TABLE VI

BOND ANGLES

Bonded atoms	Bond angle, deg	Bonded atoms	Bond angle, deg
Cl_1–Zn–Cl_2	114.7 ± 0.1	C_5–C_4–C_{12}	121.0 ± 0.9
N_1–Zn–Cl_1	108.7 ± 0.3	C_4–C_5–C_6	120.1 ± 0.9
N_1–Zn–Cl_2	115.9 ± 0.2	C_5–C_6–C_7	120.7 ± 0.8
N_2–Zn–Cl_1	124.6 ± 0.2	C_6–C_7–C_{11}	120.4 ± 0.9
N_2–Zn–Cl_2	108.2 ± 0.3	C_8–C_7–C_{11}	115.7 ± 0.8
N_1–Zn–N_2	80.4 ± 0.3	C_7–C_8–C_9	120.9 ± 0.9
C_{12}–N_1–Zn	113.2 ± 0.6	C_8–C_9–C_{10}	119.3 ± 1.0
C_{11}–N_2–Zn	112.9 ± 0.6	C_9–C_{10}–N_2	121.0 ± 0.9
C_{12}–N_1–C_1	118.8 ± 0.7	C_{10}–N_2–C_{11}	118.0 ± 0.7
N_1–C_1–C_2	121.8 ± 0.8	N_2–C_{11}–C_7	124.9 ± 0.9
C_1–C_2–C_3	119.4 ± 1.0	C_7–C_{11}–C_{12}	119.1 ± 0.8
C_2–C_3–C_4	119.7 ± 0.9	C_{11}–C_{12}–C_4	118.5 ± 0.7
C_3–C_4–C_{12}	116.4 ± 0.8	N_1–C_{12}–C_4	124.0 ± 0.9

of the fact that in $ZnCl_2 \cdot$phen the N_1 and N_2 atoms are separated by 2.67 A and fixed in a relatively rigid ring system. Thus an N_1–Zn–N_2 tetrahedral angle would require Zn–N bond distances of 1.64 A, which would represent a drastic reduction from the Zn–N bond distance of 2.04 A observed in $ZnCl_2 \cdot 2NH_3$, in which the N–N distance is not fixed.

The geometry of the phenanthroline molecule is similar to the geometry of the phenanthrene molecule determined by Trotter.[6] The latter molecule differs from the former by the replacement of nitrogen atoms by carbon atoms. In the phenanthroline molecule, it was observed that bond C_{11}–C_{12} is longer than bond C_5–C_6 while bonds C_7–C_8 and C_3–C_4 are longer than bonds C_{10}–N_2 and C_1–N_1, respectively. The corresponding bonds in phenanthrene were observed to be in the same order.

The interpretation of the paramagnetic resonance and electronic spectral data on copper(II)-doped dichloro-(1,10-phenanthroline)zinc is in progress. The hyperfine structure in the paramagnetic resonance spectrum has been shown to arise from a coupling to both the nitrogen and the chlorine nuclei. The extent of 4p admixture into the primarily 3d copper(II) orbitals, the bonding parameters, and all supporting spectroscopic data will be reported elsewhere.[2]

(6) J. Trotter, *Acta Cryst.*, **16**, 605 (1963).

CONTRIBUTION FROM THE LAWRENCE RADIATION LABORATORY AND DEPARTMENT OF CHEMISTRY,
UNIVERSITY OF CALIFORNIA, BERKELEY, CALIFORNIA

The Crystal Structure of $(B_9C_2H_{11})Re(CO)_3Cs$[1]

BY ALLAN ZALKIN, TED E. HOPKINS, AND DAVID H. TEMPLETON

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The crystal structure of the cesium salt of π-(1)-2,3-dicarbollylrhenium tricarbonyl, $(B_9C_2H_{11})Re(CO)_3Cs$, has been determined from an X-ray diffraction study of a single crystal specimen. The monoclinic cell, space group $P2_1/c$, with a = 11.435 A, b = 9.516 A, c = 12.730 A, and β = 92.87°, contains four formula units. The structure was determined by straightforward crystallographic techniques, and the atomic parameters of all but the hydrogen atoms were refined by a full-matrix least-squares procedure. The rhenium atom occupies an apex position of an icosahedron containing boron and carbon, and on the other side occupies the apex of a trigonal pyramid whose base is three carbonyls. In the icosahedron the two carbon atoms are adjacent to each other and to the rhenium.

Introduction

π-(1)-2,3-Dicarbollylrhenium tricarbonyl was synthesized by Hawthorne and Andrews.[2] The structure work was undertaken to reaffirm the results of our previous study on the dicarbollyliron structure[3] in $C_5H_5FeB_9C_2H_{11}$. In that study there was considerable thermal motion of the cyclopentadienyl ring, and to a lesser extent of the dicarbollyl portion, $B_9C_2H_{11}$. This thermal motion, evidenced by large thermal parameters, does not permit the calculation of accurate bond distances. The $B_9C_2H_{11}Re(CO)_3Cs$ crystal does not suffer these thermal effects as badly, and the resulting structure is we believe a more accurate description of the dicarbollyl geometry.

The present work confirms the geometry of this compound postulated by Hawthorne and Andrews.[2]

Experimental Section

The crystals were sent to us by Dr. M. F. Hawthorne of the Riverside campus of the University of California. A small white crystal, ~0.25 mm long and ~0.08 × ~0.08 mm in cross section, was glued to the end of a Pyrex glass fiber. The long direction of the crystal was parallel to the fiber and is the direction of the b axis. A General Electric XRD-5 X-ray diffraction setup equipped with a Molybdenum X-ray tube (Mo $K\alpha_1$, λ 0.70926 A), a scintillation counter, a pulse height discriminator, and a quarter-circle Eulerian-cradle type goniostat was used. The X-ray tube was operated at 50 kv and 20 ma, and a Zr filter was used on the receiving slit. The crystal was oriented such that the b axis was parallel to the ϕ axis. The cell dimensions were obtained from carefully measured 2θ (θ is the Bragg angle) values of the $0k0$, $h00$, and $00l$ reflections whose $\alpha1$ and $\alpha2$ components were resolved. The β angle was measured directly from the angle between the $h00$ and $00l$ sets of reflections.

A total of 2452 independent intensities were measured, of which 138 were recorded as zero. A stationary crystal, station-

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(1) Work done under the auspices of the U. S. Atomic Energy Commission.

(2) M. F. Hawthorne and T. D. Andrews, *J. Am. Chem. Soc.*, **87**, 2496 (1965).

(3) A. Zalkin, D. H. Templeton, and T. E. Hopkins, *ibid.*, **87**, 3988 (1965).

TABLE I

FINAL POSITIONAL AND THERMAL PARAMETERS[a] IN $CsB_9C_2H_{11}Re(CO)_3$[b]

Atom	x	y	z	B_{11}	B_{22}	B_{33}	B_{12}	B_{13}	B_{23}
Cs	0.2766	0.1909	−0.0065	3.77	4.57	4.65	0.19	0.53	0.08
Icosahedron									
Re(1)	−0.1495	0.1406	0.2316	2.09	1.88	2.08	0.14	0.18	0.01
C(2)	−0.232	0.356	0.267	3.4	2.6	2.0	0.1	0.0	−0.2
C(3)	−0.327	0.232	0.279	2.6	2.3	2.2	0.5	0.7	0.3
B(4)	−0.342	0.138	0.164	2.3	1.9	2.8	−0.5	−0.2	−0.1
B(5)	−0.248	0.214	0.075	2.8	2.2	2.6	0.0	0.3	−0.4
B(6)	−0.176	0.358	0.145	3.3	2.2	2.3	−0.2	−0.2	0.3
B(7)	−0.377	0.404	0.269	2.8	3.6	2.2	1.0	0.0	−0.1
B(8)	−0.449	0.263	0.200	2.1	4.0	2.7	0.7	0.6	−0.1
B(9)	−0.401	0.260	0.071	2.5	3.3	3.0	0.3	0.1	−0.7
B(10)	−0.295	0.393	0.060	3.3	3.1	2.9	−0.2	0.8	1.0
B(11)	−0.282	0.483	0.180	3.6	2.9	2.8	1.2	0.2	0.6
B(12)	−0.422	0.425	0.134	3.2	4.2	2.4	0.8	0.0	0.0
Carbonyls									
C(1)–CO	−0.043	0.167	0.349	2.7	2.8	3.6	0.5	0.3	0.2
C(2)–CO	−0.021	0.092	0.153	2.4	3.3	3.0	0.4	0.4	0.5
C(3)–CO	−0.168	−0.048	0.275	4.7	2.9	2.8	0.7	0.3	0.2
O(1)–CO	0.024	0.193	0.418	4.3	6.9	4.4	1.4	−2.1	−2.2
O(2)–CO	0.057	0.065	0.102	3.6	5.0	3.6	1.5	0.7	0.3
O(3)–CO	−0.187	−0.162	0.300	7.4	2.4	7.1	−0.1	0.8	1.4

Hydrogens[c]	x	y	z	Hydrogens[c]	x	y	z
H(2)	−0.20	0.40	0.34	H(7)	−0.40	0.46	0.34
H(3)	−0.36	0.20	0.36	H(8)	−0.54	0.28	0.20
H(4)	−0.38	0.04	0.18	H(9)	−0.46	0.20	0.02
H(5)	−0.20	0.18	0.00	H(11)	−0.26	0.60	0.20
H(6)	−0.10	0.42	0.12	H(12)	−0.50	0.48	0.10

[a] Units are A^2. The anisotropic values $B_{ij} = 4\beta_{ij}/a_i^*a_j^*$ where a_i^* is the ith reciprocal cell length. [b] Standard deviations of the positional parameters of Cs and Re are 0.0001 or less, and 0.001 or less for all the other atoms excluding hydrogens. Standard deviations of the thermal parameters are 0.04 or less for Cs and Re, and 0.7 or less for all the other atoms excluding hydrogens. [c] Hydrogen positional parameters are those from a difference Fourier and were not refined by least squares. H(10) was not found. The labeling is parallel to the labeling in the icosahedron, *i.e.*, H(5) is the hydrogen to B(5).

ary counter technique using a 10-sec count for every reflection was used. The maximum 2θ angle was 50° ($\sin\theta/\lambda = 0.595$). The maximum observed raw intensity was 7800 cps for the $11\bar{2}$ reflection. The data were corrected for the Lorentz and polarization effects. No corrections were made for either absorption or extinction.

All of the computations were performed on an IBM 7044 computer with a 32 K memory. Our unpublished least-squares program minimizes the function $\Sigma w(|F_o| - |F_c|)^2/\Sigma wF_o^2$, where F_o and F_c are the observed and calculated structure factors and w is the weighting factor. All of the reflections were given equal weight. The least-squares program has been modified to handle the anomalous dispersion, and these effects were included in the final set of refinements. The atomic scattering factors[4] for neutral Re and Cs^+ were corrected for $\Delta f'$, the real part of the anomalous dispersion,[5,6] by the amounts −1.3 and −0.5 electrons, respectively. The imaginary components of the anomalous dispersion, $\Delta f''$, were introduced into the least-squares calculations as +7.5 and +2.5 electrons, respectively, for Re and Cs. Scattering factors for neutral oxygen, carbon, boron, and hydrogen were adopted as given in the standard tables.[7] The anisotropic temperature factors used have the form $\exp(-\beta_{11}h^2 - \beta_{22}k^2 - \beta_{33}l^2 - 2\beta_{12}hk - 2\beta_{13}hl - 2\beta_{23}kl)$.

Results

Unit Cell and Space Group.—Four formula units of $(B_9C_2H_{11})Re(CO)_3Cs$ are contained in the monoclinic unit cell in space group $P2_1/c$ with dimensions $a = 11.435 \pm 0.010$ A, $b = 9.516 \pm 0.005$ A, $c = 12.730 \pm 0.010$ A, and $\beta = 92.87 \pm 0.04°$. The errors are estimates. The calculated X-ray density is 2.57 g/cc. The observed extinctions correspond to the space group $P2_1/c$. The space group is centric, and each of the atoms occupies the general fourfold position $\pm(x, y, z;\ x, {}^1/_2 - y, {}^1/_2 + z)$.

Determination of the Structure.—The positions of the Cs and Re were easily extracted from the three-dimensional Patterson function. These heavy-atom positions were refined by least squares using isotropic temperature factors, and after four cycles of refinement yielded an R factor of 0.149 where $R = \Sigma||F_o| - |F_c||/\Sigma|F_o|$. Four more cycles using anisotropic temperature factors reduced R to 0.146. A difference Fourier was calculated and the seventeen remaining atoms, excluding hydrogen, appeared as the seventeen largest peaks in the patterns. The parameters of the two heavy atoms with anisotropic temperature factors and the seventeen lighter atoms with isotropic temperature factors were refined by least squares for two cycles, and R decreased to 0.066. Several blunders in punching the data onto the IBM cards and errors in setting the angles were recognized and corrected. Two cycles with the corrected data yielded an R of 0.046. From a study of the interatomic distances and the thermal parameters it was apparent that a boron and a carbon atom were interchanged. This correction improved R very little, but the thermal parameters became more consistent.

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(4) L. H. Thomas and K. Umeda, *J. Chem. Phys.*, **26**, 293 (1957).

(5) D. T. Cromer, *Acta Cryst.*, **18**, 17 (1965).

(6) D. H. Templeton in "International Tables for X-Ray Crystallography," Kynoch Press, Birmingham, England, 1962, Vol. III, p 216.

(7) J. A. Ibers, ref 6, p 202.

TABLE II

OBSERVED AND CALCULATED STRUCTURE FACTORS IN $B_9C_2H_{11}Re(CO)_3Cs$

```
H,K= 0, 0
L FOB FCA
2 181 173
4 347 352
6 51 57
8 178 182
10 0 5
12 65 66
14 42 42

H,K= 0, 1
L FOB FCA
1 83 77
2 100 90
3 25 25
4 118 114
5 115 112
6 83 78
7 46 42
8 128 122
9 122 119
10 68 59
11 54 53
12 97 98
13 77 75
14 43 43
15 45 50

H,K= 0, 2
L FOB FCA
-0 246 233
1 237 224
2 95 90
3 187 180
4 174 166
5 134 129
6 38 41
7 142 140
8 65 63
9 48 46
10 30 34
11 55 54
12 32 32
13 10 6
14 24 27

H,K= 0, 3
L FOB FCA
1 152 145
2 94 86
3 85 81
4 47 44
5 223 218
6 37 45
7 30 28
8 44 44
9 170 168
10 73 71
11 63 59
12 40 43
13 102 104
14 45 46

H,K= 0, 4
L FOB FCA
-0 223 216
1 96 90
2 232 219
3 87 80
4 150 143
5 50 48
6 120 115
7 76 67
8 91 89
9 0 7
10 67 70
11 39 40
12 26 17
13 18 14
14 0 1

H,K= 0, 5
L FOB FCA
1 94 90
2 21 19
3 155 151
4 101 98
5 42 45
6 97 92
7 104 102
8 102 97
9 9 9
10 94 92
11 56 58
12 82 85
13 11 8

H,K= 0, 6
L FOB FCA
-0 151 149
1 143 139
2 49 45
3 144 137
4 133 129
5 105 102
6 0 8
7 54 50
8 61 66
9 56 60
10 10 5
11 10 10
12 24 25

H,K= 0, 7
L FOB FCA
1 39 29
2 24 18
3 83 81
4 25 18
5 57 49
6 9 11
7 114 114
8 21 16
9 71 76
10 10 7
11 93 96

H,K= 0, 8
L FOB FCA
-0 40 41
1 82 79
2 154 151
3 77 78
4 35 35
5 70 69
6 97 93
7 46 47
8 0 5
9 31 35
10 43 47

H,K= 0, 9
L FOB FCA
1 19 9
2 42 35
3 10 11
4 48 47
5 14 9
6 74 72
7 18 5
8 45 55
9 11 11

H,K= 0,10
L FOB FCA
-0 64 65
1 55 55
2 113 114
3 51 92
4 44 46
5 46 47
6 65 69
7 27 29

H,K= 0,11
L FOB FCA
1 11 8
2 11 8
3 42 41

H,K= 1, 0
L FOB FCA
-14 68 76
-12 77 78
-10 141 140
-8 105 102
-6 239 238
-4 81 74
-2 294 278
-0 170 168
2 71 69
4 38 39
6 13 10
8 7 9
10 48 54
12 47 50
14 68 70

H,K= 1, 1
L FOB FCA
-15 44 41
-14 35 35
-13 22 20
-12 61 64
-11 37 37
-10 30 29
-9 0 1
-8 73 76
-7 0 3
-6 162 160
-5 96 94
-4 82 80
-3 95 88
-2 358 352
-1 116 106
-0 88 82
1 152 145
2 333 342
3 184 182
4 61 54
5 120 117
6 274 276
7 97 95
8 46 44
9 94 92
10 172 176
11 44 50
12 25 29
13 39 38
14 47 52

H,K= 1, 2
L FOB FCA
-14 26 28
-13 63 67
-12 0 7
-11 140 144
-10 52 52
-9 115 115
-8 17 10
-7 271 269
-6 60 61
-5 150 140
-4 54 42
-3 290 283
-2 68 61
-1 88 84
-0 19 11
1 281 291
2 20 17
3 108 106
4 28 29
5 61 60
6 7 7
7 107 107
8 0 2
9 18 19
0 12 12
1 94 95
2 10 5
3 55 58
4 21 21

H,K= 1, 3
L FOB FCA
- 4 30 33
- 3 18 17
- 2 0 5
- 1 63 63
- 0 18 18
9 0 0
8 25 24
7 38 38
6 42 38
5 72 72
4 106 98
3 99 90
2 42 37
1 244 236
0 159 162
1 148 148
2 80 74
3 173 172
4 149 143
5 178 175
6 27 28
7 127 124
8 120 123
9 117 117
0 37 37
1 63 70
2 50 51
3 56 61
4 19 19

H,K= 1, 4
L FOB FCA
- 4 44 48
- 3 0 5
- 2 84 86
- 1 69 67
- 0 112 112
9 12 14
8 123 120
7 133 134
6 139 135
5 26 29
4 164 156
3 189 189
2 165 155
1 77 74
0 151 154
1 153 147
2 89 87
3 103 103
4 30 28
5 124 126
6 13 9
7 102 101
8 33 35
9 33 35
0 63 59
1 48 50
2 63 67
3 0 3
4 54 61

H,K= 1, 5
L FOB FCA
- 3 24 23
- 2 37 38
- 1 14 9
- 0 9 3
9 25 27
8 0 2
7 37 34
6 57 52
5 15 14
4 50 47
3 55 53
2 169 159
1 24 20
0 115 120
1 66 66
2 193 192
3 61 58
4 147 140
5 20 16
6 181 176
7 36 33
8 120 118
9 13 17
0 112 109
1 29 28
2 47 54
3 15 15

H,K= 1, 6
L FOB FCA
- 2 26 27
- 1 49 51
- 0 74 72
9 129 130
8 49 46
7 69 64
6 95 91
5 193 188
-4 76 73
-3 83 76
-2 94 90
-1 163 158
-0 70 69
1 10 8
2 51 53
3 111 110
4 19 17
5 56 55
6 0 1
7 29 27
8 13 16
9 67 67
10 31 33
11 20 22
12 24 26

H,K= 1, 7
L FOB FCA
-11 21 20
-10 23 23
-9 26 25
-8 36 34
-7 16 14
-6 22 22
-5 26 26
-4 69 65
-3 104 101
-2 49 44
-1 116 110
-0 92 97
1 118 118
2 33 35
3 116 114
4 81 80
5 122 122
6 25 27
7 120 118
8 33 34
9 85 88
10 15 15
11 57 62

H,K= 1, 8
L FOB FCA
-10 39 43
-9 71 72
-8 89 84
-7 78 75
-6 54 56
-5 95 95
-4 102 97
-3 70 69
-2 65 64
-1 66 62
-0 49 46
1 32 24
2 25 20
3 32 30
4 9 12
5 9 12
6 14 10
7 17 15
8 18 16
9 28 34
10 11 16

H,K= 1, 9
L FOB FCA
-9 0 4
-8 24 22
-7 0 5
-6 10 8
-5 14 14
-4 90 85
-3 19 14
-2 43 42
-1 23 20
-0 133 143
1 9 10
2 67 65
3 10 8
4 135 135
5 0 5
6 56 59
7 10 2
8 100 103
9 11 11

H,K= 1,10
L FOB FCA
-7 27 28
-6 52 52
-5 61 56
-4 79 76
-3 29 28
-2 53 53
-1 45 48
-0 53 53
1 10 5
2 35 34
3 40 35
4 18 16
5 0 1
6 11 7
7 0 4

H,K= 1,11
L FOB FCA
-3 50 51
-2 11 4
-1 58 58
-0 24 28
1 67 74
2 11 8
3 67 70

H,K= 2, 0
L FOB FCA
-14 102 104
-12 73 72
-10 157 156
-8 36 33
-6 175 170
-4 185 178
-2 48 48
-0 265 278
2 56 50
4 358 368
6 47 42
8 228 234
10 89 87
12 148 147
14 54 57

H,K= 2, 1
L FOB FCA
-15 0 1
-14 0 1
-13 22 27
-12 70 73
-11 34 36
-10 19 22
-9 97 99
-8 164 165
-7 66 63
-6 65 59
-5 186 181
-4 212 209
-3 118 109
-2 145 134
-1 238 241
-0 171 177
1 143 137
2 81 79
3 234 234
4 166 164
5 62 56
6 54 57
7 86 85
8 60 59
9 0 3
10 39 39
11 16 14
12 19 17
13 38 34
14 11 15

H,K= 2, 2
L FOB FCA
-14 33 32
-13 93 98
-12 10 2
-11 81 82
-10 58 59
-9 132 133
-8 36 36
-7 69 63
-6 76 73
-5 121 115
-4 77 81
-3 60 58
-2 128 125
-1 62 62
-0 132 138
1 71 69
2 84 87
3 122 121
4 127 130
5 176 174
6 45 48
7 163 162
8 107 109
9 135 134
10 9 6
11 110 110
12 46 45
13 77 78
14 0 3

H,K= 2, 3
L FOB FCA
-14 11 9
-13 49 52
-12 10 11
-11 21 19
-10 58 55
-9 129 131
-8 33 29
-7 74 70
-6 128 129
-5 260 254
-4 97 91
-3 95 89
-2 114 107
-1 342 352
-0 69 69
1 25 25
2 129 125
3 261 263
4 46 46
5 25 22
6 26 23
7 131 130
8 11 15
9 34 34
10 0 1
11 36 38
12 10 6
13 53 50
14 15 14

H,K= 2, 4
L FOB FCA
-14 62 64
-13 44 47
-12 81 84
-11 10 4
-10 78 80
-9 84 87
-8 85 85
-7 0 2
-6 48 45
-5 72 69
-4 24 21
-3 44 48
-2 34 33
-1 40 41
-0 67 62
1 70 75
2 112 109
3 16 14
4 120 115
5 64 65
6 146 144
7 66 66
8 119 119
9 47 49
10 108 109
11 40 38
12 80 82
13 24 25

H,K= 2, 5
L FOB FCA
-13 15 15
-12 42 43
-11 44 44
-10 58 60
-9 0 2
-8 116 117
-7 92 92
-6 136 133
-5 0 3
-4 190 182
-3 147 145
-2 209 204
-1 65 68
-0 208 216
1 170 178
2 126 125
3 50 51
4 112 111
5 99 99
6 93 93
7 33 34
8 48 52
9 51 50
10 19 15
11 33 32
12 15 15
13 15 18

H,K= 2, 6
L FOB FCA
-12 28 30
-11 77 78
-10 56 58
-9 40 40
-8 9 13
-7 74 73
-6 64 61
-5 0 3
-4 43 45
-3 27 24
-2 30 30
-1 56 55
-0 95 99
1 33 26
2 17 13
3 79 80
4 83 81
5 76 73
6 9 10
7 94 99
8 93 91
9 84 82
10 26 27
11 60 62
12 55 55

H,K= 2, 7
L FOB FCA
-11 54 55
-10 23 20
-9 60 58
-8 17 12
-7 120 120
-6 30 27
-5 109 106
-4 34 28
-3 185 172
-2 26 27
-1 108 102
-0 8 11
1 159 169
2 41 44
3 78 79
4 17 15
5 111 112
6 9 9
7 34 31
8 10 5
9 26 25
10 10 6
11 26 25

H,K= 2, 8
L FOB FCA
-10 34 30
-9 44 43
-8 66 66
-7 49 45
-6 10 8
-5 31 28
-4 70 66
-3 16 13
-2 58 55
-1 9 11
-0 15 9
1 13 11
2 99 99
3 45 45
4 16 11
5 62 61
6 101 98
7 69 71
8 35 38
9 64 66
10 90 88

H,K= 2, 9
L FOB FCA
-9 11 5
-8 48 49
-7 10 2
-6 104 101
-5 17 15
-4 94 91
-3 14 12
-2 130 127
-1 23 23
-0 86 89
1 10 8
2 91 96
3 26 22
4 55 58
5 0 4
6 62 63
7 15 16
8 48 45

H,K= 2,10
L FOB FCA
-6 11 8
-5 0 4
-4 28 25
-3 15 8
-2 42 42
-1 25 22
-0 0 3
1 20 26
2 68 66
3 29 31
4 28 27
5 40 38
6 66 68

H,K= 2,11
L FOB FCA
-3 87 89
-2 19 23
-1 54 54
-0 11 15
1 75 78
2 27 26

H,K= 3, 0
L FOB FCA
-14 0 5
-12 65 67
-10 42 46
-8 8 9
-6 165 166
-4 91 86
-2 329 338
-0 103 107
2 318 331
4 219 218
6 200 203
8 126 126
10 91 91
12 42 41
14 21 18

H,K= 3, 1
L FOB FCA
-14 44 46
-13 43 43
-12 99 102
-11 92 93
-10 78 79
-9 67 64
-8 190 191
-7 115 113
-6 43 40
-5 68 61
-4 251 248
-3 115 112
-2 22 20
-1 22 22
-0 205 214
1 65 71
2 128 136
3 38 33
4 72 78
5 14 14
6 188 189
7 83 81
8 16 14
9 50 46
10 129 129
11 46 46
12 39 43
13 47 46
14 76 82

H,K= 3, 2
L FOB FCA
-14 16 16
-13 35 34
-12 22 22
-11 16 12
-10 37 37
-9 0 5
-8 53 56
-7 123 121
-6 43 42
-5 98 79
-4 41 42
-3 282 280
-2 86 84
-1 68 65
-0 20 22
1 226 241
2 111 111
3 117 113
4 0 5
5 286 290
6 54 50
7 94 90
8 28 26
9 134 131
10 13 15
11 26 26
12 10 3
13 52 50
14 11 9

H,K= 3, 3
L FOB FCA
-14 36 36
-13 54 56
-12 39 39
-11 137 138
-10 84 86
-9 97 96
-8 55 53
-7 205 206
-6 98 94
-5 45 42
-4 21 20
-3 174 168
-2 88 85
-1 33 34
-0 30 29
1 82 89
2 105 102
3 23 23
4 65 63
5 0 4
6 7 3
7 83 86
8 61 60
9 62 62
10 20 20
11 80 78
12 54 55
13 76 73
14 27 27

H,K= 3, 4
L FOB FCA
-13 11 14
-12 10 11
-11 22 21
-10 9 1
-9 29 32
-8 51 52
-7 92 93
-6 84 82
-5 16 18
-4 124 121
-3 157 154
-2 165 161
-1 57 60
-0 182 188
1 157 168
2 178 182
3 35 36
4 184 183
5 128 130
6 135 136
7 20 22
8 107 105
9 99 99
10 63 61
11 20 20
12 38 36
13 30 30

H,K= 3, 5
L FOB FCA
-13 29 31
-12 83 87
-11 0 6
-10 79 83
-9 65 63
-8 120 117
-7 8 8
-6 96 90
-5 106 102
-4 125 118
-3 49 49
-2 78 76
-1 56 57
-0 79 82
1 19 23
2 25 27
3 37 37
4 0 3
5 24 26
6 58 62
7 17 14
8 45 45
9 35 37
10 82 80
11 18 15
12 58 57
13 16 15

H,K= 3, 6
L FOB FCA
-12 24 22
-11 21 21
-10 20 19
-9 37 38
-8 9 10
-7 22 22
-6 70 65
-5 146 144
-4 48 44
-3 60 55
-2 118 119
-1 172 175
-0 76 77
1 83 87
2 106 109
3 182 184
4 68 65
5 77 75
6 87 86
7 140 144
8 67 63
9 29 27
10 38 40
11 57 56
12 19 19

H,K= 3, 7
L FOB FCA
-11 73 74
-10 27 24
-9 113 110
-8 10 11
-7 90 92
-6 44 44
-5 124 121
-4 29 30
-3 57 53
-2 43 45
-1 93 96
-0 41 42
1 37 38
2 61 63
3 9 8
4 49 52
5 34 36
6 39 37
7 41 41
8 44 43
9 66 68
10 11 8
11 57 59

H,K= 3, 8
L FOB FCA
-10 15 11
-9 21 17
-8 43 42
-7 24 26
-6 10 14
-5 53 56
-4 85 81
-3 60 61
-2 37 38
-1 73 74
-0 100 107
1 67 72
2 61 63
3 89 89
4 83 83
5 61 62
6 62 60
7 63 67
8 59 64
9 30 34
10 35 33

H,K= 3, 9
L FOB FCA
-8 54 54
-7 0 4
-6 102 102
-5 10 3
-4 48 43
-3 0 10
-2 83 81
-1 0 1
-0 0 4
1 14 12
2 35 34
3 0 2
4 51 51
5 0 7
6 0 4
7 11 8
8 70 71

H,K= 3,10
L FOB FCA
-6 11 15
-5 40 38
-4 70 66
-3 18 18
-2 50 51
-1 59 59
-0 85 95
1 34 37
2 70 74
3 64 64
4 79 80
5 30 32
6 63 64

H,K= 3,11
L FOB FCA
-1 33 37
-0 0 6
1 11 11

H,K= 4, 0
L FOB FCA
-14 49 49
-12 49 51
-10 153 151
-8 116 117
-6 223 221
-4 120 120
-2 347 357
-0 35 36
2 266 281
4 19 10
6 155 156
8 53 54
10 15 17
12 82 81
14 24 21

H,K= 4, 1
L FOB FCA
-14 77 76
-13 32 34
-12 22 22
-11 55 54
-10 104 104
-9 35 37
-8 32 34
-7 39 40
-6 72 74
-5 54 55
-4 107 108
-3 6 5
-2 75 75
-1 118 123
-0 184 192
1 64 64
2 30 38
3 147 149
4 176 174
5 108 104
6 102 103
7 141 142
8 135 139
9 43 39
10 68 70
11 67 66
12 74 75
13 35 38
14 44 45

H,K= 4, 2
L FOB FCA
-14 15 17
-13 74 76
-12 14 10
-11 52 56
-10 40 42
-9 167 171
-8 11 8
-7 128 127
-6 91 91
-5 260 261
-4 9 5
-3 158 155
-2 124 122
-1 246 253
-0 60 62
1 74 77
2 106 110
3 174 175
4 85 83
5 30 29
6 42 41
7 21 19
8 45 47
9 30 32
10 27 30
11 32 30
12 39 37
13 36 39
14 11 9

H,K= 4, 3
L FOB FCA
-14 19 18
-13 46 50
-12 46 48
-11 80 80
-10 13 15
-9 27 28
-8 31 30
-7 72 70
-6 32 30
-5 93 89
-4 43 41
-3 34 35
-2 86 86
-1 147 152
-0 16 17
1 11 14
2 99 101
3 218 225
4 55 53
5 74 72
6 97 97
7 189 190
8 72 73
9 48 52
10 59 59
11 111 109
12 31 29
13 35 38

H,K= 4, 4
L FOB FCA
-13 43 44
-12 60 59
-11 10 3
-10 83 83
-9 97 99
-8 111 110
-7 12 13
-6 115 113
-5 147 146
-4 161 155
-3 22 23
-2 147 147
-1 135 140
-0 147 150
1 10 9
2 112 114
3 107 110
4 82 78
5 31 33
6 44 45
7 48 48
8 12 13
9 0 4
10 30 30
11 17 14
12 26 26
13 19 18

H,K= 4, 5
L FOB FCA
-13 29 30
-12 51 53
-11 10 7
-10 61 56
-9 42 42
-8 16 15
-7 17 19
-6 25 23
-5 38 36
-4 56 48
-3 83 83
-2 38 38
-1 43 48
-0 99 96
1 97 101
2 123 127
3 39 42
4 166 165
5 115 113
6 127 128
7 0 2
8 122 122
9 75 71
10 95 94
11 0 2
12 74 71

H,K= 4, 6
L FOB FCA
-12 27 29
-11 82 80
-10 51 52
-9 45 45
-8 31 28
-7 145 142
-6 77 72
-5 83 80
-4 35 36
-3 143 140
-2 100 99
-1 77 77
-0 21 21
1 136 142
2 97 102
3 39 40
4 8 4
5 72 75
6 51 50
7 0 3
8 13 8
9 0 1
10 10 10
11 21 20

H,K= 4, 7
L FOB FCA
-11 44 44
-10 18 19
-9 42 42
-8 30 28
-7 17 14
-6 35 32
-5 9 9
-4 25 25
-3 58 59
-2 59 60
-1 32 30
-0 15 16
1 118 122
2 43 45
3 91 94
4 13 12
5 133 132
6 19 17
7 78 77
8 0 2
9 90 89
10 11 6

H,K= 4, 8
L FOB FCA
-9 50 49
-8 83 81
-7 75 72
-6 61 59
-5 79 79
-4 107 105
-3 96 94
-2 36 34
-1 81 80
-0 106 110
1 71 76
2 13 13
3 31 33
4 66 63
5 29 29
6 20 19
7 10 8
8 18 17
9 0 2

H,K= 4, 9
L FOB FCA
-8 46 41
-7 0 3
-6 18 16
-5 14 12
-4 14 10
-3 7 5
-2 58 56
-1 17 14
-0 32 34
1 10 9
2 91 98
3 17 20
4 73 71
5 0 3
6 93 97
7 15 14

H,K= 4,10
L FOB FCA
-5 36 33
-4 70 72
-3 54 56
-2 51 54
-1 36 37
-0 79 85
1 50 51
2 18 22
3 24 26
4 49 47
5 11 14

H,K= 5, 0
L FOB FCA
-14 64 65
-12 123 127
-10 51 51
-8 168 168
-6 7 14
-4 189 195
-2 85 84
-0 58 59
2 140 143
4 0 7
6 137 133
8 64 66
10 126 129
12 78 78

H,K= 5, 1
L FOB FCA
-14 0 5
-13 10 3
-12 26 25
-11 31 29
-10 22 20
-9 0 7
-8 99 100
-7 107 109
-6 66 67
-5 76 76
-4 205 206
-3 156 156
-2 81 78
-1 127 122
-0 231 245
1 186 193
2 56 54
3 88 88
4 180 188
5 116 114
6 34 35
7 54 56
8 124 124
9 51 47
10 16 9
11 14 12
12 39 39
13 15 8

H,K= 5, 2
L FOB FCA
-14 0 2
-13 81 84
-12 42 44
-11 81 85
-10 0 8
-9 133 134
-8 69 68
-7 94 92
-6 50 52
-5 136 136
-4 116 116
-3 66 62
-2 61 63
-1 112 114
-0 55 59
1 61 67
2 39 42
3 10 10
4 25 26
5 144 145
6 54 54
7 51 48
8 32 33
9 129 127
10 34 35
11 73 73
12 21 21
13 86 88

H,K= 5, 3
L FOB FCA
-13 18 17
-12 7 4
-11 65 65
-10 26 24
-9 13 10
-8 9 10
-7 150 151
-6 62 63
-5 61 59
-4 54 54
-3 229 230
-2 105 107
-1 76 74
-0 59 62
1 245 255
2 110 113
3 114 115
4 23 25
5 177 176
6 100 99
7 59 56
8 12 18
9 64 61
10 27 27
11 10 8
12 0 1
13 11 12

H,K= 5, 4
L FOB FCA
-13 27 29
-12 77 81
-11 24 25
-10 92 93
-9 44 42
-8 89 87
-7 17 17
-6 116 113
-5 88 89
-4 70 70
-3 18 22
-2 41 40
-1 63 65
-0 26 23
1 51 55
2 70 72
3 55 57
4 88 86
5 105 106
6 76 74
7 23 23
8 102 101
9 67 61
10 83 81
11 0 4
12 76 75

H,K= 5; 5
L FOB FCA
-12 11 6
-11 10 14
-10 33 32
-9 50 53
-8 62 60
-7 13 15
-6 76 74
-5 91 92
-4 146 146
-3 34 36
-2 126 128
-1 112 115
-0 168 171
1 27 28
2 126 131
3 79 81
4 131 132
5 0 6
6 78 77
7 41 42
8 75 75
9 0 2
10 32 34
11 15 15
12 24 28

H,K= 5, 6
L FOB FCA
-11 66 69
-10 37 38
-9 53 54
-8 76 71
-7 90 90
-6 13 15
-5 26 26
-4 80 78
-3 67 67
-2 0 3
-1 14 15
-0 33 31
1 25 26
2 54 54
3 69 71
4 26 25
5 33 25
6 58 59
7 94 95
8 31 28
9 39 39
10 53 51
11 73 70

H,K= 5, 7
L FOB FCA
-10 11 10
-9 58 58
-8 10 5
-7 51 49
-6 23 23
-5 120 118
-4 9 7
-3 95 92
-2 57 57
-1 147 152
-0 20 16
1 101 104
2 51 51
3 138 142
4 18 17
5 87 86
6 41 38
7 69 70
8 14 13
9 32 33
10 27 25

H,K= 5, 8
L FOB FCA
-9 45 44
-8 21 20
-7 48 50
-6 72 71
-5 39 37
-4 0 3
-3 34 37
-2 56 56
-1 19 18
-0 25 27
1 9 6
2 13 13
3 29 34
4 53 55
5 32 34
6 25 26
7 49 48
8 55 56

H,K= 5, 9
L FOB FCA
-7 0 8
-6 70 71
-5 0 2
-4 50 53
-3 10 3
-2 110 113
-1 0 1
-0 74 76
1 14 19
2 105 111
3 14 10
4 56 55
5 21 20
6 72 73
7 11 13

H,K= 5,10
L FOB FCA
-4 15 15
-3 22 21
-2 40 44
-1 11 9
-0 24 19
1 8 7
2 11 7
3 27 26
4 35 38

H,K= 6, 0
L FOB FCA
-12 40 45
-10 18 19
-8 29 26
-6 46 39
-4 29 28
-2 181 181
-0 103 103
2 265 279
4 126 126
6 208 205
8 81 82
10 161 136
12 38 39

H,K= 6, 1
L FOB FCA
-13 41 44
-12 23 26
-11 56 56
-10 123 123
-9 65 64
-8 22 20
-7 106 105
-6 202 204
-5 106 103
-4 63 59
-3 119 119
-2 189 198
-1 51 52
-0 0 6
1 86 87
2 140 144
3 0 4
4 65 67
5 39 42
6 59 58
7 0 4
8 57 55
9 0 5
10 34 36
11 42 46
12 58 59
13 22 23

H,K= 6, 2
L FOB FCA
-13 15 20
-12 14 15
-11 50 50
- 0 9 8
9 30 29
8 9 2
7 20 21
6 11 17
5 124 123
4 37 37
3 38 38
2 81 80
1 206 213
0 10 11
1 92 92
2 72 72
3 201 210
4 11 4
5 98 100
6 64 62
7 148 142
8 9 11
9 89 88
0 46 43
1 83 84
2 0 6
3 36 36

H,K= 6, 3
L FOB FCA
- 3 51 55
- 2 60 63
- 1 84 82
- 0 27 26
9 89 89
8 86 88
7 136 135
6 59 59
5 114 111
4 106 104
3 164 164
2 18 17
1 50 48
0 82 83
1 136 138
2 39 39
3 0 4
4 26 25
5 66 65
6 36 37
7 49 45
8 9 11
9 9 6
0 28 30
1 65 63
2 32 29

H,K= 6, 4
L FOB FCA
- 2 34 36
- 1 54 55
- 0 20 21
9 41 44
8 18 19
7 37 39
6 15 12
5 92 95
4 60 60
3 44 47
2 84 83
1 123 130
0 133 136
1 15 19
2 122 127
3 123 127
4 113 112
5 22 25
6 114 110
7 75 74
8 98 96
9 0 5
0 84 81
1 45 45
2 63 63

H,K= 6, 5
L FOB FCA
- 2 62 63
- 1 21 19
- 0 117 99
9 35 37
8 91 91
7 26 23
6 139 138
5 55 54
4 114 116
3 25 24
2 141 141
1 82 80
0 52 55
1 23 24
2 43 43
3 57 59
4 9 11
5 40 39
6 13 7
7 26 24
8 37 36
9 36 35
0 36 35
1 0 1

H,K= 6, 6
L FOB FCA
- 1 11 6
- 0 11 9
9 34 36
8 0 4
7 52 50
6 23 25
5 0 4
4 0 7
-3 107 106
-2 53 54
-1 45 45
-0 43 46
1 137 139
2 83 84
3 70 70
4 39 40
5 128 129
6 78 79
7 65 63
8 28 26
9 76 77
10 53 49

H,K= 6, 7
L FOB FCA
-10 22 15
-9 87 89
-8 27 26
-7 102 100
-6 34 33
-5 108 108
-4 44 42
-3 88 90
-2 33 35
-1 91 93
-0 38 39
1 38 40
2 29 32
3 55 53
4 29 28
5 0 4
6 20 20
7 10 9
8 15 16
9 34 33

H,K= 6, 8
L FOB FCA
-8 8 10
-7 15 13
-6 0 6
-5 25 23
-4 39 39
-3 38 36
-2 31 32
-1 32 34
-0 80 84
1 65 67
2 38 42
3 61 58
4 81 82
5 66 70
6 35 40
7 53 52
8 73 70

H,K= 6, 9
L FOB FCA
-6 45 47
-5 0 4
-4 108 108
-3 0 4
-2 54 55
-1 0 2
-0 80 81
1 15 11
2 15 10
3 0 1
4 32 33
5 11 13
6 11 19

H,K= 6,10
L FOB FCA
-2 35 35
-1 27 30
-0 63 66
1 49 51
2 47 52

H,K= 7, 0
L FOB FCA
-12 67 68
-10 29 27
-8 139 141
-6 46 44
-4 248 252
-2 58 60
-0 256 270
2 56 55
4 176 176
6 19 22
8 78 75
10 10 10
12 0 2

H,K= 7, 1
L FOB FCA
-13 53 55
-12 72 76
-11 33 33
-10 66 63
-9 61 59
-8 46 49
-7 9 13
-6 88 88
-5 61 62
-4 13 12
-3 60 61
-2 21 14
-1 22 21
-0 65 70
1 76 78
2 37 38
3 44 43
4 123 126
5 88 91
6 30 30
7 51 46
8 117 119
9 79 80
10 60 61
11 46 48
12 75 74

H,K= 7, 2
L FOB FCA
-13 19 22
-12 21 20
-11 48 47
-10 24 22
-9 82 81
-8 59 63
-7 110 109
-6 26 26
-5 168 165
-4 92 94
-3 155 157
-2 45 46
-1 175 182
-0 97 96
1 118 119
2 40 41
3 163 167
4 76 69
5 65 68
6 0 8
7 86 82
8 32 30
9 10 9
10 25 21
11 21 22
12 19 17

H,K= 7, 3
L FOB FCA
-12 32 34
-11 34 34
-10 28 30
-9 106 106
-8 39 37
-7 6 5
-6 27 25
-5 109 109
-4 33 37
-3 69 72
-2 0 6
-1 35 38
-0 8 7
1 129 132
2 37 36
3 35 35
4 18 17
5 138 138
6 61 61
7 51 51
8 23 23
9 113 113
10 60 61
11 55 54

H,K= 7, 4
L FOB FCA
-12 39 41
-11 11 9
-10 62 65
-9 26 27
-8 83 84
-7 47 44
-6 120 121
-5 61 60
-4 116 115
-3 18 17
-2 142 143
-1 91 92
-0 110 113
1 27 24
2 97 95
3 77 78
4 78 81
5 0 8
6 62 62
7 48 47
8 26 28
9 14 16
10 10 13
11 24 25

H,K= 7, 5
L FOB FCA
-11 37 35
-10 60 60
-9 20 20
-8 56 57
-7 54 54
-6 40 44
-5 44 43
-4 26 24
-3 63 66
-2 9 6
-1 80 78
-0 55 55
1 38 39
2 37 37
3 70 71
4 68 66
5 6 7
6 75 72
7 62 59
8 96 95
9 0 3
10 79 77

H,K= 7, 6
L FOB FCA
-10 0 9
-9 52 51
-8 70 69
-7 82 80
-6 33 32
-5 87 84
-4 88 85
-3 118 120
-2 32 34
-1 92 95
-0 90 92
1 116 117
2 30 30
3 60 63
4 80 82
5 77 75
6 20 19
7 20 22
8 25 25
9 34 30

H,K= 7, 7
L FOB FCA
-9 52 52
-8 11 10
-7 62 64
-6 0 2
-5 0 3
-4 0 1
-3 30 31
-2 19 18
-1 41 42
-0 0 0
1 25 27
2 36 37
3 75 75
4 14 11
5 52 52
6 31 28
7 87 86
8 11 6

H,K= 7, 8
L FOB FCA
-7 61 63
-6 85 84
-5 74 72
-4 40 39
-3 64 63
-2 101 105
-1 63 65
-0 36 35
1 62 64
2 78 78
3 49 52
4 15 15
5 45 42
6 53 51
7 16 17

H,K= 7, 9
L FOB FCA
-5 11 12
-4 19 19
-3 0 0
-2 11 16
-1 0 5
-0 24 19
1 0 7
2 54 54
3 0 3
4 38 38

H,K= 8, 0
L FOB FCA
-12 88 89
-10 110 110
-8 108 107
-6 125 127
-4 113 111
-2 72 76
-0 55 54
2 30 32
4 24 30
6 58 61
8 48 42
10 75 74

H,K= 8, 1
L FOB FCA
-12 39 37
-11 18 15
-10 56 56
-9 23 22
-8 24 21
-7 38 35
-6 116 114
-5 47 44
-4 0 7
-3 77 79
-2 174 179
-1 74 76
-0 29 29
1 104 104
2 170 171
3 100 102
4 29 31
5 102 103
6 127 124
7 60 59
8 33 32
9 62 58
10 73 71
11 28 31

H,K= 8, 2
L FOB FCA
-12 19 19
-11 103 106
-10 30 28
-9 74 74
-8 30 30
-7 144 141
-6 37 38
-5 55 52
-4 8 4
-3 131 131
-2 8 7
-1 8 8
-0 27 25
1 93 95
2 27 28
3 44 48
4 17 21
5 0 4
6 16 19
7 93 91
8 14 8
9 46 46
10 21 24
11 66 66

H,K= 8, 3
L FOB FCA
-12 8 10
-11 11 14
-10 0 5
-9 22 21
-8 50 48
-7 39 36
-6 0 3
-5 57 57
-4 62 65
-3 95 96
-2 40 41
-1 92 91
-0 107 107
1 150 149
2 22 23
3 116 112
4 85 85
5 123 123
6 23 24
7 67 64
8 46 44
9 81 80
10 11 12
11 27 27

H,K= 8, 4
L FOB FCA
-11 47 50
-10 78 80
-9 10 8
-8 92 95
-7 99 96
-6 94 93
-5 20 22
-4 98 95
-3 86 87
-2 73 75
-1 34 37
-0 41 40
1 78 79
2 25 27
3 54 55
4 0 2
5 53 48
6 34 30
7 55 51
8 44 46
9 10 6
10 63 60

H,K= 8, 5
L FOB FCA
-10 11 10
-9 0 2
-8 20 19
-7 22 21
-6 72 71
-5 27 23
-4 67 65
-3 22 24
-2 117 118
-1 48 48
-0 98 95
1 24 26
2 129 131
3 48 49
4 95 97
5 14 14
6 96 94
7 40 37
8 67 65
9 0 3

H,K= 8, 6
L FOB FCA
-9 85 88
-8 46 49
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5 53 48
6 23 25
7 10 11
8 19 19

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5 11 11

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8 10 15
9 15 16
10 11 1

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7 26 24
8 11 2

H,K= 9, 6
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2 22 21
3 69 68
4 55 55
5 86 82
6 18 20
7 53 55

H,K= 9, 7
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H,K=10, 1
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3 64 63
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7 34 34
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9 49 47

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2 13 7
3 27 24
4 49 46
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7 54 51
8 43 39

H,K=10, 4
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1 92 89
2 96 95
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6 65 60
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8 42 44

H,K=10, 5
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-7 0 6
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-4 56 54
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1 0 5
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7 15 17

H,K=10, 6
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1 45 49
2 39 37
3 105 100
4 40 37
5 36 36

H,K=10, 7
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-2 21 21
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1 11 6
2 22 16
3 31 30

H,K=11, 0
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-0 13 21
2 91 87
4 40 31
6 43 39
8 38 34

H,K=11, 1
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-7 10 12
-6 0 2
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-1 66 65
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2 59 60
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4 65 62
5 53 52
6 61 63
7 58 59
8 54 59

H,K=11, 2
L FOB FCA
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-6 49 46
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-1 86 85
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6 28 25
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H,K=11, 3
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-6 10 11
-5 58 59
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4 38 41
5 50 50
6 35 34
7 92 87

H,K=11, 4
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3 15 12
4 15 13
5 0 1
6 8 9

H,K=11, 5
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2 70 68
3 0 2
4 74 72
5 45 45

H,K=11, 6
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-2 60 61
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-0 0 10
1 36 34
2 38 35
3 11 11

H,K=12, 0
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-2 39 37
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4 38 38
6 73 68

H,K=12, 1
L FOB FCA
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-6 34 36
-5 46 45
-4 104 100
-3 62 64
-2 46 43
-1 52 48
-0 105 104
1 56 53
2 20 20
3 43 41
4 88 81
5 34 33
6 24 25

H,K=12, 2
L FOB FCA
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-6 15 17
-5 42 38
-4 18 15
-3 18 20
-2 10 9
-1 0 4
-0 10 5
1 50 52
2 18 17
3 21 27
4 0 2
5 85 82

H,K=12, 3
L FOB FCA
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-5 48 48
-4 47 47
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-2 60 57
-1 61 63
-0 18 17
1 74 73
2 52 48
3 42 43
4 0 11
5 51 49

H,K=12, 4
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-3 24 19
-2 11 9
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-0 24 23
1 43 39
2 30 31
3 8 10
4 49 44

H,K=12, 5
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-3 11 6
-2 76 73
-1 27 27
-0 81 79
1 0 6

H,K=13, 0
L FOB FCA
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-2 103 101
-0 44 46
2 97 93

H,K=13, 1
L FOB FCA
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-2 56 55
-1 8 7
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1 15 13
2 22 21
3 11 12

H,K=13, 2
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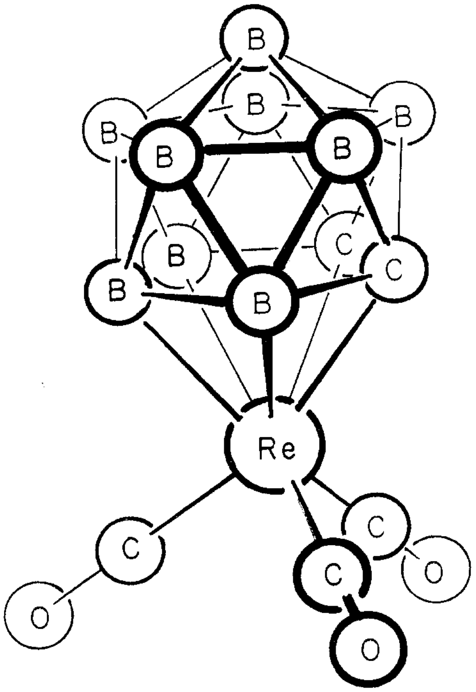

Figure 1.—$B_9C_2H_{11}Re(CO)_3^-$ ion (hydrogens excluded).

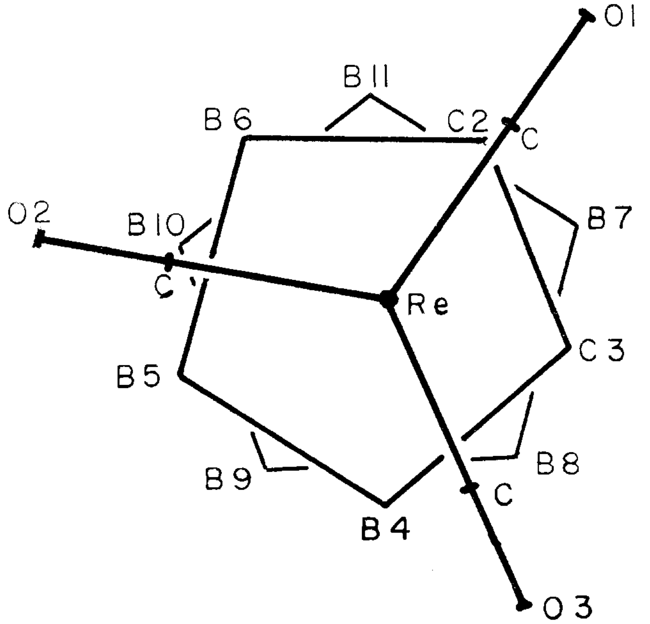

Figure 2.—Bottom view of $B_9C_2H_{11}Re(CO)_3^-$ ion (hydrogens excluded) showing the orientation of the three carbonyls to the icosahedron.

A difference function was again calculated and the patterns were studied for hydrogen peaks. Among the 35 peaks whose observed electron density was greater than 0.55 electron/A^3 at their peaks, 5 were close to Re, 6 were close to Cs, 7 were near the oxygen carbonyls, 10 were peaks in positions that would be suitable hydrogen atom locations, and 7 were peaks in the vicinity of the boron atoms which were either anisotropies or just spurious. The hydrogen atom near B(10) was not found. The ten hydrogen atoms were included in the ensuing refinements with these positions and an isotropic temperature factor of 4.0 A.^{2} No attempt was made to refine the hydrogen parameters.

For the final set of refinements, all of the atoms with the exception of the hydrogens were given anisotropic thermal parameters, the imaginary part of the anomalous dispersion for Cs and Re was added, and 10 hydrogen atoms were included but not refined. The final *R* factor was 0.042. The largest shift of any positional parameter was 0.00002 in the very last cycle. The final results are shown in Table I. Table II lists the observed and calculated structure factors.

Descripton of Structure.—The $B_9C_2H_{11}Re(CO)_3$ anion is shown in Figure 1. This structure was postulated by Hawthorne and Andrews[2] and has been confirmed by this work. The anion consists of the dicarbollide portion ($B_9C_2H_{11}$) to which the rhenium tricarbonyl is bonded *via* π-bonding to the rhenium atom; the rhenium atom occupies the no. 1 position in a completed icosahedron involving the dicarbollide portion. A bottom view of the structure is shown in Figure 2; this shows the orientation of the three carbonyls to the icosahedron. In the icosahedron the two carbon atoms are adjacent to each other and the Re atom. Lists of distances and angles are shown in Tables III and IV.

Table III

Distances in $CsB_9C_2Re(CO)_3$[a]

Distance, A		Distance, A	
Re(1)–C(1)–CO	1.90	B(6)–B(10)	1.73
Re(1)–C(2)–CO	1.88	B(6)–B(11)	1.78
Re(1)–C(3)–CO	1.90	B(7)–B(8)	1.78
Re(1)–C(2)	2.31	B(7)–B(11)	1.77
Re(1)–C(3)	2.31	B(7)–B(12)	1.77
Re(1)–B(4)	2.32	B(8)–B(9)	1.76
Re(1)–B(5)	2.35	B(8)–B(12)	1.79
Re(1)–B(6)	2.35	B(9)–B(10)	1.76
C(2)–C(3)	1.61	B(9)–B(12)	1.79
C(2)–B(6)	1.71	B(10)–B(11)	1.76
C(2)–B(7)	1.72	B(10)–B(12)	1.79
C(2)–B(11)	1.72	B(11)–B(12)	1.76
C(3)–B(4)	1.71	C(1)–CO–O(1)–CO	1.16 (1.20)[b]
C(3)–B(7)	1.71	C(2)–CO–O(2)–CO	1.16 (1.18)[b]
C(3)–B(8)	1.74	C(3)–CO–O(3)–CO	1.15 (1.19)[b]
B(4)–B(5)	1.76	Cs–O(1)–CO	3.20[c]
B(4)–B(8)	1.78	Cs–O(2)–CO	3.16[c]
B(4)–B(9)	1.77	Cs–O(3)–CO	3.20[c]
B(5)–B(6)	1.81		
B(5)–B(9)	1.80		
B(5)–B(10)	1.80		

[a] Estimated standard deviation on the distances involving Cs and Re is ~0.01 A; all other distances have standard deviations of ~0.02 A. [b] Corrected for thermal motion assuming the O rides on the C. This was the only set where the thermal effect was larger than the estimated standard deviations. [c] Nearest neighbors to the cesium ions. Each oxygen is from a different molecule.

The thermal motion of the atoms in the icosahedron in this structure is less than for comparable atoms in the $C_5H_5FeC_2B_9H_{11}$ structure,[3] and therefore we consider the resulting bond distances an improvement over the previous ones. In $B_9C_2H_{11}Re(CO)_3$ the average value of 18 B–B bonds, 1.78 A, is 0.03 A larger; the average of the 6 C–B bonds, 1.72 A, is 0.04 A larger; and the C–C bond, 1.61 A, is 0.03 A larger than the comparable values in the $C_5H_5FeC_2B_9H_{11}$ structure.

TABLE IV

ANGLES IN $B_9C_2H_{11}Re(CO)_3$

Angle, deg		Angle, deg	
O(1)CO–C(1)CO–Re(1)	175	C(3)–B(8)–B(7)	60
O(2)CO–C(2)CO–Re(1)	178	C(2)–B(11)–B(6)	58
O(3)CO–C(3)CO–Re(1)	176	C(2)–B(11)–B(7)	59
C(1)CO–Re(1)–C(2)CO	89	B(5)–B(4)–B(9)	61
C(2)CO–Re(1)–C(3)CO	92	B(8)–B(4)–B(9)	59
C(3)CO–Re(1)–C(1)CO	88	B(4)–B(5)–B(9)	60
C(2)–Re(1)–C(3)	41	B(6)–B(5)–B(10)	58
C(3)–Re(1)–B(4)	43	B(9)–B(5)–B(10)	59
B(4)–Re(1)–B(5)	44	B(5)–B(6)–B(10)	61
B(5)–Re(1)–B(6)	45	B(10)–B(6)–B(11)	60
B(6)–Re(1)–C(2)	43	B(8)–B(7)–B(12)	60
Re(1)–C(2)–C(3)	70	B(11)–B(7)–B(12)	60
Re(1)–C(2)–B(6)	70	B(4)–B(8)–B(9)	60
Re(1)–C(3)–C(2)	70	B(7)–B(8)–B(12)	60
Re(1)–C(3)–B(4)	69	B(9)–B(8)–B(12)	61
Re(1)–B(4)–C(3)	68	B(4)–B(9)–B(5)	59
Re(1)–B(4)–B(5)	69	B(4)–B(9)–B(8)	60
Re(1)–B(5)–B(4)	67	B(5)–B(9)–B(10)	60
Re(1)–B(5)–B(6)	68	B(8)–B(9)–B(12)	60
Re(1)–B(6)–C(2)	67	B(10)–B(9)–B(12)	61
Re(1)–B(6)–B(5)	67	B(5)–B(10)–B(6)	62
C(2)–B(7)–C(3)	56	B(5)–B(10)–B(9)	61
C(3)–C(2)–B(7)	63	B(6)–B(10)–B(11)	61
C(2)–C(3)–B(7)	62	B(9)–B(10)–B(12)	60
B(6)–C(2)–B(11)	63	B(11)–B(10)–B(12)	60
B(7)–C(2)–B(11)	62	B(6)–B(11)–B(10)	59
B(4)–C(3)–B(8)	63	B(7)–B(11)–B(12)	60
B(7)–C(3)–B(8)	62	B(10)–B(11)–B(12)	61
C(3)–B(4)–B(8)	59	B(7)–B(12)–B(8)	60
C(2)–B(6)–B(11)	59	B(7)–B(12)–B(11)	60
C(2)–B(7)–B(11)	59	B(8)–B(12)–B(9)	59
C(3)–B(7)–B(8)	58	B(9)–B(12)–B(10)	59
C(3)–B(8)–B(4)	59	B(10)–B(12)–B(11)	59

Such increases are expected since large motions cause the observed distance to be shorter than the true average value.

In the carbonyl portion of the ion, the Re to C to O linkages are almost linear with a slight bend of a few degrees in an outward direction away from the axis of the molecule. At the Re atom the three carbonyl carbons make very nearly right angles with respect to each other. This tricarbonyl structure is quite similar to that reported in hexamethylbenzenechromium tricarbonyl,[8] thiophenechromium tricarbonyl,[8] benzenechromium tricarbonyl,[8] and cyclopentadienylmanganese tricarbonyl.[9] The carbonyl oxygens are apparently free to flop around somewhat as their thermal parameters are larger than the carbons to which they are attached. In Table III we have included some thermally adjusted values for the C–O bond distances based on a calculation that assumes the oxygens are "riding" on the carbons. These three bonds were the only bonds in the structure where this type of a correction was larger than the estimated standard deviation of the bond length. We do not fully understand the thermal motion and report these thermally corrected bond lengths primarily as an indication of the magnitude of the thermal effect rather than as accurate values.

The cesium ion has as its closest neighbors at 3.2 A three oxygen atoms of three symmetry unrelated carbonyls from three different anions.

The hydrogen atoms were poorly resolved in this structure determination. One hydrogen atom, H(10), was not resolved at all in the difference function.

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The Crystal Structure of $AgC(CN)_3$

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Silver tricyanomethide, $AgC(CN)_3$, forms orthorhombic crystals in the space group I2cm with $a = 6.21$ A, $b = 10.19$ A, $c = 7.98$ A with four molecules per unit cell. Each Ag atom is coordinated in a flat pyramid to three N atoms, one at 2.11 ± 0.06 A and two at 2.25 ± 0.04 A, with one N–Ag–N angle of 99.7° and two of 123.9°. Owing to the large uncertainties in the light-atom positions, the $C(CN)_3^-$ group cannot be said to deviate from D_{3h} symmetry. The bonding leads to puckered, hexagonal, infinite nets of $AgC(CN)_3$. These nets interpenetrate in pairs to form a layer structure.

In the course of crystal structure studies of several silver compounds[1] and of the potassium salt of cyanoform,[2] $KC(CN)_3$, it occurred to us that $AgC(CN)_3$ might provide an example of silver atoms with coordination number three, and in particular that the planar arrangement shown in Figure 1 might exist. Accordingly, we have determined the crystal structure of $AgC(CN)_3$.

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(1) D. Britton and J. D. Dunitz, *Acta Cryst.*, **18**, 424; **19**, 662; **19**, 815 (1965).

(2) J. Witt and D. Britton, unpublished work. A preliminary report of this structure has been made by P. Andersen and B. Klewe, *Nature*, **200**, 464 (1963), who have also determined the structure of $NaC(CN_3)$ (private communication).