52.2 (2)°. There are no comparable values in the literature; the sum of the covalent radii is 2.68 Å, using 1.51 Å for Re (from $Re_2(CO)_{10}$) and 1.17 Å for Si.[19] The angle subtended at the Si atom by the two phenyl groups is within error of the tetrahedral angle, while the Re–Si–Re angle is considerably more acute at 75.7 (3)°. If the hydrogen atoms are positioned in the plane of the ReSiRe triangle such that the Re–Re–H angle is 90°, then a Re–H length of 1.68 Å[20] gives an Si–H distance of 1.59 Å and an H–Si–H angle of 156.1°. Thus an sp^3-hybridized Si atom would have two orbitals directed toward the coordination atoms of the phenyl rings and two toward the centroids of the ReHSi triangles.

Acknowledgment.—Helpful discussions with Dr. W. A. G. Graham and Dr. M. J. Bennett are gratefully acknowledged.

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The Structure of Pentakis(2-picoline N-oxide)cobalt(II) Perchlorate, $[Co(C_6H_7NO)_5](ClO_4)_2$

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The crystal structure of pentakis(2-picoline N-oxide)cobalt(II) perchlorate, $[Co(C_6H_7NO)_5](ClO_4)_2$, has been determined from X-ray counter data. The material crystallizes in the monoclinic space group C_{2h}^5-$P2_1/c$, with a = 18.667 (7) Å, b = 10.444 (8) Å, c = 18.665 (7) Å, β = 96° 21 (1)′, Z = 4, d_{obsd} = 1.45 (5) g/cm³, and d_{calcd} = 1.48 g/cm³. A least-squares refinement gave a final conventional R factor of 0.091 for those 1611 reflections above background with values of $\lambda^{-1} \sin \theta > 0.3$ Å^{-1}, whereas that for all 2293 independent reflections above background was 0.103. The compound consists of well-separated pentakis(2-picoline N-oxide)cobalt(II) and perchlorate ions. The immediate coordination about the cobalt atom for this d^7 high-spin complex is essentially trigonal bipyramidal with the axial Co–O bond length greater than the equatorial bond length by 0.123 (9) Å.

Introduction

Because of their simplicity five-coordinate transition metal complexes of the type MX_5 are of especial importance. Although fewer than a dozen such complexes have been characterized structurally, the results have provided important information on some of the factors which determine the resultant geometries.[1] Of those compounds so characterized, all have been low-spin d^8, d^9, or d^{10} systems. The present structural study of the five-coordinate Co(II) complex pentakis(2-picoline N-oxide)cobalt(II) perchlorate is the first such study of a high-spin d^7 complex containing the MX_5 group. On the basis of infrared and electronic spectra, Byers, Lever, and Parish,[2] who prepared the compound initially, characterized it as containing in solution trigonal-bipyramidal Co(II). We find this same geometry in the crystalline state. The comparison of this trigonal-bipyramidal, high-spin d^7 complex with those MX_5 complexes previously characterized adds useful information on the relative importance of the various factors (*e.g.*, ligand–ligand repulsion and d-electron–ligand repulsion) which determine the relative axial and equatorial bond lengths in MX_5 trigonal bipyramids.

Experimental Section

Collection and Reduction of X-Ray Data.—Violet crystals of pentakis(2-picoline N-oxide)cobalt(II) perchlorate were kindly supplied by Professor A. B. P. Lever and Dr. W. Byers. The crystals fell into two distinct habits: plates and prisms. Since the former gave X-ray photographs of a poorer quality, the structural study was carried out on one of the prisms, of approximate dimensions 0.2 × 0.2 × 0.8 mm, sealed in a glass capillary. Preliminary optical and X-ray examination indicated that the crystals belong to the monoclinic system. The systematic absences, as determined from $hk0$ and $h0l$ through $h3l$ photographs (hkl, none; $h0l$, $l = 2n + 1$; $0k0$, $k = 2n + 1$) are consistent with the space group C_{2h}^5-$P2_1/c$. The lattice parameters at 23°, obtained using Mo $K\alpha_1$ radiation (λ 0.7093 Å) are a = 18.667 (7) Å, b = 10.444 (8) Å, c = 18.665 (7) Å, and β = 96° 21 (1)′. The least-squares refinement of cell parameters was carried out as previously described.[3] The setting angles χ, ϕ, and 2θ of eight high-angle (2θ) reflections, as obtained from a narrow-source and narrow-counter aperture, were used. The density, as measured by flotation in a hexane–carbon tetrachloride mixture, of 1.45 (5) g/cm³ agrees with a value of 1.48 g/cm³ calculated for four formula units per cell. The large uncertainty in the observed density results from the rapid dissolution of the crystals in halocarbons commonly used for density measurement. Since the order of the space group is 4, no crystallographic symmetry need be imposed on the structure.

The crystal was mounted on an automatic Picker four-circle diffractometer, and the unique axis b (the 0.8-mm dimension of the crystal) was slightly offset from coincidence with the polar (ϕ) axis of the instrument, in order to decrease the probability of multiple diffraction effects.[4] At a low takeoff angle and wide counter aperture, representative peaks showed a maximum width at half-height of 0.1° in ω. Intensity data were collected as previously described using Mo $K\alpha$ radiation filtered

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TABLE I

FINAL ATOMIC POSITIONAL AND THERMAL PARAMETERS FOR $[Co(C_6H_7NO)_5](ClO_4)_2$

Atom	x	y	z	β_{11}[b] or B	β_{22}	β_{33}	β_{12}	β_{13}	β_{23}
Co	−0.23507 (9)[a]	0.0869 (2)	0.00462 (9)	0.00232 (6)	0.0091 (2)	0.00278 (7)	−0.00026 (9)	0.00030 (4)	−0.00002 (10)
Cl(1)	0.44477 (19)	0.0830 (5)	0.32589 (21)	0.00370 (12)	0.0133 (4)	0.00420 (14)	−0.00045 (23)	0.00061 (10)	0.00073 (25)
Cl(2)	0.13251 (26)	0.2064 (4)	0.22439 (27)	0.00490 (17)	0.0133 (5)	0.00520 (19)	0.00078 (23)	−0.00071 (14)	−0.00315 (26)
O(1)	−0.3460 (4)	0.439 (1)	0.4759 (5)	0.0022 (3)	0.0141 (13)	0.0039 (3)	0.0001 (5)	0.0006 (2)	0.0008 (5)
O(2)	−0.1275 (5)	0.132 (1)	0.0392 (5)	0.0021 (3)	0.0205 (16)	0.0029 (3)	−0.0012 (5)	0.0010 (2)	0.0004 (5)
O(3)	0.2101 (5)	0.095 (1)	0.0092 (7)	0.0025 (3)	0.0089 (11)	0.0070 (5)	0.0010 (5)	−0.0001 (3)	−0.0011 (7)
O(4)	−0.2561 (5)	0.133 (1)	0.1024 (5)	0.0031 (3)	0.0159 (14)	0.0026 (3)	−0.0007 (5)	−0.0002 (2)	−0.0014 (5)
O(5)	−0.2176 (6)	0.302 (2)	0.4229 (9)	0.0024 (3)	0.036 (3)	0.0072 (7)	−0.0010 (8)	0.0008 (4)	−0.0121 (13)
C(1)[c]	−0.3933 (11)	0.3048 (16)	−0.0063 (13)	0.0048 (7)	0.0067 (16)	0.0087 (9)	0.0006 (8)	−0.0001 (6)	0.0001 (11)
C(2)	−0.0388 (11)	0.3301 (27)	0.0700 (13)	0.0044 (7)	0.022 (3)	0.0061 (8)	0.0005 (12)	0.0000 (6)	0.0002 (14)
C(3)	0.2606 (14)	0.2458 (29)	0.4099 (14)	0.0068 (9)	0.023 (3)	0.0054 (9)	0.0043 (15)	−0.0008 (7)	−0.0017 (14)
C(4)	−0.2388 (15)	0.3842 (23)	0.1441 (14)	0.0069 (9)	0.017 (3)	0.0067 (9)	0.0037 (13)	0.0003 (8)	0.0020 (13)
C(5)	−0.1849 (13)	0.0557 (26)	0.4055 (11)	0.0064 (9)	0.022 (3)	0.0039 (6)	0.0021 (14)	−0.0004 (6)	0.0001 (12)
O(11)[d]	0.4993 (12)	−0.0061 (22)	0.3124 (12)	17.2 (6)					
O(12)	0.4656 (11)	0.1950 (22)	0.2972 (11)	16.8 (6)					
O(13)	0.3817 (12)	0.0543 (21)	0.2826 (12)	17.2 (6)					
O(14)	0.4412 (12)	0.0676 (24)	0.3951 (14)	21.3 (7)					
O(21)	0.1631 (11)	0.0940 (23)	0.2125 (11)	15.9 (6)					
O(22)	0.1169 (12)	0.2533 (22)	0.1512 (13)	19.4 (7)					
O(23)	0.1907 (12)	0.2831 (21)	0.2460 (11)	14.5 (6)					
O(24)	0.0749 (14)	0.2704 (25)	0.2349 (14)	21.8 (8)					

Group	x_c[e]	y_c	z_c	δ	ϵ	η	B_N	B_1	B_2	B_3	B_4	B_5
R_1	0.5576 (3)	0.0907 (7)	0.0708 (3)	1.440 (7)	−2.307 (5)	2.922 (9)	3.4 (2)	5.3 (3)	5.5 (3)	5.3 (3)	5.3 (3)	4.0 (3)
R_2	0.9778 (4)	0.3483 (7)	0.4549 (4)	−1.662 (7)	2.424 (6)	−2.453 (8)	4.0 (2)	4.2 (3)	5.4 (3)	6.0 (4)	6.4 (4)	5.0 (3)
R_3	0.3112 (4)	0.2624 (7)	0.0631 (4)	−0.810 (8)	−2.834 (5)	−1.840 (8)	4.5 (2)	6.1 (4)	7.0 (4)	7.2 (4)	6.2 (4)	4.1 (3)
R_4	0.8509 (4)	0.1817 (7)	0.2073 (4)	−1.335 (6)	−2.441 (6)	−0.012 (8)	4.0 (2)	4.7 (3)	5.3 (3)	6.2 (4)	5.9 (4)	5.1 (3)
R_5	0.7003 (4)	0.1849 (7)	0.3169 (4)	2.268 (7)	2.384 (7)	2.971 (9)	5.1 (3)	6.7 (4)	6.4 (4)	6.5 (4)	5.9 (4)	4.6 (3)

[a] In all tables, numbers in parentheses are the standard deviations in the least significant digits. [b] The expression for the anisotropic temperature factor is $\exp[-\beta_{11}h^2 - \beta_{22}k^2 - \beta_{33}l^2 - 2\beta_{12}hk - 2\beta_{13}hl - 2\beta_{23}kl]$. [c] Each methyl carbon atom C(n) is bonded to the ring carbon atom R(n)C(5). [d] The perchlorate oxygen atoms O(n1) through O(n4) are bonded to chlorine atom Cl(n). [e] x_c, y_c, z_c are the fractional coordinates of the group centers. The angles δ, ϵ, and η (in radians) have been described previously.[8]

through 0.08 mm of zirconium foil. At a takeoff angle α of 1.6°, where 80% of the maximum peak height as a function of α was observed for a typical peak, a 2θ scan of 1.5° symmetrically located about the $K\alpha_1$ peak maximum was used at a scan rate of 1°/min. Background counts, each of 10 sec duration, were taken at each end of the scan. A counter aperture 7 × 7 mm was placed 35 cm from the crystal, and the pulse-height analyzer was set to admit 90% of the Mo $K\alpha$ radiation. Copper foil attenuators were automatically inserted if the diffracted beam exceeded an intensity of about 7000 counts/sec. Independent reflections were measured out to a 2θ value of 42°; few reflections were observed to have significant intensity past this angle. Four standards were checked every 200 observations, and their constancy (variation <1%) provided evidence of crystal and electronic stability. The intensities were processed as previously described[3] using a value of $p = 0.03$ in the expression for $\sigma(I)$. Of the 3949 reflections collected and corrected for Lorentz and polarization effects 2293 had $F^2 > 3\sigma(F^2)$. Only these were used in subsequent calculations. Of the weak reflections, 317 had $2\sigma(F^2) < F^2 < 3\sigma(F^2)$ and 462 had $\sigma(F^2) < F^2 < 2\sigma(F^2)$. Trial calculations for reflections chosen to give the widest variations led to values for the transmission factors of 0.86–0.89, and consequently no absorption correction was carried out ($\mu = 7.14$ cm^{-1}).

Solution and Refinement.—The cobalt and both chlorine atoms were located from a sharpened, origin-removed Patterson map.[5] Three cycles of least-squares refinement (in which the scattering[6] and dispersion[7] factors used were taken from the usual compilations), each followed by a difference Fourier synthesis, successfully led to the location of all nonhydrogen atoms. Because of the large number (51) of independent nonhydrogen atoms (all in general positions) to be refined, the rings were refined as rigid groups,[8] having the geometry of free pyridine.[9] Initially each ring was given an overall isotropic thermal parameter. With the other atoms refined with individual isotropic parameters, the agreement factors at this stage were $R_1 = 0.148$ and $R_2 = 0.176$, where $R_1 = \Sigma(||F_o| - |F_c||)/\Sigma|F_o|$ and $R_2 = (\Sigma w(|F_o| - |F_c|)^2/\Sigma wF_o^2)^{1/2}$ and the function minimized was $\Sigma w(|F_o| - |F_c|)^2$. Here $|F_o|$ and $|F_c|$ are the observed and calculated structure amplitudes, respectively, and the weights w are taken as $4F_o^2/\sigma^2(F_o^2)$. A further least-squares calculation was performed in which all individual atoms (except the anionic oxygen atoms) were refined with anisotropic thermal parameters and the group atoms were assigned individual thermal parameters. The scattering from the hydrogen atoms was also included as a fixed contribution, using the scattering factors of Stewart, *et al.*[10] (It was assumed that the C–H bond length is 1.0 Å and that $B_H = 6$ Å^2.) Contributions from the methyl hydrogen atoms were not included. The agreement factors were now 0.103 and 0.129, respectively, for this refinement of 210 variables with 2293 observations.

A difference Fourier map at this stage exhibited, as the highest features, peaks of 0.7, 0.8, and 1.0 e$^-$/Å^3 within 1.3–1.6 Å of Cl(1) and peaks of 0.5, 0.8, and 1.2 e$^-$/Å^3 within 1.3–1.6 Å of Cl(2). Peak heights of 1.5–2.5 e$^-$/Å^3 were found for the original perchlorate oxygen atoms. Both the unsatisfactory geometry for perchlorate group 2, as obtained from the previous refinement where O–Cl–O angles ranging from 83 to 149° were found, and the presence of these residual peaks suggest that there may be some disorder of one or both of the perchlorate groups. However, such disorder cannot be of major importance, as the residual peak heights are lower than the original ones. Moreover around neither of the chlorine atoms is it possible to discern a model of perchlorate disorder with the use of the four original oxygen positions together with the residual peaks noted above. The derived geometry of perchlorate group 1 seems acceptable, particularly in view of the presence of residual peaks. The geometry of perchlorate group 2 would also be reasonable if O(24) were displaced by about 0.5 Å. There is considerable density in the vicinity of O(24) and it seems possible that the position derived from the refinement corresponds to an artificial peak center formed by the near overlap of two separate half-oxygen positions. This point was not pursued because of the insensitivity of the

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(5) In addition to local programs for a CDC 6400 computer, including NUCLS, which in its nongroup form resembles the Busing–Levy least-squares program ORFLS, those used in this work were local modifications of Busing and Levy's ORFFE error function program, Johnson's ORTEP thermal ellipsoid plotting program, and Zalkin's FORDAP Fourier program.

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TABLE II

FINAL POSITIONAL AND THERMAL PARAMETERS OF GROUP ATOMS $[Co(C_6H_7NO)_5](ClO_4)_2$

Group and atom	x	y	z	B, Å^2
R(1)N	0.6078 (4)	0.0790 (8)	0.0208 (4)	3.4 (2)
R(1)C(1)	0.5847 (7)	−0.0232 (7)	0.0551 (6)	5.3 (3)
R(1)C(2)	0.5348 (7)	−0.0168 (8)	0.1054 (6)	5.5 (3)
R(1)C(3)	0.5070 (5)	0.1026 (10)	0.1213 (5)	5.3 (3)
R(1)C(4)	0.5305 (7)	0.2099 (8)	0.0861 (6)	5.3 (3)
R(1)C(5)	0.5806 (7)	0.1929 (7)	0.0367 (5)	4.0 (3)
R(2)N	0.9212 (4)	0.3575 (8)	0.4979 (5)	4.0 (2)
R(2)C(1)	0.9283 (6)	0.4411 (10)	0.4447 (5)	4.2 (3)
R(2)C(2)	0.9836 (7)	0.4362 (9)	0.4002 (5)	5.4 (3)
R(2)C(3)	1.0348 (5)	0.3390 (11)	0.4114 (6)	6.0 (4)
R(2)C(4)	1.0282 (6)	0.2512 (11)	0.4666 (6)	6.4 (4)
R(2)C(5)	0.9708 (6)	0.2647 (8)	0.5080 (5)	5.0 (3)
R(3)N	0.2592 (5)	0.1743 (9)	0.0347 (5)	4.5 (2)
R(3)C(1)	0.2835 (7)	0.1754 (10)	0.1050 (5)	6.1 (4)
R(3)C(2)	0.3353 (7)	0.2611 (13)	0.1360 (4)	7.0 (4)
R(3)C(3)	0.3637 (6)	0.3512 (12)	0.0918 (6)	7.2 (4)
R(3)C(4)	0.3389 (7)	0.3513 (10)	0.0185 (6)	6.2 (4)
R(3)C(5)	0.2870 (5)	0.2615 (9)	−0.0071 (4)	4.1 (3)
R(4)N	0.7949 (4)	0.1579 (8)	0.1527 (5)	4.0 (2)
R(4)C(1)	0.8377 (6)	0.0637 (7)	0.1812 (5)	4.7 (3)
R(4)C(2)	0.8943 (6)	0.0823 (9)	0.2356 (6)	5.3 (3)
R(4)C(3)	0.9074 (5)	0.2058 (10)	0.2623 (6)	6.2 (4)
R(4)C(4)	0.8632 (7)	0.3049 (8)	0.2333 (6)	5.9 (4)
R(4)C(5)	0.8081 (6)	0.2759 (8)	0.1790 (5)	5.1 (3)
R(5)N	0.7423 (5)	0.2474 (9)	0.3730 (5)	5.1 (3)
R(5)C(1)	0.6878 (7)	0.3068 (8)	0.3336 (6)	6.7 (4)
R(5)C(2)	0.6443 (6)	0.2490 (12)	0.2771 (6)	6.4 (4)
R(5)C(3)	0.6579 (6)	0.1219 (11)	0.2602 (6)	6.5 (4)
R(5)C(4)	0.7144 (8)	0.0586 (8)	0.3007 (6)	5.9 (4)
R(5)C(5)	0.7547 (6)	0.1253 (10)	0.3561 (5)	4.6 (4)

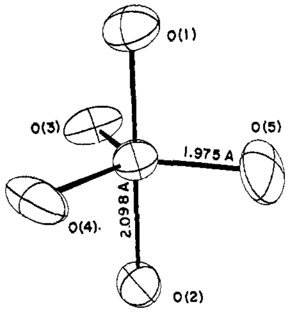

Figure 1.—The CoO_5 chromophore in $[Co(C_6H_7NO)_5](ClO_4)_2$. Average axial and equatorial bond distances are shown.

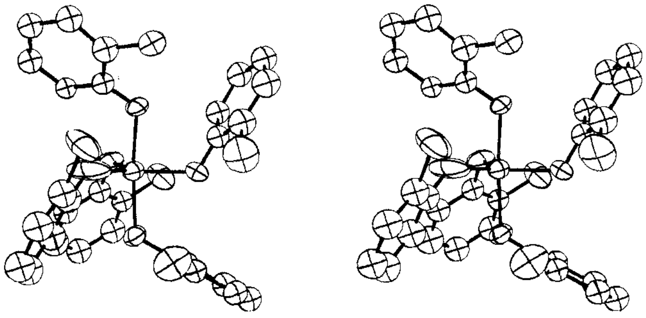

Figure 2.—Stereoview of the cation in $[Co(C_6H_7NO)_5](ClO_4)_2$. The hydrogen atoms are omitted for the sake of clarity.

cation geometry to minor perturbations in the anion geometry. This insensitivity was established in the following manner. Because of the high thermal motion and the low atomic number, the oxygen atoms of the perchlorate groups scatter principally at low Bragg angles, whereas the high-angle data are important for the precise determination of the structure of the cation. Hence a final least-squares cycle was performed in which the perchlorate oxygen atoms were set at the positions initially found, and only the high-angle reflections ($\lambda^{-1} \sin \theta > 0.3$ Å^{-1}) were used. This refinement of 178 variables with 1611 observations converged to values for R_1 and R_2 of 0.091 and 0.094, respectively. Of importance, no parameter for the cation changed by more than one standard deviation from the value obtained when all the data were used. Thus although the scattering from the perchlorate anions may not have been satisfactorily described, the cation geometry is correctly determined within the derived limits of error. Based on these high-angle data alone, the highest peak in a final difference Fourier map is 0.4 e$^-$/Å^3. There are no obvious trends of $\Sigma w(|F_o| - |F_c|)^2$ with $|F_o|$ or $\lambda^{-1} \sin \theta$. An examination of $|F_c|$ for the 1656 reflections below background (*i.e.*, where $F_o^2 < 3\sigma(F_o^2)$) revealed only 21 instances where $|F_o^2 - F_c^2|$ was above $3\sigma(F_o^2)$. The final error in an observation of unit weight is 2.6 e$^-$.

The fact that the final agreement factors for the high-angle data are higher than we would anticipate on the basis of experience with similar compounds we believe results not from difficulties with the perchlorate anion geometry but rather from our failure to refine the parameters of the atoms of the pyridine rings individually. Our imposition of a fixed geometry for the pyridine ring has prevented us from refining anisotropic thermal parameters and individual positional parameters for 30 of the 41 atoms of the cation. Total anisotropic refinement of the cation and the two chlorine atoms (together with fixed positions for the perchlorate oxygen atoms) would involve 388 variable parameters, far in excess of the capacity of our computer. Such a refinement could have been split into two or more blocks, but the convergence properties of such a process are difficult to assess.

The following lines of evidence suggest that the group refinement carried out here has not resulted in an underestimation of the errors quoted for the cation geometry. First of all, the geometry chosen for the pyridine portion of the ligand appears to be reasonable. Recent X-ray data on various pyridine N-oxide–metal systems[11,12] indicate that the lengths of the three independent bonds within the pyridine ring range from 1.326 to 1.364, 1.352 to 1.407, and 1.328 to 1.418 Å, respectively, for the N–C(α), C(α)–C(β), and C(β)–C(γ) bonds. The estimated standard deviations of individual determinations of these bond lengths are greater than 0.01 Å. The values of 1.340, 1.395, and 1.395 Å were chosen for our rigid-group refinement. Second, in the present refinement the average C(α)–C(methyl) bond distance is 1.55 (2) Å, and the individual values range from 1.53 (2) to 1.57 (2) Å. (These distances would be about 0.02–0.04 Å shorter had the methyl hydrogen atoms been included in the calculations.) Thus for all five ligands the methyl carbon atoms, refined individually, have achieved plausible positions with respect to the rigid groups to which they are attached. Third, the standard deviation of a single observation, as estimated from the agreement among presumably equivalent bond distances (*e.g.*, the five C(α)–C(methyl) bond distances), agrees very well with that estimated from the inverse matrix. Fourth, there is no significant residual electron density in the vicinity of any of the rings.

The final atomic and group parameters and their estimated standard deviations are given in Table I, while Table II lists the final positional parameters of the heterocyclic atoms derived from the group parameters. The values of $|F_o|$ and $|F_c|$ in electrons (×10) for all reflections above background are given in Table III. Selected bond distances and angles are given in Table IV, together with their standard deviations as derived from the variance–covariance matrix for functions involving nongroup atoms and from variances alone for those involving group atoms.

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TABLE III

OBSERVED AND CALCULATED STRUCTURE AMPLITUDES FOR $[Co(C_6H_7NO)_5](ClO_4)_2$ IN ELECTRONS (×10)

H	K	FO	FC
***** L = -18 *****			
1	1	161	145
3	1	143	117
3	3	188	211
4	0	225	239
4	1	147	114
4	2	248	240
5	1	162	173
6	0	208	233
6	1	251	259
6	2	155	148
***** L = -17 *****			
1	4	293	299
2	1	190	207
4	1	192	173
5	1	141	83
5	2	443	460
5	4	241	233
6	1	218	216
7	2	177	210
8	1	158	146
***** L = -16 *****			
2	0	221	219
2	1	261	289
2	2	140	105
2	5	236	213
3	3	282	287
3	5	225	201
5	1	276	276
5	3	361	345
5	5	169	123
6	0	527	497
6	2	259	300
7	0	147	113
7	1	221	267
8	1	136	109
8	3	240	233
9	1	316	290
9	3	153	122
10	2	154	149
11	0	224	207
***** L = -15 *****			
1	2	179	211
1	5	257	233
2	3	195	232
2	6	198	184
3	1	133	87
3	2	309	352
4	1	271	245
4	2	143	159
4	5	268	298
5	2	271	310
5	4	201	221
6	1	302	317
7	2	266	280
7	3	224	254
7	4	206	216
9	1	219	176
10	1	201	164
10	4	157	136
11	2	197	206
12	1	139	156
12	2	178	221
***** L = -14 *****			
1	1	248	194
1	3	262	310
1	6	193	181
2	0	479	489
2	1	256	189
2	2	321	316
2	3	170	244
2	6	338	303
3	0	269	240
3	1	434	398
4	0	379	364
4	2	174	152
4	3	204	187
4	4	373	366
4	6	233	220
5	0	409	395
5	1	519	545
5	2	138	161
5	3	464	457
5	4	155	115
5	5	155	163
6	0	318	305
6	2	143	174
6	3	333	342
6	4	162	195
6	5	173	180
6	6	142	137
7	0	288	301
7	3	361	323
7	4	176	183
7	6	185	76
8	0	211	188
8	2	153	179
8	3	191	209
8	6	230	254
10	3	332	285
10	5	136	168
11	0	307	365
11	1	209	176
11	3	267	272
12	2	216	216
12	3	176	148
13	0	255	274
14	0	177	128
14	1	159	165
***** L = -13 *****			
1	3	216	80
1	4	177	154
2	1	551	514
2	5	247	213
2	7	370	348
3	2	653	646
3	3	222	222
3	4	214	217
3	5	241	250
3	6	155	175
4	1	269	264
4	5	165	137
4	7	226	188
5	1	159	203
5	2	541	523
5	4	192	249
5	5	186	174
6	1	472	512
6	4	185	196
6	5	480	508
6	7	146	165
7	2	154	110
7	3	138	163
7	4	285	316
8	2	302	328
8	4	155	136
9	1	165	144
9	4	317	287
10	4	160	203
11	1	143	162
11	4	165	142
12	1	214	233
12	4	223	212
14	2	186	187
***** L = -12 *****			
1	0	225	271
1	2	145	165
1	3	388	426
1	5	136	143
1	6	321	360
2	0	433	504
2	5	199	167
3	0	298	301
3	3	733	674
3	8	210	215
4	0	729	746
4	1	206	229
4	2	240	262
4	4	256	196
4	6	368	372
4	8	179	145
5	1	223	252
5	3	214	228
6	0	169	134
6	3	169	148
6	6	393	391
7	0	306	278
7	1	260	265
7	3	446	488
7	5	164	167
7	7	137	141
8	0	174	128
8	2	284	226
8	3	144	161
9	0	164	173
9	2	269	241
9	4	176	177
9	6	162	210
10	0	158	173
10	2	163	159
10	4	193	246
10	5	372	369
10	6	231	175
11	3	542	510
12	2	246	288
12	4	267	187
13	0	342	337
13	1	206	243
13	3	352	369
14	0	220	256
14	2	183	160
14	3	155	130
***** L = -11 *****			
1	2	751	776
1	4	170	165
1	8	204	232
2	1	577	590
2	2	317	314
2	4	382	385
2	5	537	522
2	6	154	116
3	1	147	127
3	2	518	476
3	4	327	332
3	6	196	175
3	8	138	160
4	1	708	741
4	3	254	260
4	4	369	355
4	5	389	340
4	7	227	293
5	2	639	632
5	4	487	503
5	8	253	269
6	1	144	128
6	2	248	252
6	3	244	227
6	4	176	115
6	5	171	220
6	6	288	253
7	1	265	262
7	2	187	258
7	3	195	171
7	4	232	232
8	1	314	332
8	5	329	326
8	7	168	167
9	2	146	159
9	7	223	154
10	1	163	192
10	2	297	275
10	3	213	214
10	4	379	413
10	6	186	160
11	1	265	271
11	2	667	692
11	4	277	285
11	5	269	260
12	1	411	412
12	2	180	200
12	3	152	145
12	5	196	223
13	1	355	383
13	2	193	226
13	4	162	193
14	1	243	255
14	2	344	346
14	4	274	253
***** L = -10 *****			
1	0	181	180
1	2	232	261
1	3	170	228
1	5	203	215
2	0	493	489
2	2	486	540
2	4	287	336
2	5	130	99
2	6	566	560
3	1	518	543
3	2	220	197
3	3	864	833
3	4	136	121
3	5	196	236
3	7	151	136
4	0	973	950
4	2	148	102
4	3	200	216
4	4	211	182
5	1	289	256
5	2	123	246
5	3	625	627
5	4	354	364
5	6	177	184
5	7	248	230
6	0	297	464
6	1	186	136
6	3	344	362
6	4	248	264
6	6	385	384
7	0	193	198
7	1	189	218
7	2	177	176
7	3	424	452
7	4	126	44
7	7	129	88
8	0	196	209
8	2	187	223
8	4	156	111
9	0	163	102
9	1	392	437
9	3	271	247
9	5	177	225
9	7	143	143
10	0	369	340
10	3	160	176
10	5	303	333
11	0	426	437
11	1	529	523
11	2	209	201
11	4	152	120
11	6	371	410
12	0	485	455
12	1	243	210
12	2	167	152
12	3	341	326
12	4	292	341
12	6	177	184
13	0	167	303
13	1	269	309
13	3	193	185
13	5	159	177
14	0	207	196
14	1	215	265
14	3	162	194
14	5	129	33
15	0	370	338
16	3	150	97
17	0	141	122
***** L = -9 *****			
1	1	109	137
1	2	551	583
1	4	388	476
1	5	244	301
1	6	163	200
2	1	373	250
2	2	177	240
2	4	223	201
2	5	320	317
3	1	526	650
3	2	563	669
3	3	153	69
3	4	352	298
3	5	146	191
3	7	322	265
3	8	301	317
4	1	1155	1192
4	2	367	338
4	3	295	225
4	5	554	514
4	7	175	175
5	2	1014	892
5	3	122	116
5	5	208	221
5	8	221	206
6	1	432	488
6	2	212	311
6	3	346	357
6	5	326	369
6	7	158	141
6	8	137	127
7	2	809	832
7	4	694	712
7	6	242	209
7	8	174	180
8	1	533	482
8	3	201	207
8	4	205	169
8	7	137	168
9	1	457	533
9	2	483	464
9	4	302	272
9	6	139	122
9	7	323	335
10	1	611	617
10	2	277	245
10	3	232	199
10	4	521	563
10	5	188	136
10	6	151	133
11	1	165	218
11	2	531	523
12	1	138	151
12	2	387	377
12	3	149	75
12	4	323	315
12	5	258	284
12	6	212	188
13	1	262	289
13	2	442	433
13	4	343	312
13	5	168	206
14	1	208	220
14	2	166	190
15	1	178	176
15	4	140	54
16	2	225	237
***** L = -8 *****			
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1	1	290	181
1	2	143	25
1	3	1129	1219
1	4	137	80
1	7	321	295
2	0	1569	1853
2	1	462	467
2	3	217	258
2	4	348	272
2	5	204	258
2	6	354	374
3	3	542	564
3	4	212	295
3	7	132	82
4	0	1232	1171
4	2	573	564
4	3	298	330
4	4	718	627
4	6	529	508
4	7	179	198
5	0	436	297
5	1	1089	1204
5	2	128	70
5	3	660	725
5	4	247	201
5	5	237	228
5	7	214	208
5	9	293	297
6	0	1051	850
6	3	206	286
6	4	195	141
6	6	177	242
7	0	659	742
7	1	966	1012
7	2	368	465
7	3	131	130
7	4	521	514
7	5	149	168
7	6	400	385
7	7	200	216
8	0	414	589
8	1	178	230
8	3	322	288
8	4	396	439
8	6	273	281
9	0	581	605
9	1	723	644
9	2	361	334
9	3	138	89
9	7	254	262
9	8	146	107
10	0	493	508
10	1	298	297
10	3	651	646
10	5	359	393
11	0	597	642
11	1	389	398
11	2	141	153
11	3	592	575
11	4	289	306
11	6	335	301
11	7	235	227
12	0	323	330
12	3	441	435
12	4	331	340
12	5	138	89
12	6	140	145
12	7	131	114
13	0	670	656
13	1	201	162
13	3	259	258
13	4	295	285
13	5	156	159
14	0	316	308
14	1	238	281
14	2	227	224
14	3	288	287
14	6	256	263
15	0	177	230
16	1	142	126
16	3	281	257
17	2	167	173
***** L = -7 *****			
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1	3	320	208
1	4	291	233
1	5	134	74
2	1	873	909
2	2	447	520
2	4	531	520
2	5	600	651
2	6	151	137
2	7	371	346
3	1	127	180
3	2	551	515
3	3	216	225
3	4	704	704
3	5	144	65
3	7	127	195
3	8	154	126
4	1	801	677
4	2	153	205
4	3	146	251
4	4	298	341
4	6	175	237
4	7	267	312
5	1	494	699
5	2	795	786
5	3	258	342
5	4	408	431
5	5	245	217
5	7	214	226
5	8	143	201
6	1	319	341
6	4	166	211
6	5	469	481
6	6	209	217
6	7	318	311
6	8	178	169
7	1	373	251
7	2	392	367
7	3	207	212
7	5	208	219
8	1	381	338
8	3	241	233
8	4	396	336
8	5	414	393
8	6	196	200
9	1	327	243
9	2	392	375
9	3	143	36
9	4	322	356
9	5	155	177
9	8	308	322
10	1	285	293
10	2	251	254
10	3	130	108
11	1	462	509
11	2	326	317
11	5	513	517
11	7	153	193
12	1	371	384
12	2	548	551
12	3	220	196
12	4	395	403
12	6	210	162
12	7	281	260
13	1	160	213
13	2	245	235
13	3	307	273
13	4	455	451
14	2	224	237
15	1	322	325
15	4	140	139
16	4	210	208
17	1	139	115
***** L = -6 *****			
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1	1	1333	1442
1	3	779	751
1	5	206	236
1	6	298	284
1	8	208	248
1	9	298	277
2	0	1095	632
2	2	647	618
2	3	158	125
2	4	561	587
2	5	201	258
2	6	288	341
3	0	515	595
3	1	1220	1125
3	2	762	797
3	3	707	745
3	4	892	897
3	5	679	720
3	7	339	332
3	9	304	298
4	0	1164	1339
4	1	337	437
4	2	579	606
4	4	336	381
4	6	510	502
4	8	180	194
5	0	429	317
5	1	360	267
5	2	366	391
5	3	584	454
5	4	402	497
5	5	117	125
5	7	310	289
6	0	495	691
6	1	402	414
6	2	477	448
6	3	517	559
6	4	460	407
6	6	402	397
6	7	136	85
6	8	128	105
7	1	252	243
7	3	780	871
7	5	138	132
7	7	250	260
7	9	175	212
8	0	708	715
8	1	537	630
8	2	433	399
8	3	239	311
8	4	157	156
9	0	502	624
9	2	283	297
9	3	611	621
9	4	355	318
9	5	147	126
9	6	220	183
9	7	194	163
10	0	569	605
10	2	565	580
10	3	291	311
10	4	282	259
10	5	253	250
10	6	389	376
10	7	161	132
11	0	682	586
11	1	347	348
11	2	170	219
11	3	304	284
11	4	250	235
11	5	260	133
11	6	228	256
12	0	135	219
12	1	286	328
12	2	145	94
12	3	723	737
12	4	220	245
12	5	181	149
12	6	166	137
12	7	173	201
13	0	313	362
13	2	276	258
13	3	433	404
13	4	559	554
13	5	321	298
13	7	248	224
14	0	228	207
14	5	135	127
15	0	177	188
15	2	155	77
16	0	212	167
16	3	521	493
17	1	183	153
18	0	151	102
***** L = -5 *****			
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1	2	966	362
1	3	212	242
1	4	1222	1248
1	5	183	309
1	6	156	156
1	7	175	116
1	8	219	297
1	10	177	194
2	1	811	890
2	2	528	632
2	3	642	659
2	4	370	325
2	5	788	766
2	6	305	286
2	7	385	355
2	8	265	278
3	1	1018	969
3	2	111	165
3	3	326	403
3	4	120	80
3	5	378	393
3	6	390	209
3	7	146	80
3	8	269	292
4	1	113	135
4	2	377	443
4	3	405	457
4	4	579	605
4	5	555	621
4	7	349	339
4	8	175	178
5	1	648	521
5	2	368	367
5	3	123	90
5	4	388	442
5	5	422	410
5	7	196	170
5	8	433	402
6	4	300	281
7	1	404	477
7	3	201	167
7	4	964	1017
7	5	385	398
7	6	251	251
7	7	211	147
7	8	345	368
8	1	170	326
8	2	169	179
8	3	276	319
8	4	373	345
8	5	269	302
8	7	410	417
9	1	462	501
9	2	170	195
9	3	177	203
9	4	414	408
9	5	207	196
9	7	315	313
9	8	166	170
9	9	135	113
10	1	565	524
10	2	553	536
10	4	536	517
10	5	171	183
10	8	237	245
11	1	576	555
11	2	581	600
11	4	441	408
11	5	212	221
11	7	390	420
11	8	228	257
12	1	159	171
12	2	255	251
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13	1	328	330
13	2	154	138
13	5	565	551
14	1	199	189
14	2	298	299
14	5	145	136
15	4	278	268
16	2	235	239
16	3	211	179
16	4	241	224
16	5	240	231
17	1	356	320
18	2	253	236
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1	7	151	133
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2	2	997	971
2	3	316	327
2	4	758	824
2	6	568	602
2	7	176	167
2	8	261	212
2	10	264	271
3	0	137	196
3	1	1925	2008
3	2	1248	1331
3	3	274	316
3	4	122	182
3	5	338	353
3	6	421	458
3	7	255	194
3	8	138	102
3	9	246	282
3	10	167	154
4	0	3118	2973
4	1	653	874
4	2	1116	1026
4	6	200	205
4	7	168	137
4	9	132	5
5	1	802	648
5	3	681	720
5	4	138	70
5	5	317	318
5	6	566	572
5	7	192	131
5	9	325	392
5	10	215	204
6	1	109	156
6	2	553	606
6	3	705	703
6	4	273	396
6	6	380	374
6	8	284	281
7	0	304	146
7	1	198	253
7	2	216	359
7	3	228	185
7	4	276	205
7	5	211	243
7	6	122	139
7	7	148	182
7	9	214	241
8	0	396	286
8	1	158	235
8	2	253	364
8	3	154	229
8	5	570	569
8	6	224	202
8	7	236	230
8	8	211	265
8	9	196	181
9	1	125	88
9	2	620	568
9	3	630	686
9	4	362	391
9	5	307	325
9	7	286	288
9	8	203	154
9	9	157	132
10	0	432	455
10	3	156	155
10	5	381	362
10	7	220	185
10	8	139	145
11	0	901	898
11	2	323	332
11	3	339	326
11	4	211	165
11	6	383	377
11	7	149	133
11	8	161	225
12	0	428	362
12	2	343	364
12	3	643	679
12	4	358	335
12	5	310	262
12	7	161	110
12	8	212	176
13	4	172	150
13	5	254	232
13	6	157	168
14	0	408	400
14	1	221	198
14	3	283	297
14	6	127	32
15	0	159	171
15	2	145	135
15	3	174	133
15	4	135	127
15	5	178	165
15	6	325	303
16	1	183	119
17	0	229	205
17	3	222	173
18	1	219	215
18	2	140	125
18	3	390	422
***** L = -3 *****			
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1	3	296	303
1	4	927	832
1	6	273	252
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1	8	241	198
2	1	376	227
2	2	113	44
2	3	295	276
2	4	284	207
2	5	849	750
2	7	267	281
2	8	269	300
2	9	199	161
3	1	680	558
3	2	1634	1415
3	3	959	828
3	4	1078	1226
3	5	493	446
3	7	156	82
3	8	350	352
4	1	1886	1855
4	2	1588	1493
4	3	145	208
4	4	132	216
4	5	260	210
4	7	599	604
5	1	726	726
5	3	516	479
5	4	320	295
5	7	496	550
5	8	264	278
5	9	158	136
6	1	1271	1307
6	4	725	789
6	5	912	1008
6	7	176	100
6	8	191	259
7	1	436	373
7	2	470	659
7	3	230	173
7	4	857	774
7	7	273	298
7	8	420	446
8	1	206	111
8	4	170	220
8	5	165	223
8	6	150	152
8	7	177	140
9	1	366	439
9	2	216	289
9	3	400	353
9	4	484	433
9	5	737	705
9	6	212	153
9	7	330	299
9	8	141	147
10	1	383	473
10	2	379	454
10	3	464	426
10	7	221	226
10	8	146	180
11	1	404	363
11	2	442	433
11	3	161	119
11	4	343	343
11	5	302	235
11	6	246	242
12	1	272	284
12	2	470	452
12	3	142	210
12	4	598	603
12	5	174	186
12	6	198	185
13	1	292	304
13	2	262	265
13	4	284	296
13	5	384	355
13	7	148	147
14	1	171	145
14	5	192	157
14	6	146	188
15	2	192	185
15	4	144	126
15	5	152	94
16	2	143	182
16	4	218	198
18	2	396	391
***** L = -2 *****			
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1	3	1174	1072
1	4	116	35
1	5	526	626
1	6	203	215
1	7	217	182
1	9	430	409
2	0	488	360
2	1	605	549
2	2	88	94
2	3	1256	1400
2	4	818	839
2	5	201	84
2	6	340	342
2	7	208	186
2	9	199	255
3	0	553	656
3	1	839	560
3	2	1143	1182
3	3	500	495
3	4	343	433
3	5	304	280
3	7	284	299
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4	1	1759	1880
4	2	868	735
4	3	536	525
4	4	265	261
4	5	458	550
4	6	744	828
4	7	158	182
4	8	248	234
4	9	212	185
4	10	219	212
5	0	101	172
5	1	246	267
5	2	321	260
5	3	645	636
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5	6	275	256
5	7	278	289
5	8	228	284
5	9	205	181
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6	3	147	186
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6	10	150	97
7	0	1241	1373
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7	2	259	271
7	3	788	816
7	4	377	414
7	6	361	371
7	7	320	333
7	8	330	298
8	0	433	518
8	1	176	249
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8	3	353	335
8	4	492	509
8	5	354	371
8	6	420	406
9	1	121	212
9	2	492	482
9	5	269	281
9	6	218	262
9	7	199	181
10	0	271	203
10	1	559	596
10	2	171	296
10	3	158	197
10	4	353	348
10	5	272	346
10	7	240	233
11	0	906	823
11	1	238	241
11	3	653	703
11	4	174	172
11	5	478	434
11	6	339	383
11	7	296	268
12	0	295	287
12	1	630	597
12	2	240	210
12	8	177	149
13	0	248	292
13	1	203	200
13	2	252	259
13	4	259	270
13	5	217	187
13	6	394	364
13	7	173	153
14	0	166	148
14	1	169	198
14	3	376	401
14	6	198	196
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15	2	210	161
15	3	197	209
15	5	170	146
16	0	265	232
16	3	227	241
17	0	321	333
17	1	214	143
17	2	296	261
18	1	169	176
18	3	343	328
***** L = -1 *****			
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1	3	678	638
1	4	312	345
1	5	111	64
1	6	129	24
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1	8	179	211
2	1	1208	1232
2	2	468	546
2	4	308	311
2	5	804	993
2	7	298	317
2	9	187	173
3	1	573	434
3	2	731	547
3	3	657	647
3	4	109	65
3	5	130	125
3	6	109	168
3	7	229	237
3	8	307	310
4	1	326	136
4	2	420	336
4	3	534	348
4	4	218	86
4	6	201	220
4	8	247	248
4	10	156	159
5	1	655	573
5	2	274	44
5	3	406	446
5	4	802	853
5	5	675	789
5	7	227	263
5	8	359	332
5	10	149	142
6	1	1026	1031
6	2	275	185
6	3	1066	1051
6	4	535	408
6	7	169	166
7	1	457	367
7	3	166	231
7	4	550	481
7	5	391	360
7	6	442	472
7	7	237	241
8	1	674	773
8	2	768	791
8	3	361	383
8	4	260	369
8	5	373	346
8	7	221	264
9	1	465	496
9	2	586	585
9	4	490	556
9	7	389	390
9	8	315	342
10	1	113	154
10	2	289	208
10	3	263	243
10	5	162	135
11	1	603	660
11	2	220	233
11	4	182	160
11	5	527	485
11	7	343	317
12	1	269	278
12	2	422	397
12	3	229	282
12	4	186	211
12	5	329	299
12	7	165	134
12	8	159	174
13	3	185	212
13	4	257	208
13	5	262	289
14	1	210	209
14	2	284	334
14	4	251	241
15	1	142	150
15	4	402	377
15	5	158	165
17	1	272	276
17	4	146	120
18	2	411	403
***** L = 0 *****			
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1	2	1494	1553
1	3	1819	1724
1	4	107	67
1	5	111	107
1	7	267	254
1	9	208	198
2	0	1575	1404
2	1	111	139
2	2	733	714
2	3	1207	1373
2	4	846	819
2	6	547	516
2	9	158	145
3	0	1115	1190
3	1	860	800
3	2	703	595
3	3	1247	1141
3	4	215	213
3	5	247	360
3	6	142	168
3	7	365	358
3	8	196	145
3	9	138	109
3	10	298	268
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4	1	261	206
4	2	324	296
4	3	1041	1130
4	4	375	419
4	5	306	296
4	6	448	446
4	8	149	169
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5	2	699	661
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5	4	200	324
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5	6	396	372
5	7	268	252
5	8	146	119
6	0	1227	1077
6	1	1250	1310
6	2	134	115
6	4	626	627
6	5	393	489
6	6	310	305
6	9	268	228
7	0	579	567
7	1	655	772
7	2	445	367
7	3	894	1024
7	4	522	505
7	6	127	204
7	7	450	449
7	9	196	171
8	0	1082	1010
8	1	534	566
8	3	183	191
8	4	289	283
8	6	227	225
9	0	799	865
9	2	123	211
9	3	669	686
9	4	460	445
9	5	243	200
9	6	443	411
9	7	406	438
10	0	709	815
10	1	248	289
10	3	342	339
10	4	313	296
10	6	262	279
11	0	394	418
11	1	139	96
11	3	252	260
11	4	237	232
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12	1	485	447
12	2	350	335
12	3	542	521
12	4	160	170
12	7	144	134
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13	2	475	437
13	3	370	368
13	4	266	232
13	5	157	190
13	6	284	265
13	7	175	209
15	0	151	60
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15	4	157	184
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16	4	164	152
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17	2	222	212
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18	3	385	411
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1	6	106	197
1	7	247	243
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2	2	488	404
2	3	1052	833
2	5	358	267
2	6	299	248
2	7	319	313
2	8	332	406
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3	2	1521	1487
3	3	650	586
3	5	274	321
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4	2	121	18
4	3	817	856
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4	6	197	272
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4	10	230	191
5	2	774	650
5	3	122	77
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6	3	342	327
6	4	103	184
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7	5	819	910
7	7	432	406
7	8	314	295
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8	2	1042	979
8	3	131	231
8	4	463	451
8	5	685	682
8	6	217	196
8	7	299	322
9	1	330	262
9	2	278	248
9	4	658	605
9	5	322	354
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10	4	207	225
10	7	245	315
10	8	287	293
11	1	520	461
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11	3	162	165
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12	8	147	116
13	1	597	591
13	2	159	153
13	4	146	134
13	5	281	256
13	7	333	349
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14	2	319	329
14	3	145	107
14	4	356	362
14	5	229	236
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16	1	262	235
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16	3	132	61
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17	1	201	215
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18	2	243	248
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1	6	136	145
1	7	137	125
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2	1	1369	1211
2	2	1518	1255
2	3	619	431
2	4	326	285
2	5	550	447
2	6	714	780
2	8	206	214
2	9	128	175
2	10	267	291
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3	1	1889	1823
3	2	553	491
3	3	467	588
3	4	491	405
3	7	193	235
3	8	292	260
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4	3	354	413
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4	6	512	441
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4	10	194	176
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5	1	814	747
5	2	220	151
5	3	773	800
5	4	143	61
5	6	417	421
5	7	332	335
5	8	196	227
5	9	184	198
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6	2	533	562
6	3	648	481
6	4	374	334
6	5	117	102
6	6	378	414
6	8	148	108
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7	1	322	246
7	2	1012	911
7	3	348	201
7	4	724	722
7	5	140	126
7	6	446	417
7	8	223	262
7	9	149	162
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8	1	436	440
8	3	859	889
8	4	376	357
8	5	238	248
8	6	353	338
8	9	178	158
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9	1	392	509
9	2	716	678
9	3	765	788
9	4	298	313
9	5	200	249
9	6	196	198
9	9	277	278
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12	1	466	485
12	3	350	362
12	7	156	159
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13	1	146	140
13	3	143	137
13	6	183	197
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14	3	498	502
14	5	176	123
15	0	361	396
15	1	258	244
15	6	213	223
16	0	284	222
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0	7	565	550
0	9	144	80
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1	2	1797	1554
1	3	744	661
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1	7	303	310
1	8	495	519
1	9	159	168
2	1	793	722
2	2	1397	1352
2	3	421	323
2	4	405	377
2	5	652	677
2	6	169	141
2	7	253	268
3	1	109	30
3	2	160	129
3	4	704	733
3	5	485	605
3	8	484	479
3	10	133	114
4	1	464	317
4	3	300	210
4	4	271	347
4	5	444	421
4	6	150	120
4	7	188	213
4	8	137	236
4	9	155	132
5	1	351	242
5	2	190	69
5	3	379	317
5	4	224	206
5	5	544	636
5	6	239	293
5	7	278	231
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6	1	1575	1485
6	2	621	796
6	3	724	794
6	4	343	489
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6	6	151	130
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6	8	254	214
7	1	667	654
7	2	1244	1176
7	5	341	310
7	6	259	252
7	7	257	263
7	8	195	208
7	9	143	104
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8	2	511	439
8	3	197	241
8	4	473	434
8	5	184	192
8	6	220	253
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9	2	849	760
9	3	515	526
9	4	121	144
9	5	374	378
9	7	423	420
9	8	174	255
9	9	186	167
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11	4	242	207
11	5	344	359
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12	5	303	107
12	7	155	128
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13	2	272	278
13	4	311	260
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15	5	254	211
16	2	456	487
16	4	213	218
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17	3	206	179
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0	6	699	654
0	8	286	313
0	9	178	181
0	10	220	236
1	0	1470	1411
1	1	1399	1325
1	2	948	922
1	3	923	951
1	4	177	232
1	5	701	726
1	6	270	264
1	7	210	201
1	8	172	245
1	9	506	494
1	10	154	138
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2	1	1407	1249
2	2	1627	1618
2	3	393	400
2	5	357	438
2	6	605	598
2	8	243	272
2	9	202	206
2	10	162	183
3	0	584	697
3	1	637	626
3	2	493	551
3	4	359	458
3	5	280	313
3	6	390	363
3	8	160	184
3	9	239	234
4	0	836	758
4	1	259	192
4	3	239	198
4	4	184	46
4	5	292	290
4	6	641	636
4	9	264	262
5	0	447	303
5	1	288	238
5	2	127	206
5	3	517	540
5	4	132	168
5	6	244	237
5	9	207	219
6	0	1220	1103
6	1	508	521
6	2	335	238
6	3	183	133
6	4	125	28
6	5	238	283
6	8	176	239
6	9	244	238
7	0	963	952
7	1	592	693
7	2	857	846
7	3	658	753
7	4	473	438
7	6	630	667
7	9	319	333
8	0	1229	1358
8	1	340	251
8	3	546	532
8	5	237	249
8	6	247	231
8	8	310	319
9	0	980	900
9	2	140	116
9	3	117	68
9	4	280	320
9	5	160	131
9	6	333	348
10	0	341	246
10	1	512	455
10	2	221	233
10	3	303	355
10	5	168	136
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11	0	478	469
11	1	409	381
11	3	154	144
11	5	189	184
12	0	258	267
12	1	226	162
12	6	218	216
13	0	567	537
13	4	308	296
13	6	263	267
14	1	452	447
14	2	156	147
14	3	231	236
15	0	163	182
16	0	319	300
16	1	255	262
16	3	320	343
17	0	389	413
***** L = 5 *****			
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0	4	407	418
0	5	848	819
0	7	359	360
0	8	192	220
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1	2	407	377
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1	4	503	608
1	5	281	263
1	7	122	111
1	9	148	215
1	10	154	215
2	1	2149	2016
2	2	506	245
2	4	242	324
2	5	419	439
2	6	296	320
2	7	581	582
3	3	245	173
3	4	122	160
3	5	409	230
3	8	254	311
4	1	709	669
4	2	528	561
4	3	197	86
4	4	962	976
4	5	298	298
5	1	914	995
5	2	858	907
5	3	409	376
5	4	435	391
5	5	348	376
5	7	456	469
5	8	325	250
6	1	683	714
6	2	451	336
6	3	238	80
6	5	618	604
7	1	775	698
7	2	398	303
7	3	247	266
7	4	161	177
7	5	742	726
7	6	172	154
8	1	292	276
8	2	746	813
8	4	526	553
8	5	173	127
8	7	274	256
8	8	139	105
9	1	189	196
9	4	493	495
9	5	507	471
10	2	177	122
10	3	143	130
10	5	247	272
10	6	148	165
10	7	204	230
11	1	424	426
11	2	209	157
11	3	134	137
11	4	167	148
11	5	187	189
11	7	210	265
12	1	270	290
12	2	178	214
12	7	168	157
13	1	312	298
13	3	186	162
13	5	163	152
14	2	504	509
14	3	157	114
14	4	300	267
15	1	328	329
15	2	214	179
15	5	243	245
16	2	223	280
17	1	197	185
17	2	175	188
***** L = 6 *****			
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0	1	259	379
0	2	740	733
0	4	579	641
0	5	125	134
0	6	861	870
1	0	938	857
1	3	220	277
1	4	204	290
1	8	322	370
1	9	143	185
2	0	1163	1398
2	1	525	637
2	2	356	225
2	3	259	123
2	4	166	161
2	6	466	343
2	7	279	328
1	8	199	214
3	0	525	399
3	1	120	211
3	2	409	400
3	3	514	618
3	4	288	252
3	6	253	270
3	7	319	301
3	9	232	284
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4	3	280	119
4	4	138	175
4	5	300	310
4	6	411	418
4	9	136	89
5	0	724	875
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5	6	467	515
5	7	203	216
5	9	141	118
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6	5	194	199
6	6	317	303
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6	9	184	149
7	0	579	527
7	1	839	921
7	2	576	613
7	3	502	491
7	4	513	457
7	5	190	224
7	7	188	188
7	9	258	245
8	0	409	334
8	2	393	370
8	3	366	308
8	6	155	176
9	0	403	413
9	2	294	333
9	3	144	198
9	4	461	476
9	5	337	331
9	6	360	405
9	7	179	174
10	0	128	101
10	1	238	283
10	2	321	288
10	6	332	299
11	0	174	152
11	1	195	231
11	2	132	160
11	3	129	138
11	5	170	180
11	6	183	239
11	7	137	134
12	0	259	225
12	1	245	255
12	2	181	143
12	3	458	469
12	5	190	144
13	0	601	597
13	1	160	172
13	6	311	324
14	0	176	135
14	1	140	173
14	3	394	379
15	0	443	449
15	1	220	202
15	2	182	171
15	3	251	220
16	1	201	240
16	3	227	238
17	1	148	112
***** L = 7 *****			
0	1	779	801
0	2	388	452
0	4	237	204
0	5	662	660
0	7	172	126
1	1	230	341
1	2	655	756
1	3	145	112
1	4	366	390
1	6	325	313
1	7	166	113
1	8	433	371
2	1	444	376
2	3	465	463
2	4	483	536
2	5	398	379
2	7	343	331
3	1	213	149
3	2	281	285
3	3	220	287
3	4	449	482
3	5	474	489
3	8	201	202
4	1	389	486
4	3	348	152
4	4	619	594
4	5	337	361
4	6	141	157
4	7	473	423
5	2	425	460
5	3	267	277
5	4	484	504
5	5	263	243
5	6	229	249
6	2	364	382
6	3	279	254
6	4	200	258
6	6	147	179
7	1	975	995
7	2	330	330
7	3	187	233
7	4	540	592
7	5	245	224
7	7	292	310
7	8	272	284
8	1	765	725
8	3	386	360
8	4	247	220
8	5	265	312
8	6	193	124
8	7	367	370
9	5	231	231
9	6	243	213
9	7	251	257
10	1	227	211
10	2	398	411
10	3	300	326
10	4	139	112
10	5	237	208
10	6	217	172
11	3	216	198
11	4	225	236
11	5	175	248
11	7	137	133
12	1	199	233
13	1	256	249
13	3	161	191
13	5	326	356
14	4	273	284
***** L = 8 *****			
0	0	1428	1393
0	1	322	158
0	2	285	326
0	3	205	236
0	4	410	471
0	6	361	417
1	0	696	951
1	1	237	282
1	3	461	486
1	5	149	143
1	6	152	164
1	7	230	265
1	8	152	120
1	9	169	139
2	0	643	583
2	1	149	80
2	2	351	451
2	4	541	546
2	6	538	532
2	7	170	154
3	0	478	569
3	2	488	505
3	3	208	183
3	4	251	227
3	7	217	205
3	9	216	171
4	0	172	238
4	2	360	294
4	3	495	434
4	5	232	243
4	6	385	432
4	8	231	250
4	9	231	249
5	0	282	307
5	1	113	103
5	2	657	702
5	3	307	366
5	4	141	170
5	6	388	405
5	7	305	335
5	8	189	188
6	0	162	356
6	1	208	257
6	2	171	125
6	4	415	345
6	6	284	254
6	7	126	80
7	0	624	679
7	2	472	428
7	3	438	378
7	4	424	444
8	0	1072	1062
8	2	302	275
8	3	734	707
8	6	477	492
8	7	159	157
8	8	191	177
9	1	242	260
9	2	226	272
9	3	272	237
9	5	374	397
9	6	308	328
9	7	218	219
10	0	269	254
10	3	179	194
10	5	273	232
10	7	149	114
11	1	302	286
11	2	316	325
11	4	184	187
11	6	329	345
12	0	269	253
12	4	139	84
13	0	135	128
13	1	364	320
13	2	330	322
14	1	261	245
14	3	287	271
15	2	255	236
15	3	156	141
***** L = 9 *****			
0	1	716	840
0	2	441	448
0	4	279	280
0	5	724	682
0	7	328	349
0	9	145	156
1	3	538	585
1	4	580	572
1	5	209	197
1	6	286	330
2	1	206	258
2	4	142	19
2	5	347	389
2	6	238	225
2	7	181	182
3	2	548	616
3	4	264	249
3	7	157	109
3	8	356	358
3	9	146	147
4	1	669	622
4	4	164	131
4	5	496	472
5	1	286	303
5	2	366	365
5	5	366	372
5	7	301	357
6	1	381	383
6	2	720	777
6	5	677	687
6	6	357	298
6	8	248	252
7	1	393	374
7	2	381	363
7	3	163	189
7	4	458	454
7	5	317	346
7	6	164	141
8	1	223	237
8	2	529	548
8	4	188	224
8	7	137	201
9	1	406	408
9	2	158	226
9	3	302	298
9	4	276	257
9	5	490	487
9	7	260	279
10	4	346	332
10	6	137	77
11	4	142	145
11	6	144	100
12	4	312	341
12	5	152	112
13	1	261	267
13	2	347	367
14	2	214	217
15	1	255	268
***** L = 10 *****			
0	0	783	874
0	1	486	607
0	2	413	393
0	3	429	464
0	4	270	205
0	6	400	422
1	0	604	651
1	2	384	379
1	3	734	727
1	4	286	291
1	5	242	249
1	7	133	138
2	0	469	411
2	1	158	201
2	2	204	123
2	3	177	135
2	4	154	109
2	5	189	196
2	6	288	291
2	8	147	165
3	2	320	302
3	3	382	418
3	6	228	229
4	0	971	944
4	2	328	302
4	3	496	492
4	4	135	138
4	5	134	110
4	6	448	452
5	0	336	350
5	1	345	387
5	3	321	307
5	6	294	308
6	1	384	379
6	3	360	371
6	4	356	332
6	5	402	373
7	0	577	554
7	1	405	408
7	2	439	450
7	3	325	307
7	4	479	511
7	6	206	188
8	0	386	386
8	1	219	235
8	6	264	283
9	0	210	218
9	2	412	423
9	4	244	200
9	6	141	178
10	0	194	124
10	2	190	151
10	5	183	154
11	0	256	236
11	1	227	170
11	3	283	284
11	5	137	112
12	0	312	271
12	3	151	177
13	0	464	412
13	2	140	183
13	4	174	184
14	2	149	152
***** L = 11 *****			
0	1	249	217
0	2	397	385
0	3	131	99
0	5	357	356
0	6	160	131
0	8	172	153
1	1	430	426
1	2	654	639
1	5	264	272
1	8	173	174
2	1	649	676
2	2	215	230
2	3	155	134
2	5	527	553
2	6	262	246
2	7	254	250
2	8	210	191
3	2	283	271
3	3	204	223
3	4	172	117
3	6	194	123
4	1	460	473
4	2	423	440
4	3	319	345
4	4	316	337
4	5	141	111
5	1	551	551
5	2	480	443
5	4	316	288
5	5	447	416
5	6	266	225
5	7	236	291
6	1	324	343
6	2	258	249
6	3	137	116
6	4	361	345
6	5	313	330
6	6	172	161
7	1	475	452
7	2	341	372
7	3	257	221
7	4	172	170
7	5	218	244
7	7	221	200
8	1	301	329
8	2	474	465
8	5	345	323
8	6	218	160
9	1	257	226
9	2	580	605
9	6	142	105
10	1	187	144
10	2	160	163
10	3	150	151
11	1	217	241
11	5	286	317
12	2	158	202
13	1	305	281
***** L = 12 *****			
0	0	747	754
0	4	355	358
0	6	207	243
0	7	162	143
1	0	567	489
1	1	500	501
1	2	244	202
1	3	163	235
1	5	178	104
2	0	268	220
2	1	486	493
2	2	235	255
2	3	336	308
2	4	286	261
2	5	146	106
2	6	259	281
2	7	182	144
3	1	313	302
3	3	485	518
3	5	138	191
3	6	237	190
4	0	301	307
4	1	219	230
4	6	195	179
5	0	661	620
5	2	273	298
5	3	236	238
5	4	270	267
5	5	313	296
5	6	283	273
6	0	477	451
6	1	379	406
6	2	135	154
6	3	423	401
6	4	169	240
6	5	140	150
6	6	139	140
7	0	538	533
7	1	179	187
7	3	385	402
7	4	268	293
8	0	217	131
8	1	241	237
8	3	318	329
8	6	139	49
9	0	659	617
9	1	137	153
9	2	160	171
9	4	217	243
9	5	226	170
10	1	156	129
10	2	346	336
11	0	163	174
11	4	185	216
12	0	164	189
12	1	360	356
12	3	246	229
13	0	304	315
***** L = 13 *****			
0	1	220	211
0	2	310	304
0	4	306	328
0	7	227	213
1	1	291	297
1	2	353	351
1	3	160	153
1	4	255	202
2	4	183	185
2	5	209	203
2	6	172	169
3	1	241	237
3	2	250	278
3	4	245	228
3	5	226	177
3	6	219	174
4	1	304	308
4	2	172	176
4	5	270	273
5	2	287	271
6	2	530	542
7	1	340	357
7	2	194	204
7	3	144	159
7	4	292	231
7	5	172	241
8	2	165	230
9	1	280	305
9	3	169	204
10	4	244	261
12	1	198	169
***** L = 14 *****			
0	2	144	99
0	6	154	182
1	0	423	386
1	3	260	272
1	6	228	230
2	0	423	420
2	2	151	156
2	3	262	205
2	5	163	112
2	6	352	359
3	0	209	210
3	3	246	279
3	5	137	9
4	0	188	197
4	2	187	186
4	3	228	230
4	6	189	179
5	0	568	586
5	1	366	383
5	3	305	262
5	4	221	182
5	5	148	135
6	0	215	193
6	1	354	334
6	2	217	234
6	3	160	151
6	5	186	157
7	0	475	499
7	2	255	211
7	4	286	287
8	0	303	254
8	1	278	316
8	3	214	211
9	0	152	200
11	0	288	310
***** L = 15 *****			
0	1	172	126
0	3	137	143
0	5	251	308
2	2	355	361
3	1	241	200
3	2	183	149
3	4	386	341
4	4	159	151
5	1	349	345
6	2	229	240
6	4	376	352
7	1	265	248
8	2	208	187
***** L = 16 *****			
0	2	236	204
0	3	216	209
1	0	138	21
1	1	267	267
1	3	157	197
3	0	208	197
3	1	148	155
3	2	217	204
3	3	155	81
4	0	421	408
6	3	281	204
7	0	262	289
***** L = 17 *****			
0	1	145	162
0	3	154	81
0	4	195	218
1	1	206	211
1	2	178	187
1	4	172	201
2	1	247	235
2	4	220	217
3	1	164	124
3	2	193	188
4	1	190	150
4	2	140	118
5	2	221	215
***** L = 18 *****			
0	0	264	257
3	0	155	177

Table IV

Selected Bond Lengths (in Å) and Angles (in deg) in $[Co(C_6H_7NO)_5](ClO_4)_2$

	Cations		
Co–O(1)	2.100 (9)	O(1)–Co–O(2)	173.4 (4)
Co–O(2)	2.095 (9)	O(1)–Co–O(3)	94.7 (4)
Co–O(ax)(av)	2.098 (4)[a]	O(1)–Co–O(4)	88.6 (4)
		O(1)–Co–O(5)	96.9 (4)
Co–O(3)	1.99 (1)	O(2)–Co–O(3)	91.4 (4)
Co–O(4)	1.97 (1)	O(2)–Co–O(4)	86.7 (4)
Co–O(5)	1.97 (1)	O(2)–Co–O(5)	82.6 (4)
Co–O(eq)(av)	1.975 (8)	O(3)–Co–O(4)	115.4 (5)
		O(3)–Co–O(5)	113.7 (8)
O(1)–N(1)	1.28 (1)	O(4)–Co–O(5)	129.8 (8)
O(2)–N(2)	1.26 (1)		
O(3)–N(3)	1.28 (1)	O(1)–N(1)–R(1)C(1)	118 (1)
O(4)–N(4)	1.29 (1)	O(2)–N(2)–R(2)C(1)	122 (1)
O(5)–N(5)	1.26 (2)	O(3)–N(3)–R(3)C(1)	121 (1)
O–N(av)	1.275 (12)	O(4)–N(4)–R(4)C(1)	120 (1)
		O(5)–N(5)–R(5)C(1)	123 (1)
C(1)–R(1)C(5)	1.53 (2)	O(1)–N(1)–R(1)C(5)	125 (1)
C(2)–R(2)C(5)	1.55 (2)	O(2)–N(2)–R(2)C(5)	121 (1)
C(3)–R(3)C(5)	1.57 (2)	O(3)–N(3)–R(3)C(5)	122 (1)
C(4)–R(4)C(5)	1.53 (2)	O(4)–N(4)–R(4)C(5)	123 (1)
C(5)–R(5)C(5)	1.56 (2)	O(5)–N(5)–R(5)C(5)	120 (1)
C(*n*)–R(n)C(5)(av)	1.55 (2)		
		Co–O(3)–N(3)	120 (1)
Co–O(1)–N(1)	122 (1)	Co–O(4)–N(4)	121 (1)
Co–O(2)–N(2)	124 (1)	Co–O(5)–N(5)	134 (1)
	Anions		
Cl(1)–O(11)	1.42 (2)	Cl(2)–O(21)	1.34 (2)
Cl(1)–O(12)	1.36 (2)	Cl(2)–O(22)	1.45 (2)
Cl(1)–O(13)	1.38 (2)	Cl(2)–O(23)	1.37 (2)
Cl(1)–O(14)	1.31 (2)	Cl(2)–O(24)	1.30 (3)
		Cl–O(av)	1.37 (5)
O(11)–Cl(1)–O(12)	105 (1)	O(21)–Cl(2)–O(22)	101 (1)
O(11)–Cl(1)–O(13)	109 (1)	O(21)–Cl(2)–O(23)	103 (1)
O(11)–Cl(1)–O(14)	102 (1)	O(21)–Cl(2)–O(24)	149 (1)
O(12)–Cl(1)–O(13)	102 (1)	O(22)–Cl(2)–O(23)	99 (1)
O(12)–Cl(1)–O(14)	122 (1)	O(22)–Cl(2)–O(24)	83 (1)
O(13)–Cl(1)–O(14)	114 (1)	O(23)–Cl(2)–O(24)	107 (1)
		O–Cl–O(av)	108 (16)

[a] Standard deviations following average quantities are for single observations and thus may be compared directly with standard deviations estimated from the inverse matrix to provide an indication of the reliability of the latter estimates or the equivalence of the averaged distances. In particular while the estimated standard deviations on the cation appear to be reasonable, those on the anions are not. As discussed in the text, there are indications of disorder of the perchlorate groups and this disorder has not been included in the refinement model.

Description of the Structure

The crystal is composed of discrete pentakis(2-picoline N-oxide)cobalt(II) and perchlorate ions as suggested by the results of the earlier experiments.[2] The CoO_5 chromophore, which has a slightly distorted trigonal-bipyramidal structure, may be viewed in Figure 1, while Figure 2 provides a stereoview of the cation. All thermal ellipsoids are drawn for 50% probability.

The extensive literature on the complexes of various metals with pyridine N-oxide and its substituted derivatives has been recently reviewed.[13,14] Table V compares the average metal–oxygen and oxygen–nitrogen distances and the metal–oxygen–nitrogen angles found here with those for similar heterocyclic amine oxide complexes of metals which have been examined structurally. Generally the observations made here fall within the range of those observed by others, with the exception of the markedly shorter N–O bond lengths. Presumably the N–O bond length is a sensitive function of the electronic configuration in this region. Thus the N–O bond lengths in selected compounds are 1.39 Å in $(CH_3)_3NO$[15] (formal single bond), 1.19 Å in N_2O[16] (formal double bond), and 1.06 Å in NO^+ [17] (formal triple bond). We conclude that the N–O bond in the compound studied here has slightly more double-bond character than have those studied previously.

In none of the five ligands of the present compound does the oxygen atom or the carbon atom of the methyl group deviate significantly from the plane of the ring. The maximum deviations are 0.06 (2) Å for O(2) and 0.07 (2) Å for C(1). On the other hand, the Co atom deviates significantly from these ligand planes, with respective deviations of 1.77, 1.15, 1.65, 1.59, and 1.01 Å. This can be indicated in another way by the values of the dihedral angles between the Co–O–N planes and the aromatic planes, which are 84, 41, 76, 71, and 49° for the five ligands. Thus even though the Co–O–N angles are fairly close to 120° in this compound, as well as in the other compounds of Table V, the labeling of the oxygen atom as sp^2 seems somewhat arbitrary in view of the deviation of the metal from the ligand plane. This point has been discussed previously.[12] As a comparison it may be noted that Co–O–P bond angles of 139.6 and 133.2° have been found in bis(trimethylphosphine oxide)dinitratocobalt(II).[18]

Discussion

The inner coordination sphere about the Co atom is distorted from regular trigonal-bipyramidal geometry (Figure 1) as one of the equatorial O–Co–O angles is significantly greater than the other two. This type of distortion is similar to that noted previously[19,20] in which a significantly longer M–X equatorial bond is opposite the largest X–M–X equatorial angle, but in the present case the "longer" bond is longer than the others only by little more than a standard deviation. Also, the Co atom lies 0.114 (7) Å from the equatorial plane defined by the three oxygen atoms. (Alternatively, the O atoms lie 0.067 (9), 0.093 (9), and 0.151 (12) Å and the Co lies 0.009 (2) Å from the weighted least-squares plane through the four atoms, which has the equation $17.44X + 1.66Y + 4.01Z + 3.93 = 0$ in monoclinic coordinates.) Presumably these small angular distortions result from various packing forces, as do the variations in Co–O–N bond angles, although "packing forces" are probably invoked here in the usual spirit of ignorance. In Table VI the shortest interligand distances (less than 3.5 Å) are quoted. The observed distortions are not easily related to distances in this tabulation nor to intermolecular contacts, all of which appear to be normal.

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TABLE V

DISTANCES (Å) AND ANGLES (DEG) INVOLVING THE OXYGEN ATOMS IN HETEROCYCLIC AMINE OXIDE COMPLEXES

Compound	M–O[a]	N–O	M–O–N	Angle between M–O–N plane and aromatic ring	Coordn	Ref
$[CuCl_2(C_5H_5NO)]_2$	2.01 (1)	1.35 (2)	124, 128 (2)	70	Bridged	*b*
$[Cu(NO_3)_2(C_5H_5NO)_2]_2$	1.96	...	...	...	Bridged	*c*
$Cu_3Cl_6(H_2O)_2(C_6H_7NO)_2$[d]	1.99 (1)	1.36 (2)	121.6, 127.1 (8)	89	Bridged	*e*
$[Cu(C_5H_5NO)_4](ClO_4)_2$	1.93	...	...	...	Sq planar	*f*
$[Cu(C_5H_5NO)_4](BF_4)_2$	1.92	...	...	...	Sq planar	*f*
$ZnCl_2(C_7H_9NO)_2$	2.01 (1)	1.35 (3)	118.6 (7)	83	Tetrahedral	*g*, *h*
$Ni(C_5H_7O_2)_2(C_5H_5NO)_2$	2.096 (5)	1.33 (1)	122.4, 119.2 (4)	48, 67	Octahedral	*i*
$SnCl_2(CH_3)_2(C_5H_5NO)_2$	2.25 (2)	1.37 (2)	117 (1)	83	Octahedral	*j*
$[Co(C_6H_7NO)_5](ClO_4)_2$	2.098 (4) 1.975 (8)	1.275 (12)	122, 124, 120 121, 134 (1)	84, 41, 76 71, 49	Trigonal bipyramidal	*k*

[a] All structurally equivalent distances in this table have been averaged. [b] Reference 11. [c] S. Scavnicar and B. Matkovik, *Chem. Commun.*, 297 (1967). [d] Substituents in the pyridine rings in all these compounds are α-methyl groups. [e] R. S. Sager and W. H. Watson, *Inorg. Chem.*, **7**, 2035 (1968). [f] D. S. Brown, J. D. Lee, and B. G. A. Melsom, *Chem. Commun.*, 852 (1968). [g] H. L. Schafer, J. C. Morrow, and H. M. Smith, *J. Chem. Phys.*, **42**, 504 (1965). [h] R. S. Sager and W. H. Watson, *Inorg. Chem.*, **7**, 1358 (1968). [i] Reference 12. [j] E. A. Blom, B. R. Penfold, and W. T. Robinson, *J. Chem. Soc., A*, 913 (1969). [k] This work.

TABLE VI

INTERLIGAND DISTANCES LESS THAN 3.5 Å

O(1)–N(3)	2.96	O(4)–R(1)C(1)	3.42
O(1)–N(5)	3.33	O(4)–R(1)C(5)	3.22
O(1)–R(3)C(1)	3.18	O(5)–N(2)	2.87
O(1)–R(5)C(1)	3.12	O(5)–R(2)C(1)	3.07
O(2)–N(4)	2.71	N(4)–R(5)C(4)	3.44
O(2)–R(4)C(1)	2.89	N(4)–R(5)C(3)	3.44
O(2)–R(4)C(5)	3.35	R(1)C(4)–R(3)C(3)	3.46
O(3)–N(2)	3.48	R(3)C(3)–R(5)C(4)	3.39
O(3)–R(2)C(1)	3.24	R(3)C(2)–R(5)C(4)	3.49
O(4)–N(1)	2.87	R(4)C(1)–R(5)C(4)	3.38

In this high-spin d^7 complex, the average Co–O axial bond length is 2.098 (4) Å, while the average Co–O equatorial bond length is 1.975 (8) Å, so that the difference of 0.123 (9) Å is highly significant. In a recent tabulation[1] it was pointed out that for the known d^8 and d^9 trigonal-bipyramidal MX_5 complexes no axial lengthening is observed, but rather that in some cases, such as the $CuCl_5^{3-}$ ion (d^9), significant axial shortening is observed. This is in keeping with the notion that d-electron–ligand repulsions are the determining factor here,[1,21] since ligand–ligand repulsions favor axial lengthening. In going from a d^9 system to a high-spin d^7 system, electrons are removed from the *xy* plane, and one expects, and finds here, that since d-electron repulsions are decreased, shortening of the M–X equatorial bonds results.

A related trend has been observed in the d^{10} $CdCl_5^{3-}$ ion,[22] where the Cd–Cl axial bond length is greater than the equatorial bond length. Here in going from a d^9 to a d^{10} system the extra electron fills the d_{z^2} orbital with consequent lengthening of the axial bond.

On the basis of the known structures of trigonal-bipyramidal MX_5 complexes, it thus appears that d-electron–ligand repulsion effects are of great importance in determining the differences between axial and equatorial bond lengths.

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