8 | 46 | 46 |
| 3 | -7 | 35 | -46 * |
| 3 | -6 | 286 | 285 |
| 3 | -5 | 192 | 193 |
| 3 | -4 | 91 | 92 |
| 3 | -3 | 134 | 135 |
| 3 | -2 | 269 | 257 |
| 3 | -1 | 193 | 206 |
| 3 | 0 | 185 | 196 |
| 3 | 1 | 66 | 58 |
| 3 | 2 | 38 | 28 * |
| 3 | 3 | 67 | -80 |
| 3 | 4 | 58 | 57 |
| 3 | 5 | 108 | 141 |
| 3 | 6 | 45 | 7 |
| 3 | 7 | 51 | 29 |
| 3 | 8 | 36 | 11 * |
| 3 | 9 | 41 | -46 |
| 3 | 10 | 99 | -106 |
| 3 | 11 | 20 | -31 * |
| 4 | -16 | 23 | 10 * |
| 4 | -15 | 68 | 62 |
| 4 | -14 | 14 | 11 * |
| 4 | -13 | 56 | 48 |
| 4 | -12 | 22 | -12 * |
| 4 | -11 | 81 | 76 |
| 4 | -10 | 68 | -67 |
| 4 | -9 | 40 | 29 |
| 4 | -8 | 51 | 20 |
| 4 | -7 | 74 | -44 * |
| 4 | -6 | 39 | 33 |
| 4 | -5 | 184 | 198 |
| 4 | -4 | 70 | -94 |
| 4 | -3 | 135 | -145 |
| 4 | -2 | 122 | -123 |
| 4 | -1 | 138 | -131 |
| 4 | 0 | 119 | -113 |
| 4 | 1 | 128 | -127 |
| 4 | 2 | 49 | -29 |
| 4 | 3 | 143 | -148 |
| 4 | 4 | 44 | -84 |
| 4 | 5 | 40 | -35 |
| 4 | 6 | 42 | -34 |
| 4 | 7 | 29 | -23 * |
| 4 | 8 | 55 | -64 |
| 5 | -13 | 75 | -72 |
| 5 | -12 | 108 | 104 |
| 5 | -11 | 105 | -113 |
| 5 | -10 | 47 | 31 |
| 5 | -9 | 110 | -109 |
| 5 | -8 | 55 | 54 |
| 5 | -7 | 90 | -81 |
| 5 | -6 | 43 | 44 |
| 5 | -5 | 42 | -29 |
| 5 | -4 | 45 | 27 |
| 5 | -3 | 34 | 45 * |
| 5 | -2 | 47 | -42 |
| 5 | -1 | 120 | 124 |
| 5 | 0 | 30 | 5 * |
| 5 | 1 | 90 | 97 |
| 5 | 2 | 73 | -89 |
| K = 8 | | | |
| 0 | 0 | 96 | -77 |
| 0 | 1 | 218 | -187 |
| 0 | 2 | 156 | -148 |
| 0 | 3 | 180 | -167 |
| 0 | 4 | 74 | -77 |
| 0 | 5 | 291 | -276 |
| 0 | 6 | 43 | -10 |
| 0 | 7 | 234 | -164 |
| 0 | 8 | 108 | 122 |
| 0 | 9 | 283 | -278 |
| 0 | 10 | 78 | -109 |
| 0 | 11 | 180 | -177 |
| 0 | 12 | 40 | -36 |
| 0 | 13 | 177 | -168 |
| 0 | 14 | 16 | -16 * |
| 0 | 15 | 69 | -59 |
| 0 | 16 | 23 | -3 * |
| 1 | -16 | 24 | 21 * |
| 1 | -15 | 16 | 22 * |
| 1 | -14 | 24 | 20 * |
| 1 | -13 | 18 | 14 * |
| 1 | -12 | 21 | -7 * |
| 1 | -11 | 18 | -3 * |
| 1 | -10 | 42 | -77 |
| 1 | -9 | 114 | -149 |
| 1 | -8 | 45 | 52 |
| 1 | -7 | 217 | -221 |
| 1 | -6 | 17 | 21 * |
| 1 | -5 | 254 | 273 |
| 1 | -4 | 106 | -124 |
| 1 | -3 | 255 | -247 |
| 1 | -2 | 108 | 85 |
| 1 | -1 | 256 | -250 |
| 1 | 0 | 82 | 90 |
| 1 | 1 | 268 | -304 |
| 1 | 2 | 137 | 170 |
| 1 | 3 | 196 | -131 |
| 1 | 4 | 26 | -7 * |
| 1 | 5 | 163 | 105 |
| 1 | 6 | 92 | -19 |
| 1 | 7 | 189 | 167 |
| 1 | 8 | 96 | 87 |
| 1 | 9 | 138 | 182 |
| 1 | 10 | 18 | 9 * |
| 1 | 11 | 169 | 203 |
| 1 | 12 | 90 | 57 |
| 1 | 13 | 206 | 228 |
| 1 | 14 | 60 | 75 |
| 2 | -17 | 91 | 96 |
| 2 | -16 | 58 | -50 |
| 2 | -15 | 37 | -11 * |
| 2 | -14 | 19 | 15 * |
| 2 | -13 | 65 | 75 |
| 2 | -12 | 52 | -18 |
| 2 | -11 | 101 | 81 |
| 2 | -10 | 47 | -48 |
| 2 | -9 | 107 | 105 |
| 2 | -8 | 71 | 53 |
| 2 | -7 | 18 | -13 * |
| 2 | -6 | 18 | 7 * |
| 2 | -5 | 112 | -122 |
| 2 | -4 | 100 | 112 |
| 2 | -3 | 57 | 59 |
| 2 | -2 | 141 | -144 |
| 2 | -1 | 215 | 213 |
| 2 | 0 | 69 | 79 |
| 2 | 1 | 65 | 45 |
| 2 | 2 | 18 | 16 * |
| 2 | 3 | 38 | 9 * |
| 2 | 4 | 168 | -178 |
| 2 | 5 | 33 | -47 * |
| 2 | 6 | 95 | 95 |
| 2 | 7 | 153 | 156 |
| 2 | 8 | 18 | -19 * |
| 2 | 9 | 27 | 37 * |
| 2 | 10 | [illegible] | [illegible] * |
| 2 | 11 | 88 | -71 |
| 2 | 12 | 78 | -85 |
| 3 | -16 | 28 | -9 * |
| 3 | -15 | 105 | -101 |
| 3 | -14 | 113 | 130 |
| 3 | -13 | 162 | -171 |
| 3 | -12 | 21 | -11 * |
| 3 | -11 | 132 | -128 |
| 3 | -10 | 24 | -11 * |
| 3 | -9 | 86 | -77 |
| 3 | -8 | 18 | 18 * |
| 3 | -7 | 10 | -36 * |
| 3 | -6 | 84 | 80 |
| 3 | -5 | 142 | 122 |
| 3 | -4 | 35 | 37 * |
| 3 | -3 | 60 | 48 |
| 3 | -2 | 35 | -27 * |
| 3 | -1 | 55 | 51 |
| 3 | 0 | 29 | -2 * |
| 3 | 1 | 172 | 165 |
| 3 | 2 | 50 | 45 |
| 3 | 3 | 59 | -73 |
| 3 | 4 | 16 | -27 * |
| 3 | 5 | 31 | -38 * |
| 3 | 6 | 78 | -79 |
| 3 | 7 | 31 | 31 * |
| 3 | 8 | 37 | 1 * |
| 3 | 9 | 23 | -19 * |
| 4 | -14 | 25 | -28 |
| 4 | -13 | 52 | 78 |
| 4 | -12 | 45 | 15 |
| 4 | -11 | 110 | 102 |
| 4 | -10 | 49 | 22 |
| 4 | -9 | 203 | 205 |
| 4 | -8 | 109 | -92 |
| 4 | -7 | 243 | 248 |
| 4 | -6 | 18 | 27 * |
| 4 | -5 | 195 | 217 |
| 4 | -4 | 72 | -73 |
| 4 | -3 | 103 | 95 |
| 4 | -2 | 86 | -106 |
| 4 | -1 | 42 | 64 |
| 4 | 0 | 53 | -50 |
| 4 | 1 | 53 | 78 |
| 4 | 2 | 21 | 25 * |
| 4 | 3 | 78 | -81 |
| 4 | 4 | 16 | 2 * |
| 4 | 5 | 76 | -92 |
| 4 | 6 | 39 | -13 |
| 5 | -10 | 55 | -37 |
| 5 | -9 | 96 | -103 |
| 5 | -8 | 67 | -84 |
| 5 | -7 | 118 | -113 |
| 5 | -6 | 55 | 28 |
| 5 | -5 | 182 | -178 |
| 5 | -4 | 59 | 71 |
| 5 | -3 | 149 | -154 |
| 5 | -2 | 58 | 32 |
| 5 | -1 | 115 | -131 |
| K = 9 | | | |
| 0 | 1 | 230 | 224 |
| 0 | 2 | 35 | -7 |
| 0 | 3 | 234 | 219 |
| 0 | 4 | 117 | -87 |
| 0 | 5 | 180 | 157 |
| 0 | 6 | 209 | -218 |
| 0 | 7 | 130 | 139 |
| 0 | 8 | 66 | -70 |
| 0 | 9 | 31 | -14 * |
| 0 | 10 | 42 | 45 |
| 0 | 11 | 39 | -5 * |
| 0 | 12 | 16 | -11 |
| 0 | 13 | 50 | -52 |
| 0 | 14 | 32 | 36 |
| 1 | -15 | 46 | -67 |
| 1 | -14 | 149 | 171 |
| 1 | -13 | 16 | -9 * |
| 1 | -12 | 156 | 169 |
| 1 | -11 | 24 | -35 * |
| 1 | -10 | 88 | 53 |
| 1 | -9 | 48 | 79 |
| 1 | -8 | 35 | 11 * |
| 1 | -7 | 98 | 114 |
| 1 | -6 | 104 | 100 |
| 1 | -5 | 84 | -102 |
| 1 | -4 | 62 | -54 |
| 1 | -3 | 159 | -155 |
| 1 | -2 | 167 | -157 |
| 1 | -1 | 83 | -77 |
| 1 | 0 | 184 | -231 |
| 1 | 1 | 93 | -31 |
| 1 | 2 | 35 | 10 * |
| 1 | 3 | 200 | -206 |
| 1 | 4 | 68 | 8 |
| 1 | 5 | 164 | -179 |
| 1 | 6 | 106 | -155 |
| 1 | 7 | 122 | -136 |
| 1 | 8 | 67 | -25 |
| 1 | 9 | 90 | -110 |
| 1 | 10 | 101 | -45 |
| 1 | 11 | 41 | -29 |
| 1 | 12 | 61 | 39 |
| 2 | -15 | 14 | 0 * |
| 2 | -14 | 113 | -122 |
| 2 | -13 | 24 | 19 * |
| 2 | -12 | 77 | -77 |
| 2 | -11 | 32 | 41 * |
| 2 | -10 | 188 | -189 |
| 2 | -9 | 60 | 43 |
| 2 | -8 | 200 | -217 |
| 2 | -7 | 85 | 91 |
| 2 | -6 | 87 | -95 |
| 2 | -5 | 27 | 17 * |
| 2 | -4 | 107 | -90 |
| 2 | -3 | 51 | -31 |
| 2 | -2 | 18 | 0 * |
| 2 | -1 | 168 | 166 |
| 2 | 0 | 77 | -59 |
| 2 | 1 | 58 | 55 |
| 2 | 2 | 162 | 145 |
| 2 | 3 | 168 | 179 |
| 2 | 4 | 118 | 124 |
| 2 | 5 | 21 | -0 * |
| 2 | 6 | 128 | 116 |
| 2 | 7 | 161 | 166 |
| 2 | 8 | 131 | 147 |
| 2 | 9 | 185 | 202 |
| 2 | 10 | 161 | 159 |
| 3 | -14 | 14 | 14 * |
| 3 | -13 | 19 | 33 * |
| 3 | -12 | 40 | 27 |
| 3 | -11 | 37 | -46 * |
| 3 | -10 | 17 | 14 * |
| 3 | -9 | 45 | -60 |
| 3 | -8 | 59 | 65 |
| 3 | -7 | 32 | -13 * |
| 3 | -6 | 33 | 28 * |
| 3 | -5 | 64 | -52 |
| 3 | -4 | 209 | 206 |
| 3 | -3 | 185 | -181 |
| 3 | -2 | 130 | 117 |
| 3 | -1 | 191 | -209 |
| 3 | 0 | 68 | 51 |
| 3 | 1 | 68 | -69 |
| 3 | 2 | 190 | 200 |
| 3 | 3 | 72 | -59 |
| 3 | 4 | 48 | 53 |
| 3 | 5 | 65 | -68 |
| 3 | 6 | 40 | 31 |
| 3 | 7 | 94 | -86 |
| 4 | -11 | 43 | -44 |
| 4 | -10 | 56 | 36 |
| 4 | -9 | 15 | 20 * |
| 4 | -8 | 22 | -2 * |
| 4 | -7 | 16 | -16 * |
| 4 | -6 | 49 | 30 |
| 4 | -5 | 94 | 60 |
| 4 | -4 | 51 | 98 |
| 4 | -3 | 90 | 72 |
| 4 | -2 | 81 | -74 |
| 4 | -1 | 76 | 46 |
| 4 | 0 | 129 | 143 |
| 4 | 1 | 104 | 119 |
| 4 | 2 | 136 | -115 |
| 4 | 3 | 117 | 124 |
| K = 10 | | | |
| 0 | 0 | 133 | -148 |
| 0 | 1 | 48 | -16 |
| 0 | 2 | 76 | -72 |
| 0 | 3 | 77 | -60 |
| 0 | 4 | 69 | 80 |
| 0 | 5 | 71 | -41 |
| 0 | 6 | 79 | -48 |
| 0 | 7 | 54 | -62 |
| 0 | 8 | 170 | -179 |
| 0 | 9 | 35 | -1 * |
| 0 | 10 | 137 | -130 |
| 0 | 11 | 28 | -69 * |
| 0 | 12 | 14 | -25 * |
| 1 | -12 | 66 | 81 |
| 1 | -11 | 78 | 69 |
| 1 | -10 | 143 | 154 |
| 1 | -9 | 52 | 52 |
| 1 | -8 | 112 | 116 |
| 1 | -7 | 35 | 21 * |
| 1 | -6 | 121 | 136 |
| 1 | -5 | 55 | -2 * |
| 1 | -4 | 218 | 221 |
| 1 | -3 | 95 | -92 |
| 1 | -2 | 141 | 137 |
| 1 | -1 | 41 | -42 |
| 1 | 0 | 101 | 75 |
| 1 | 1 | 82 | -57 |
| 1 | 2 | 157 | -95 |
| 1 | 3 | 43 | -8 |
| 1 | 4 | 152 | 118 |
| 1 | 5 | 36 | -60 |
| 1 | 6 | 81 | -20 |
| 1 | 7 | 49 | -53 |
| 1 | 8 | 105 | -51 |
| 1 | 9 | 50 | -41 |
| 1 | 10 | 46 | -3 |
| 2 | -12 | 79 | 89 |
| 2 | -11 | 127 | -132 |
| 2 | -10 | 85 | 89 |
| 2 | -9 | 105 | -103 |
| 2 | -8 | 80 | -93 |
| 2 | -7 | 95 | -79 |
| 2 | -6 | 85 | -82 |
| 2 | -5 | 64 | -75 |
| 2 | -4 | 113 | -117 |
| 2 | -3 | 18 | 2 * |
| 2 | -2 | 64 | -42 |
| 2 | -1 | 67 | -84 |
| 2 | 0 | 180 | -174 |
| 2 | 1 | 75 | 60 |
| 2 | 2 | 248 | -251 |
| 2 | 3 | 83 | 55 |
| 2 | 4 | 127 | -135 |
| 2 | 5 | 72 | 45 |
| 2 | 6 | 132 | 123 |
| 3 | -11 | 71 | 77 |
| 3 | -10 | 92 | -91 |
| 3 | -9 | 42 | 30 |
| 3 | -8 | 33 | -26 * |
| 3 | -7 | 62 | 59 |
| 3 | -6 | 16 | -24 * |
| 3 | -5 | 112 | 107 |
| 3 | -4 | 36 | 10 * |
| 3 | -3 | 78 | 72 |
| 3 | -2 | 113 | 116 |
| 3 | -1 | 120 | 130 |
| 3 | 0 | 37 | -5 * |
| 3 | 1 | 35 | 13 * |
| 3 | 2 | 164 | 160 |
| 3 | 3 | 90 | 113 |
| 3 | 4 | 189 | 193 |
| K = 11 | | | |
| 0 | 1 | 151 | 138 |
| 0 | 2 | 91 | -78 |
| 0 | 3 | 71 | 63 |
| 0 | 4 | 52 | -48 |
| 0 | 5 | 104 | 113 |
| 0 | 6 | 34 | 60 * |
| 0 | 7 | 60 | -69 |
| 0 | 8 | 69 | -62 |
| 0 | 9 | 50 | -46 |
| 1 | -9 | 130 | 137 |
| 1 | -8 | 39 | -73 * |
| 1 | -7 | 111 | 141 |
| 1 | -6 | 165 | -180 |
| 1 | -5 | 85 | 63 |
| 1 | -4 | 104 | -105 |
| 1 | -3 | 17 | 9 * |
| 1 | -2 | 49 | -31 |
| 1 | -1 | 57 | 28 |
| 1 | 0 | 38 | 15 * |
| 1 | 1 | 61 | -72 |
| 1 | 2 | 77 | -61 |
| 1 | 3 | 52 | -20 |
| 1 | 4 | 125 | -73 |
| 1 | 5 | 141 | -137 |
| 1 | 6 | 77 | 67 |
| 1 | 7 | 105 | -65 |
| 2 | -8 | 91 | 93 |
| 2 | -7 | 77 | -76 |
| 2 | -6 | 96 | 93 |
| 2 | -5 | 74 | -85 |
| 2 | -4 | 43 | 31 |
| 2 | -3 | 67 | -49 |
| 2 | -2 | 47 | 11 |
| 2 | -1 | 54 | -61 |
| 2 | 0 | 190 | 137 |
| 2 | 1 | 64 | -66 |
| 2 | 2 | 54 | -74 |
| 2 | 3 | 78 | -81 |
| 2 | 4 | 39 | 14 |
| K = 12 | | | |
| 0 | 0 | 200 | 188 |
| 0 | 1 | 58 | 36 |
| 0 | 2 | 173 | 168 |
| 0 | 3 | 65 | 69 |

In the chain of atoms S(1) to O, differences in bond length from desaurin, *i.e.* C(3)=O and C(1)–C(2), longer, and C(2)–C(3), shorter, are of marginal significance. This chain of atoms is also, as in desaurin, closely coplanar; S(2) is closely planar with them also. Various least-squares planes and deviations from them are given in Table 3. The bond angles in this chain of atoms are quite different from those in desaurin, the net effect being a significantly longer S···O distance 2·727 (10) Å compared with 2·640 (6) Å in desaurin, but still well within the range of interaction. The benzene ring (closely coplanar, see Table 3, with mean C–C, 1·402 Å) makes an angle 19·3° with the central plane of the molecule, plane *D*. The bond C(4)–C(3) by which the phenyl group is attached is, at 1·511 (13) Å, only marginally longer than the corresponding bond in desaurin, 1·495 (8) Å. Sulphur atom S(2) is closely coplanar with the central molecular plane, being 0·13 Å from plane *C* (Table 3). In the analogous system in 2-desylidene-1,3-dithiolane (II) Schmidt & Tulinsky, 1967; Tulinsky, 1967), S(2) is quite substantially (0·24 Å) out of the mean plane O=C–C=C–S(1) which is itself closely coplanar with mean atomic deviation 0·034 Å. This difference is presumably attributable to constraints exerted by the ring ethylene group.

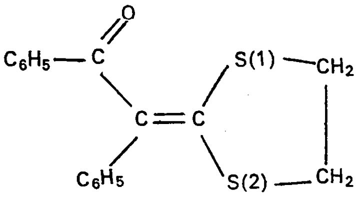
Table 5. *Non-bonded interatomic distances less than* 3·90 Å

Atom *B* is generated from the coordinates of Table 1 using the unit-cell translation shown together with the following symmetry operations:

i $x, y, z$ iii $x, \frac{1}{2}-y, \frac{1}{2}+z$

ii $-x, -y, z$ iv $-x, \frac{1}{2}+y, \frac{1}{2}-z$.

| Atom *A* | Atom *B* | Unit cell translation of atom *B* | Distance |
|---|---|---|---|
| S(1) | S(1$^{ii}$) | ( 1, 0, 1) | 3·41 Å |
| S(1) | C(10$^{ii}$) | ( 1, 0, 1) | 3·89 |
| S(2) | S(2$^{ii}$) | ( 2, 1, 1) | 3·57 |
| S(2) | C(2$^{ii}$) | ( 1, 1, 1) | 3·88 |
| S(2) | C(3$^{i}$) | ( 1, 0, 0) | 3·69 |
| S(2) | C(4$^{i}$) | ( 1, 0, 0) | 3·77 |
| S(2) | C(9$^{i}$) | ( 1, 0, 0) | 3·79 |
| S(2) | C(11$^{ii}$) | ( 2, 1, 1) | 3·80 |
| O | C(5$^{iv}$) | ( 0, −1, 0) | 3·88 |
| O | C(6$^{iv}$) | ( 0, −1, 0) | 3·41 |
| O | C(10$^{i}$) | (−1, 0, 0) | 3·53 |
| O | C(10$^{ii}$) | ( 1, 0, 1) | 3·47 |
| C(1) | C(9$^{i}$) | ( 1, 0, 0) | 3·46 |
| C(1) | C(11$^{ii}$) | ( 1, 1, 1) | 3·71 |
| C(2) | C(8$^{i}$) | ( 1, 0, 0) | 3·56 |
| C(2) | C(9$^{i}$) | ( 1, 0, 0) | 3·56 |
| C(3) | C(8$^{i}$) | ( 1, 0, 0) | 3·88 |
| C(4) | C(11$^{i}$) | (−1, 0, 0) | 3·80 |
| C(6) | C(9$^{iv}$) | (−1, 0, 0) | 3·74 |
| C(6) | C(10$^{iii}$) | (−1, 0, −1) | 3·68 |
| C(7) | C(9$^{iv}$) | (−1, 0, 0) | 3·89 |
| C(7) | C(11$^{iv}$) | ( 0, −1, 0) | 3·74 |
| C(8) | C(11$^{iv}$) | ( 1, −1, 0) | 3·45 |



(II)

Intermolecular interatomic distances of less than 3·9 Å are listed in Table 5, and the packing illustrated in Fig. 2. Because of the shortness of the *a* cell dimension there is no overlap in *x* projection. No intermolecular contacts are unusual save perhaps C(8)–Me(11) which, at 3·45 Å, is somewhat shorter than the expected 3·65 Å.

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