Table 1. *Positional and thermal parameters in* $BaTbO_3$

Space group $R\bar{3}c$, $a=6{\cdot}050\ (5)^*$ Å, $\alpha=60{\cdot}13\ (5)^\circ$ at 298 °K.

| Temperature (°K) | 11 | 46 | 80 | 298 |
|---|---|---|---|---|
| Wavelength (Å) | 1·2016 | 1·2016 | 1·3642 | 1·2016 |
| Oxygen $x$ parameter | 0·7073 (3) | 0·7096 (12) | 0·7104 (4) | 0·7131 (15) |
| Ba occupancy factor | 1·000 (†) | 1·000 (4) | 1·000 (†) | 1·000 (†) |
| Tb occupancy factor | 1·002 (20) | 0·979 (3) | 0·979 (†) | 0·979 (†) |
| Ba temperature factor | 0·13 (†) | 0·26 (26) | 0·28 (†) | 0·54 (9) |
| Tb temperature factor | 0·06 (†) | 0·12 (18) | 0·13 (†) | 0·40 (7) |
| O temperature factor | 0·33 (†) | 0·65 (13) | 0·70 (†) | 1·06 (24) |
| $R=\frac{\sum\omega(I_{\rm obs}-I_{\rm calc})^2}{\sum I^2_{\rm obs}}$ | 0·031 (‡) | 0·044 | 0·108 | 0·027 |
| Number of observations | 11 | 20 | 9 | 12 |

* Figures in parentheses give the estimated standard deviation in the last significant figure.

† This parameter not varied in refinement.

‡ Simultaneous refinement of nuclear and magnetic intensities (the magnetic moment is an additional variable here).

scattering vector); if one of the parity classes is absent, however, it follows that $\mathbf{K}_{hkl}$ is zero since $\mathbf{e}\times\mathbf{K}$ must vanish for constant $\mathbf{K}$ and variable $\mathbf{e}$. Thus, setting $\mathbf{K}_{hkl}$ in equation (1) equal to zero for all but the all-odd class of reflections, we obtain a set of eight relations connecting the individual moments, which on further manipulation yield the following relations among the atomic moments: $\mathbf{K}_1=-\mathbf{K}_2=-\mathbf{K}_3=-\mathbf{K}_4=\mathbf{K}_5=\mathbf{K}_6=\mathbf{K}_7=-\mathbf{K}_8$. These relations demonstrate that the moments must be collinear; placing the moments at the positions as labeled above shows them to be arranged in the *G*-type antiferromagnetic structure. The magnetic moment of $Tb^{4+}$ was obtained by a least-squares refinement of the magnetic and positional parameters from the data at 11 °K. The form factor for $Tb^{4+}$ was estimated by a linear extrapolation of theoretical values for the isoelectronic $Eu^{2+}$ and $Gd^{3+}$ (Blume, Freeman & Watson, 1962). The value of $\langle q^2\rangle$, the parameter related to spin orientation, was taken to be $\frac{2}{3}$, the average over cubic forms (Shirane, 1959), inasmuch as the rhombohedral splittings of the magnetic reflections were not resolved. The refined value of the $Tb^{4+}$ moment is 6·66 (11)$\mu_B$, which is less than 5% below the free-ion value for an $^8S_{7/2}$ ground state.

At 11 °K, the temperature is about one third of the Néel temperature. For an ion with $S=\frac{7}{2}$, the reduced magnetization at this temperature should be about 0·95. Applying this factor to the calculated value of the terbium moment yields a value of 7·01$\mu_B$ for $Tb^{4+}$ at 0 °K, which is the theoretical value within 0·15%.

It is of some interest to compare the Néel temperature of 36 °K for this compound with the value of 2·4 °K in $LaErO_3$ (Moreau, Mareschal & Bertaut, 1968). Although the magnetic moment of $Er^{3+}$ is larger than that of $Tb^{4+}$, and the distances are comparable, the $Tb^{4+}$ compound has a 15-fold stronger magnetic interaction. This may be due to the appearance of superexchange mechanisms resulting from the polarization of the metal–oxygen bond induced by the higher formal charge on the $Tb^{4+}$ (greater covalency).

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## 2,4,5-Trichloro-6-(methylthio)isophthalonitrile.

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$C_9H_3N_2SCl_3$, monoclinic, $P2_1/c$, $a=7{\cdot}705\ (6)$, $b=32{\cdot}356\ (28)$, $c=8{\cdot}901\ (7)$ Å, $\beta=99{\cdot}86\ (4)^\circ$, 25 °C, $M=277{\cdot}56$, $Z=8$, $D=1{\cdot}682$ g.cm$^{-3}$. Bond distances and angles are normal but the molecules show significant deviations from planarity. Unusually short intermolecular contacts are found between cyanide and chloride functions.

### Introduction

This crystal structure determination was undertaken to identify positively the substituent positions in a compound known to be a trichloro(methylthio)isophthalonitrile (Domenico, 1970), but which could not be unambiguously identified by conventional spectroscopic methods. Solution of the structure showed the isomer to be 2,4,5-trichloro-6-(methylthio)isophthalonitrile. The structure study also revealed the presence of unusually short interatomic dis-

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tances, 2·995 and 3·000 Å, between cyanide groups and chlorides on adjacent molecules. These distances represent a shortening of about 0·3 Å from the sum of the van der Waals radii (Pauling, 1960) for N (1·5 Å) and Cl (1·8 Å). This observation appears to be of considerable interest because our N···Cl distances are comparable to the linear donor–acceptor interaction in $\mathrm{ClC{\equiv}N}$ (N···Cl = 3·01 Å) found by Heiart & Carpenter (1956); by contrast, Britton (1967) had been unable to detect any such shortening in an aromatic system, *p*-chlorophenyl cyanide (N···Cl = 3·3 Å), even though a linear structure suggestive of an interaction was observed. While an N···Cl distance of 3·08 Å was reported by Golder, Zhdanov & Umanskij (1952) for 2,4,6-trichlorophenyl cyanide from projection the reliability of this determination has since questioned (Britton, 1967). A very recent redetermination of this structure using three-

Table 1. *Atomic parameters with standard errors*

Errors in parentheses refer to last significant figures. Thermal parameters are of the form $\exp\,[-(\beta_{11}h^2+\beta_{22}k^2+\beta_{33}l^2+2\beta_{12}hk+2\beta_{13}hl+2\beta_{23}kl)]$

| | $x$ | $y$ | $z$ | $10^4\,\beta_{11}$ | $10^4\,\beta_{22}$ | $10^4\,\beta_{33}$ | $10^4\,\beta_{12}$ | $10^4\,\beta_{13}$ | $10^4\,\beta_{23}$ |
|---|---|---|---|---|---|---|---|---|---|
| Cl(1) | 0·6941 (5) | 0·0770 (1) | −0·0137 (3) | 224 (9) | 106 (6) | 118 (5) | −2 (2) | 22 (5) | −2 (1) |
| Cl(2) | 0·6264 (5) | 0·0562 (1) | 0·5695 (4) | 196 (8) | 100 (6) | 136 (6) | −1 (1) | 62 (5) | 12 (1) |
| Cl(3) | 0·7833 (5) | 0·1434 (1) | 0·6506 (4) | 220 (9) | 109 (6) | 115 (5) | 3 (2) | 40 (5) | −1 (1) |
| S(1) | 0·8938 (5) | 0·2011 (1) | 0·3893 (4) | 189 (8) | 81 (5) | 193 (6) | − 12 (1) | 60 (5) | −4 (1) |
| Cl(4) | 0·1871 (5) | 0·4195 (1) | 0·5679 (4) | 215 (9) | 106 (6) | 115 (5) | 0 (1) | 21 (5) | −3 (1) |
| Cl(5) | 0·1308 (5) | 0·4461 (1) | −0·0318 (4) | 195 (8) | 88 (5) | 125 (5) | 4 (1) | 9 (5) | 14 (1) |
| Cl(6) | 0·2879 (5) | 0·3588 (1) | −0·0739 (4) | 184 (7) | 107 (6) | 103 (4) | −3 (1) | 37 (4) | 2 (1) |
| S(2) | 0·3689 (5) | 0·2968 (1) | 0·2014 (4) | 220 (9) | 77 (5) | 183 (6) | 12 (1) | 107 (6) | 8 (1) |
| C(1) | 0·7936 (15) | 0·1338 (4) | 0·2048 (13) | 98 (25) | 92 (15) | 117 (19) | 0 (5) | 27 (17) | 1 (4) |
| C(2) | 0·7236 (16) | 0·0951 (3) | 0·1700 (13) | 133 (27) | 51 (10) | 106 (18) | 1 (4) | 0 (16) | 3 (4) |
| C(3) | 0·6652 (14) | 0·0719 (3) | 0·2813 (13) | 79 (21) | 51 (10) | 125 (18) | 3 (4) | 6 (15) | 7 (4) |
| C(4) | 0·6867 (16) | 0·0865 (4) | 0·4297 (12) | 152 (29) | 81 (16) | 86 (17) | 6 (5) | 25 (17) | 4 (4) |
| C(5) | 0·7569 (15) | 0·1263 (4) | 0·4633 (12) | 116 (24) | 85 (16) | 68 (15) | 5 (5) | 27 (16) | −7 (4) |
| C(6) | 0·8100 (16) | 0·1509 (4) | 0·3528 (14) | 127 (26) | 79 (16) | 132 (19) | −3 (5) | 47 (17) | −2 (4) |
| C(7) | 0·8565 (16) | 0·1587 (4) | 0·0862 (16) | 137 (29) | 75 (16) | 169 (23) | −1 (5) | 62 (20) | 0 (5) |
| N(1) | 0·9017 (17) | 0·1765 (4) | −0·0073 (13) | 300 (37) | 124 (18) | 159 (22) | 2 (6) | 102 (22) | 8 (5) |
| C(8) | 0·5863 (16) | 0·0316 (4) | 0·2443 (13) | 149 (27) | 53 (9) | 111 (18) | −2 (5) | 22 (17) | 1 (4) |
| N(2) | 0·5249 (17) | 0·0006 (4) | 0·2197 (14) | 230 (33) | 86 (9) | 231 (25) | − 15 (5) | 48 (21) | 0 (5) |
| C(9) | 0·7021 (21) | 0·2290 (5) | 0·4298 (22) | 184 (38) | 114 (15) | 433 (46) | 17 (7) | 24 (32) | − 13 (7) |
| C(10) | 0·2762 (15) | 0·3623 (4) | 0·3722 (12) | 123 (35) | 55 (9) | 108 (18) | − 10 (4) | 34 (17) | 4 (4) |
| C(11) | 0·2067 (15) | 0·4017 (4) | 0·3890 (12) | 115 (26) | 70 (14) | 100 (18) | −6 (4) | 7 (16) | −7 (4) |
| C(12) | 0·1596 (15) | 0·4266 (4) | 0·2631 (13) | 103 (23) | 85 (16) | 121 (20) | −3 (5) | 16 (17) | −1 (4) |
| C(13) | 0·1879 (14) | 0·4132 (4) | 0·1202 (13) | 84 (23) | 63 (10) | 123 (19) | −6 (4) | −11 (16) | 9 (4) |
| C(14) | 0·2547 (15) | 0·3742 (4) | 0·1049 (12) | 129 (26) | 78 (14) | 85 (17) | −6 (5) | 25 (16) | 3 (4) |
| C(15) | 0·2939 (15) | 0·3477 (3) | 0·2293 (13) | 98 (23) | 62 (9) | 113 (17) | −1 (4) | 32 (16) | 7 (4) |
| C(16) | 0·3410 (17) | 0·3385 (4) | 0·5073 (15) | 169 (30) | 77 (11) | 128 (21) | 0 (5) | 49 (20) | 7 (5) |
| N(3) | 0·3952 (16) | 0·3203 (4) | 0·6138 (13) | 242 (32) | 149 (20) | 147 (20) | 5 (6) | 41 (20) | 18 (5) |
| C(17) | 0·0786 (17) | 0·4669 (5) | 0·2807 (13) | 148 (30) | 112 (20) | 117 (20) | 0 (6) | 22 (19) | 6 (5) |
| N(4) | 0·0156 (17) | 0·4987 (4) | 0·2930 (14) | 246 (36) | 117 (16) | 215 (25) | 18 (6) | 40 (22) | 3 (5) |
| C(18) | 0·2108 (19) | 0·2651 (4) | 0·2811 (17) | 249 (37) | 58 (8) | 250 (28) | − 11 (6) | 144 (26) | 12 (5) |

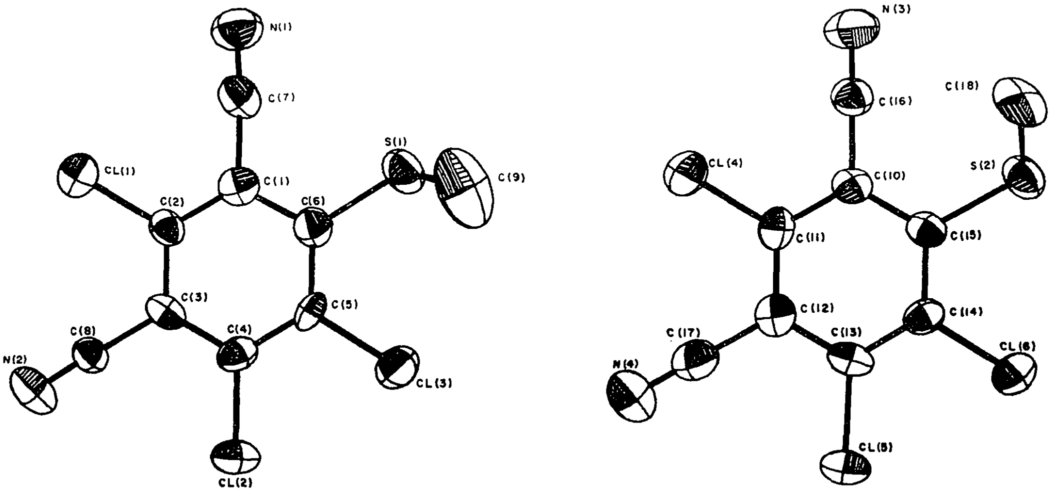

Fig. 1. The molecular structures and numbering system for the two independent molecules (left *A*, right *B*) of 2,4,5-trichloro-6-(methylthio)isophthalonitrile. Thermal ellipsoids are drawn at 50% probability.

dimensional data shows the shortest N···Cl contact to be 3·22 Å (Carter & Britton, 1972). The present results thus provide important evidence proving that appreciable donor–acceptor interactions can occur in the solid state between the C≡N group and an aromatic chloride.

## Experimental

Considerable difficulty was encountered in obtaining single crystals suitable for an X-ray diffraction study and this problem was never completely solved. The sample was impure as received and contained no usable crystals, but purification by recrystallization from acetonitrile gave crystals (m.p. 157·5–159°) which almost always appeared twinned under the optical microscope. An acceptable crystal was finally grown by slow evaporation of an acetone solution of the purified material. This specimen was an irregular triangular slab, 0·35 mm long, a maximum of 0·18 mm wide, and 0·10 mm thick. The crystal was aligned on the *c* axis, and the space group was determined from the reciprocal lattice symmetry $C_{2h}$ and the systematic absences of *h*0*l* reflections for *l* odd and 0*k*0 for *k* odd exhibited on Weissenberg photographs. Lattice constants were determined by least-squares refinement of the setting angles of 24 carefully centered reflections using a four-circle goniostat. Intensity data were gathered by a Picker automatic diffractometer (θ–2θ scan mode) using Mo $K\bar{\alpha}$ radiation monochromatized by the 002 reflection of a highly oriented

Table 2. *Observed and calculated structure factors in e*

| H | L | FOBS | FCAL |
|---|---|---|---|
| ** K = 0 ** | | | |
| 0 | 2 | 91 | 90 |
| 0 | 6 | 38 | 40 |
| 1 | 2 | 45 | 47 |
| 1 | 4 | 41 | 39 |
| 1 | -6 | 22 | 20 |
| 1 | 8 | 21 | 19 |
| 2 | 0 | 313 | 309 |
| 2 | -2 | 83 | 78 |
| 2 | 2 | 94 | 94 |
| 2 | -4 | 132 | 128 |
| 2 | 4 | 33 | 32 |
| 2 | -6 | 48 | 46 |
| 2 | 6 | 40 | 40 |
| 2 | 8 | 21 | 20 |
| 2 | -10 | 22 | 22 |
| 2 | 10 | 30 | 28 |
| 3 | -2 | 71 | 68 |
| 3 | 2 | 32 | 32 |
| 3 | 4 | 77 | 81 |
| 3 | -6 | 48 | 49 |
| 3 | 6 | 30 | 40 |
| 3 | -8 | 23 | 23 |
| 4 | 0 | 49 | 49 |
| 4 | -2 | 32 | 32 |
| 4 | 2 | 29 | 29 |
| 4 | -4 | 70 | 67 |
| 4 | -6 | 27 | 27 |
| 5 | -2 | 82 | 86 |
| 5 | -4 | 26 | 26 |
| 5 | 4 | 56 | 58 |
| 6 | -4 | 27 | 30 |
| 7 | -2 | 31 | 31 |
| 7 | -4 | 28 | 30 |
| 7 | -8 | 22 | 19 |
| 8 | -4 | 22 | 19 |
| ** K = 1 ** | | | |
| 0 | 1 | 59 | 62 |
| 0 | 4 | 75 | 76 |
| 0 | 5 | 52 | 53 |
| 0 | 9 | 25 | 22 |
| 1 | -1 | 79 | 74 |
| 1 | 1 | 87 | 82 |
| 1 | 2 | 81 | 77 |
| 1 | -3 | 103 | 100 |
| 1 | 3 | 139 | 135 |
| 1 | 4 | 29 | 28 |
| 1 | -5 | 35 | 33 |
| 1 | 5 | 59 | 57 |
| 1 | -6 | 42 | 44 |
| 1 | 6 | 43 | 44 |
| 1 | 7 | 78 | 76 |
| 1 | -8 | 23 | 22 |
| 2 | 0 | 90 | 93 |
| 2 | -2 | 39 | 41 |
| 2 | 2 | 27 | 26 |
| 2 | -3 | 99 | 96 |
| 2 | 4 | 76 | 75 |
| 2 | -6 | 28 | 28 |
| 2 | 7 | 32 | 30 |
| 3 | -1 | 26 | 23 |
| 3 | -2 | 25 | 26 |
| 3 | 2 | 42 | 41 |
| 3 | -3 | 62 | 61 |
| 3 | -4 | 69 | 67 |
| 3 | -5 | 46 | 47 |
| 3 | 5 | 34 | 34 |
| 3 | -6 | 47 | 45 |
| 3 | 6 | 40 | 39 |
| 3 | -7 | 93 | 84 |
| 3 | 7 | 47 | 47 |
| 3 | -9 | 21 | 16 |
| 3 | -10 | 22 | 19 |
| 4 | -1 | 28 | 27 |
| 4 | 1 | 43 | 44 |
| 4 | -2 | 24 | 23 |
| 4 | 2 | 30 | 30 |
| 4 | 4 | 21 | 18 |
| 4 | -5 | 24 | 23 |
| 4 | -6 | 40 | 39 |
| 4 | -7 | 22 | 21 |
| 4 | -8 | 21 | 22 |
| 5 | -2 | 60 | 63 |
| 5 | 2 | 65 | 68 |
| 5 | -3 | 22 | 22 |
| 5 | 3 | 30 | 26 |
| 5 | -4 | 51 | 52 |
| 5 | -5 | 50 | 52 |
| 5 | -6 | 32 | 31 |
| 5 | -7 | 45 | 46 |
| 6 | -1 | 26 | 25 |
| 6 | -3 | 25 | 24 |
| 6 | -10 | 24 | 18 |
| 7 | -2 | 34 | 35 |
| 8 | 0 | 20 | 20 |
| 8 | -1 | 26 | 25 |
| ** K = 2 ** | | | |
| 0 | 2 | 44 | 43 |
| 0 | 3 | 94 | 95 |
| 0 | 4 | 81 | 81 |
| 0 | 5 | 64 | 65 |
| 0 | 9 | 25 | 22 |
| 1 | 1 | 39 | 37 |
| 1 | -2 | 69 | 69 |
| 1 | 2 | 25 | 23 |
| 1 | -3 | 110 | 108 |
| 1 | -4 | 27 | 27 |
| 1 | -5 | 72 | 74 |
| 1 | 5 | 25 | 24 |
| 1 | 6 | 24 | 21 |
| 1 | 7 | 21 | 21 |
| 1 | 9 | 20 | 16 |
| 1 | -11 | 21 | 17 |
| 2 | 0 | 41 | 32 |
| 2 | -1 | 27 | 25 |
| 2 | -2 | 44 | 51 |
| 2 | 2 | 98 | 93 |
| 2 | -3 | 32 | 31 |
| 2 | 3 | 70 | 70 |
| 2 | -5 | 67 | 67 |
| 2 | 5 | 48 | 51 |
| 2 | -8 | 20 | 20 |
| 2 | -9 | 31 | 29 |
| 2 | 9 | 22 | 23 |
| 2 | -10 | 24 | 21 |
| 3 | -2 | 89 | 86 |
| 3 | 2 | 77 | 74 |
| 3 | -3 | 22 | 23 |
| 3 | -4 | 32 | 30 |
| 3 | 5 | 46 | 45 |
| 3 | -6 | 21 | 24 |
| 3 | 6 | 20 | 22 |
| 3 | 7 | 34 | 34 |
| 3 | -11 | 24 | 20 |
| 4 | -1 | 54 | 54 |
| 4 | 1 | 71 | 70 |
| 4 | -2 | 62 | 63 |
| 4 | 3 | 23 | 24 |
| 4 | -5 | 35 | 35 |
| 4 | -8 | 21 | 16 |
| 4 | -9 | 34 | 36 |
| 4 | -10 | 22 | 21 |
| 5 | -1 | 24 | 25 |
| 5 | 1 | 26 | 26 |
| 5 | -2 | 36 | 39 |
| 5 | -3 | 35 | 34 |
| 5 | 3 | 31 | 29 |
| 5 | -4 | 25 | 23 |
| 5 | 4 | 29 | 30 |
| 5 | -6 | 22 | 21 |
| 5 | 6 | 31 | 27 |
| 6 | 0 | 28 | 26 |
| 6 | -1 | 56 | 57 |
| 6 | 1 | 58 | 60 |
| 7 | 2 | 23 | 23 |
| 7 | -3 | 29 | 31 |
| 7 | 3 | 22 | 20 |
| 7 | -4 | 33 | 34 |
| 7 | -6 | 27 | 27 |
| 8 | 1 | 27 | 26 |
| ** K = 3 ** | | | |
| 0 | 1 | 40 | 41 |
| 0 | 2 | 69 | 67 |
| 0 | 3 | 123 | 128 |
| 0 | 6 | 41 | 43 |
| 0 | 7 | 22 | 19 |
| 0 | 10 | 27 | 24 |
| 1 | -1 | 71 | 66 |
| 1 | 1 | 45 | 40 |
| 1 | -2 | 37 | 29 |
| 1 | 2 | 89 | 85 |
| 1 | -3 | 30 | 28 |
| 1 | 3 | 48 | 46 |
| 1 | -4 | 37 | 35 |
| 1 | 4 | 66 | 64 |
| 1 | -5 | 20 | 20 |
| 1 | 5 | 49 | 48 |
| 1 | -6 | 41 | 43 |
| 1 | 6 | 65 | 61 |
| 2 | 0 | 252 | 255 |
| 2 | -1 | 61 | 59 |
| 2 | 1 | 68 | 68 |
| 2 | -2 | 103 | 95 |
| 2 | 2 | 39 | 40 |
| 2 | -3 | 61 | 60 |
| 2 | 3 | 64 | 62 |
| 2 | 4 | 54 | 51 |
| 2 | -5 | 37 | 36 |
| 2 | -6 | 32 | 33 |
| 2 | -7 | 26 | 27 |
| 2 | -9 | 26 | 22 |
| 3 | -2 | 54 | 55 |
| 3 | 2 | 39 | 39 |
| 3 | -3 | 82 | 79 |
| 3 | 3 | 30 | 31 |
| 3 | -4 | 28 | 24 |
| 3 | 4 | 25 | 25 |
| 3 | 5 | 21 | 19 |
| 3 | -6 | 60 | 60 |
| 3 | 6 | 33 | 32 |
| 3 | -7 | 26 | 25 |
| 3 | 7 | 32 | 29 |
| 3 | 8 | 20 | 17 |
| 4 | 0 | 45 | 45 |
| 4 | -1 | 80 | 82 |
| 4 | 1 | 48 | 48 |
| 4 | -2 | 39 | 40 |
| 4 | 2 | 42 | 41 |
| 4 | -3 | 22 | 24 |
| 4 | 3 | 34 | 36 |
| 4 | -4 | 35 | 35 |
| 4 | 4 | 48 | 47 |
| 4 | -5 | 32 | 32 |
| 4 | -6 | 23 | 23 |
| 5 | -1 | 47 | 50 |
| 5 | -2 | 40 | 41 |
| 5 | -4 | 50 | 51 |
| 5 | 4 | 24 | 24 |
| 5 | -5 | 27 | 26 |
| 5 | 5 | 24 | 24 |
| 5 | -6 | 43 | 46 |
| 5 | -7 | 24 | 26 |
| 5 | 7 | 22 | 23 |
| 6 | 0 | 34 | 36 |
| 6 | -5 | 32 | 34 |
| 6 | -9 | 25 | 25 |
| 7 | -4 | 22 | 24 |
| 7 | 4 | 24 | 24 |
| 9 | -5 | 20 | 15 |
| ** K = 4 ** | | | |
| 0 | 0 | 189 | 210 |
| 0 | 2 | 116 | 115 |
| 0 | 3 | 94 | 98 |
| 0 | 4 | 72 | 75 |
| 0 | 7 | 44 | 41 |
| 1 | -1 | 45 | 45 |
| 1 | 1 | 97 | 95 |
| 1 | -2 | 90 | 92 |
| 1 | 2 | 46 | 44 |
| 1 | -3 | 108 | 108 |
| 1 | 3 | 64 | 62 |
| 1 | -4 | 24 | 23 |
| 1 | 4 | 33 | 30 |
| 1 | -5 | 58 | 62 |
| 1 | -6 | 22 | 25 |
| 1 | 6 | 28 | 28 |
| 1 | -7 | 106 | 117 |
| 1 | 7 | 54 | 52 |
| 1 | -9 | 21 | 20 |
| 2 | 0 | 260 | 263 |
| 2 | 1 | 82 | 83 |
| 2 | -3 | 57 | 56 |
| 2 | 3 | 41 | 41 |
| 2 | -4 | 38 | 35 |
| 2 | -6 | 26 | 28 |
| 2 | -7 | 29 | 32 |
| 3 | -1 | 45 | 40 |
| 3 | 1 | 32 | 31 |
| 3 | -2 | 69 | 69 |
| 3 | -3 | 78 | 77 |
| 3 | 3 | 78 | 80 |
| 3 | -4 | 21 | 21 |
| 3 | 4 | 40 | 37 |
| 3 | -5 | 99 | 99 |
| 3 | -7 | 36 | 36 |
| 4 | 0 | 73 | 73 |
| 4 | -1 | 43 | 45 |
| 4 | 2 | 29 | 28 |
| 4 | -3 | 89 | 89 |
| 4 | -4 | 61 | 61 |
| 4 | -5 | 20 | 21 |
| 4 | -7 | 27 | 24 |
| 4 | 7 | 22 | 22 |
| 5 | -3 | 29 | 29 |
| 5 | 3 | 29 | 30 |
| 5 | -4 | 39 | 42 |
| 5 | -6 | 27 | 28 |
| 5 | -7 | 33 | 32 |
| 6 | -1 | 38 | 38 |
| 6 | 1 | 46 | 49 |
| 6 | 3 | 26 | 27 |
| 6 | -4 | 39 | 42 |
| 7 | -5 | 23 | 25 |
| 7 | -6 | 20 | 21 |
| 8 | 0 | 22 | 17 |
| ** K = 5 ** | | | |
| 0 | 1 | 39 | 39 |
| 0 | 4 | 78 | 80 |
| 0 | 8 | 23 | 22 |
| 0 | 10 | 34 | 33 |
| 1 | -1 | 60 | 58 |
| 1 | -2 | 22 | 17 |
| 1 | 2 | 101 | 99 |
| 1 | 3 | 78 | 28 |
| 1 | 4 | 30 | 29 |
| 1 | -5 | 22 | 27 |
| 1 | 5 | 82 | 82 |
| 1 | -6 | 62 | 68 |
| 1 | 7 | 24 | 21 |
| 2 | 0 | 330 | 327 |
| 2 | -1 | 42 | 41 |
| 2 | 1 | 31 | 29 |
| 2 | -2 | 89 | 89 |
| 2 | 2 | 79 | 76 |
| 2 | -3 | 78 | 76 |
| 2 | 3 | 57 | 57 |
| 2 | -4 | 97 | 92 |
| 2 | -5 | 45 | 45 |
| 2 | 5 | 25 | 24 |
| 2 | -6 | 22 | 21 |
| 2 | -10 | 25 | 23 |
| 3 | -1 | 64 | 59 |
| 3 | 1 | 82 | 80 |
| 3 | 2 | 73 | 76 |
| 3 | 4 | 39 | 39 |
| 3 | -5 | 47 | 46 |
| 3 | 5 | 42 | 41 |
| 3 | 7 | 30 | 32 |
| 3 | -10 | 29 | 24 |
| 4 | 0 | 136 | 133 |
| 4 | -2 | 26 | 25 |
| 4 | 2 | 30 | 29 |
| 4 | -3 | 44 | 47 |
| 4 | 4 | 25 | 23 |
| 4 | -5 | 20 | 20 |
| 5 | -1 | 21 | 21 |
| 5 | 3 | 24 | 23 |
| 5 | -4 | 26 | 26 |
| 5 | 4 | 23 | 20 |
| 5 | 6 | 25 | 24 |
| 5 | -7 | 41 | 42 |
| 6 | 0 | 33 | 35 |
| 6 | -2 | 26 | 27 |
| 6 | 3 | 27 | 28 |
| 6 | 4 | 20 | 17 |
| 7 | 4 | 27 | 29 |
| 7 | -7 | 27 | 27 |
| 8 | 0 | 22 | 22 |
| 8 | -3 | 20 | 18 |
| 9 | -2 | 24 | 23 |
| 9 | -5 | 25 | 20 |
| ** K = 6 ** | | | |
| 0 | 0 | 35 | 25 |
| 0 | 2 | 104 | 111 |
| 0 | 3 | 46 | 45 |
| 0 | 4 | 31 | 33 |
| 0 | 5 | 48 | 52 |
| 0 | 7 | 25 | 26 |
| 0 | 9 | 34 | 34 |
| 1 | 1 | 47 | 44 |
| 1 | -2 | 39 | 40 |
| 1 | 2 | 32 | 80 |
| 1 | -3 | 85 | 85 |
| 1 | 3 | 64 | 66 |
| 1 | -4 | 57 | 56 |
| 1 | 4 | 42 | 43 |
| 1 | -5 | 71 | 77 |
| 1 | 5 | 44 | 46 |
| 1 | 6 | 23 | 24 |
| 1 | -7 | 64 | 70 |
| 1 | 7 | 36 | 34 |
| 2 | 0 | 118 | 109 |
| 2 | -1 | 59 | 55 |
| 2 | 1 | 65 | 61 |
| 2 | 2 | 41 | 41 |
| 2 | -3 | 79 | 76 |
| 2 | 3 | 56 | 55 |
| 2 | -4 | 40 | 40 |
| 2 | 4 | 37 | 36 |
| 2 | 5 | 43 | 44 |
| 2 | 6 | 21 | 17 |
| 2 | -9 | 34 | 37 |
| 2 | -10 | 23 | 23 |
| 3 | -1 | 60 | 62 |
| 3 | -2 | 56 | 57 |
| 3 | 2 | 58 | 59 |
| 3 | -3 | 41 | 38 |
| 3 | 3 | 71 | 72 |
| 3 | -4 | 56 | 56 |
| 3 | 4 | 44 | 46 |
| 3 | 5 | 37 | 39 |
| 3 | -6 | 29 | 30 |
| 3 | 6 | 32 | 32 |
| 3 | -7 | 44 | 45 |
| 4 | 0 | 24 | 24 |
| 4 | 1 | 46 | 48 |
| 4 | 3 | 31 | 31 |
| 4 | 5 | 28 | 30 |
| 4 | -6 | 23 | 24 |
| 5 | -1 | 22 | 21 |
| 5 | -5 | 34 | 35 |
| 5 | -6 | 41 | 42 |
| 5 | 6 | 31 | 33 |
| 6 | 0 | 34 | 36 |
| 6 | -3 | 49 | 49 |
| 6 | 3 | 22 | 22 |
| 7 | -1 | 21 | 20 |
| 7 | -2 | 27 | 28 |
| 7 | -4 | 25 | 30 |
| 7 | 5 | 21 | 21 |
| 7 | -6 | 39 | 44 |
| ** K = 7 ** | | | |
| 0 | 3 | 36 | 39 |
| 0 | 7 | 27 | 24 |
| 1 | -1 | 80 | 77 |
| 1 | 1 | 54 | 49 |
| 1 | -2 | 79 | 77 |
| 1 | 2 | 75 | 74 |
| 1 | 3 | 59 | 59 |
| 1 | -4 | 76 | 77 |
| 1 | 4 | 28 | 27 |
| 1 | -5 | 61 | 65 |
| 1 | 5 | 46 | 47 |
| 1 | -6 | 58 | 60 |
| 1 | 7 | 35 | 34 |
| 1 | 9 | 22 | 16 |
| 2 | 0 | 72 | 66 |
| 2 | -1 | 116 | 114 |
| 2 | 1 | 128 | 128 |
| 2 | -4 | 47 | 45 |
| 2 | 4 | 24 | 25 |
| 2 | -5 | 28 | 29 |
| 2 | 5 | 32 | 32 |
| 2 | -7 | 33 | 38 |
| 2 | 7 | 20 | 22 |
| 2 | 9 | 22 | 20 |
| 3 | -2 | 77 | 71 |
| 3 | 2 | 30 | 28 |
| 3 | -3 | 91 | 88 |
| 3 | 3 | 26 | 25 |
| 3 | -4 | 42 | 42 |
| 3 | 4 | 21 | 21 |
| 3 | -6 | 26 | 24 |
| 3 | 6 | 22 | 19 |
| 3 | -7 | 31 | 30 |
| 3 | -11 | 20 | 14 |
| 4 | 0 | 50 | 47 |
| 4 | -1 | 90 | 89 |
| 4 | 1 | 109 | 110 |
| 4 | -3 | 50 | 52 |
| 4 | 3 | 33 | 34 |
| 4 | -5 | 46 | 47 |
| 4 | -9 | 25 | 24 |
| 4 | 9 | 24 | 23 |
| 5 | -1 | 27 | 31 |
| 5 | -2 | 24 | 22 |
| 5 | -3 | 71 | 76 |
| 5 | -5 | 34 | 34 |
| 6 | -2 | 25 | 25 |
| 6 | -3 | 49 | 51 |
| 6 | -9 | 25 | 21 |
| 7 | -7 | 27 | 26 |
| 8 | 1 | 30 | 31 |
| ** K = 8 ** | | | |
| 0 | 0 | 123 | 128 |
| 0 | 2 | 122 | 125 |
| 0 | 3 | 24 | 27 |
| 0 | 4 | 51 | 50 |
| 1 | 1 | 74 | 71 |
| 1 | -2 | 132 | 129 |
| 1 | 2 | 43 | 45 |
| 1 | -3 | 58 | 59 |
| 1 | 3 | 34 | 34 |
| 1 | -4 | 33 | 31 |
| 1 | 4 | 29 | 32 |
| 1 | -5 | 52 | 54 |
| 1 | 5 | 45 | 47 |
| 1 | -7 | 52 | 56 |
| 1 | 7 | 58 | 59 |
| 1 | 8 | 20 | 17 |
| 2 | 0 | 48 | 41 |
| 2 | -1 | 110 | 110 |
| 2 | 1 | 76 | 74 |
| 2 | -2 | 31 | 29 |
| 2 | -3 | 29 | 26 |
| 2 | 3 | 39 | 38 |
| 2 | -4 | 29 | 28 |
| 2 | 4 | 70 | 68 |
| 2 | 5 | 26 | 26 |
| 2 | -6 | 39 | 41 |
| 2 | 6 | 21 | 22 |
| 2 | -10 | 26 | 21 |
| 3 | 1 | 24 | 22 |
| 3 | -2 | 56 | 52 |
| 3 | 3 | 23 | 24 |
| 3 | 4 | 34 | 34 |
| 3 | -7 | 65 | 66 |
| 3 | 7 | 25 | 26 |
| 3 | -10 | 21 | 20 |
| 4 | 0 | 174 | 173 |
| 4 | -1 | 31 | 29 |
| 4 | 3 | 44 | 45 |
| 4 | 5 | 29 | 28 |
| 4 | -6 | 30 | 29 |
| 4 | -9 | 20 | 18 |
| 5 | -1 | 28 | 28 |
| 5 | 1 | 37 | 38 |
| 5 | -3 | 28 | 27 |
| 5 | 3 | 29 | 28 |
| 5 | 4 | 25 | 23 |
| 5 | -6 | 34 | 37 |
| 5 | 6 | 29 | 28 |
| 5 | -7 | 28 | 28 |
| 5 | -8 | 23 | 20 |
| 6 | 0 | 28 | 26 |
| 6 | 1 | 37 | 38 |
| 6 | -4 | 26 | 26 |
| 6 | 4 | 24 | 23 |
| 7 | -4 | 32 | 32 |
| 7 | -6 | 35 | 40 |
| 7 | -7 | 22 | 22 |
| 9 | -4 | 22 | 23 |
| ** K = 9 ** | | | |
| 0 | 2 | 30 | 28 |
| 0 | 3 | 29 | 27 |
| 0 | 4 | 29 | 31 |
| 0 | 6 | 25 | 29 |
| 0 | 7 | 21 | 21 |
| 1 | -1 | 78 | 76 |
| 1 | 1 | 79 | 78 |
| 1 | -2 | 26 | 27 |
| 1 | 2 | 109 | 110 |
| 1 | -3 | 91 | 91 |
| 1 | 3 | 91 | 90 |
| 1 | -4 | 44 | 45 |
| 1 | 4 | 22 | 22 |
| 1 | 5 | 46 | 50 |
| 1 | 6 | 23 | 24 |
| 1 | 7 | 36 | 37 |
| 1 | -8 | 20 | 21 |
| 1 | -10 | 21 | 20 |
| 2 | 0 | 55 | 53 |
| 2 | -1 | 42 | 41 |
| 2 | -2 | 89 | 85 |
| 2 | 2 | 28 | 26 |
| 2 | -3 | 53 | 48 |
| 2 | -4 | 45 | 47 |
| 2 | 4 | 50 | 51 |
| 2 | -8 | 23 | 22 |
| 2 | -9 | 22 | 18 |
| 2 | -10 | 26 | 27 |
| 3 | -1 | 31 | 30 |
| 3 | -2 | 43 | 40 |
| 3 | -3 | 26 | 25 |
| 3 | -4 | 74 | 73 |
| 3 | -5 | 53 | 55 |
| 3 | 6 | 25 | 26 |
| 3 | -7 | 35 | 35 |
| 4 | 0 | 170 | 168 |
| 4 | 1 | 27 | 27 |
| 4 | -2 | 37 | 36 |
| 4 | -3 | 69 | 69 |
| 4 | 3 | 36 | 36 |
| 4 | -4 | 30 | 31 |
| 4 | 4 | 35 | 34 |
| 4 | -6 | 27 | 26 |
| 4 | -9 | 23 | 17 |
| 5 | 0 | 21 | 21 |
| 5 | -1 | 20 | 20 |
| 5 | 1 | 21 | 22 |
| 5 | 2 | 22 | 21 |
| 5 | 4 | 25 | 24 |
| 5 | -7 | 22 | 18 |
| 5 | -8 | 22 | 21 |
| 6 | 0 | 94 | 95 |
| 6 | -4 | 21 | 22 |
| 7 | -4 | 32 | 35 |
| 7 | -5 | 24 | 24 |
| 8 | -3 | 20 | 15 |
| 8 | -4 | 22 | 24 |
| 8 | -6 | 20 | 23 |
| 9 | -2 | 26 | 26 |
| ** K = 10 ** | | | |
| 0 | 0 | 80 | 77 |
| 0 | 2 | 78 | 80 |
| 0 | 3 | 21 | 19 |
| 0 | 5 | 22 | 25 |
| 0 | 10 | 23 | 22 |
| 1 | -1 | 26 | 21 |
| 1 | -2 | 177 | 176 |
| 1 | 2 | 104 | 104 |
| 1 | -3 | 43 | 43 |
| 1 | -4 | 21 | 19 |
| 1 | 4 | 83 | 86 |
| 1 | -5 | 70 | 74 |
| 1 | 6 | 48 | 49 |
| 1 | -7 | 54 | 60 |
| 1 | 7 | 44 | 45 |
| 2 | 0 | 111 | 103 |
| 2 | 1 | 45 | 46 |
| 2 | -2 | 24 | 21 |
| 2 | 2 | 36 | 34 |
| 2 | -3 | 31 | 28 |
| 2 | 5 | 24 | 24 |
| 2 | -6 | 20 | 22 |
| 3 | 2 | 50 | 50 |
| 3 | -3 | 49 | 47 |
| 3 | 3 | 54 | 56 |
| 3 | -4 | 32 | 33 |
| 3 | -5 | 41 | 40 |
| 3 | -6 | 62 | 64 |
| 3 | 6 | 26 | 26 |
| 3 | -7 | 37 | 36 |
| 4 | -1 | 34 | 34 |
| 4 | 1 | 24 | 23 |
| 4 | -2 | 54 | 53 |
| 4 | 2 | 29 | 28 |
| 4 | -3 | 24 | 24 |
| 4 | 3 | 29 | 28 |
| 4 | -4 | 61 | 61 |
| 4 | 5 | 26 | 28 |
| 5 | -2 | 21 | 20 |
| 5 | 2 | 28 | 29 |
| 5 | -3 | 22 | 21 |
| 5 | 3 | 27 | 29 |
| 5 | 4 | 27 | 27 |
| 5 | -5 | 22 | 22 |
| 5 | -6 | 42 | 43 |
| 6 | -1 | 28 | 28 |
| 6 | 1 | 21 | 23 |
| 6 | -4 | 33 | 33 |
| 6 | 4 | 27 | 26 |
| 7 | -1 | 21 | 18 |
| 7 | -2 | 29 | 28 |
| 8 | -2 | 33 | 32 |
| ** K = 11 ** | | | |
| 0 | 1 | 223 | 223 |
| 0 | 2 | 41 | 42 |
| 0 | 3 | 44 | 45 |
| 0 | 4 | 45 | 47 |
| 0 | 6 | 37 | 39 |
| 1 | -1 | 23 | 24 |
| 1 | -2 | 33 | 32 |
| 1 | 2 | 54 | 55 |
| 1 | -3 | 28 | 29 |
| 1 | 3 | 55 | 57 |
| 1 | -4 | 30 | 31 |
| 1 | -5 | 30 | 30 |
| 1 | -6 | 25 | 27 |
| 1 | 6 | 28 | 29 |
| 2 | 0 | 113 | 112 |
| 2 | -1 | 84 | 84 |
| 2 | 1 | 90 | 88 |
| 2 | 2 | 27 | 27 |
| 2 | -5 | 53 | 56 |
| 2 | -6 | 21 | 20 |
| 2 | 8 | 21 | 15 |
| 2 | 9 | 32 | 35 |
| 3 | -2 | 68 | 67 |
| 3 | 2 | 23 | 21 |
| 3 | -4 | 30 | 30 |
| 3 | 4 | 20 | 17 |
| 3 | -5 | 34 | 34 |
| 3 | 5 | 27 | 26 |
| 3 | -6 | 21 | 18 |
| 3 | -7 | 24 | 23 |
| 3 | -8 | 21 | 22 |
| 3 | 8 | 23 | 23 |
| 4 | 0 | 21 | 19 |
| 4 | 2 | 23 | 23 |
| 4 | -3 | 62 | 60 |
| 4 | 4 | 53 | 56 |
| 4 | -5 | 35 | 34 |
| 4 | -6 | 31 | 30 |
| 4 | -9 | 20 | 24 |
| 4 | 9 | 22 | 17 |
| 5 | -2 | 26 | 25 |
| 5 | -3 | 20 | 20 |
| 5 | 3 | 28 | 26 |
| 5 | -4 | 34 | 33 |
| 5 | 4 | 28 | 28 |
| 5 | 5 | 33 | 34 |
| 5 | -8 | 30 | 32 |
| 6 | 0 | 38 | 38 |
| 6 | -2 | 26 | 26 |
| 6 | -5 | 25 | 26 |
| 7 | -4 | 24 | 28 |
| 8 | -2 | 20 | 20 |
| ** K = 12 ** | | | |
| 0 | 0 | 29 | 26 |
| 0 | 1 | 42 | 33 |
| 0 | 2 | 26 | 27 |
| 0 | 4 | 28 | 28 |
| 0 | 5 | 37 | 43 |
| 1 | 2 | 53 | 56 |
| 1 | -3 | 97 | 94 |
| 1 | 3 | 36 | 36 |
| 1 | -4 | 55 | 58 |
| 1 | 4 | 49 | 53 |
| 1 | 5 | 34 | 34 |
| 1 | 6 | 40 | 41 |
| 1 | 7 | 25 | 23 |
| 1 | 8 | 27 | 25 |
| 2 | 0 | 29 | 25 |
| 2 | -1 | 53 | 50 |
| 2 | 1 | 23 | 21 |
| 2 | -2 | 41 | 42 |
| 2 | -3 | 39 | 39 |
| 2 | 3 | 42 | 45 |
| 2 | -4 | 46 | 47 |
| 2 | -5 | 33 | 37 |
| 2 | 5 | 27 | 27 |
| 2 | -6 | 31 | 30 |
| 2 | 7 | 27 | 25 |
| 3 | 2 | 53 | 52 |
| 3 | -3 | 78 | 76 |
| 3 | -4 | 39 | 38 |
| 3 | 4 | 21 | 21 |
| 3 | -5 | 20 | 19 |
| 3 | -6 | 41 | 43 |
| 3 | 6 | 25 | 27 |
| 3 | -7 | 25 | 26 |
| 3 | 7 | 29 | 29 |
| 3 | -8 | 37 | 39 |
| 4 | 0 | 42 | 43 |
| 4 | -1 | 22 | 22 |
| 4 | 1 | 35 | 36 |
| 4 | -2 | 42 | 43 |
| 4 | -3 | 23 | 24 |
| 4 | 3 | 28 | 28 |
| 4 | -7 | 28 | 28 |
| 4 | -9 | 23 | 25 |
| 5 | -1 | 20 | 21 |
| 5 | -4 | 71 | 72 |
| 5 | -5 | 24 | 24 |
| 5 | -6 | 32 | 33 |
| 5 | -7 | 32 | 30 |
| 6 | 0 | 48 | 52 |
| 6 | -1 | 33 | 32 |
| 6 | 1 | 54 | 56 |
| 6 | -2 | 21 | 22 |
| 6 | -4 | 38 | 37 |
| 6 | -7 | 20 | 15 |
| 7 | 2 | 27 | 31 |
| 7 | -3 | 34 | 34 |
| 8 | 0 | 35 | 36 |
| ** K = 13 ** | | | |
| 0 | 1 | 82 | 83 |
| 0 | 3 | 54 | 55 |
| 0 | 4 | 48 | 54 |
| 0 | 5 | 30 | 33 |
| 1 | -1 | 33 | 35 |
| 1 | -2 | 50 | 49 |
| 1 | 2 | 22 | 22 |
| 1 | -3 | 56 | 55 |
| 1 | 3 | 55 | 55 |
| 1 | -4 | 62 | 65 |
| 1 | -5 | 27 | 26 |
| 1 | 5 | 42 | 40 |
| 1 | 7 | 25 | 24 |
| 2 | -2 | 77 | 75 |
| 2 | 2 | 71 | 71 |
| 2 | -3 | 26 | 24 |
| 2 | 3 | 86 | 88 |
| 2 | 4 | 60 | 62 |
| 2 | -5 | 20 | 21 |
| 2 | 10 | 21 | 8 |
| 3 | 1 | 28 | 27 |
| 3 | -2 | 38 | 38 |
| 3 | -3 | 45 | 44 |
| 3 | 3 | 30 | 29 |
| 3 | 4 | 56 | 56 |
| 3 | -5 | 32 | 29 |
| 3 | 5 | 32 | 31 |
| 3 | -7 | 26 | 26 |
| 3 | 7 | 46 | 46 |
| 4 | 0 | 59 | 58 |
| 4 | -1 | 26 | 28 |
| 4 | 1 | 23 | 23 |
| 4 | -4 | 22 | 24 |
| 4 | 4 | 26 | 25 |
| 4 | -8 | 20 | 21 |
| 4 | -9 | 23 | 20 |
| 5 | -2 | 40 | 37 |
| 5 | 2 | 43 | 45 |
| 5 | -4 | 26 | 26 |
| 5 | -6 | 29 | 30 |
| 5 | -7 | 52 | 54 |
| 5 | 7 | 23 | 25 |
| 6 | 0 | 54 | 59 |
| 6 | -2 | 37 | 35 |
| 6 | 2 | 23 | 22 |
| 6 | 3 | 21 | 18 |
| 6 | -5 | 20 | 18 |
| 7 | -1 | 22 | 23 |
| 7 | 1 | 21 | 24 |
| 7 | -2 | 42 | 42 |
| 7 | 2 | 25 | 25 |
| 7 | -7 | 31 | 31 |
| 8 | 0 | 30 | 30 |
| 8 | -1 | 21 | 21 |
| ** K = 14 ** | | | |
| 0 | 0 | 217 | 213 |
| 0 | 9 | 38 | 29 |
| 1 | -1 | 83 | 79 |
| 1 | 1 | 47 | 41 |
| 1 | -2 | 31 | 29 |
| 1 | -3 | 23 | 23 |
| 1 | 3 | 21 | 23 |
| 1 | -4 | 32 | 34 |
| 1 | 4 | 22 | 23 |
| 1 | -5 | 38 | 38 |
| 1 | 6 | 28 | 28 |
| 1 | 7 | 20 | 19 |
| 2 | 0 | 118 | 115 |
| 2 | -1 | 38 | 36 |
| 2 | 1 | 24 | 26 |
| 2 | 2 | 52 | 52 |
| 2 | -3 | 83 | 84 |
| 2 | -4 | 49 | 52 |
| 2 | 4 | 30 | 31 |
| 2 | -6 | 21 | 23 |
| 2 | 6 | 22 | 22 |
| 2 | -9 | 25 | 28 |
| 2 | 10 | 21 | 13 |
| 3 | -1 | 67 | 65 |
| 3 | -2 | 44 | 44 |
| 3 | 3 | 28 | 28 |
| 3 | 4 | 35 | 37 |
| 3 | -5 | 47 | 47 |
| 3 | 5 | 45 | 46 |
| 3 | 7 | 22 | 19 |
| 4 | 0 | 24 | 23 |
| 4 | 1 | 32 | 31 |
| 4 | 3 | 21 | 20 |
| 4 | -4 | 40 | 39 |
| 4 | 4 | 34 | 35 |
| 5 | -1 | 26 | 25 |
| 5 | -2 | 46 | 47 |
| 5 | -3 | 30 | 29 |
| 5 | -5 | 53 | 55 |
| 6 | 0 | 33 | 35 |
| 6 | -3 | 46 | 49 |
| 6 | -4 | 35 | 36 |
| 6 | -9 | 22 | 21 |
| 7 | -2 | 25 | 24 |
| 7 | -6 | 21 | 16 |
| ** K = 15 ** | | | |
| 0 | 1 | 99 | 99 |
| 0 | 3 | 39 | 42 |
| 0 | 4 | 20 | 23 |
| 0 | 5 | 26 | 24 |
| 0 | 8 | 21 | 20 |
| 1 | 1 | 22 | 25 |
| 1 | -2 | 47 | 47 |
| 1 | 2 | 42 | 45 |
| 1 | -3 | 43 | 41 |
| 1 | 3 | 58 | 61 |
| 1 | -4 | 50 | 52 |
| 1 | 4 | 45 | 46 |
| 1 | -5 | 34 | 36 |
| 1 | -6 | 65 | 67 |
| 1 | 6 | 33 | 33 |
| 1 | 7 | 22 | 23 |
| 1 | -8 | 30 | 32 |
| 1 | 8 | 20 | 18 |
| 2 | 0 | 27 | 30 |
| 2 | -1 | 30 | 30 |
| 2 | -3 | 64 | 67 |
| 2 | 7 | 22 | 19 |
| 3 | -1 | 33 | 34 |
| 3 | 1 | 40 | 42 |
| 3 | -2 | 53 | 53 |
| 3 | 2 | 63 | 64 |
| 3 | 3 | 27 | 26 |
| 3 | -4 | 60 | 53 |
| 3 | 4 | 60 | 60 |
| 3 | 5 | 23 | 25 |
| 3 | -6 | 42 | 44 |
| 3 | -7 | 27 | 29 |
| 3 | 7 | 22 | 20 |
| 4 | -1 | 22 | 23 |
| 4 | 1 | 40 | 41 |
| 4 | -2 | 35 | 33 |
| 4 | -3 | 21 | 21 |
| 4 | 4 | 20 | 22 |
| 4 | -5 | 30 | 29 |
| 5 | -1 | 28 | 26 |
| 5 | 2 | 32 | 34 |
| 5 | -3 | 26 | 26 |
| 5 | 4 | 23 | 22 |
| 5 | -5 | 25 | 25 |
| 6 | 0 | 21 | 23 |
| 6 | -2 | 31 | 30 |
| 6 | 2 | 34 | 34 |
| 6 | -5 | 23 | 21 |
| 6 | -7 | 21 | 24 |
| ** K = 16 ** | | | |
| 0 | 0 | 20 | 22 |
| 0 | 2 | 28 | 29 |
| 0 | 3 | 64 | 64 |
| 0 | 4 | 23 | 23 |
| 0 | 5 | 42 | 43 |
| 0 | 7 | 26 | 23 |
| 0 | 9 | 34 | 36 |
| 1 | -1 | 30 | 28 |
| 1 | 1 | 26 | 26 |
| 1 | -3 | 25 | 24 |
| 1 | 3 | 25 | 25 |
| 1 | 4 | 34 | 47 |
| 1 | 5 | 34 | 33 |
| 1 | 6 | 28 | 28 |
| 1 | -7 | 30 | 31 |
| 2 | 0 | 44 | 43 |
| 2 | -1 | 128 | 126 |
| 2 | 1 | 124 | 127 |
| 2 | 2 | 21 | 22 |
| 2 | -3 | 34 | 33 |
| 2 | 4 | 28 | 25 |
| 2 | -5 | 46 | 48 |
| 2 | 5 | 23 | 26 |
| 2 | -9 | 26 | 29 |
| 3 | -1 | 44 | 44 |
| 3 | -3 | 29 | 29 |
| 3 | 3 | 39 | 39 |
| 3 | -4 | 53 | 53 |
| 4 | -1 | 50 | 50 |
| 4 | 1 | 42 | 43 |
| 4 | 3 | 38 | 39 |
| 4 | -5 | 29 | 27 |
| 4 | -9 | 26 | 23 |
| 5 | 1 | 25 | 24 |
| 5 | 2 | 26 | 27 |
| 5 | -4 | 31 | 28 |
| 6 | -2 | 30 | 30 |
| 7 | -7 | 22 | 22 |
| 8 | 0 | 26 | 26 |
| ** K = 17 ** | | | |
| 0 | 3 | 86 | 89 |
| 1 | -1 | 42 | 41 |
| 1 | 1 | 25 | 23 |
| 1 | -4 | 47 | 47 |
| 1 | 4 | 27 | 25 |
| 1 | 5 | 21 | 19 |
| 1 | -6 | 55 | 67 |
| 1 | 6 | 25 | 24 |
| 1 | 7 | 21 | 17 |
| 1 | -8 | 33 | 35 |
| 1 | 9 | 21 | 22 |
| 2 | 1 | [illegible] | [illegible] |
| 2 | -3 | 46 | 48 |
| 2 | -9 | 21 | 25 |
| 3 | -1 | 64 | 63 |
| 3 | 1 | 48 | 50 |
| 3 | -2 | 24 | 24 |
| 3 | 2 | 45 | 44 |
| 3 | -3 | 68 | 66 |
| 3 | 3 | 28 | 26 |
| 3 | -4 | 40 | 39 |
| 3 | -5 | 37 | 37 |
| 3 | -6 | 33 | 33 |
| 3 | -7 | 27 | 27 |
| 3 | 7 | 25 | 25 |
| 4 | 0 | 31 | 30 |
| 4 | -1 | 33 | 33 |
| 4 | -4 | 26 | 26 |
| 4 | 4 | 25 | 24 |
| 4 | -9 | 23 | 20 |
| 5 | -1 | 41 | 42 |
| 5 | -2 | 33 | 33 |
| 5 | 2 | 39 | 41 |
| 5 | -3 | 44 | 47 |
| 5 | -5 | 26 | 25 |
| 5 | 5 | 26 | 26 |
| 5 | -7 | 22 | 18 |
| 5 | 7 | 24 | 24 |
| 6 | 4 | 21 | 23 |
| 6 | -5 | 22 | 20 |
| 7 | -1 | 20 | 18 |
| 7 | -5 | 33 | 33 |
| 8 | 0 | 22 | 25 |
| ** K = 18 ** | | | |
| 0 | 0 | 91 | 93 |
| 0 | 2 | 27 | 25 |
| 0 | 3 | 29 | 25 |
| 0 | 4 | 38 | 38 |
| 1 | -1 | 22 | 22 |
| 1 | 1 | 36 | 35 |
| 1 | -2 | 21 | 20 |
| 1 | 2 | 21 | 22 |
| 1 | 4 | 72 | 77 |
| 1 | 6 | 38 | 40 |
| 1 | -7 | 33 | 35 |
| 1 | 7 | 25 | 25 |
| 2 | 0 | 94 | 94 |
| 2 | 1 | 24 | 22 |
| 2 | 2 | 31 | 30 |
| 2 | -3 | 55 | 57 |
| 2 | 3 | 53 | 53 |
| 2 | -4 | 46 | 47 |
| 2 | 4 | 22 | 21 |
| 3 | -1 | 26 | 28 |
| 3 | 1 | 24 | 23 |
| 3 | -2 | 69 | 69 |
| 3 | 2 | 40 | 40 |
| 3 | 3 | 33 | 32 |
| 3 | -4 | 40 | 42 |
| 4 | 0 | 35 | 35 |
| 4 | -2 | 43 | 42 |
| 4 | 2 | 55 | 58 |
| 4 | -3 | 51 | 54 |
| 4 | -4 | 33 | 32 |
| 5 | -2 | 59 | 59 |
| 5 | -3 | 20 | 19 |
| 5 | 3 | 35 | 36 |
| 5 | 4 | 22 | 22 |
| 6 | -2 | 21 | 21 |
| 6 | -8 | 22 | 22 |
| 7 | -1 | 23 | 20 |
| 8 | 0 | 24 | 25 |
| 8 | -2 | 22 | 23 |
| ** K = 19 ** | | | |
| 0 | 1 | 75 | 78 |
| 0 | 3 | 29 | 28 |
| 0 | 4 | 54 | 54 |
| 0 | 5 | 26 | 27 |
| 0 | 6 | 22 | 27 |
| 1 | -2 | 27 | 26 |
| 1 | -3 | 29 | 29 |
| 1 | 4 | 42 | 44 |
| 1 | -6 | 26 | 25 |
| 1 | 6 | 23 | 24 |
| 2 | 0 | 63 | 61 |
| 2 | -2 | 26 | 25 |
| 2 | -3 | 41 | 43 |
| 2 | 3 | 37 | 34 |
| 2 | 4 | 38 | 38 |
| 2 | -5 | 23 | 25 |
| 2 | 5 | 21 | 22 |
| 2 | 7 | 20 | 18 |
| 2 | -8 | 21 | 22 |
| 2 | -9 | 20 | 17 |
| 3 | 2 | 39 | 39 |
| 3 | -3 | 22 | 22 |
| 3 | -4 | 36 | 35 |
| 3 | -5 | 24 | 24 |
| 3 | 5 | 24 | 25 |
| 3 | -6 | 22 | 21 |
| 3 | 6 | 23 | 22 |
| 3 | 7 | 21 | 20 |
| 4 | 0 | 32 | 30 |
| 4 | -1 | 48 | 45 |
| 4 | 1 | 47 | 49 |
| 4 | -2 | 27 | 26 |
| 4 | -3 | 28 | 28 |
| 4 | -6 | 24 | 23 |
| 4 | -7 | 23 | 21 |
| 5 | 2 | 37 | 37 |
| 5 | -7 | 26 | 25 |
| 7 | -3 | 24 | 24 |
| 7 | -5 | 22 | 19 |
| 7 | -7 | 29 | 24 |
| ** K = 20 ** | | | |
| 0 | 0 | 62 | 63 |
| 0 | 2 | 26 | 29 |
| 0 | 4 | 39 | 37 |
| 0 | 5 | 33 | 35 |
| 0 | 7 | 28 | 29 |
| 1 | 1 | 26 | 25 |
| 1 | -2 | 26 | 27 |
| 1 | 2 | 65 | 67 |
| 1 | 3 | 35 | 37 |
| 1 | -4 | 75 | 75 |
| 1 | 4 | 40 | 40 |
| 1 | 6 | 27 | 24 |
| 1 | 8 | 32 | 34 |
| 2 | 0 | 21 | 20 |
| 2 | -1 | 42 | 38 |
| 2 | 1 | 43 | 43 |
| 2 | -2 | 35 | 36 |
| 2 | -3 | 35 | 36 |
| 2 | -4 | 40 | 41 |
| 2 | 5 | 30 | 30 |
| 2 | -6 | 26 | 25 |
| 2 | -9 | 29 | 28 |
| 3 | -1 | 33 | 33 |
| 3 | 1 | 27 | 29 |
| 3 | 2 | 59 | 59 |
| 3 | 3 | 31 | 32 |
| 3 | -6 | 34 | 35 |
| 3 | -8 | 31 | 33 |
| 4 | 0 | 32 | 32 |
| 4 | 1 | 27 | 26 |
| 4 | -2 | 22 | 21 |
| 4 | 2 | 43 | 43 |
| 5 | -4 | 34 | 34 |
| 6 | -6 | 27 | 23 |
| ** K = 21 ** | | | |
| 0 | 1 | 71 | 77 |
| 0 | 3 | 42 | 46 |
| 0 | 4 | 21 | 17 |
| 0 | 6 | 30 | 30 |
| 1 | 1 | 23 | 20 |
| 1 | -2 | 38 | 41 |
| 1 | 2 | 52 | 53 |
| 1 | -3 | 28 | 25 |
| 1 | -4 | 80 | 84 |
| 1 | 4 | 38 | 39 |
| 1 | -5 | 49 | 47 |
| 2 | 0 | 52 | 53 |
| 2 | -1 | 30 | 28 |
| 2 | 1 | 38 | 39 |
| 2 | -2 | 37 | 36 |
| 2 | 2 | 28 | 29 |
| 2 | 3 | 23 | 21 |
| 2 | 9 | 24 | 18 |
| 3 | -2 | 68 | 67 |
| 3 | 2 | 42 | 43 |
| 3 | -3 | 35 | 36 |
| 3 | 4 | 33 | 32 |
| 3 | 6 | 23 | 24 |
| 4 | 0 | 28 | 29 |
| 4 | -1 | 20 | 18 |
| 4 | -2 | 25 | 22 |
| 4 | 2 | 22 | 22 |
| 4 | -5 | 25 | 26 |
| 5 | 1 | 27 | 26 |
| 5 | -3 | 34 | 33 |
| 6 | -2 | 26 | 27 |
| 6 | -3 | 21 | 21 |
| 7 | -3 | 21 | 21 |
| ** K = 22 ** | | | |
| 0 | 0 | 27 | 25 |
| 0 | 2 | 23 | 26 |
| 1 | 1 | 32 | 31 |
| 1 | -2 | 56 | 57 |
| 1 | 2 | 32 | 34 |
| 1 | -3 | 30 | 29 |
| 1 | -4 | 50 | 52 |
| 1 | -5 | 20 | 21 |
| 1 | 6 | 27 | 27 |
| 1 | -7 | 31 | 33 |
| 1 | 7 | 25 | 27 |
| 2 | 0 | 30 | 29 |
| 2 | -1 | 43 | 45 |
| 2 | -3 | 45 | 43 |
| 2 | 3 | 36 | 39 |
| 2 | -4 | 21 | 21 |
| 2 | 4 | 38 | 41 |
| 2 | -5 | 31 | 34 |
| 3 | -2 | 23 | 24 |
| 3 | -4 | 27 | 29 |
| 3 | 5 | 23 | 21 |
| 3 | -5 | 28 | 29 |
| 3 | -7 | 25 | 24 |
| 4 | 0 | 53 | 57 |
| 4 | -2 | 40 | 40 |
| 4 | -3 | 27 | 26 |
| 4 | 3 | 28 | 29 |
| 4 | -4 | 25 | 28 |
| 5 | -1 | 36 | 38 |
| 5 | 1 | 25 | 23 |
| 5 | -3 | 30 | 28 |
| 5 | 3 | 26 | 25 |
| 5 | -5 | 24 | 25 |
| 5 | -6 | 21 | 16 |
| 6 | -6 | 24 | 20 |
| 7 | 3 | 21 | 17 |
| ** K = 23 ** | | | |
| 0 | 1 | 22 | 30 |
| 0 | 3 | 31 | 33 |
| 0 | 4 | 24 | 24 |
| 1 | -1 | 21 | 27 |
| 1 | -2 | 35 | 40 |
| 1 | 2 | 35 | 37 |
| 1 | -4 | 48 | 47 |
| 1 | 5 | 21 | 21 |
| 1 | -6 | 22 | 24 |
| 2 | 0 | 24 | 23 |
| 2 | 2 | 34 | 34 |
| 2 | -3 | 37 | 39 |
| 2 | 3 | 22 | 23 |
| 2 | -4 | 40 | 36 |
| 2 | 4 | 22 | 22 |
| 2 | 8 | 24 | 21 |
| 3 | 1 | 20 | 19 |
| 3 | -4 | 54 | 52 |
| 3 | -9 | 21 | 25 |
| 4 | 0 | 27 | 25 |
| 4 | -2 | 22 | 30 |
| 4 | -4 | 21 | 21 |
| 4 | -6 | 27 | 22 |
| 6 | 0 | 52 | 53 |
| 6 | 2 | 26 | 27 |
| 7 | -4 | 22 | 19 |
| ** K = 24 ** | | | |
| 0 | 0 | 20 | 20 |
| 0 | 5 | 21 | 21 |
| 0 | 7 | 21 | 22 |
| 1 | -2 | 80 | 83 |
| 1 | 2 | 57 | 59 |
| 1 | 4 | 37 | 39 |
| 2 | -1 | 52 | 56 |
| 2 | 1 | 62 | 62 |
| 2 | -2 | 25 | 26 |
| 2 | 2 | 33 | 32 |
| 2 | 4 | 20 | 18 |
| 2 | 5 | 28 | 27 |
| 3 | -1 | 25 | 20 |
| 3 | -2 | 31 | 30 |
| 3 | -3 | 27 | 27 |
| 3 | -6 | 34 | 34 |
| 3 | -7 | 22 | 19 |
| 3 | 7 | 25 | 19 |
| 4 | 3 | 26 | 24 |
| 5 | -5 | 22 | 20 |
| 5 | -6 | 22 | 22 |
| 5 | -7 | 26 | 25 |
| 7 | 3 | 20 | 17 |
| ** K = 25 ** | | | |
| 0 | 1 | 43 | 43 |
| 0 | 9 | 20 | 19 |
| 1 | -1 | 53 | 56 |
| 1 | 1 | 31 | 32 |
| 1 | -3 | 21 | 27 |
| 1 | -6 | 29 | 27 |
| 1 | -8 | 20 | 24 |
| 2 | -1 | 22 | 21 |
| 2 | 1 | 39 | 36 |
| 2 | -2 | 41 | 42 |
| 2 | 2 | 25 | 26 |
| 2 | -3 | 25 | 25 |
| 2 | -5 | 27 | 22 |
| 2 | -9 | 21 | 14 |
| 3 | 1 | 32 | 30 |
| 3 | -2 | 23 | 23 |
| 3 | 3 | 27 | 27 |
| 3 | 4 | 22 | 21 |
| 4 | -3 | 43 | 43 |
| 4 | 4 | 21 | 17 |
| 6 | 1 | 22 | 19 |
| 6 | -2 | 22 | 21 |
| 6 | -3 | 23 | [illegible] |
| ** K = 26 ** | | | |
| 0 | 4 | 26 | 29 |
| 1 | -1 | 31 | 28 |
| 1 | 1 | 39 | 39 |
| 1 | -2 | 32 | 40 |
| 1 | 2 | 49 | 48 |
| 1 | 3 | 42 | 40 |
| 1 | 4 | 43 | 46 |
| 1 | -5 | 25 | 28 |
| 1 | 6 | 27 | 26 |
| 1 | -7 | 21 | 18 |
| 2 | -3 | 25 | 26 |
| 2 | 4 | 22 | 16 |
| 2 | -9 | 21 | 16 |
| 3 | -1 | 32 | 32 |
| 3 | 1 | 27 | 27 |
| 3 | 3 | 26 | 25 |
| 3 | -4 | 33 | 34 |
| 3 | 5 | 24 | 24 |
| 3 | -7 | 26 | 26 |
| 4 | 1 | 26 | 27 |
| 4 | -3 | 20 | 18 |
| 6 | -3 | 26 | 23 |
| 6 | 3 | 22 | 15 |
| ** K = 27 ** | | | |
| 0 | 1 | 53 | 55 |
| 0 | 2 | 20 | 16 |
| 1 | 1 | 22 | 19 |
| 1 | 2 | 20 | 16 |
| 1 | -3 | 21 | 26 |
| 1 | -5 | 23 | 23 |
| 2 | -2 | 34 | 36 |
| 2 | 3 | 47 | 46 |
| 2 | -4 | 26 | 25 |
| 2 | 4 | 22 | 20 |
| 2 | -7 | 24 | 20 |
| 2 | -8 | 23 | 17 |
| 3 | -2 | 23 | 21 |
| 3 | -3 | 27 | 27 |
| 3 | -4 | 30 | 30 |
| 3 | 5 | 21 | 17 |
| 4 | 0 | 38 | 41 |
| 4 | -1 | 34 | 34 |
| 4 | 1 | 28 | 26 |
| 4 | -6 | 23 | 24 |
| 5 | -7 | 21 | 16 |
| 6 | 0 | 23 | 22 |
| ** K = 28 ** | | | |
| 0 | 2 | 32 | 33 |
| 1 | -3 | 23 | 23 |
| 1 | -7 | 22 | 20 |
| 1 | 8 | 22 | 14 |
| 2 | -3 | 36 | 34 |
| 3 | -2 | 35 | 31 |
| 3 | -4 | 27 | 28 |
| 3 | -5 | 20 | 23 |
| 3 | -6 | 20 | 13 |
| 4 | 0 | 33 | 34 |
| 4 | 2 | 21 | 22 |
| 4 | -4 | 23 | 20 |
| 5 | -2 | 23 | 21 |
| 7 | -1 | 20 | 20 |
| ** K = 29 ** | | | |
| 1 | 2 | 29 | 31 |
| 1 | -4 | 22 | 22 |
| 1 | 5 | 31 | 28 |
| 1 | -6 | 31 | 34 |
| 3 | -1 | 26 | 25 |
| 3 | 1 | 22 | 21 |
| 3 | -2 | 32 | 32 |
| 3 | 2 | 24 | 24 |
| 3 | 4 | 30 | 26 |
| 3 | -5 | 32 | 31 |
| 3 | -8 | 21 | 13 |
| 4 | 3 | 25 | 24 |
| 4 | 4 | 26 | 25 |
| 4 | -5 | 25 | 23 |
| 6 | -2 | 26 | 23 |
| 6 | -5 | 23 | 21 |
| ** K = 30 ** | | | |
| 0 | 2 | 39 | 45 |
| 1 | 3 | 34 | 36 |
| 2 | -1 | 37 | 35 |
| 2 | 1 | 42 | 45 |
| 2 | -3 | 21 | 17 |
| 2 | -4 | 20 | 14 |
| 2 | -7 | 23 | 22 |
| 3 | -2 | 26 | 27 |
| 3 | 2 | 23 | 20 |
| 3 | 3 | 24 | 21 |
| 4 | -1 | 26 | 26 |
| 4 | 1 | 29 | 27 |
| 4 | -2 | 32 | 31 |
| 5 | -3 | 24 | 23 |
| ** K = 31 ** | | | |
| 1 | -1 | 24 | 23 |
| 1 | -3 | 26 | 29 |
| 1 | 3 | 21 | 23 |
| 2 | 0 | 41 | 39 |
| 3 | 2 | 21 | 18 |
| 3 | -4 | 22 | 23 |
| ** K = 32 ** | | | |
| 0 | 0 | 41 | 41 |
| 2 | 0 | 29 | 27 |
| 2 | -1 | 21 | 25 |
| 2 | 3 | 22 | 24 |
| 2 | 4 | 24 | 26 |
| 3 | -2 | 35 | 30 |
| 3 | 2 | 25 | 25 |
| 4 | -4 | 22 | 20 |
| 5 | -2 | 30 | 34 |
| ** K = 33 ** | | | |
| 1 | -2 | 33 | 33 |
| 2 | 2 | 28 | 27 |
| 3 | 3 | 26 | 26 |
| 5 | -2 | 24 | 23 |
| 5 | 2 | 29 | 28 |
| ** K = 34 ** | | | |
| 0 | 0 | 36 | 37 |
| 1 | -5 | 24 | 23 |
| 1 | 5 | 21 | 15 |
| 2 | -4 | 23 | 23 |
| 2 | 5 | 25 | 22 |
| 3 | 5 | 24 | 16 |
| ** K = 35 ** | | | |
| 0 | 1 | 36 | 39 |
| 1 | 2 | 23 | 21 |
| 2 | 0 | 23 | 21 |
| 3 | -1 | 21 | 23 |
| ** K = 36 ** | | | |
| 0 | 2 | 23 | 24 |
| 2 | 2 | 27 | 25 |
| ** K = 37 ** | | | |
| 1 | 5 | 29 | 26 |
| ** K = 39 ** | | | |
| 2 | 0 | 24 | 19 |
| 3 | -3 | 21 | 18 |
| ** K = 40 ** | | | |
| 0 | 0 | [illegible] | [illegible] |
| 1 | -2 | 22 | 21 |

graphite crystal. A test reflection was monitored after every 50 measurements, and an additional group of 8 test reflections was monitored once daily. Variations were within ±3% of the mean intensity. An error $\sigma(I)=[(0\cdot03I)^2+N_0+k^2N_b]^{1/2}$ was assigned to the net intensity $I=N_0-kN_b$ of each reflection where $N_0$ is the gross count, $N_b$ the background count, and $k$ the ratio of scan time to background time. These $\sigma$ values were used to calculate the weights $w=4F^2/\sigma^2(F^2)$ for the least-squares refinement, where the quantity $\sum[w(|F_o|-|F_c|)^2]$ was minimized. A total of 4973 unique reflections (within the sphere sin $\leq 0\cdot461$) were measured, but because maximum attainable precision in bond distances and angles was not an objective of this study and because the accuracy of the data was limited by experimental factors, only the 1333 reflections for which $|F|>15$ were used in the refinement. Absorption corrections were not applied ($\mu=9\cdot76$ cm$^{-1}$) and neglect of this effect may introduce errors approaching 5% in some $F$'s. Phases determined by iterative application of the $\sum_2$ formula (Dewar & Stone, 1968) were used to generate an $E$ map in which the Cl and S atoms were located. A difference Fourier then yielded the remaining C and N atoms. Full-matrix least-squares refinement of atomic positions and anisotropic temperature factors converged at $R_1=4\cdot6\%$ and $R_2=5\cdot2\%$. (A ratio of 5 observations to each parameter was maintained in the refinement.) Scattering factors, including $\Delta f'$ and $\Delta f''$ for chlorine and sulfur, were obtained from *International Tables for X-ray Crystallography* (1962). Table 1 lists the final atomic parameters and Table 2 gives the observed and calculated structure factors.

Table 3. *Bond distances and angles*

(*a*) Bond distances

Standard errors (in parentheses) were computed from the variance-covariance matrix calculated after the final least-squares cycle.

| Molecule *A* | | Molecule *B* | |
|---|---|---|---|
| C(1)–C(2) | 1·379 (16) Å | C(10)–C(11) | 1·399 (16) Å |
| C(2)–C(3) | 1·379 (15) | C(11)–C(12) | 1·379 (16) |
| C(3)–C(4) | 1·386 (15) | C(12)–C(13) | 1·396 (15) |
| C(4)–C(5) | 1·410 (16) | C(13)–C(14) | 1·376 (16) |
| C(5)–C(6) | 1·380 (15) | C(14)–C(15) | 1·393 (15) |
| C(6)–C(1) | 1·414 (16) | C(15)–C(10) | 1·386 (15) |
| C(1)–C(7) | 1·473 (17) | C(10)–C(16) | 1·445 (17) |
| C(3)–C(8) | 1·453 (16) | C(12)–C(17) | 1·465 (19) |
| C(2)–Cl(1) | 1·716 (12) | C(11)–Cl(4) | 1·724 (11) |
| C(4)–Cl(2) | 1·711 (12) | C(13)–Cl(5) | 1·719 (11) |
| C(5)–Cl(3) | 1·735 (11) | C(14)–Cl(6) | 1·729 (11) |
| C(7)–N(1) | 1·116 (14) | C(16)–N(3) | 1·133 (14) |
| C(8)–N(2) | 1·113 (14) | C(17)–N(4) | 1·150 (16) |
| C(6)–S(1) | 1·757 (13) | C(15)–S(2) | 1·775 (12) |
| C(9)–S(1) | 1·818 (15) | C(18)–S(2) | 1·827 (12) |

(*b*) Bond angles *

| | | | |
|---|---|---|---|
| C(6)–C(1)–C(2) | 122·2° | C(15)–C(10)–C(11) | 120·6° |
| C(6)–C(1)–C(7) | 117·8 | C(15)–C(10)–C(16) | 120·4 |
| C(2)–C(1)–C(7) | 120·0 | C(11)–C(10)–C(16) | 118·8 |
| C(1)–C(2)–C(3) | 119·9 | C(10)–C(11)–C(12) | 119·9 |
| C(1)–C(2)–Cl(1) | 120·5 | C(10)–C(11)–Cl(4) | 119·9 |
| C(3)–C(2)–Cl(1) | 119·5 | C(12)–C(11)–Cl(4) | 120·2 |
| C(2)–C(3)–C(4) | 119·8 | C(11)–C(12)–C(13) | 119·8 |
| C(2)–C(3)–C(8) | 120·1 | C(11)–C(12)–C(17) | 119·4 |
| C(4)–C(3)–C(8) | 120·0 | C(13)–C(12)–C(17) | 120·7 |
| C(3)–C(4)–C(5) | 119·6 | C(12)–C(13)–C(14) | 119·6 |
| C(3)–C(4)–Cl(2) | 119·6 | C(12)–C(13)–Cl(5) | 117·7 |
| C(5)–C(4)–Cl(2) | 120·8 | C(14)–C(13)–Cl(5) | 122·6 |
| C(4)–C(5)–C(6) | 121·6 | C(13)–C(14)–C(15) | 121·3 |
| C(4)–C(5)–Cl(3) | 118·2 | C(13)–C(14)–Cl(6)) | 118·1 |
| C(6)–C(5)–Cl(3) | 120·2 | C(15)–C(14)–Cl(6) | 120·5 |
| C(5)–C(6)–C(1) | 116·7 | C(14)–C(15)–C(10 | 118·4 |
| C(5)–C(6)–S(1) | 123·0 | C(14)–C(15)–S(2) | 119·5 |
| C(1)–C(6)–S(1) | 120·3 | C(10)–C(15)–S(2) | 122·1 |
| C(1)–C(7)–N(1) | 177·5 | C(10)–C(16)–N(3) | 178·5 |
| C(3)–C(8)–N(2) | 178·1 | C(12)–C(17)–N(4) | 179·1 |
| C(6)–S(1)–C(9) | 102·1 | C(15)–S(2)—C(18) | 102·2 |

* Errors in the bond angles are ±1·0° at ring carbons, ±1·4° at the nitrile carbons, and ±0·7° at the sulfur atoms.

## Results and discussion

The crystal structure contains two independent molecules, labeled *A* and *B*. Bond lengths [Table 3(*a*)] in the two molecules agree closely with each other (within 2·3$\sigma$ for corresponding bonds) and with literature values. Average distances for the six bond types are: C–C(ring), 1·390 Å; C–CN, 1·459 Å; C–Cl, 1·772 Å; C≡N, 1·128 Å; C($sp^2$)–S, 1·766 Å; and C($sp^3$)–S, 1·823 Å. Bond angles at the twelve ring carbons range from 116·7 to 123·0° (±1·1°) and are thus all within about three standard deviations of the ideal trigonal angle [Table 3(*b*)]. Likewise the C–C≡N angles (177·5, 178·1, 178·5 and 179·1°, all ±1·4°, at C(7), C(8), C(16) and C(17) respectively) are linear within experimental error. The bond angles at sulfur are 102·1 and 102·2±0·7° at S(1) and S(2) respectively.

Although bond distances and angles in the two molecules are individually very close to normal, a series of cumulative distortions arising from substituent crowding and/or crystal packing forces leads to very significant deviations of individual atoms from the least-squares planes defined by the ring atoms (see Table 4). Note that the deviations from plane are substantially larger in the case of molecule *B* and that, with the exception of one chloride substituent, the deviations are in the same direction for both molecules. The conformation of the methylthio substituents can be defined by the dihedral angles between the C–S–C planes and the ring planes of Table 4; these angles are 67·4 (*A*) and 56·0° (*B*) in the respective directions shown in Fig. 1.

Table 4. *Deviations from least-squares planes through the ring atoms* (Å)

The equations of plane are $A$: $6\cdot854x-12\cdot958y+0\cdot572z=3\cdot813$; $B$: $7\cdot043x+12\cdot072y-0\cdot004z=6\cdot297$.

| Molecule *A* | | Molecule *B* | |
|---|---|---|---|
| C(1) | 0·009 | C(10) | 0·021 |
| C(2) | 0·011 | C(11) | 0·006 |
| C(3) | −0·024 | C(12) | −0·024 |
| C(4) | 0·017 | C(13) | 0·014 |
| C(5) | 0·003 | C(14) | 0·014 |
| C(6) | −0·015 | C(15) | −0·031 |
| Cl(1) | −0·061 | Cl(4) | 0·083 |
| Cl(2) | 0·078 | Cl(5) | 0·010 |
| Cl(3) | 0·070 | Cl(6) | 0·062 |
| S(1) | −0·070 | S(2) | −0·116 |
| C(7) | 0·051 | C(16) | 0·188 |
| N(1) | 0·076 | N(3) | 0·350 |
| C(8) | −0·064 | C(17) | −0·109 |
| N(2) | −0·098 | N(4) | −0·168 |

Table 5. *Intermolecular distances less than* 3·7 Å

| | | | | | |
|---|---|---|---|---|---|
| C(1) | N(3) | $x$ | $\frac{1}{2}-y$ | $z-\frac{1}{2}$ | 3·38 Å |
| C(2) | N(4) | $1-x$ | $y-\frac{1}{2}$ | $\frac{1}{2}-z$ | 3·69 |
| C(3) | N(4) | $1-x$ | $y-\frac{1}{2}$ | $\frac{1}{2}-z$ | 3·56 |
| C(4) | Cl(6) | $x$ | $\frac{1}{2}-y$ | $\frac{1}{2}+z$ | 3·54 |
| C(4) | Cl(5) | $1+x$ | $\frac{1}{2}-y$ | $\frac{1}{2}+z$ | 3·54 |
| C(5) | Cl(6) | $x$ | $\frac{1}{2}-y$ | $\frac{1}{2}+z$ | 3·60 |
| C(5) | C(13) | $1+x$ | $\frac{1}{2}-y$ | $\frac{1}{2}+z$ | 3·61 |
| C(6) | Cl(6) | $1+x$ | $\frac{1}{2}-y$ | $\frac{1}{2}+z$ | 3·64 |
| C(6) | N(3) | $x$ | $\frac{1}{2}-y$ | $z-\frac{1}{2}$ | 3·64 |
| C(10) | N(1) | $x-1$ | $\frac{1}{2}-y$ | $\frac{1}{2}+z$ | 3·48 |
| C(11) | N(1) | $x-1$ | $\frac{1}{2}-y$ | $\frac{1}{2}+z$ | 3·68 |
| C(12) | N(2) | $1-x$ | $\frac{1}{2}+y$ | $\frac{1}{2}-z$ | 3·40 |
| C(12) | Cl(3) | $x-1$ | $\frac{1}{2}-y$ | $z-\frac{1}{2}$ | 3·68 |
| C(13) | Cl(2) | $x$ | $\frac{1}{2}-y$ | $z-\frac{1}{2}$ | 3·62 |
| C(13) | Cl(3) | $x-1$ | $\frac{1}{2}-y$ | $z-\frac{1}{2}$ | 3·66 |
| C(14) | Cl(2) | $x$ | $\frac{1}{2}-y$ | $z-\frac{1}{2}$ | 3·70 |
| Cl(1) | N(2) | $1-x$ | $-y$ | $-z$ | 3·38 Å |
| Cl(2) | N(2) | $1-x$ | $-y$ | $1-z$ | 3·00 |
| Cl(3) | N(1) | $x$ | $y$ | $1+z$ | 3·21 |
| S(1) | C(18) | $1+x$ | $y$ | $z$ | 3·46 |
| S(1) | Cl(6) | $1+x$ | $\frac{1}{2}-y$ | $\frac{1}{2}+z$ | 3·57 |
| Cl(4) | N(4) | $-x$ | $1-y$ | $1-z$ | 3·41 |
| Cl(4) | C(8) | $x$ | $\frac{1}{2}-y$ | $\frac{1}{2}+z$ | 3·57 |
| Cl(4) | C(7) | $x-1$ | $\frac{1}{2}-y$ | $\frac{1}{2}+z$ | 3·61 |
| Cl(5) | N(4) | $-x$ | $1-y$ | $-z$ | 2·99 |
| Cl(6) | N(3) | $x$ | $y$ | $z-1$ | 3·28 |
| S(2) | C(9) | $x$ | $y$ | $z$ | 3·71 |
| N(2) | N(4) | $1-x$ | $y-\frac{1}{2}$ | $\frac{1}{2}-z$ | 3·56 |
| C(7) | N(3) | $x$ | $\frac{1}{2}-y$ | $z-\frac{1}{2}$ | 3·67 |
| C(8) | N(4) | $1-x$ | $y-\frac{1}{2}$ | $\frac{1}{2}-z$ | 3·31 |
| C(8) | C(17) | $1-x$ | $y-\frac{1}{2}$ | $\frac{1}{2}-z$ | 3·36 |
| C(9) | N(1) | $x$ | $\frac{1}{2}-y$ | $\frac{1}{2}+z$ | 3·43 |
| C(16) | N(1) | $x-1$ | $\frac{1}{2}-y$ | $\frac{1}{2}+z$ | 3·40 |
| C(17) | N(2) | $1-x$ | $\frac{1}{2}+y$ | $\frac{1}{2}-z$ | 3·24 |
| C(18) | N(3) | $x$ | $\frac{1}{2}-y$ | $z-\frac{1}{2}$ | 3·55 |

Errors are ±0·01–0·02 Å.

The crystal structure is shown in Fig. 2. The ring systems of the two independent molecules can be seen to be approximately parallel and to be related by an approximate translation of $a/2$–$c/2$; however, a chloride and a cyanide group are interchanged with respect to this translation. Table 5 lists the intermolecular contacts, the shortest of which are the Cl(2)···N(2) distances of 3·000±0·011 Å and the Cl(5)···N(4) distances of 2·995±0·011 Å mentioned above. These interactions occur pairwise between molecules about the inversion centers at $\frac{1}{2},0,\frac{1}{2}$ (for the *A* molecules) and $0,\frac{1}{2},0$ (for *B*). The Cl···N≡C angles for these short interactions are 128·7° for *A* and 124·6° for *B*. Two other Cl···N distances are shorter than 3·3 Å, the nominal sum of Cl and N van der Waals radii, namely Cl(3)···N(1) = 3·208 Å (*A* molecules) and Cl(6)···N(3) = 3·278 Å (*B*). These interactions are generated by the lattice translation along **c**. Finally, there exist pairs of interactions about the inversion centers at $\frac{1}{2},0,0$ [*A*: Cl(1)···N(2), 3·384 Å] and $0,\frac{1}{2},\frac{1}{2}$ [*B*: Cl(4)···N(4), 3·412 Å] which are longer than the sum of van der Waals radii but otherwise are similar to the short pairwise interactions at $\frac{1}{2},0,\frac{1}{2}$ and $0,\frac{1}{2},0$. The 3·384 Å pair of contacts can be seen in Fig. 2 at the center of the unit cell.

We are grateful to E. C. Steiner for his skilful assistance in purifying and recrystallizing this material.

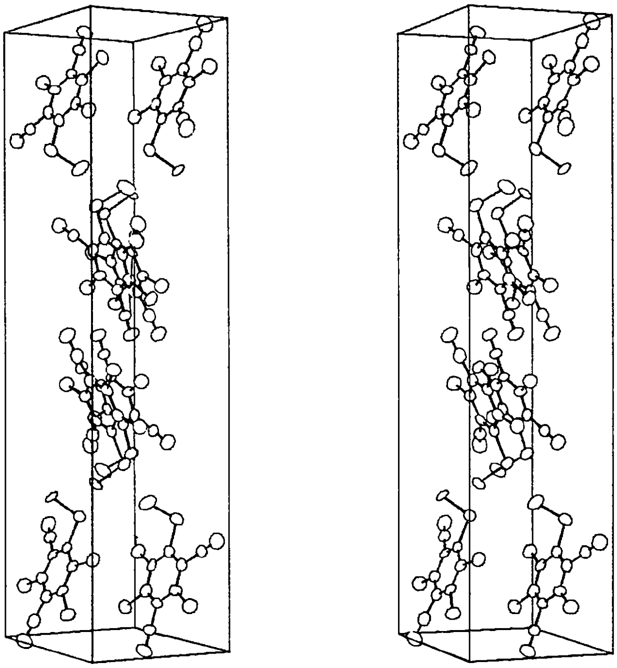

Fig. 2. The crystal structure of 2,4,5-trichloro-6-(methylthio)-isophthalonitrile. The *y* axis is vertical and *x* runs approximately left to right.

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