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The Crystal and Molecular Structure of the Perchlorate and Chloride of $[(NH_3)_5(CN)Co^{III}]^{2+}$ *

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The structures of the perchlorate and chloride of $[(NH_3)_5(CN)Co^{III}]^{2+}$ *have been determined by three-dimensional single-crystal x-ray analysis. Final conventional and weighted R factors are 0.082 and 0.119 respectively for the perchlorate and 0.080 and 0.105 respectively for the chloride. These structure determinations indicate the cyanide bonding mode is Co—C—N.*

Both structures are orthorhombic belonging to space group Cmcm. Reduced cell parameters for the perchlorate compound are a=*8.164(1),* b=*20.737 (4),* c=*7.724(1) Å, and those for the chloride are* a=*10.190(1),* b=*8.740(1),* c=*10.335(2) Å.*

Introduction

Transition metal cyanide ion coordination has long been the subject of much conjecture between experimenters from various fields. In many cyanide complexes, metal to carbon bonding is often assumed and this assumption is found in many textbooks.[1]

Spectral studies attempted thus far have been unable to unambiguously determine the cyanide ion coordination. Results of infrared studies on a series of cyanides favor the metal-ion to carbon atom coordination; however, the alternate coordination cannot be completely rejected.[2,3] Kuroda and Gentile[4] have recently analyzed the visible and ultraviolet spectra of two cobalt-cyanide complexes and they interpret their results in terms of Co—N coordination.

Early x-ray diffraction studies of transition metal cyanide complexes, such as the ferrocyanide ion or $KAg(CN)_2$,[5] were interpreted to indicate that the metal ion is attached to the carbon atom. However, even with today's modern instrumentation and high speed computers, atoms differing by only one electron can still be difficult to distinguish from one another. Even though neutron diffraction is better suited to this type of problem, only the molecular structures of $K_3Co(CN)_6$,[6] $K_2Zn(CN)_4$,[7] and $Hg(CN)_2$[8] have been attempted thus far by neutron diffraction. All of these studies have indicated metal to carbon bonding.

In 1968, Birk and Espenson[9] reported the chromium(II) oxidation by $[Co(NH_3)_5(CN)]^{2+}$. The kinetics and mechanism of the reaction were explained in terms of a C-bonded cobalt(III). However, the N-bonded model is not entirely excluded. Therefore, we decided to undertake the single-crystal x-ray diffraction analysis of $[(NH_3)_5(CN)Co^{III}](ClO_4)_2 \cdot 0.5H_2O$.

During the refinement of the above complex the perchlorate ions were found to be disordered. Consequently, we decided to carry on the single-crystal x-ray study of $[(NH_3)_5(CN)Co^{III}]Cl_2$ in conjunction with the above analysis.

Data Taking Procedure. All x-ray intensity data were taken on a Hilger-Watts four-circle diffractometer interfaced to an SDS 910 computer in a real time mode. Zirconium-filtered molybdenum radiation was used.

Data were taken using a θ-2θ step scan procedure with steps of 0.01 degrees in theta and a counting time of 0.4096 seconds per step. The number of steps through a given reflection varies with theta; $[50+(2\times\theta)]$ where θ is the peak center in degrees. Stationary-crystal, stationary-counter background measurements were made at the beginning and end of the step scan, each measurement being made for one-half the total scan time.

As a general check on electronic and crystal stability, the intensities of three standard reflections were measured periodically during the data collection period. Approximately 25 reflections per hour were obtained and logged on an IBM seven track tape.

Experimental Section

$[(NH_3)_5(CN)Co^{III}](ClO_4)_2 \cdot 0.5H_2O$ ———— X-ray.

Crystals of pentaaminecyanocobalt^{III} perchlorate were prepared by the method of Siebert.[10] Recrystallization from a water solution yielded red-orange crystals.

(*) Work was performed in the Ames Laboratory of the U. S. Atomic Energy Commission. Contribution No. 2698.

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(3) L. Jones, *J. Chem. Phys.*, *27*, 468 (1957).

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(7) A. Sequeria and R. Chidamboram, *Acta. Cryst.*, *20*, 910 (1966).

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(10) H. Siebert, Z. *Anorg. Allgem. Chem.*, *327*, 63 (1964).

Preliminary precession photographs (Mo Kα) showed the unit cell to be orthorhombic with systematic absences $hk\ell$ when $h+k \neq 2n$, and $h0\ell$ when $\ell \neq 2n$. These absences are consistent with space groups Cmcm, Cmc2_1, or Ama2 (alternate setting). The unit cell parameters at 25°C are $a = 8.164(1)$, $b = 20.737(4)$, $c = 7.724(1)$ Å. These parameters and their standard deviations were obtained by a least-squares fit to 15 independent reflections. The center of each reflection was found by left-right top-bottom beam splitting on the previously described Hilger-Watts diffractometer. Any error in the instrumental zero was eliminated by centering the reflection at both $+2\theta$ and -2θ. The calculated density of 1.92 g/cm^3 based on four molecules per unit cell agrees quite well with the observed density of 1.90 g/cm^3 which was determined by flotation techniques.

For data collection a cylindrical crystal with radius 0.08 mm and a height of 0.34 mm was mounted on a glass fiber. The latter direction was the c crystal axis and was coincident with the spindle axis. Complete three-dimensional data to $\sin\theta/\lambda = 0.7035$ at 25°C were taken for the four octants with positive ℓ index. The rest of the experimental arrangement for intesity collection has been discussed in some detail above.

The intensity data were corrected for Lorentz-polarization effects. The absorption coefficient, μ, is 18.14 cm^{-1}. The maximum and minimum transmission factors are 78.58 and 77.16% respectively, which were calculated using a modified version of Busing and Levy's ABCOR program.[11] Therefore, no absorption correction was made.

Of the 4543 possible observations, 1488 were found to be less than three times the standard deviation in the background and were subsequently disregarded. The three sigma criteria were tested on 1154 symmetry extinct reflections and were found to hold 96% of the time. Since four octants of equivalent intensity data were collected, a confidence test[12] was applied. This test was used to determine if any piece of a set of equivalent data should be disregarded. Only 112 of the remaining 3055 possible observations failed this confidence test. The individual values of F_o^2 from given equivalent sets were then averaged to yield 750 independent F_o^2 values. The standard deviations of F_o^2 were estimated from the averages of the individual intensities and their standard deviations.

$[(NH_3)_5(CN)Co^{III}]Cl_2$----------X-ray.

Crystals of pentaaminecyanocobalt(III) chloride, prepared by the method of Siebert[10] and recrystallized from a water solution, are orthorhombic with cell dimensions $a = 10.190(1)$, b = 8.740(1), $c = 10.335(2)$ Å, $D_m = 1.78$ gm cm^3 (by flotation), for $Z = 4$, $D_c = 1.76$ gm cm^3. Systematic absences ($hk\ell$ when $h+k \neq 2n$ and $h0\ell$ when $\ell \neq 2n$) indicate space groups Cmcm, Cmcm2_1, or Ama2 (alternate setting).

Complete three-dimensional X-ray diffraction intensity data to $\sin\theta/\lambda = 0.904$ were taken at room temperature (Mo Kα) using a crystal with dimensions $0.18 \times 0.28 \times 0.28$ mm along the a, b, and c crystal axes respectively, such that the c axis was along the spindle axis. The rest of the experimental arrangement for intensity collection has been previously described.

The intensity data were corrected for Lorentz-polarization effects and effects due to absorption. The three sigma test was applied to the intensity data and 682 of the 2003 possible observable reflections were rejected.

Solution and Refinement.

$[(NH_3)_5(CN)Co^{III}](ClO_4)_2 \cdot 0.5H_2O$---------X-ray.

A Howells', Phillips' and Rogers' plot[13] was obtained using all the collected data and indicated the presence of a center of symmetry and hence the appropriate space group was assumed to be Cmcm. An unsharpened Patterson function was calculated and a vector which was assumed to be a Co–Co vector resulting from the c-glide was located on the Harker line. The positions of the cobalt ligand atoms were also indicated from this three-dimensional Patterson function. However, the direction of the cyanide group could not be determined; hence the immediate ligand atoms were all assigned nitrogen scattering factors. Two cycles of positional refinement on the cobalt and immediate ligand atoms produced a conventional R-factor of 0.43.

The initial structure factor and electron density calculation indicated the direction of the cyanide group. It was also evident the perchlorate ions were in two four-fold sets (mm symmetry) instead of an eight-fold set and were disordered. After accounting for all the perchlorate oxygens in disordered positions there was still one peak left about the size of one-fourth an oxygen. This peak was assumed to be part of the water molecule. A difference Fourier was then computed, and it was verified that all non-hydrogen atoms had been accounted for, and some anisotropic motion was evident.

A full-matrix least-squares refinement minimizing the weighted R-factor, $wR = (\Sigma w(|F_o|-|F_c|)^2/\Sigma w|F_o|^2)^{1/2}$, was initiated with all atoms isotropic using the program of Busing *et al.*[11] and the atomic scattering factors of Hanson *et al.*[14] Two trial structures were assumed for refinement, one having the carbon atom of the cyanide group adjacent to the cobalt and the other having the nitrogen atom next to the cobalt. When the conventional R-factor ($R = \Sigma|F_o|-|F_c|/\Sigma|F_o|$) in both cases fell below 0.15, anisotropic refinement on all atoms except the disordered oxygens was begun. Since the temperature factors are a function of the occupancy numbers, it did not seem justifiable to refine the oxygens anisotropically. At this time the weighting scheme was modified from one based on counting statistics such that a plot of $\omega\Delta^2$ *versus* F_o^2 was a constant. The final convention-

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[11] In addition to programs written at this Laboratory, other programs used in this work were Johnson's ORTEP to prepare Figures 1 and 2, Busing and Levy's ORFFE to calculate errors, a modified version of Busing and Levy's ABCOR program and Busing, Martin and Levy's ORFLS program.

[12] R. B. Dean and W. J. Dixon, *Anal. Chem.*, *23*, 636 (1951).

[13] E. R. Howells, D. C. Phillips, and D. Rogers, *Acta, Cryst.*, *3*, 210 (1950).

[14] H. P. Hanson, F. Herman, J. D. Lee, and S. Skillman, *Acta Cryst. 17*, 1040 (1964).

Table Ia. Observed and calculated structure factors for $[(NH_3)_5(CN)Co^{III})](ClO_4)_2 . 0.5H_2O$

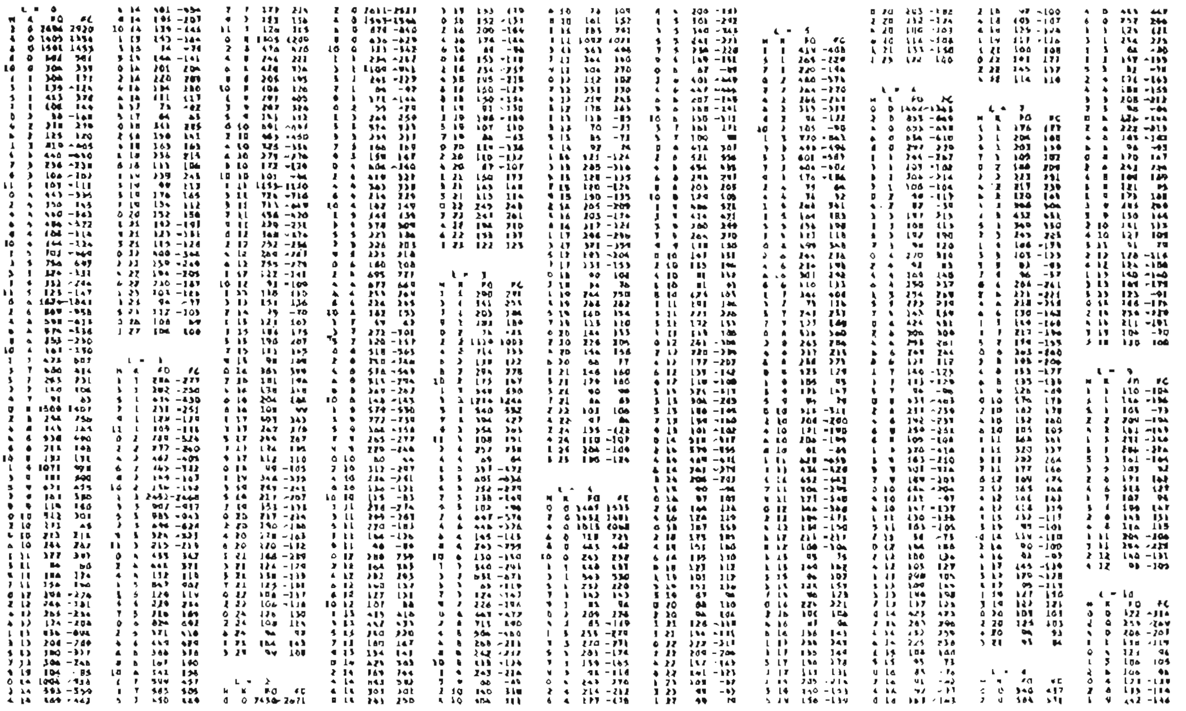

Table Ib. Final positional parameters for $[(NH_3)_5(CN)Co^{III})](ClO_4)_2 . 0.5H_2O$ [a]

Atom	x	y	z
Co	0.0	0.11100(6)	0.25 [b]
Cl(1)	0.0	0.74530(17)	0.25
Cl(2)	0.0	0.45085(41)	0.25
Cl(3)	0.0	0.38648(35)	0.25
C	0.0	0.02018(65)	0.25
N(1)	0.0	0.20740(53)	0.25
N(2)	0.0	−0.03473(59)	0.25
N(3)	0.17077(64)	0.11000(29)	0.06931(69)
O(1)	0.1442(24)	0.3483(09)	0.25
O(2	0.1360(30)	0.4828(12)	0.25
O(3)	0.0	0.4239(06)	0.4000(15)
O(4)	0.1214(20)	0.7373(08)	0.1172(15)
O(5)	0.0	0.8113(13)	0.25
O(6)	0.0	0.6767(28)	0.25
O(7)	0.0	0.5569(13)	0.25

[a] Numbers in parenthesis represent standard deviations occurring in the last digits of the parameter. [b] Numbers not followed by standard deviations are fixed by symmetry in this and subsequent tables.

al and weighted R-factors are 0.082 and 0.119 respectively for the Co—C—N model, 0.085 and 0.123 respectively for the Co—N—C model.

The observed and calculated structure factors for the Co—C—N model in space group Cmcm are given in Table Ia. The final positional, anisotropic temperature factors and standard errors are given in Tables Ib and Ic. In Table Ib, Cl(2) and Cl(3) are the half chlorines and O(7) is the water molecule. The more important interatomic distances, angles and their errors (calculated using the function and error program of Busing *et all.*[11]) are summarized in Table Id.

It may be noted here that the average effective isotropic B for the ammonia nitrogens is 4.2 Å· In the Co—C—N model the effective isotropic B's for C and N are 4.4 and 7.5 $Å^2$, respectively, while in the Co—N—C model the effective isotropic B's for C and N are 6.0 and 6.0 $Å^2$ respectively. Also, the experimental ratio of C:N integrated electron densities for the Co—C—N model is 0.864 while the calculated value is 0.857. For the Co—N—C model the experimental ratio of N:C integrated electron densities is 0.867.

$[(NH_3)_5(CN)Co^{III}]Cl_2$———X-ray.

An unsharpened Patterson map was calculated using all observed reflections. All non-hydrogen atomic positional parameters were found and placed accordingly in the unit cell. The direction of the cyanide group was assumed to be the same as in the perchlorate case.

Using the full-matrix least-squares program of Busing *et al.*[11] and the scattering factors of Hanson *et al.*[14] an isotropic refinement was undertaken on all atoms· After four iterations using a Co—C—N model in space group Cmcm the conventional and weighted R-factors were 0.112 and 0.094 respectively. After four cycles of anisotropic refinement the weighting scheme was modified such that a plot of $\omega\Delta^2$ *versus* F_o^2 was a constant. The final conventional and weighted R-factors are 0.076 and 0.101 respectively.

Refinement in space groups $Cmc2_1$ and Ama2 using a Co—C—N model gave weighted discrepancy factors of 0.095 and 0.091. However, both of these cases resulted in meaningless distortions of the cations and shifts in the anion positions· The centric space group Cmcm was also indicated by the HPR statistical test.[13]

Also, refinement of a Co—N—C model was carried out in space group Cmcm. Final conventional and

Table Ic. Final anisotropic temperature coefficients ×10^5 (Standard errors ×10^5 are given in parenthesis after the parameter)[a]

Atom	β_{11}	β_{22}	β_{33}	β_{12}	β_{13}	β_{23}
Co(1)	716(20)	197(3)	919(25)	0	0	0
Cl(1)	1799(61)	261(8)	1883(63)	0	0	0
Cl(2)	838(72)	390(20)	1398(98)	0	0	0
Cl(3)	1436(06)	298(18)	1979(127)	0	0	0
C	2723(308)	227(33)	1064(181)	0	0	0
N(1)	1826(196)	238(27)	1526(187)	0	0	0
N(2)	5392(492)	228(35)	1620(219)	0	0	0
N(3)	1336(79)	375(16)	1559(187)	3(27)	374(70)	−50(28)
O(1)	74(4)	—	—	—	—	—
O(2)	95(5)	—	—	—	—	—
O(3)	98(3)	—	—	—	—	—
O(4)	123(3)	—	—	—	—	—
O(5)	100(6)	—	—	—	—	—
O(6)	76(3)	—	—	—	—	—
O(7)	67(5)	—	—	—	—	—

[a] Dashed lines indicate that the β_{11} term is the isotropic B×10 followed by the errors ×10. The form of the anisotropic temperature factor expression is $[-(\beta_{11}h^2+\beta_{22}k^2+\beta_{33}l^2+2\beta_{12}hk+2\beta_{13}hl+2\beta_{23}kl)]$.

Table Id. Selected interatomic distances and angles in $[(NH_3)_5(CN)Co^{III}](ClO_4)_2 . 0.5H_2O$ [a]

Atoms	Distance, Å	Atoms	Angle, deg.
Co—C	1.883(0.013)	C—Co—N(3)	89.3(0.2)
Co—N(1)	1.999(0.011)	N(3)[b]—Co—N(3)	89.9(0.3)
Co—N(3)	1.972(0.005)	O(4)—Cl(1)—O(6)	83.3(0.7)
C—N(2)	1.138(0.017)	O(4)—Cl(1)—O(4)[b]	87.3(1.1)
Cl(1)—O(4)	1.435(0.015)	O(3)—Cl(2)—O(2)	102.8(0.5)
Cl(1)—O(5)	1.369(0.028)	O(2)—Cl(2)—O(2)[b]	118.3(2.4)
Cl(1)—O(6)	1.421(0.058)	O(3)—Cl(2)—O(3)[c]	128.5(1.2)
Cl(2)—O(2)	1.293(0.026)	O(3)—Cl(3)—O(1)	108.1(0.4)
Cl(2)—O(3)	1.286(0.012)	O(1)—Cl(3)—O(1)[b]	112.2(1.6)
Cl(3)—O(1)	1.418(0.021)	O(3)—Cl(3)—O(3)[c]	112.3(1.0)
Cl(3)—O(3)	1.395(0.013)		

[a] See Table Ib. [b] Implies atom transformed to (x, y, z). [c] Implies atom transformed to $(x, y, \frac{1}{2}-z)$.

weighted R-factors in this case are 0.080 and 0.105.

The observed and calculated structure factors for the Co–C–N model in space group Cmcm are given in Table IIa. The final positional, anisotropic temperature factors and standard errors are given in Tables IIb and IIc respectively. The more important distances, angles and their errors are summarized in Table IId·

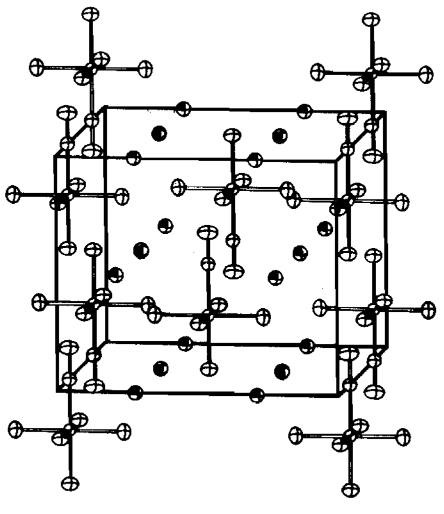

Figure 1. Crystal structure of $[(NH_3)_5(CN)Co^{III})]Cl_2$, the x-axis points (left to right) across the page, the y-axis points up the page and the z-axis points out of the page.

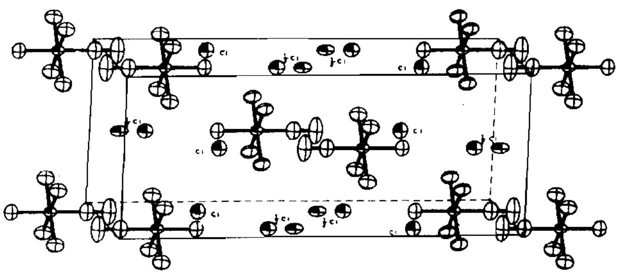

Figure 2. Crystal structure of $[(NH_3)_5(CN)Co^{III}](ClO_4)_2 . 0.5H_2O$, the x-axis points up the page, the y-axis points across the page (right to left) and the z-axis points out of the page.

For this compound the average isotropic B of the ammonia nitrogen is 2.4 Å^2. In the Co–C–N model the effective isotropic B's for C and N are 2.1 and 3.0 A^2 respectively and the experimental ratio of C:N integrated electron densities is 0.873. In the Co–N–C model the effective isotropic B's for C and N are 2.5 and 2.6 Å^2 respectively, while the experimental ratio of N:C integrated electron densities is 0.900.

Description of the Structure· The crystal structures of $[(NH_3)_5(CN)Co^{III}]Cl_2$ and $[(NH_3)_5(CN)Co^{III}](ClO_4)_2$ are depicted in Figures 1 and 2 respectively. In both cases the cobalt atom lies in a position of mm crystallographic symmetry with the $[(NH_3)_5(CN)Co^{III}]^{2+}$ having approximately C4v symmetry. In Figure 2 the mirror plane at a quarter in z bisects the four nitrogens in the equatorial plane while in Figure 1 the four-fold nitrogens lie in the mirror planes.

The disordered oxygens have been left out of Figure 2. The two chlorines labeled one half in Figure 2 share two oxygen atoms. Hence, one can imagine two tetrahedron joined together on an edge. The disorder about the other chlorine leads to an approximately octahedral arrangement of oxygen atoms. This by no means indicates that the geometry of a perchlorate ion is anything other tetrahedral.

Table IIa. Observed and calculated structure factors for $[(NH_3)_5(CN)Co^{III}]Cl_2$

H	K	FO	FC
L = 0			
2	0	832	699
4	0	2627	2259
6	0	1158	1070
8	0	651	570
10	0	919	801
12	0	148	128
14	0	476	389
16	0	120	88
18	0	169	132
1	1	223	253
3	1	1031	923
5	1	372	-324
7	1	803	715
9	1	278	-240
11	1	358	313
15	1	60	44
17	1	78	67
0	2	356	-226
2	2	1587	-1557
4	2	325	-247
6	2	921	-858
8	2	421	-366
10	2	242	-211
12	2	441	-385
16	2	281	-227
1	3	1304	-1125
5	3	1291	-1242
7	3	174	131
9	3	677	-620
13	3	193	-168
15	3	151	-112
19	3	79	-70
0	4	1838	1692
2	4	179	-191
4	4	1012	984
6	4	362	350
8	4	215	206
10	4	494	448
14	4	294	294
18	4	100	89
1	5	767	767
3	5	970	968
5	5	297	316
7	5	855	824
9	5	83	75
11	5	504	463
13	5	107	96
15	5	178	148
17	5	134	117
0	6	421	357
2	6	597	-574
4	6	196	184
6	6	254	-231
8	6	89	-90
10	6	55	49
12	6	199	-177
14	6	85	88
16	6	118	-100
1	7	605	-578
3	7	65	-63
5	7	780	-771
9	7	454	-450
11	7	98	-84
13	7	161	-144
15	7	132	-120
0	8	356	334
2	8	385	-378
4	8	185	181
6	8	111	-118
10	8	74	71
12	8	126	-122
14	8	87	75
16	8	87	-64
1	9	456	444
3	9	576	569
5	9	229	223
7	9	525	513
9	9	110	91
11	9	315	307
13	9	90	86
15	9	141	111
0	10	469	459
2	10	93	-82
4	10	318	310
6	10	105	89
8	10	86	77
10	10	174	170
14	10	120	112
1	11	224	-227
5	11	329	-325
7	11	62	43
9	11	215	-205
15	11	66	-68
2	12	336	-333
4	12	122	-93
6	12	201	-210
8	12	124	-132
10	12	83	-77
12	12	114	-125
1	13	73	57
3	13	134	138
7	13	141	144
11	13	81	82
0	14	312	301
2	14	71	77
4	14	221	225
6	14	145	131
8	14	119	101
10	14	140	133
7	15	67	72
2	16	110	-115
6	16	100	-81
1	17	74	-54
L = 1			
H	K	FO	FC
1	1	1265	-1235
3	1	594	-580
5	1	1147	-495
7	1	482	-450
9	1	467	-403
11	1	391	-353
13	1	180	-152
15	1	211	-176
17	1	111	-95
19	1	78	-59
0	2	332	-270
2	2	94	21
4	2	171	-145
6	2	182	-178
8	2	76	-70
10	2	146	-132
12	2	74	-65
14	2	72	-51
16	2	69	-53
1	3	882	835
3	3	437	439
5	3	730	705
7	3	351	339
9	3	329	294
11	3	286	262
13	3	114	112
15	3	146	132
17	3	91	72
19	3	70	45
0	4	1100	991
2	4	624	591
4	4	643	644
6	4	540	550
8	4	302	289
10	4	340	317
12	4	195	172
14	4	136	124
16	4	127	109
1	5	624	-593
3	5	419	-401
5	5	466	-471
7	5	267	-261
9	5	222	-211
11	5	196	-174
13	5	88	-82
15	5	105	-84
0	6	775	-761
2	6	490	-471
4	6	510	-527
6	6	488	-472
8	6	248	-253
10	6	298	-296
12	6	176	-162
14	6	132	-119
16	6	115	-110
18	6	90	-49
3	7	50	-44
0	8	609	585
2	8	411	398
4	8	425	432
6	8	384	391
8	8	220	229
10	8	252	257
12	8	156	149
14	8	107	112
16	8	109	98
1	9	175	184
3	9	147	150
5	9	164	156
7	9	107	109
9	9	90	89
11	9	79	73
0	10	286	-283
2	10	193	-190
4	10	217	-214
6	10	208	-204
8	10	132	-121
10	10	149	-147
12	10	98	-89
14	10	65	-68
16	10	93	-63
1	11	155	-159
3	11	119	-119
5	11	132	-151
7	11	95	-98
9	11	95	-92
11	11	107	-83
15	11	73	-49
0	12	92	100
4	12	76	75
6	12	71	75
10	12	66	60
1	13	169	174
3	13	148	140
5	13	152	163
11	13	93	93
1	15	95	-105
3	15	102	-84
5	15	89	-100
1	17	84	80
L = 2			
H	K	FO	FC
0	0	693	-613
2	0	1813	-1877
4	0	598	-465
6	0	1149	-1031
8	0	548	-461
10	0	341	-294
12	0	495	-439
16	0	292	-256
1	1	472	-520
3	1	462	414
5	1	933	-832
7	1	442	415
9	1	523	-455
11	1	145	120
13	1	113	-109
15	1	68	-49
19	1	82	-52
0	2	1758	1679
2	2	1014	-862
4	2	833	828
6	2	229	214
8	2	92	72
10	2	483	433
12	2	85	-75
14	2	272	244
18	2	84	83
1	3	336	296
3	3	717	697
5	3	119	-104
7	3	478	463
9	3	171	-156
11	3	370	343
15	3	95	75
17	3	85	77
0	4	224	217
2	4	892	-871
4	4	91	64
6	4	450	-474
8	4	197	-206
10	4	89	-77
12	4	301	-286
14	4	185	-172
1	5	681	-660
3	5	81	49
5	5	908	-918
7	5	123	125
9	5	516	-522
11	5	78	-71
13	5	170	-151
15	5	136	-129
0	6	716	672
2	6	415	-420
4	6	373	380
10	6	183	181
12	6	111	-112
14	6	125	131
1	7	184	156
3	7	367	348
7	7	401	416
9	7	87	-86
11	7	269	269
15	7	96	86
17	7	82	75
0	8	387	370
2	8	356	-338
4	8	211	212
6	8	90	-83
10	8	82	96
12	8	102	-101
14	8	83	88
1	9	450	-443
3	9	112	-135
5	9	558	-571
9	9	341	-351
11	9	98	-86
13	9	105	-124
15	9	111	-133
0	10	144	136
2	10	288	-298
4	10	72	59
6	10	138	-147
8	10	66	-77
12	10	116	-119
16	10	71	-73
1	11	79	90
3	11	198	200
7	11	220	216
11	11	126	132
0	12	321	330
4	12	224	226
6	12	91	98
8	12	66	66
10	12	132	132
14	12	86	84
1	13	113	-103
5	13	167	-165
9	13	112	-110
0	14	79	-61
2	14	206	-208
4	14	83	-73
6	14	135	-142
8	14	101	-92
5	15	67	-66
0	16	109	119
L = 3			
H	K	FO	FC
1	1	549	576
3	1	108	163
5	1	652	628
7	1	272	261
9	1	307	270
11	1	294	265
13	1	110	104
15	1	174	143
17	1	89	77
0	2	32	49
2	2	204	-168
6	2	82	76
10	2	78	87
1	3	452	-457
3	3	141	-179
5	3	442	-472
7	3	198	-201
9	3	202	-205
11	3	200	-199
13	3	88	-78
15	3	131	-109
0	4	656	-622
2	4	327	-313
4	4	371	-403
6	4	363	-378
8	4	179	-184
10	4	237	-240
12	4	121	-127
14	4	95	-94
16	4	93	-91
1	5	462	438
3	5	273	288
5	5	338	365
7	5	194	232
9	5	161	166
11	5	154	146
13	5	57	65
15	5	96	73
0	6	524	511
2	6	270	256
4	6	321	342
6	6	304	326
8	6	155	157
10	6	216	275
12	6	116	116
14	6	99	92
16	6	94	91
3	7	40	32
0	8	442	-427
2	8	280	-270
4	8	298	-309
6	8	282	-294
8	8	148	-161
10	8	202	-203
12	8	111	-117
14	8	95	-89
16	8	85	-85
1	9	125	-125
3	9	98	-95
5	9	89	-113
7	9	73	-70
9	9	68	-65
0	10	216	219
2	10	121	126
4	10	160	160
6	10	150	156
8	10	84	87
10	10	117	121
1	11	109	100
3	11	62	70
5	11	101	101
7	11	79	65
9	11	59	62
11	11	74	64
0	12	82	-78
4	12	67	-58
1	13	134	-131
3	13	90	-100
5	13	129	-129
7	13	91	-86
9	13	90	-83
11	13	72	-76
1	15	91	81
5	15	99	79
L = 4			
H	K	FO	FC
0	0	2655	2625
2	0	294	251
4	0	1617	1524
6	0	774	725
8	0	446	400
10	0	735	647
12	0	90	81
14	0	390	330
16	0	85	69
18	0	141	114
1	1	113	101
3	1	619	632
5	1	316	-307
7	1	616	585
9	1	257	-229
11	1	294	268
0	2	62	51
2	2	999	-1005
4	2	79	-62
6	2	582	-605
8	2	248	-247
10	2	171	-136
12	2	352	-315
16	2	215	-195
1	3	788	-711
3	3	55	48
5	3	839	-929
7	3	186	182
9	3	514	-503
13	3	154	-135
15	3	102	-92
19	3	76	-61
0	4	1316	1229
2	4	242	-237
4	4	700	742
6	4	229	238
8	4	140	143
10	4	377	372
14	4	235	221
1	5	493	491
3	5	694	701
5	5	145	167
7	5	638	657
11	5	374	384
13	5	80	69
15	5	121	124
17	5	119	100
0	6	351	325
2	6	485	-479
4	6	164	176
6	6	190	-191
8	6	70	-72
12	6	154	-155
14	6	82	80
16	6	135	-89
1	7	424	-406
3	7	46	49
5	7	586	-637
7	7	99	107
9	7	344	-365
13	7	119	-115
15	7	97	-100
0	8	342	321
2	8	320	-311
4	8	187	183
6	8	80	-88
8	8	43	-37
10	8	62	72
12	8	94	-103
1	9	350	341
3	9	458	450
5	9	169	159
7	9	401	430
9	9	79	62
11	9	235	263
13	9	65	70
15	9	104	56
0	10	380	376
2	10	113	-106
4	10	253	249
6	10	71	57
10	10	145	140
14	10	88	96
1	11	185	-185
9	11	155	-176
2	12	398	-272
4	12	85	-61
6	12	160	-170
8	12	110	-104
10	12	75	-60
12	12	97	-106
3	13	124	124
7	13	134	130
11	13	73	74
0	14	263	255
2	14	65	56
4	14	199	190
6	14	117	108
8	14	93	84
10	14	123	115
3	15	69	58
7	15	71	62
2	16	82	-98
L = 5			
H	K	FO	FC
1	1	1083	-1019
3	1	585	-631
5	1	763	-852
7	1	433	-452
9	1	377	-385
11	1	333	-330
13	1	156	-155
15	1	168	-167
17	1	99	-92
0	2	328	-294
2	2	144	-128
4	2	151	-190
6	2	170	-190
8	2	86	-91
10	2	130	-128
12	2	76	-69
1	3	739	719
3	3	435	461
5	3	519	410
7	3	301	333
9	3	255	281
11	3	236	247
13	3	117	114
15	3	111	126
17	3	47	70
0	4	841	817
2	4	550	548
4	4	502	576
6	4	434	492
8	4	249	282
10	4	252	296
12	4	155	166
14	4	122	121
16	4	107	102
1	5	486	-482
3	5	318	-344
5	5	353	-398
7	5	207	-232
9	5	167	-194
11	5	145	-158
13	5	73	-79
15	5	64	-78
17	5	60	-43
0	6	690	-672
2	6	461	-466
4	6	452	-489
6	6	412	-441
8	6	228	-254
10	6	243	-279
12	6	150	-161
14	6	103	-117
16	6	89	-105
0	8	547	536
2	8	372	379
4	8	398	408
6	8	323	366
8	8	204	225
10	8	209	244
12	8	117	144
14	8	97	109
16	8	82	93
1	9	172	174
3	9	142	148
5	9	133	146
7	9	103	109
9	9	70	85
11	9	79	72
0	10	272	-265
2	10	195	-193
4	10	205	-206
6	10	196	-197
8	10	110	-123
10	10	124	-140
12	10	69	-88
1	11	170	-162
3	11	122	-124
5	11	150	-153
7	11	97	-100
9	11	84	-95
11	11	90	-81
0	12	104	99
2	12	60	59
6	12	74	73
1	13	159	171
3	13	133	143
5	13	145	157
7	13	117	117
9	13	89	100
11	13	78	90
1	15	86	-104
5	15	76	-99
L = 6			
H	K	FO	FC
0	0	689	-700
2	0	1412	-1486
4	0	541	-572
6	0	935	-914
8	0	506	-483
10	0	316	-312
12	0	426	-410
14	0	59	-53
16	0	230	-233
1	1	405	-379
3	1	154	178
5	1	569	-626
7	1	262	274
9	1	381	-381
11	1	82	79
13	1	59	-79
15	1	62	-47
0	2	1448	1349
2	2	158	-156
4	2	704	818
6	2	279	318
8	2	160	169
10	2	349	413
14	2	225	229
1	3	385	384
3	3	611	653
7	3	533	593
11	3	293	313
15	3	65	79
17	3	63	73
2	4	772	-776
4	4	79	-84
6	4	392	-446
8	4	236	-228
10	4	99	-104
12	4	227	-261
16	4	137	-153
1	5	704	-668
3	5	158	-160
5	5	726	-826
9	5	420	-488
11	5	108	-108
13	5	146	-165
15	5	114	-129
0	6	580	528
2	6	285	-288
4	6	298	314
10	6	135	155
12	6	77	-83
14	6	100	110
1	7	269	257
3	7	408	405
5	7	71	75
7	7	371	414
11	7	230	261
15	7	69	91
0	8	335	324
2	8	237	-234
4	8	191	196
10	8	68	90
14	8	89	77
1	9	443	-429
3	9	156	-157
5	9	485	-520
7	9	63	-60
9	9	279	-324
11	9	85	-101
13	9	99	-122
15	9	76	-96
0	10	50	58
2	10	287	-291
6	10	145	-157
8	10	98	-94
12	10	81	-113
1	11	105	105
3	11	181	191
7	11	180	197
11	11	102	120
0	12	300	313
4	12	221	224
6	12	86	107
10	12	101	129
1	13	89	-90
5	13	129	-139
0	14	92	-83
2	14	202	-201
4	14	73	-89
6	14	128	-141
8	14	89	-96
0	16	100	114
L = 7			
H	K	FO	FC
1	1	481	493
3	1	239	274
5	1	429	479
7	1	246	243
9	1	230	251
11	1	223	222
13	1	92	97
15	1	122	124
17	1	42	69
0	2	113	121
4	2	58	72
6	2	86	87
10	2	71	78
1	3	376	-373
3	3	191	-211
5	3	290	-341
7	3	153	-179
9	3	155	-175
11	3	142	-166
13	3	72	-73
15	3	68	-94
0	4	463	-451
2	4	301	-286
4	4	289	-321
6	4	281	-300
8	4	145	-144
10	4	187	-198
12	4	87	-113
14	4	68	-83
16	4	74	-79
18	4	64	-36
1	5	319	303
3	5	217	217
5	5	250	262
7	5	134	161
9	5	116	131
11	5	111	119
13	5	59	56
0	6	446	403
2	6	247	233
4	6	289	288
6	6	253	268
8	6	127	144
10	6	166	191
12	6	105	104
14	6	73	46
16	6	63	79
0	8	360	-338
2	8	244	-235
4	8	253	-255
6	8	236	-245
8	8	137	-144
10	8	163	-172
12	8	72	-105
14	8	78	-78
16	8	65	-74
1	9	114	-107
3	9	87	-82
5	9	95	-99
9	9	61	-60
0	10	191	187
2	10	127	112
4	10	150	140
6	10	119	134
8	10	73	83
10	10	96	105
1	11	89	94
3	11	74	72
5	11	81	91
7	11	66	65
0	12	59	-65
2	12	61	-44
1	13	122	-118
3	13	95	-92
5	13	117	-115
7	13	68	-78
9	13	71	-76
1	15	65	73
5	15	71	70
L = 8			
H	K	FO	FC
0	0	1300	1199
4	0	714	774
6	0	354	352
8	0	204	207
10	0	406	411
14	0	228	227
16	0	82	47
18	0	77	83
3	1	316	344
5	1	217	-227
7	1	358	380
9	1	174	-174
11	1	173	185
17	1	68	42
0	2	158	140
2	2	549	-521
4	2	69	68
6	2	286	-315
8	2	116	-119
12	2	193	-204
16	2	126	-137
1	3	347	-327
3	3	101	103
5	3	481	-530
7	3	153	179
9	3	286	-321
13	3	89	-86
15	3	70	-62
0	4	797	692
2	4	211	-198
4	4	421	439
6	4	110	117
8	4	66	74
10	4	224	247
14	4	134	156
1	5	247	222
3	5	413	392
7	5	368	412
11	5	221	256
17	5	67	73
0	6	294	242
2	6	336	-315
4	6	132	137
6	6	122	-123
12	6	88	-110
1	7	222	-208
3	7	90	92
5	7	364	-371
7	7	102	118
9	7	211	-234
15	7	75	-70
0	8	262	247
2	8	217	-202
4	8	151	147
10	8	58	59
1	9	214	202
3	9	302	294
5	9	101	85
7	9	288	289
11	9	156	184
0	10	252	244
2	10	108	-100
4	10	157	158
10	10	85	94
1	11	117	-118
5	11	187	-189
9	11	96	-123
2	12	175	-177
6	12	104	-110
3	13	101	92
7	13	93	97
0	14	171	177
4	14	134	131
6	14	74	74
L = 9			
H	K	FO	FC
1	1	451	-425
3	1	247	-270
5	1	344	-435
7	1	203	-223
9	1	193	-210
11	1	182	-196
13	1	91	-93
15	1	114	-111
0	2	130	-115
2	2	68	-47
4	2	69	-77
6	2	74	-86
10	2	61	-70
1	3	329	319
3	3	197	208
5	3	264	301
7	3	154	171
9	3	131	155
11	3	142	150
13	3	65	69
15	3	93	84
0	4	404	379
2	4	249	246
4	4	260	280
6	4	217	255
8	4	119	149
10	4	159	176
12	4	95	100
14	4	72	79
16	4	66	69
1	5	248	-250
3	5	173	-179
5	5	203	-226
7	5	118	-133
9	5	104	-121
11	5	71	-101
0	6	351	-332
2	6	238	-226
4	6	237	-248
6	6	222	-239
8	6	127	-137
10	6	144	-167
12	6	90	-101
14	6	65	-75
16	6	74	-73
0	8	319	306
2	8	216	204
4	8	241	235
6	8	209	216
8	8	134	134
10	8	124	157
12	8	91	93
14	8	68	75
1	9	101	91
3	9	83	79
5	9	90	78
7	9	64	62
9	9	60	47
11	9	66	45
0	10	162	-159
2	10	121	-117
4	10	132	-125
6	10	129	-126
8	10	80	-79
10	10	95	-93
12	10	69	-61
1	11	94	-90
5	11	83	-91
9	11	76	-59
0	12	70	70
2	12	59	39
1	13	102	108
3	13	86	91
5	13	94	100
7	13	70	78
9	13	64	67
1	15	72	-70
L = 10			
H	K	FO	FC
0	0	360	-365
2	0	785	-857
4	0	291	-343
6	0	521	-570
8	0	330	-334
10	0	231	-225
12	0	289	-290
14	0	65	-55
16	0	151	-167
1	1	230	-214
3	1	89	92
5	1	314	-379
7	1	147	164
9	1	221	-250
11	1	52	45
0	2	846	777
2	2	46	-43
4	2	440	514
6	2	180	216
8	2	117	133
10	2	261	285
14	2	156	165
1	3	223	226
3	3	389	401
7	3	331	387
11	3	197	215
2	4	519	-499
4	4	74	-74
6	4	254	-300
8	4	143	-168
10	4	76	-86
12	4	165	-185
16	4	81	-110
1	5	463	-432
3	5	126	-132
5	5	512	-542
9	5	302	-339
11	5	90	-92
13	5	114	-125
15	5	84	-98
0	6	355	333
2	6	181	-172
4	6	213	205
10	6	77	105
12	6	61	-49
1	7	204	192
3	7	294	290
5	7	79	73
7	7	288	292
11	7	144	189
13	7	63	45
0	8	215	211
2	8	148	-146
4	8	139	130
1	9	337	-304
3	9	150	-130
5	9	361	-362
9	9	209	-233
11	9	67	-84
2	10	218	-204
6	10	102	-116
8	10	74	-73
1	11	85	84
3	11	155	139
7	11	129	141
11	11	87	88
0	12	227	222
4	12	176	163
6	12	98	86
8	12	68	68
10	12	75	96
5	13	100	-98
0	14	73	-73
2	14	153	-149
4	14	86	-75
L = 11			
H	K	FO	FC
1	1	421	412
3	1	261	300
5	1	314	379
7	1	211	237
9	1	232	210
11	1	164	190
13	1	94	100
15	1	83	105
0	2	162	140
2	2	83	81
4	2	99	103
6	2	76	99
10	2	88	75
1	3	321	-307
3	3	220	-220
5	3	261	-286
7	3	157	-173
9	3	140	-159
11	3	129	-141
13	3	67	-75
15	3	73	-79
0	4	361	-343
2	4	274	-263
4	4	269	-268
6	4	218	-248
8	4	149	-158
10	4	155	-167
12	4	95	-105
14	4	69	-76
16	4	90	-66
1	5	214	211
3	5	169	167
5	5	162	186
7	5	97	120
9	5	84	104
11	5	89	94
0	6	359	332
2	6	242	232
4	6	262	257
6	6	231	234
8	6	133	148
10	6	148	166
12	6	88	100
14	6	71	78
0	8	298	-277
2	8	239	-219
4	8	232	-222
6	8	215	-210
8	8	136	-139
10	8	122	-146
12	8	94	-95
1	9	108	-98
3	9	75	-80
5	9	84	-89
0	10	175	163
2	10	121	112
4	10	126	129
6	10	119	119
8	10	81	80
10	10	77	90
1	11	100	99
3	11	99	84
5	11	94	90
7	11	93	71
1	13	121	-110
3	13	114	-91
5	13	99	-104
7	13	83	-74
L = 12			
H	K	FO	FC
0	0	750	692
2	0	72	76
4	0	440	483
6	0	230	247
8	0	156	166
10	0	270	276
12	0	73	52
14	0	141	156
3	1	190	207
5	1	100	-114
7	1	199	230
9	1	77	-90
11	1	110	116
2	2	369	-353
6	2	189	-221
8	2	94	-106
10	2	73	-63
12	2	123	-143
1	3	234	-213
5	3	286	-327
7	3	67	76
9	3	193	-208
0	4	474	422
2	4	74	-69
4	4	276	282
6	4	91	98
10	4	155	166
14	4	93	105
1	5	201	179
3	5	294	270
5	5	55	64
7	5	254	279
11	5	156	177
0	6	135	133
2	6	200	-186
4	6	85	73
6	6	137	-77
12	6	64	-68
1	7	177	-165
5	7	259	-254
9	7	152	-166
0	8	139	131
2	8	147	-128
4	8	72	74
12	8	67	-45
1	9	171	154
3	9	228	206
5	9	87	83
7	9	192	198
11	9	127	128
0	10	172	167
4	10	119	115
1	11	97	-85
5	11	133	-125
9	11	103	-84
2	12	130	-127
6	12	88	-85
L = 13			
H	K	FO	FC
1	1	207	-177
3	1	93	-110
5	1	150	-184
7	1	103	-102
9	1	98	-105
11	1	115	-106
15	1	74	-67
0	2	60	-43
1	3	143	135
3	3	78	86
5	3	125	137
7	3	65	80
9	3	82	78
0	4	181	171
2	4	107	105
4	4	130	129
6	4	124	123
8	4	79	73
10	4	91	95
14	4	81	47
1	5	130	-120
3	5	94	-85
5	5	109	-115
7	5	90	-68
9	5	88	-67
11	5	65	-57
0	6	155	-151
2	6	110	-100
4	6	125	-114
6	6	128	-118
8	6	75	-69
10	6	91	-91
0	8	176	157
2	8	106	100
4	8	130	122
6	8	109	115
10	8	88	90
12	8	70	56
0	10	82	-86
2	10	72	-65
6	10	94	-72
1	13	74	63
L = 14			
H	K	FO	FC
0	0	137	-115
2	0	381	-376
4	0	108	-126
6	0	270	-258
8	0	162	-153
10	0	117	-110
12	0	165	-150
1	1	118	-94
3	1	64	58
5	1	182	-185
7	1	100	90
9	1	120	-127
0	2	367	336
2	2	71	-69
4	2	208	219
6	2	67	80
10	2	141	139
14	2	112	87
1	3	75	74
3	3	190	170
7	3	178	181
11	3	108	137
2	4	258	-237
6	4	133	-145
8	4	103	-82
12	4	114	-99
1	5	211	-188
5	5	263	-258
9	5	173	-170
11	5	64	-47
13	5	97	-67
0	6	179	168
2	6	89	-92
4	6	109	104
10	6	66	55
1	7	86	74
3	7	150	127
7	7	133	141
11	7	105	98
0	8	116	99
2	8	74	-86
1	9	165	-153
5	9	199	-187
9	9	132	-125
2	10	101	-98
3	11	89	73
0	12	115	112
L = 15			
H	K	FO	FC
1	1	230	221
3	1	169	170
5	1	213	208
7	1	161	141
9	1	134	127
11	1	129	115
13	1	74	66
0	2	83	77
2	2	53	49
1	3	167	-167
3	3	142	-126
5	3	164	-159
7	3	113	-103
9	3	137	-97
11	3	107	-86
0	4	203	-183
2	4	167	-147
4	4	162	-149
6	4	146	-141
8	4	88	-96
10	4	97	-99
12	4	72	-66
1	5	116	116
3	5	102	96
5	5	96	104
0	6	200	185
2	6	145	135
4	6	152	149
6	6	125	137
8	6	94	92
10	6	110	101
0	8	173	-161
2	8	154	-133
4	8	136	-133
6	8	135	-127
8	8	86	-89
0	10	107	102
2	10	70	74
4	10	99	83
6	10	79	76
L = 16			
H	K	FO	FC
0	0	441	403
2	0	112	117
4	0	319	301
6	0	197	184
8	0	132	135
10	0	202	177
3	1	119	115
7	1	134	122
0	2	66	-60
2	2	249	-230
4	2	88	-72
6	2	160	-158
8	2	103	-95
10	2	82	-67
1	3	162	-144
5	3	210	-192
9	3	138	-125
0	4	275	245
4	4	190	176
6	4	97	86
8	4	84	64
10	4	98	105
1	5	170	149
3	5	215	192
5	5	91	87
7	5	192	179
2	6	111	-99
1	7	155	-134
5	7	193	-168
9	7	119	-113
2	8	84	-71
1	9	131	118
3	9	146	140
5	9	79	79
0	10	124	106
L = 17			
H	K	FO	FC
1	1	173	-136
3	1	127	-104
5	1	144	-133
7	1	84	-89
9	1	96	-84
1	3	113	102
3	3	84	79
5	3	108	98
7	3	76	68
9	3	73	62
0	4	135	121
2	4	98	89
4	4	103	98
6	4	104	90
8	4	71	63
1	5	74	-75
5	5	76	-71
0	6	125	-112
2	6	114	-89
4	6	115	-92
6	6	108	-90
8	6	80	-62
0	8	127	110
2	8	92	82
4	8	89	91
L = 18			
H	K	FO	FC
2	0	169	-165
6	0	115	-119
5	1	92	-80
0	2	157	143
4	2	103	95
3	3	91	73
7	3	83	80
2	4	128	-106
6	4	76	-69
1	5	89	-88
5	5	129	-118
4	6	67	46
3	7	82	60
L = 19			
H	K	FO	FC
1	1	106	79
5	1	85	79
5	3	71	-62
L = 20			
H	K	FO	FC
0	0	187	175

Table IIb. Final positional parameters for $[(NH_3)_5(CN)Co^{III})]Cl_2$ [a]

Atom	x	y	z
Co	0.0	0.21599(09)	0.25
N(1)	0.0	0.44441(56)	0.25
N(2)	0.0	−0.13299(74)	0.25
N(3)	0.19289(38)	0.21765(46)	0.25
N(4)	0.0	0.21253(43)	0.05886(31)
C	0.0	−0.00230(68)	0.25
Cl	0.28386(10)	0.0	0.0

[a] See Table Ib.

However, since the perchlorate ion is almost spherical by nature, it is not surprising in this case that it has little preference regarding its orientation in packing.

The average values of the Co–C, Co–N, and C–N bond lengths agree quite well with previously reported values in the literature.[15-17]

Conclusion

The main interest in these structure determinations lies in the attempt to distinguish between the Co–C–N and Co–N–C models. We conclude that the former is the correct bonding mode on the following evidence:

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(15) N. A. Curry and W. A. Runciman, *Acta Cryst.*, *12*, 674 (1959).

(16) Y. Tanito, Y. Saito, and H. Kuroya, *Bull. Chem. Soc. Japan*, *25*, 188 (1925).

(17) Y. Tanito, Y. Saito, and H. Kuyoya, *Bull. Chem. Soc. Japan*, *26*, 420 (1953).

Table IIc. Final anisotropic coefficients $\times 10^5$ (Standard errors $\times 10^5$ are given in parenthesis after the parameter)[a]

Atom	β_{11}	β_{22}	β_{33}	β_{12}	β_{13}	β_{23}
Co	409(5)	470(6)	302(4)	0	0	0
N(1)	857(53)	579(49)	488(35)	0	0	0
N(2)	1046(66)	668(57)	616(43)	0	0	0
N(3)	490(25)	909(42)	535(26)	6(26)	0	0
N(4)	756(33)	813(37)	332(20)	0	0	17(23)
C	561(43)	682(53)	401(35)	0	0	0
Cl	556(8)	735(11)	494(7)	0	0	20(6)

[a] See footnote in Table Ic.

Table IId. Selected interatomic distances and angles in $[(NH_3)_5(CN)Co^{III})Cl_2$[a]

Atoms	Distance, Å	Atoms	Angles, deg.
Co—N(1)	1.996(0.0005)	C—Co—N(3)	90.42(0.12)
Co—N(3)	1.965(0.004)	C—Co—N(4)	89.12(0.10)
Co—N(4)	1.975(0.003)	C—Co—N(3)	90.04(0.17)
Co—C	1.908(0.006		
C—N(2)	1.142(0.008)		

[a] See Table Ib.

a) Integrated electron densities of both structures favored the Co—C—N model.

b) In both cases, the Co—C—N model gave better agreement factors.

c) In both structures, the effective isotropic temperature factor of the atom bonded to the cobalt atom had a tendency to increase when the Co—N—C model was involked. The trend would, of course, be observed if a nitrogen were input where a carbon should be located.