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The Crystal Structure of $Cs_2(B_9C_2H_{11})Co(B_8C_2H_{10})Co(B_9C_2H_{11})\cdot H_2O$, a Salt of a Three-Icosahedral-Fragment Metallocarborane[1]

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The crystal structure of the monohydrated cesium salt of the bis[π-(3)-1,2-dicarbollylcobalt]-π-(3,6)-1,2-dicarbacanastide ion, $Cs_2Co_2B_{26}C_6H_{32}\cdot H_2O$, has been determined from 3649 independent X-ray data obtained from a single crystal by counter methods. The crystals are monoclinic, space group $P2_1/c$. Four molecules are in the unit cell with a = 7.089 (4) Å, b = 19.240 (14) Å, c = 20.682 (4) Å, and β = 98.00 (6)°. The calculated density is 1.871 g/cm³. The structure was refined by least squares to a conventional R factor of 3.4%. The carborane anion, $(B_9C_2H_{11})Co(B_8C_2H_{10})Co(B_9C_2H_{11})^{2-}$, consists of three linked icosahedra. Two corners of a central 10-light-atom icosahedron are occupied by cobalts each of which is common to another icosahedron containing 11 light atoms. Five of the positions in the icosahedra are occupied by carbons but, because of disorder, two positions contain half-boron–half-carbon atoms. The cages are staggered across the cobalts and all carbons are as close to each other as is possible in this configuration. All hydrogens except those in the water molecule were located.

Introduction

A novel anion of the carborane type $(B_9C_2H_{11})Co(B_8C_2H_{10})Co(B_9C_2H_{11})^{2-}$, the bis(undecahydro-1,2-dicarba-3-cobalta-*closo*-dodecaborano)-[3′,3′:3,6]-*commo*-decahydro-1,2-dicarba-3,6-dicobalta-*closo*-dodecaborate(2−) ion, has recently been prepared.[2,3] Francis and Hawthorne proposed that the anion consisted of two of the previously known 11-atom icosahedral fragments each having a cobalt atom bonded to the open face with the cobalts linked together *via* a new 10-atom icosahedral fragment. In this paper, we report the results of an X-ray analysis of the cesium salt of this anion, $Cs_2(Co_2B_{26}C_6H_{32})\cdot H_2O$, shown in Figure 1. We confirm the structure assigned for the anion by Francis and Hawthorne. We show that the rotational configuration of the cages in the crystal are those in which the cages are staggered and that the carbons are as close to each other as possible in this staggered arrangement.

Experimental Section

The dark red crystals were sent to us by Professor Hawthorne of the University of California, Riverside, Calif. A single crystal, which was cut from a larger one and trimmed to a fragment with dimensions 0.11 × 0.12 × 0.23 mm, was glued to a glass fiber with its crystallographic b axis parallel to the fiber axis.

Approximate cell dimensions were calculated from oscillation and zero-level Weissenberg films, and the space group was ascertained from precession photographs. The crystal was mounted on a manual General Electric XRD-5 diffractometer with its b axis parallel to the φ axis of the goniostat. With the use of Mo X-rays ($\lambda_{K\alpha_1}$ 0.70926 Å) space group absences were rechecked, and accurate cell dimensions were obtained from 2θ measurements along the $h00$, $0k0$, and $00l$ rows of reflections; β was measured directly from the observed angle between the $h00$ and $00l$ rows. Intensity data were measured with this manually operated diffractometer equipped with a quarter-circle Eulerian cradle, a scintillation counter, and a pulse height discriminator. The molybdenum X-rays were filtered by a 0.003-in. Zr foil placed in front of the receiving slit. One complete set of independent reflections (including space group absences), with $2\theta \leqq 45°$ ($(\sin\theta)/\lambda = 0.538$), was measured using the stationary-crystal, stationary-counter technique by counting for 10 sec on the peak. Background was plotted as a function of 2θ and subtracted from the gross intensity; however, individual backgrounds were measured for those reflections whose counts were seriously affected by streaking from other orders. Excluding space group extinctions, there were 3649 independent reflections of which 344 had intensities less than their estimated standard deviations. The absorption coefficient is μ = 38 cm^{-1}. Absorption effects on the data were neglected. It is estimated that the maximum absorption correction of an intensity differs by less than 12% from the minimum correction.

Calculations were done on a CDC 6600 computer. Lorentz and polarization corrections were applied and the data were converted to structure factors. Refinements of parameters were accomplished with our least-squares program which minimizes the quantity $\Sigma w(|F_o| - |F_c|)^2/\Sigma w|F_o|^2$, where F_o and F_c are the observed and calculated structure factors, respectively. The weighting factor, $w = [\sigma(F_o)]^{-2}$, is derived from the standard deviation of the intensity, $\sigma(I)$, estimated by the equation $\sigma(I) = [I + 2I_b + (0.05I)^2]^{1/2}$, where I_b is the number of counts in the background and I is the number of counts on the peak minus I_b.

All atoms were considered to be in their neutral valence state. The scattering factors of Cromer and Waber[4] were used for all except the hydrogen atoms whose scattering factors are those of Stewart, Davidson, and Simpson.[5] Cromer's corrections for anomalous dispersion[6] applied to the scattering factors of the Cs and Co are $\Delta f' = -0.5$ and $\Delta f'' = +2.6$ electrons and $\Delta f' = +0.4$ and $\Delta f'' = +1.0$ electron, respectively. The anisotropic temperature factors were of the form $\exp(-\beta_{11}h^2 - \beta_{22}k^2 - \beta_{33}l^2 - 2\beta_{12}hk - 2\beta_{13}hl - 2\beta_{23}kl)$.

Crystal Data

The crystals were found to be monoclinic with unit cell dimensions, measured at room temperature (~22°), a = 7.089 ± 0.004 Å, b = 19.240 ± 0.014 Å, c = 20.682 ± 0.004 Å, and β = 98.00 ± 0.06°. There are

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[1] Work done under the auspices of the U. S. Atomic Energy Commission.

[2] J. M. Francis and M. F. Hawthorne, *J. Am. Chem. Soc.*, **90**, 1663 (1968).

[3] This name is an extension of the ACS-approved nomenclature rules given in *Inorg. Chem.*, **7**, 1945 (1968), which do not explicitly cover the naming of ions in which a single polyhedron is completed by two identical groups attached at two different positions in the cage. The name originally given by Francis and Hawthorne in ref 2 is the bis-[π-(3)-1,2-dicarbollylcobalt]-π-(3,6)-1,2-dicarbacanastide ion. Both names fail to describe the rotational isomerism of the π bonding.

[4] D. T. Cromer and J. T. Waber, *Acta Cryst.*, **18**, 104 (1965).

[5] R. F. Stewart, E. R. Davidson, and W. T. Simpson, *J. Chem. Phys.*, **42**, 3175 (1965); see especially Table II.

[6] D. T. Cromer, *Acta Cryst.*, **18**, 17 (1965).

TABLE I

COORDINATES ($\times 10^5$) AND THERMAL PARAMETERS ($\times 10^2$)[a] OF HEAVY ATOMS[b]

Atom	x	y	z	B_{11}	B_{22}	B_{33}	B_{12}	B_{13}	B_{23}
Cs(1)	21468 (6)	27505 (2)	17044 (2)	434 (2)	336 (2)	318 (2)	017 (1)	054 (1)	−012 (1)
Cs(2)	05321 (6)	02870 (2)	34230 (2)	503 (2)	280 (2)	449 (2)	031 (2)	106 (2)	−044 (1)
Co(1)	23982 (10)	76225 (4)	58130 (3)	250 (3)	195 (3)	229 (3)	020 (2)	−002 (2)	010 (2)
Co(2)	25769 (10)	57752 (4)	64795 (3)	231 (3)	214 (3)	239 (3)	−002 (2)	002 (2)	019 (2)

[a] Anisotropic thermal parameters, B, in units of Å^2, are given by $B = 4\beta_{ij}/a_i^*a_j^*$, where a_i^* is the ith reciprocal cell length. [b] Estimated standard deviations are given in parentheses following the parameter.

TABLE II

COORDINATES ($\times 10^4$) AND THERMAL PARAMETERS ($\times 10^2$) OF THE LIGHT ATOMS[a,b]

Atom	x	y	z	B, Å^2
O(1)	7075 (8)	5640 (3)	8419 (3)	643 (12)
Atoms in Cage I				
B(1)	3781 (10)	8967 (4)	4548 (3)	329 (13)
B(2)	3175 (10)	8098 (4)	4321 (3)	321 (13)
B(3)	5330 (10)	8283 (4)	4825 (3)	326 (13)
B(4)	4890 (9)	8951 (4)	5360 (3)	294 (12)
B(5)	2461 (9)	9202 (4)	5183 (3)	292 (12)
B(6)	1410 (10)	8660 (4)	4538 (3)	309 (13)
C(7)	3825 (8)	7631 (3)	5016 (3)	293 (11)
C(8)	4806 (8)	8116 (3)	5604 (3)	295 (11)
B(9)	3196 (9)	8664 (3)	5870 (3)	278 (12)
B(10)	0994 (9)	8496 (3)	5351 (3)	266 (12)
B(11)	1482 (9)	7788 (4)	4818 (3)	294 (12)
Atoms in Cage II				
C(12)	1689 (7)	6581 (3)	5850 (3)	232 (9)
C(13)	3550 (8)	6763 (3)	6316 (2)	236 (10)
B(14)	3294 (9)	7459 (3)	6797 (3)	264 (12)
B(15)	0822 (9)	7708 (4)	6597 (3)	299 (12)
B(16)	−0137 (9)	7143 (3)	5945 (3)	251 (11)
B(17)	3360 (9)	6575 (3)	7117 (3)	264 (12)
B(18)	1585 (10)	7179 (4)	7298 (3)	318 (13)
B(19)	−0546 (9)	6978 (3)	6762 (3)	275 (12)
B(20)	−0047 (9)	6259 (3)	6267 (3)	260 (11)
B(21)	0951 (9)	6289 (3)	7108 (3)	284 (12)
Atoms in Cage III				
C(22)	4005 (8)	5193 (3)	5879 (3)	297 (11)
BC(23)	5182 (9)	5261 (3)	6618 (3)	292 (11)
B(24)	3661 (9)	5032 (3)	7168 (3)	256 (12)
B(25)	1423 (9)	4807 (3)	6691 (3)	265 (12)
BC(26)	1816 (9)	4931 (3)	5893 (3)	306 (12)
B(27)	5659 (11)	4569 (4)	6115 (4)	363 (14)
B(28)	5409 (10)	4434 (4)	6947 (3)	337 (13)
B(29)	3074 (9)	4136 (3)	6982 (3)	284 (12)
B(30)	1870 (10)	4088 (4)	6165 (3)	312 (13)
B(31)	3488 (10)	4355 (4)	5649 (4)	339 (14)
B(32)	4321 (10)	3856 (4)	6337 (3)	325 (13)

[a] Numbering system used is shown in Figure 1. [b] BC refers to disordered atoms, half boron and half carbon.

TABLE III

COORDINATES ($\times 10^3$) OF THE HYDROGEN ATOMS[a−c]

Atom	x	y	z	Atom	x	y	z
H(1)	410	931	415	H(17)	473	650	745
H(2)	326	787	385	H(18)	142	741	786
H(3)	677	687	973	H(19)	−200	703	687
H(4)	615	927	556	H(20)	−123	592	601
H(5)	200	975	526	H(21)	038	601	753
H(6)	038	885	415	H(22)	420	551	552
H(7)	430	725	498	H(23)	623	559	667
H(8)	603	793	587	H(24)	379	516	767
H(9)	352	892	635	H(25)	000	484	684
H(10)	956	864	548	H(26)	105	507	556
H(11)	049	738	458	H(27)	701	455	589
H(12)	189	642	544	H(28)	662	430	733
H(13)	457	671	617	H(29)	269	376	738
H(14)	439	777	697	H(30)	067	372	601
H(15)	027	821	675	H(31)	331	424	518
H(16)	860	722	555	H(32)	466	332	628

[a] Number refers to the position in the cage occupied by the atom to which the hydrogen atom is attached. See Figure 1. [b] Refined average temperature factor is $B = 2.6 \pm 0.2$ Å^2. [c] Standard deviations for x, y, and z are ± 0.007, ± 0.003, and ± 0.003, respectively.

four formula units, $Cs_2Co_2B_{26}C_6OH_{34}$, per unit cell. The density is calculated to be $\rho = 1.87$ g/cm^3. No density measurement was made because the sample was lost. The observed extinction rules, $h0l$, $l = 2n$, and $0k0$, $k = 2n$, correspond to space group $P2_1/c$. All atoms lie on the general symmetry-related positions.

Determination of the Structure

The positions of the cesium and cobalt atoms were deduced from sections through a three-dimensional Patterson function synthesis. Full-matrix, least-squares refinement of a scale factor and the positional and isotropic thermal parameters of the Cs and Co atoms gave $R = 0.208$. These atoms were used to calculate approximate phases for the reflections and a three-dimensional difference Fourier map was synthesized from which the coordinates of the 32 boron and carbon atoms were found. Since a water of crystallization was not expected, the oxygen atom which appeared in this Fourier map was ignored. When the positions and isotropic thermal parameters of these 32 light atoms, all with the scattering power of boron, were incorporated into the refinement, the R value, $R = \Sigma||F_o| - |F_c||/\Sigma|F_o|$, dropped to 0.105. Anisotropic thermal parameters were introduced for the cesium and cobalt atoms, and further refinement reduced the R value to 0.073. Five of the light atoms had thermal parameters (1.2–2.0 Å^2) that were substantially lower than the average for all of the light atoms (average $B = 2.8$ Å^2). These atoms were deduced to be five of the six carbon atoms in the structure, and a list of interatomic distances showed this to be reasonable in that distances involving these carbon atoms were as expected shorter than for the comparable boron atoms. In this type carborane cage the anticipated interatomic distances for C–C, B–C, and B–B, are ~1.6, ~1.7, and ~1.8 Å, respectively.[7] At this stage in the structure determination the two identifiable C–C distances were 1.62 and 1.57 Å. Further refinement, which included

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(7) A. Zalkin, T. E. Hopkins, and D. H. Templeton, *Inorg. Chem.*, **5**, 1189 (1966).

TABLE IV: OBSERVED AND CALCULATED STRUCTURE FACTORS[a]

L	FOB	FCA
H,K= -1, -6		
21	0	8*
H,K= -1, -5		
21	62	65
H,K= -1, -4		
21	106	110
H,K= -1, -3		
21	0	1*
22	0	13*
H,K= -1, -2		
21	33	37
22	93	100
H,K= -1, -1		
21	80	79
22	17	19*
H,K= 0, 0		
2	199	181
4	737	761
6	637	648
8	328	333
10	341	353
12	531	539
14	42	61
16	264	273
18	68	74
20	42	53
22	38	37
H,K= 0, 1		
1	78	69
3	84	76
4	365	356
5	201	196
6	88	85
7	210	208
8	295	291
9	325	320
10	73	77
11	46	42
12	168	168
13	105	103
14	34	31
15	164	168
16	256	256
17	41	30
18	93	95
19	34	64
20	122	121
21	64	63
22	0	34*
H,K= 0, 2		
0	117	112
1	218	199
2	187	172
3	40	37
4	219	212
5	147	150
6	176	174
7	56	56
8	264	262
9	67	68
10	269	270
11	64	69
12	174	173
13	0	17*
14	155	153
15	30	34
16	142	144
17	0	22*
18	21	20
19	0	2*
20	219	215
21	0	12*
H,K= 0, 3		
1	192	178
2	296	291
3	307	296
4	572	575
5	8	6*
6	120	116
7	247	243
8	626	623
9	46	36
10	76	77
11	152	152
12	85	85
13	79	82
14	194	193
15	0	23*
16	126	125
17	70	70
18	78	77
19	60	63
20	114	117
21	0	21*
H,K= 0, 4		
0	694	708
1	418	402
2	260	247
3	44	44
4	328	321
5	183	180
6	363	354
7	259	255
8	295	299
9	45	46
10	65	67
11	35	31
12	514	521
13	197	199
14	47	48
15	73	73
16	136	131
17	80	77
18	119	124
19	163	153
20	101	99
21	0	4*
H,K= 0, 5		
1	331	324
2	160	164
3	538	529
4	111	106
5	146	142
6	176	173
7	328	318
8	105	100
9	340	335
10	39	39
11	49	46
12	217	223
13	218	223
14	166	164
15	75	60
16	176	173
17	0	4*
18	108	113
19	65	63
20	36	34
21	69	65
H,K= 0, 6		
0	369	353
1	19	16
2	15	14
3	101	99
4	123	122
5	49	48
6	139	137
7	89	86
8	82	85
9	16	25
10	16	22
11	48	49
12	152	156
13	124	127
14	0	9*
15	118	116
16	0	11*
17	0	7*
18	38	34
19	73	78
20	28	35
21	90	85
H,K= 0, 7		
1	137	134
2	277	275
3	88	84
4	401	403
5	94	95
6	67	63
7	137	137
8	367	363
9	84	84
10	91	92
11	270	272
12	67	70
13	0	18*
14	82	84
15	101	103
16	150	156
17	116	124
18	66	63
19	54	50
20	104	99
H,K= 0, 8		
0	169	173
1	501	501
2	28	25
3	37	37
4	14	2
5	586	591
6	97	100
7	422	421
8	115	115
9	192	191
10	94	97
11	336	340
12	124	125
13	192	192
14	44	42
15	25	21
16	40	47
17	196	209
18	0	4*
19	75	73
20	73	76
H,K= 0, 9		
1	252	248
2	253	248
3	217	241
4	0	3*
5	71	70
6	20	18
7	52	48
8	17	13
9	225	224
10	162	156
11	146	147
12	36	37
13	89	86
14	137	136
15	81	78
16	40	39
17	31	33
18	32	37
19	0	18*
H,K= 0, 10		
0	116	120
1	133	132
2	0	23*
3	210	216
4	52	48
5	193	190
6	17	16
7	101	96
8	67	67
9	166	166
10	19	27
11	175	172
12	105	104
13	111	108
14	33	29
15	255	259
16	22	25
17	16	12
18	23	25
19	147	157
H,K= 0, 11		
1	303	301
2	26	24
3	420	418
4	159	160
5	73	78
6	12	14*
7	154	151
8	124	120
9	276	270
10	27	11
11	152	156
12	32	22
13	188	182
14	37	35
15	133	138
16	74	73
17	16	10*
18	44	45
H,K= 0, 12		
0	0	6*
1	339	335
2	104	105
3	75	71
4	22	24
5	424	418
6	130	133
7	289	288
8	48	49
9	162	157
10	59	55
11	190	187
12	41	41
13	104	105
14	126	117
15	0	1*
16	0	9*
17	153	151
H,K= 0, 13		
1	18	21
2	277	277
3	54	56
4	127	127
5	29	26
6	33	36
7	88	93
8	176	173
9	0	5*
10	163	163
11	204	202
12	78	68
13	62	64
13	69	64
14	128	126
15	54	50
16	0	8*
17	110	107
H,K= 0, 14		
0	0	10*
1	19	26
2	50	53
3	91	91
4	36	37
5	63	63
6	28	29
7	73	71
8	14	4
9	25	6
10	15	19
11	0	5*
12	15	18
13	45	42
14	23	22
15	68	70
16	0	7*
H,K= 0, 15		
1	245	246
2	34	32
3	279	279
4	28	9
5	91	84
6	73	76
7	118	113
8	53	46
9	213	205
10	108	107
11	78	77
12	116	108
13	178	170
14	33	26
15	91	92
H,K= 0, 16		
0	228	229
1	14	10*
2	129	130
3	103	98
4	114	115
5	55	49
6	266	261
7	112	107
8	40	37
9	0	21*
10	114	114
11	28	24
12	145	142
13	80	65
14	82	75
H,K= 0, 17		
1	37	40
2	195	197
3	50	49
4	121	128
5	40	44
6	27	44
7	113	105
8	137	132
9	16	21
10	75	74
11	108	106
12	29	20
H,K= 0, 18		
0	82	80
1	51	45
2	0	1*
3	60	56
4	95	96
5	135	127
6	50	46
7	76	73
8	37	35
9	110	103
10	107	102
H,K= 0, 19		
1	114	112
2	114	109
3	28	52
4	109	105
5	23	23
6	44	41
7	58	55
8	121	112
H,K= 0, 20		
0	252	253
1	74	70
2	107	98
3	67	67
4	155	153
5	34	15
H,K= 1, 0		
-20	0	20*
-18	114	119
-16	143	142
-14	203	210
-12	205	204
-10	534	530
-8	25	30
-6	345	338
-4	588	568
-2	631	609
0	306	286
2	1033	1106
4	18	23
6	334	327
8	169	173
10	100	101
12	238	240
14	276	277
16	193	187
18	43	41
20	0	30*
H,K= -1, 0		
22	163	171
H,K= 1, 1		
-20	74	72
-19	181	172
-18	191	189
-17	0	20*
-16	74	70
-15	217	205
-14	250	246
-13	282	283
-12	77	75
-11	83	87
-10	61	64
-9	332	329
-8	150	148
-7	238	235
-6	450	443
-5	243	241
-4	95	89
-3	573	574
-2	293	288
-1	113	109
0	165	154
1	528	523
2	467	448
3	322	308
4	76	72
5	41	41
6	506	499
7	244	236
8	104	106
9	96	93
10	114	114
11	126	128
12	103	99
13	55	53
14	285	284
15	36	33
16	0	3*
17	81	82
18	232	227
19	0	15*
20	36	47
21	29	26
H,K= 1, 2		
-20	32	35
-19	46	49
-18	45	45
-17	89	90
-16	78	74
-15	0	6*
-14	119	112
-13	167	171
-12	26	25
-11	123	124
-10	203	208
-9	41	49
-8	25	23
-7	298	298
-6	176	174
-5	31	34
-4	110	103
-3	438	437
-2	413	414
-1	20	25
0	89	92
1	30	31
2	371	366
3	387	371
4	345	339
5	219	213
6	283	277
7	146	144
8	145	140
9	217	219
10	514	517
11	26	30
12	128	128
13	100	96
14	268	266
15	98	98
16	177	167
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8	130	135
9	174	174
10	259	253
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18	96	93
19	103	104
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13	55	55
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11	117	112
12	141	143
13	0	10*
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17	0	3*
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14	168	167
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7	371	376
8	147	155
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13	110	110
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15	44	34
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7	126	127
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9	47	51
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11	237	236
12	120	123
13	78	84
14	46	46
15	37	38
16	62	56
17	32	29
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H,K= 1, 10		
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7	55	64
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11	299	290
12	14	13*
13	88	91
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16	79	81
17	243	237
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10	58	51
11	197	195
12	221	208
13	87	82
14	15	13
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-10	54	57
-9	169	173
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3	200	198
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6	83	79
7	213	210
8	0	18*
9	108	103
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11	102	97
12	26	20
13	43	26
14	66	63
15	0	25*
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17	38	37
H,K= 1, 13		
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3	35	33
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5	53	52
6	33	29
7	225	218
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9	137	143
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11	110	106
12	40	33
13	225	221
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3	263	257
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5	193	194
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14	129	122
15	119	114
H,K= 1, 15		
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10	31	32
11	115	107
12	130	128
13	40	40
14	94	92
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3	0	3*
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12	47	49
13	94	92
H,K= 1, 17		
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7	149	143
8	16	23
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11	131	126
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7	144	135
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6	62	63
7	129	126
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3	208	210
4	236	239
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6	109	108
7	272	275
8	335	331
9	106	106
10	95	100
11	218	220
12	0	4*
13	228	224
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15	0	19*
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20	124	126
H,K= 2, 2		
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5	293	292
6	167	165
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8	119	110
9	206	204
10	223	223
11	203	204
12	219	223
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15	70	65
16	122	114
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3	325	317
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7	307	303
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9	123	121
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3	181	178
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7	156	153
8	29	34
9	263	261
10	191	188
11	184	188
12	195	199
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14	107	108
15	63	64
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17	147	142
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12	109	113
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3	213	216
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8	349	347
9	213	203
10	73	70
11	58	61
12	238	230
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15	91	88
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7	109	111
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9	150	149
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13	83	88
14	22	18
15	28	34
16	23	26
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1	198	199
2	356	358
3	195	194
4	0	13*
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6	122	122
7	27	29
8	207	206
9	141	140
10	38	39
11	66	68
12	182	180
13	127	123
14	144	150
15	76	79
16	113	113
H,K= 2, 12		
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-12	70	70
-11	112	114
-10	14	17*
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-8	41	40
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-6	75	72
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-1	36	36
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1	90	89
2	26	24
3	132	130
4	119	125
5	134	132
6	0	3*
7	163	166
8	55	63
9	14	14*
10	95	101
11	67	66
12	44	37
13	85	84
14	135	133
15	77	74
16	68	63
H,K= 2, 13		
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-14	16	21
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-10	15	20*
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-7	148	154
-6	14	11
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-4	84	86
-3	78	83
-2	23	25
-1	33	36
0	123	119
1	265	265
2	0	9*
3	97	91
4	24	18
5	65	67
6	84	81
7	71	67
8	33	32
9	135	133
10	112	106
11	83	81
12	45	38
13	91	94
14	40	39
15	75	78
H,K= 2, 14		
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-15	47	49
-14	59	61
-13	66	74
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-11	78	82
-10	120	124
-9	39	31
-8	102	102
-7	241	241
-6	306	311
-5	177	189
-4	20	23
-3	154	157
-2	216	216
-1	179	180
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1	130	128
2	14	7
3	0	13*
4	246	238
5	297	293
6	221	221
7	90	85
8	89	90
9	178	177
10	203	198
11	120	115
12	65	64
13	33	24
14	51	53
H,K= 2, 15		
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-12	101	113
-11	35	32
-10	148	152
-9	27	28
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-7	71	72
-6	68	70
-5	108	107
-4	137	139
-3	0	2*
-2	57	58
-1	66	67
0	80	66
1	25	27
2	163	159
3	21	13
4	15	1*
5	0	6*
6	37	35
7	73	71
8	35	34
9	75	70
10	88	84
11	94	95
12	17	7
13	41	41
H,K= 2, 16		
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-10	51	56
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-2	21	19
-1	15	8
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1	45	46
2	42	42
3	93	88
4	76	74
5	22	28
6	38	43
7	50	53
8	39	42
9	0	1*
10	47	46
11	50	46
H,K= 2, 17		
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-6	0	17*
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-4	89	91
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-2	99	100
-1	41	41
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1	241	240
2	136	142
3	157	150
5	105	102
6	39	48
7	81	82
8	127	126
9	74	78
10	61	60
H,K= 2, 18		
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1	45	23
2	0	18*
3	72	72
4	141	139
5	124	113
6	106	107
7	53	50
8	17	11
H,K= 2, 19		
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2	68	60
3	132	133
4	37	38
5	17	18
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6	105	101
8	394	392
10	334	338
12	163	157
14	358	360
16	22	13
18	79	75
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-18	141	136
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-11	166	169
-10	69	60
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-8	243	237
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-5	40	46
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-3	198	197
-2	340	343
-1	82	88
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1	223	218
2	27	28
3	131	126
4	153	146
5	90	87
6	200	202
7	166	181
8	93	94
9	93	96
10	85	81
11	53	56
12	53	52
13	148	142
14	99	105
15	0	30*
16	22	33
17	62	68
18	160	160
19	76	81
H,K= 3, 2		
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-18	232	220
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-15	47	50
-14	0	13*
-13	62	65
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-11	0	11*
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-9	62	68
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-7	52	51
-6	366	373
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-3	68	73
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0	315	312
1	96	99
2	108	113
3	134	134
4	228	237
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6	36	34
7	169	171
8	114	119
9	140	142
10	66	70
11	105	114
12	14	2*
13	90	95
14	33	34
15	0	4*
16	22	23
17	23	29
18	62	60
H,K= 3, 3		
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-19	69	73
-18	88	88
-17	77	69
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-13	53	52
-12	41	38
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-9	265	270
-8	43	39
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-6	441	449
-5	177	177
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0	287	290
1	210	206
2	171	176
3	199	199
4	269	273
5	34	31
6	569	584
7	195	196
8	130	132
9	58	58
10	308	314
11	36	38
12	180	184
13	25	31
14	0	13*
15	0	17*
16	132	130
17	16	27*
18	133	130
H,K= 3, 4		
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-20	23	32
-19	28	28
-18	31	32
-17	109	108
-16	15	10
-15	111	108
-14	133	135
-13	105	113
-12	54	57
-11	91	93
-10	209	208
-9	132	131
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-7	16	7
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-3	88	89
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1	69	67
2	384	385
3	149	151
4	82	87
5	135	133
6	12	12*
7	64	64
8	145	148
9	95	95
10	230	234
11	127	130
12	59	53
13	41	33
14	175	174
15	126	127
16	32	38
17	78	80
18	0	11*
H,K= 3, 5		
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-19	23	23
-18	109	112
-17	15	19
-16	210	204
-15	85	87
-14	275	274
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-12	73	75
-11	153	151
-10	279	281
-9	36	45
-8	163	176
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-1	334	333
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2	98	101
3	85	82
4	30	29
5	291	294
6	43	45
7	152	152
8	129	128
9	34	35
10	0	3*
11	246	247
12	20	27
13	102	104
14	66	68
15	110	110
16	32	32
17	91	94
18	88	82
H,K= 3, 6		
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-19	89	83
-18	62	60
-17	183	182
-16	26	26
-15	39	39
-14	62	66
-13	148	148
-12	30	26
-11	178	177
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-9	111	117
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-6	105	102
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-3	11	4*
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2	380	374
3	94	90
4	74	77
5	40	42
6	60	61
7	166	163
8	41	40
9	48	48
10	69	69
11	31	32
12	54	54
13	21	22
14	96	94
15	16	25*
16	84	88
17	29	23
18	24	24
H,K= 3, 7		
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-19	111	115
-18	80	76
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-16	22	26
-15	170	170
-14	25	27
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-12	55	52
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-5	110	120
-4	62	62
-3	159	154
-2	118	123
-1	115	110
0	125	132
1	150	149
2	194	193
3	169	166
4	17	7
5	66	68
6	322	323
7	18	19
8	44	51
9	13	10
10	151	149
11	122	120
12	81	84
13	78	77
14	95	98
15	16	7*
16	67	71
17	0	7*
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-11	38	43
-10	151	161
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-2	12	15
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2	12	18*
3	505	512
4	168	168
5	161	158
6	38	38
7	323	323
8	36	36
9	279	282
10	80	81
11	38	34
12	0	7*
13	147	140
14	35	41
15	153	163
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17	17	24
H,K= 3, 9		
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-18	17	10
-17	23	17
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-14	52	54
-13	86	92
-12	70	73
-11	14	10*
-10	93	95
-9	171	172
-8	13	18*
-7	124	127
-6	0	9*
-5	12	7
-4	166	174
-3	55	53
-2	122	123
-1	268	267
0	80	81
1	139	142
2	136	131
3	190	192
4	0	3*
5	135	130
6	62	66
7	70	72
8	159	155
9	37	39
10	46	47
11	178	171
12	130	119
13	73	72
14	16	15
15	102	97
16	0	6*
H,K= 3, 10		
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-15	61	64
-14	59	50
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-12	25	32
-11	240	252
-10	52	55
-9	27	31
-8	67	66
-7	218	224
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-2	102	100
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0	0	9*
1	96	92
2	86	82
3	93	95
4	29	31
5	44	43
6	41	31
7	123	120
8	42	39
9	83	80
10	85	85
11	34	37
12	0	14*
13	108	100
14	28	28
15	23	30
16	34	32
H,K= 3, 11		
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-16	16	19
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-13	90	90
-12	21	20
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-10	135	135
-9	114	115
-8	66	67
-7	148	143
-6	79	82
-5	166	166
-4	42	42
-3	37	38
-2	47	43
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0	26	19
1	204	204
2	183	181
3	137	133
4	14	19*
5	156	155
6	175	174
7	110	118
8	29	25
9	26	24
10	26	27
11	228	227
12	16	7
13	93	94
14	108	108
15	111	111
H,K= 3, 12		
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-14	16	20
-13	41	40
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-11	0	2*
-10	47	44
-9	142	144
-8	57	61
-7	183	183
-6	68	72
-5	78	79
-4	33	33
-3	283	285
-2	52	59
-1	73	69
0	0	5*
1	128	131
2	31	39
3	216	217
4	151	143
5	186	181
6	29	23
7	254	246
8	73	74
9	185	182
10	27	19
11	16	15
12	85	88
13	96	93
14	17	8
H,K= 3, 13		
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-14	33	31
-13	161	153
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-11	69	66
-10	50	50
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-7	38	37
-6	79	79
-5	219	223
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-3	145	140
-2	40	43
-1	52	57
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1	94	98
2	69	69
3	169	165
4	38	37
5	44	45
6	149	143
7	52	54
8	84	79
9	73	70
10	90	84
11	16	15
12	139	133
13	50	49
H,K= 3, 14		
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-10	31	28
-9	53	55
-8	15	21
-7	33	28
-6	82	86
-5	223	221
-4	81	82
-3	54	56
-2	46	44
-1	133	136
0	87	81
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2	59	61
3	68	67
4	15	15
5	0	9*
6	118	116
7	156	159
8	78	75
9	16	23
10	54	62
11	70	69
12	41	41
H,K= 3, 15		
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-11	111	116
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-7	44	49
-6	46	48
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-2	78	79
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0	0	2*
1	195	197
2	97	100
3	83	77
4	0	6*
5	150	150
6	52	49
7	115	117
8	28	23
9	16	16
10	17	6
11	200	193
H,K= 3, 16		
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-11	33	31
-10	52	53
-9	0	2*
-8	125	128
-7	22	2
-6	0	5*
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-3	27	15
-2	125	128
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1	22	34
2	129	132
3	27	18
4	143	145
5	55	56
6	32	31
7	43	47
8	115	120
9	24	15
H,K= 3, 17		
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-9	143	145
-8	33	40
-7	16	8
-6	93	97
-5	68	76
-4	48	52
-3	42	42
-2	50	58
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0	169	159
1	42	47
2	16	19
3	141	139
4	120	117
5	52	45
6	123	120
7	82	78
H,K= 3, 18		
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-6	173	169
-5	60	56
-4	23	26
-3	70	63
-2	128	127
-1	23	16
0	126	120
1	23	27
2	23	31
3	85	87
4	71	69
5	61	59
H,K= 3, 19		
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-1	56	49
0	85	87
H,K= 4, 0		
-20	94	89
-18	28	32
-16	26	23
-14	197	193
-12	276	279
-10	109	105
-8	319	310
-6	242	240
-4	105	108
-2	395	403
0	360	345
2	228	239
4	399	399
6	94	97
8	90	93
10	291	297
12	155	160
14	179	185
16	135	143
H,K= 4, 1		
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-19	0	17*
-18	112	109
-17	124	118
-16	141	136
-15	120	117
-14	89	85
-13	14	12*
-12	140	136
-11	228	220
-10	53	55
-9	82	78
-8	35	36
-7	251	253
-6	211	205
-5	237	239
-4	313	316
-3	45	46
-2	155	157
-1	178	185
0	114	118
1	203	203
2	53	52
3	12	13*
4	167	164
5	148	146
6	119	123
7	52	54

TABLE IV (*Continued*)

H,K= 4, 1		
8	144	140
9	75	76
10	28	32
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14	49	46
15	0	19*
16	118	116
17	0	10*
H,K= 4, 2		
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-18	95	88
-17	22	25
-16	68	67
-15	21	16
-14	32	24
-13	28	25
-12	45	49
-11	23	15
-10	172	169
-9	90	88
-8	116	116
-7	69	68
-6	238	244
-5	179	180
-4	50	51
-3	60	64
-2	12	17*
-1	67	70
0	114	114
1	86	82
2	39	42
3	45	49
4	39	43
5	169	169
6	57	59
7	99	101
8	219	222
9	69	67
10	0	8*
11	143	145
12	173	174
13	34	33
14	54	61
15	48	45
16	37	39
17	45	35
H,K= 4, 3		
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-19	64	66
-18	74	74
-17	38	37
-16	141	141
-15	76	79
-14	61	57
-13	20	16
-12	78	74
-11	48	47
-10	90	93
-9	76	79
-8	183	181
-7	12	15*
-6	208	213
-5	100	107
-4	362	373
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-2	0	15*
-1	93	94
0	219	218
1	64	65
2	266	269
3	74	78
4	151	154
5	105	112
6	277	278
7	35	36
8	386	394
9	106	104
10	103	98
11	74	78
12	160	159
13	22	19
14	83	95
15	36	34
16	58	56
H,K= 4, 4		
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-18	56	59
-17	22	34
-16	0	14*
-15	220	220
-14	201	200
-13	259	260
-12	183	182
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-10	182	178
-9	257	260
-8	328	323
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-6	17	28
-4	76	77
-3	315	327
-2	271	278
-1	107	108
0	168	165
1	182	183
2	254	259
3	150	156
4	252	255
5	48	42
6	29	25
7	78	73
8	33	34
9	107	108
10	130	140
11	21	18
12	72	80
13	0	2*
14	91	91
15	28	26
16	60	62
H,K= 4, 5		
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-18	80	80
-17	55	56
-16	79	81
-15	48	43
-14	173	177
-13	45	44
-12	90	87
-11	134	134
-10	30	22
-9	191	191
-8	0	1*
-7	66	77
-6	51	54
-5	187	189
-4	71	75
-3	257	265
-2	131	138
-1	17	14
0	105	107
1	314	314
2	95	97
3	169	166
4	135	135
5	161	161
6	35	27
7	160	160
8	86	83
9	81	85
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H,K= 5, 9		
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6	205	208
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H,K= 5, 15		
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H,K= 6, 7		
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H,K= 6 12		
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2	170	169
4	0	7*
H,K= 7, 1		
-11	0	10*
-10	55	57
-9	72	70
-8	52	48
-7	76	76
-6	0	1*
-5	0	9*
-4	118	117
-3	74	74
-2	62	55
-1	51	50
0	90	86
1	51	56
2	0	4*
3	62	63
4	33	33
5	0	8*
H,K= 7, 2		
-11	41	42
-10	0	12*
-9	29	21
-8	160	160
-7	23	17
-6	67	69
-5	16	8
-4	62	64
-3	0	8*
-2	58	56
-1	0	11*
0	76	73
1	23	10
2	0	7*
3	86	81
4	140	136
5	34	29
H,K= 7, 3		
-11	48	47
-10	44	40
-9	33	24
-8	40	35
-7	59	61
-6	94	91
-5	46	43
-4	61	64
-3	16	15
-2	104	101
-1	0	10*
0	54	51
1	16	12
2	0	6*
3	17	5*
4	124	122
5	24	30
H,K= 7, 4		
-10	110	108
-9	53	50
-8	66	68
-7	76	79
-6	80	84
-5	123	119
-4	43	44
-3	16	15
-2	28	29
-1	99	101
0	127	124
1	44	40
2	117	113
3	17	15
4	103	105
H,K= 7, 5		
-9	45	45
-8	0	4*
-7	24	25
-6	23	24
-5	33	31
-4	111	114
-3	28	25
-2	0	10*
-1	97	96
0	126	127
1	33	31
2	17	14*
3	92	87
4	54	47
H,K= 7, 6		
-8	72	74
-7	44	50
-6	33	30
-5	0	19*
-4	41	38
-3	52	53
-2	76	73
-1	41	34
0	29	18
1	17	9
2	45	38
3	17	13
H,K= 7, 7		
-7	34	28
-6	94	98
-5	101	108
-4	84	84
-3	79	73
-2	102	102
-1	0	10*
0	29	23
1	68	71
H,K= 7, 8		
-5	113	109
-4	29	31
-3	68	65
-2	29	20
-1	29	28

[a] Reflections given zero weight in the final refinement are marked with an asterisk.

five of the atoms with carbon scattering factors, reduced R to 0.070 and resulted in larger thermal parameters for these atoms (2.1–3.0 Å^2). A difference Fourier map was prepared in which appeared the water oxygen atom as well as 32 of the 34 hydrogen atoms; the two hydrogen atoms of the water molecule were not found. The sixth carbon atom in the structure was assumed to be disordered and occupied positions adjacent to either side of C(22) (Figure 1). Both of these positions, which up to now had been assumed to be occupied by boron atoms, had smaller than average thermal parameters and also had associated with them interatomic distances that were shorter than expected for boron atoms and longer than expected for carbon atoms. In the subsequent refinements each of the disordered atoms was assigned the scattering power of an atom that was half boron and half carbon.

After some blunders in the intensity data were corrected, a final series of full-matrix, least-squares refinement was executed. The scattering factors of the Cs and Co atoms were corrected for anomalous dispersion, and zero weight was assigned to all reflections which had $I < \sigma(I)$. A scale factor, three positional parameters for each of the 69 atoms, six anisotropic thermal parameters for each Cs and Co atom, individual isotropic thermal parameters for 33 nonhydrogen light atoms, and an average thermal parameter for all 32 hydrogens were refined. The R value for the 3305 statistically observable data became 0.034. For all 3649 data the R value is 0.041. The weighted R_2 factor, $(\Sigma w(|F_o| - |F_c|)^2/\Sigma wF_o^2)^{1/2}$, is 0.039. The standard deviation of an observation of unit weight is 1.2 and the rms values of $(|F_o| - |F_c|)/\sigma(F_o)$ averaged over small intensity intervals approximate this value over the entire intensity range. No parameter in the final refinement differed from that of the previous refinement cycle by an amount greater than one-tenth of its standard deviation.

Results and Discussion of the Structure

The final values for positional and thermal parameters are given in Table I for the heavy atoms, in Table II for the oxygen, carbon, and boron atoms, and in Table III for the hydrogen atoms. The observed and calculated structure factors are given in Table IV.

A drawing of the anion skeleton is given in Figure 1. It consists of two 11-light-atom icosahedral fragments, arbitrarily labeled cages I and III, each having a cobalt ion completing the icosahedron by bonding to the apex position of each cage. The cobalts are linked *via* the

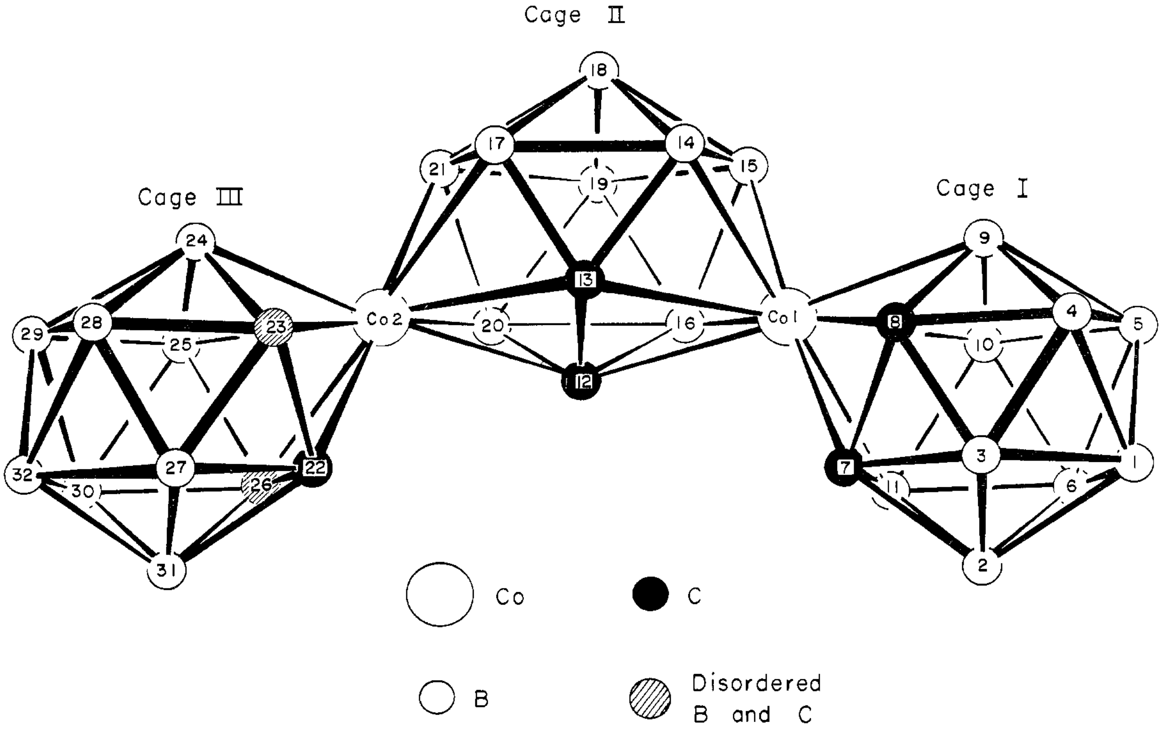

Figure 1.—Drawing of the $Co_2B_{26}C_6H_{32}^{2-}$ anion. Hydrogen atoms are not shown.

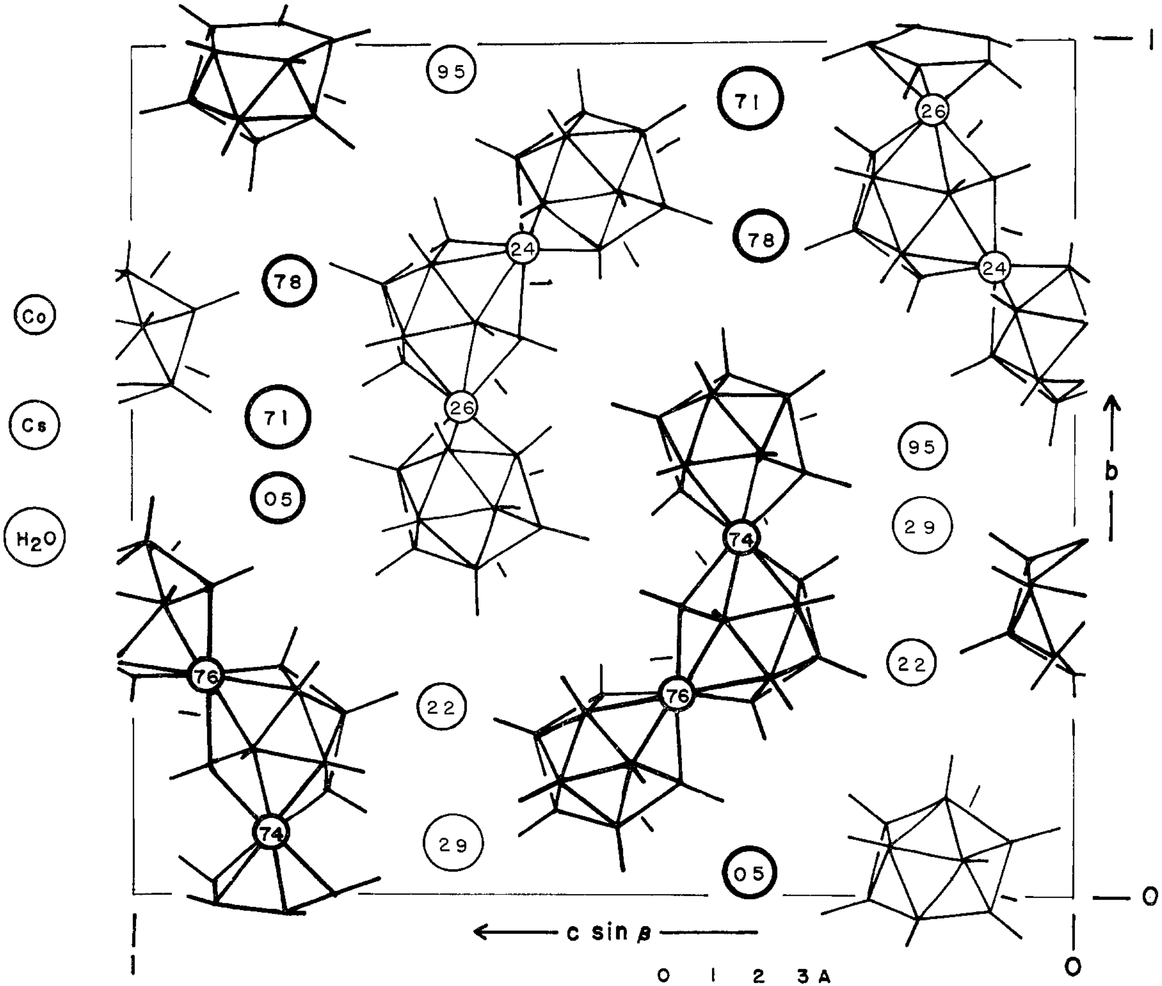

Figure 2.—Framework drawing of the unit cell contents projected down the *a* axis. Numbers in the circles represent the *x* coordinate of the atom ×100.

TABLE V

BOND DISTANCES

Atom 1	Atom 2	Distance, Å	Atom 1	Atom 2	Distance, Å
Co(1)	C(8)	2.051 ± 0.006	C(7)	B(2)	1.702 ± 0.009
Co(1)	C(7)	2.051 ± 0.006	B(11)	B(10)	1.815 ± 0.009
Co(1)	B(11)	2.094 ± 0.007	B(11)	B(2)	1.787 ± 0.009
Co(1)	B(10)	2.113 ± 0.007	B(11)	B(6)	1.772 ± 0.009
Co(1)	B(9)	2.081 ± 0.007	B(10)	B(9)	1.797 ± 0.009
Co(1)	C(12)	2.070 ± 0.005	B(10)	B(6)	1.775 ± 0.009
Co(1)	C(13)	2.061 ± 0.005	B(10)	B(5)	1.774 ± 0.009
Co(1)	B(14)	2.070 ± 0.006	B(9)	B(5)	1.776 ± 0.009
Co(1)	B(15)	2.100 ± 0.007	B(9)	B(4)	1.792 ± 0.009
Co(1)	B(16)	2.072 ± 0.006	B(3)	B(2)	1.762 ± 0.010
Co(2)	C(12)	2.065 ± 0.005	B(3)	B(4)	1.754 ± 0.009
Co(2)	C(13)	2.065 ± 0.005	B(2)	B(6)	1.759 ± 0.009
Co(2)	B(17)	2.053 ± 0.007	B(6)	B(5)	1.772 ± 0.009
Co(2)	B(20)	2.072 ± 0.006	B(5)	B(4)	1.776 ± 0.009
Co(2)	B(21)	2.101 ± 0.007	B(1)	B(3)	1.759 ± 0.010
Co(2)	C(22)	2.043 ± 0.006	B(1)	B(2)	1.775 ± 0.010
Co(2)	BC(23)	2.080 ± 0.006	B(1)	B(6)	1.779 ± 0.009
Co(2)	B(24)	2.087 ± 0.007	B(1)	B(5)	1.774 ± 0.009
Co(2)	B(25)	2.105 ± 0.007	B(1)	B(4)	1.754 ± 0.010
Co(2)	BC(26)	2.055 ± 0.006	C(12)	C(13)	1.561 ± 0.007
C(8)	C(7)	1.613 ± 0.008	C(12)	B(16)	1.719 ± 0.008
C(8)	B(9)	1.700 ± 0.008	C(12)	B(20)	1.713 ± 0.008
C(8)	B(3)	1.734 ± 0.009	C(13)	B(14)	1.695 ± 0.008
C(8)	B(4)	1.688 ± 0.009	C(13)	B(17)	1.720 ± 0.008
C(7)	B(11)	1.682 ± 0.008	B(14)	B(15)	1.808 ± 0.009
C(7)	B(3)	1.727 ± 0.009	B(14)	B(17)	1.823 ± 0.009
B(14)	B(18)	1.783 ± 0.009	BC(23)	B(28)	1.728 ± 0.009
B(15)	B(16)	1.791 ± 0.009	B(24)	B(25)	1.801 ± 0.009
B(15)	B(18)	1.791 ± 0.009	B(24)	B(28)	1.797 ± 0.009
B(15)	B(19)	1.768 ± 0.009	B(24)	B(29)	1.804 ± 0.009
B(16)	B(19)	1.783 ± 0.009	B(25)	BC(26)	1.729 ± 0.009
B(16)	B(20)	1.824 ± 0.009	B(25)	B(29)	1.790 ± 0.009
B(17)	B(18)	1.790 ± 0.009	B(25)	B(30)	1.814 ± 0.009
B(18)	B(19)	1.786 ± 0.009	BC(26)	B(30)	1.715 ± 0.009
B(19)	B(20)	1.786 ± 0.009	BC(26)	B(31)	1.747 ± 0.009
B(21)	B(17)	1.792 ± 0.009	B(27)	B(28)	1.772 ± 0.010
B(21)	B(18)	1.800 ± 0.009	B(27)	B(31)	1.748 ± 0.010
B(21)	B(19)	1.783 ± 0.009	B(28)	B(29)	1.764 ± 0.009
B(21)	B(20)	1.786 ± 0.009	B(29)	B(30)	1.787 ± 0.009
C(22)	BC(23)	1.643 ± 0.008	B(30)	B(31)	1.749 ± 0.010
C(22)	BC(26)	1.636 ± 0.008	B(32)	B(27)	1.764 ± 0.010
C(22)	B(27)	1.702 ± 0.009	B(32)	B(28)	1.775 ± 0.010
C(22)	B(31)	1.706 ± 0.009	B(32)	B(29)	1.784 ± 0.009
BC(23)	B(24)	1.729 ± 0.009	B(32)	B(30)	1.782 ± 0.009
BC(23)	B(27)	1.752 ± 0.009	B(32)	B(31)	1.750 ± 0.010

TABLE VI

HYDROGEN TO CARBON OR BORON DISTANCES (Å)[a]

Atoms in cage I		Atoms in cage II		Atoms in cage III	
Atom	Distance	Atom	Distance	Atom	Distance
C(8)	1.02	C(12)	0.94	C(22)	0.99
C(7)	0.81	C(13)	0.82	BC(23)	0.97
B(11)	1.12	B(14)	1.01	B(24)	1.05
B(10)	1.12	B(15)	1.11	B(25)	1.10
B(9)	1.10	B(16)	1.14	BC(26)	0.86
B(3)	1.11	B(17)	1.12	B(27)	1.12
B(2)	1.08	B(18)	1.26	B(28)	1.11
B(6)	1.07	B(19)	1.09	B(29)	1.15
B(5)	1.13	B(20)	1.14	B(30)	1.12
B(4)	1.11	B(21)	1.14	B(31)	0.98
B(1)	1.09			B(32)	1.07

[a] Estimated standard deviations on all distances are ±0.05 (Å).

TABLE VII

AVERAGES OF EQUIVALENT BOND DISTANCES (Å)[a,b]

Type	No.	Av	σ
Co–C	7	2.06	0.01
Co–B	11	2.09	0.02
C–B	12	1.71	0.02
B–B	48	1.78	0.02
C–H	5	0.92	0.10
B–H	25	1.11	0.05

[a] An average is given only if there are five or more values to include in the calculation of that average. [b] The root-mean-square deviation from the average is given by $\sigma = [\Sigma\Delta^2/(n-1)]^{1/2}$, where Δ_i is the difference between the ith bond distance and the average of n distances of the ith type.

TABLE VIII

ANGLES INVOLVING THE COBALTS AND THE CANASTIDE ION

Atom 1	Atom 2	Atom 3	Angle, deg	Atom 1	Atom 2	Atom 3	Angle, deg
C(12)	Co(1)	C(13)	44.4 ± 0.2	Co(1)	B(16)	B(15)	65.4 ± 0.3
C(12)	Co(2)	C(13)	44.4 ± 0.2	Co(2)	B(17)	B(21)	65.9 ± 0.3
C(12)	Co(1)	B(16)	49.0 ± 0.2	Co(2)	B(21)	B(17)	63.1 ± 0.3
C(13)	Co(1)	B(14)	48.5 ± 0.2	Co(2)	B(21)	B(20)	63.8 ± 0.3
C(12)	Co(2)	B(20)	48.9 ± 0.2	Co(2)	B(20)	B(21)	65.5 ± 0.3
C(13)	Co(2)	B(17)	49.4 ± 0.2	C(12)	C(13)	B(14)	112.9 ± 0.4
B(14)	Co(1)	B(15)	51.4 ± 0.2	C(12)	C(13)	B(17)	112.0 ± 0.4
B(15)	Co(1)	B(16)	50.8 ± 0.2	C(13)	C(12)	B(16)	112.0 ± 0.4
B(17)	Co(2)	B(21)	51.1 ± 0.2	C(13)	C(12)	B(20)	112.1 ± 0.4
B(20)	Co(2)	B(21)	50.7 ± 0.2	B(14)	C(13)	B(17)	64.5 ± 0.4
Co(1)	C(12)	C(13)	67.5 ± 0.2	B(16)	C(12)	B(20)	64.2 ± 0.4
Co(1)	C(13)	C(12)	68.1 ± 0.2	C(13)	B(14)	B(17)	58.4 ± 0.3
Co(2)	C(12)	C(13)	67.8 ± 0.2	C(13)	B(17)	B(14)	57.1 ± 0.3
Co(2)	C(13)	C(12)	67.8 ± 0.2	C(12)	B(16)	B(20)	57.7 ± 0.3
Co(1)	C(12)	B(16)	65.5 ± 0.3	C(12)	B(20)	B(16)	58.1 ± 0.3
Co(1)	C(13)	B(14)	66.1 ± 0.3	C(13)	B(14)	B(15)	104.7 ± 0.4
Co(2)	C(12)	B(20)	65.8 ± 0.3	C(12)	B(16)	B(15)	104.7 ± 0.4
Co(2)	C(13)	B(17)	64.9 ± 0.3	C(13)	B(17)	B(21)	104.9 ± 0.4
Co(1)	B(14)	C(13)	65.5 ± 0.3	C(12)	B(20)	B(21)	105.3 ± 0.4
Co(1)	B(16)	C(12)	65.4 ± 0.3	B(14)	B(15)	B(16)	105.5 ± 0.4
Co(2)	B(17)	C(13)	65.7 ± 0.3	B(17)	B(21)	B(20)	105.5 ± 0.4
Co(2)	B(20)	C(12)	65.3 ± 0.2	C(13)	B(14)	B(18)	103.9 ± 0.4
Co(1)	B(14)	B(15)	65.2 ± 0.3	C(13)	B(17)	B(18)	102.5 ± 0.4
Co(1)	B(15)	B(14)	63.5 ± 0.3	C(12)	B(16)	B(19)	102.7 ± 0.4
Co(1)	B(15)	B(16)	63.8 ± 0.3	C(12)	B(20)	B(19)	102.8 ± 0.4
B(15)	B(14)	B(18)	59.8 ± 0.4	B(16)	B(19)	B(21)	110.3 ± 0.4
B(21)	B(17)	B(18)	60.3 ± 0.4	B(18)	B(19)	B(20)	107.9 ± 0.5
B(15)	B(16)	B(19)	59.3 ± 0.4	Co(1)	C(13)	B(17)	125.1 ± 0.3
B(21)	B(20)	B(19)	59.9 ± 0.4	Co(1)	B(14)	B(17)	119.1 ± 0.3
B(14)	B(15)	B(18)	59.4 ± 0.4	Co(1)	B(14)	B(18)	118.5 ± 0.4
B(17)	B(21)	B(18)	59.8 ± 0.4	Co(1)	B(15)	B(18)	116.6 ± 0.3
B(16)	B(15)	B(19)	60.1 ± 0.4	Co(1)	B(15)	B(19)	116.9 ± 0.3
B(20)	B(21)	B(19)	60.0 ± 0.4	Co(1)	B(16)	B(19)	117.6 ± 0.3
B(14)	B(17)	B(18)	59.1 ± 0.4	Co(1)	B(16)	B(20)	118.4 ± 0.3
B(17)	B(14)	B(18)	59.5 ± 0.4	Co(1)	C(12)	B(20)	124.3 ± 0.3
B(16)	B(20)	B(19)	59.2 ± 0.4	Co(2)	C(12)	B(16)	124.7 ± 0.3
B(20)	B(16)	B(19)	59.3 ± 0.4	Co(2)	B(20)	B(16)	118.8 ± 0.3
B(17)	B(18)	B(15)	110.0 ± 0.5	Co(2)	B(20)	B(19)	118.0 ± 0.3
B(17)	B(18)	B(19)	106.7 ± 0.5	Co(2)	B(21)	B(19)	116.7 ± 0.3
B(14)	B(18)	B(19)	106.9 ± 0.5	Co(2)	B(21)	B(18)	116.2 ± 0.3
B(14)	B(18)	B(21)	109.3 ± 0.5	Co(2)	B(17)	B(18)	119.1 ± 0.3
B(15)	B(18)	B(21)	109.0 ± 0.5	Co(2)	B(17)	B(14)	118.4 ± 0.3
B(15)	B(19)	B(21)	110.9 ± 0.5	Co(2)	C(13)	B(14)	124.4 ± 0.3
B(15)	B(19)	B(20)	110.3 ± 0.5	Co(1)	C(12)	Co(2)	134.1 ± 0.2
B(16)	B(19)	B(18)	108.3 ± 0.5	Co(1)	C(13)	Co(2)	134.7 ± 0.2

basket-shaped canastide ion completing a third icosahedron, labeled cage II, by bonding to the open faces in this bridging fragment. The cages are staggered with respect to each other across the cobalts. That is, atoms 7 and 22 are equidistant from atoms 12 and 13. The two carbon atoms in each of cages I and II were located at positions 7 and 8 and 12 and 13, respectively. Disorder was found, however, in cage III, one carbon being localized at position 22 and the other being equally distributed between positions 23 and 26 adjacent to position 22. This disorder indicates the presence of three rotational isomers in the crystal differing only in the directions of rotation of the end cages. Beginning from a hypothetical configuration in which the carbons are all eclipsed, each end cage is rotated 36° either to the right or to the left. The isomers consist of an enantiomorphic pair with point symmetry 2 and a third isomer with point symmetry m. Since the external shape is not sensitive to the carbon positions, one might expect disorder at both ends of the anion. We have no explanation for the fact that all the disorder seems to be at cage III. Ignoring the distinction between boron and carbon, the anion has approximately 2mm (C_{2v}) point symmetry in which one of the mirror planes contains atoms in positions 12, 13, 18, and 19 of cage II and the other mirror plane is perpendicular to the first one and bisects the bonds between atoms 12–13 and 18–19. The twofold rotation axis is along the intersection of these two mirror planes. If the carbon atom in position 8 of cage I were disordered equally between positions 8 and 11, the anion would have 2mm point symmetry with respect to all atoms including borons and carbons. The axis of cage I, Co(1)–B(1), makes an angle of 117° with the axis of cage III, Co(2)–B(32); the ideal angle for regular icosahedra is 116.5°. The cages are arranged such that all of the carbon atoms lie on the interior side of this angle and are as close to each other as is possible in this staggered configuration.

The bond distances between all the atoms in the icosahedral framework except hydrogens are listed in Table V and the distances between the hydrogen atoms and the atoms to which they are bonded are given in Table VI. The standard deviations quoted on the bond distances in these tables are calculated from the least-squares estimates of the accuracy of the final positional parameters. Probably a better estimate of their accuracy is given by the larger root-mean-square deviations of equivalent bond distances from their average values, given in Table VII. A complete list of bond angles would be a rather long list indeed. Therefore, since both the cages I and III are analogous to the previously investigated 11-atom icosahedral fragments,[7] only the angles involving the 10-atom fragment, cage II, are reported in Table VIII.

The molecular packing in the crystal is shown in Figure 2 by a framework drawing of the projection of the unit cell contents along the *a* axis. This drawing, together with the distances given in Table IX, reveals a series of interactions among the cesium ions, the oxygens of the water molecules, and the hydrogen atoms attached to the anion. The cesium ions and the anion cages are held in their relative orientations by the balance of the attraction of their unlike charges with the repulsive forces of the electrons in the cesium ions and the hydrogen atoms attached to the cages. All of the shortest distances to the oxygen, given in Table IX, correspond to reasonable van der Waals contacts expected for a normal water of hydration.

TABLE IX

SHORTEST DISTANCES (Å) TO CESIUMS AND OXYGEN[a]

Atom	To O(1)	Atom	To Cs(1)	Atom	To Cs(2)
H(1)	2.76	H(18)	2.82	H(15)	2.95
H(24)	2.78	H(32)	2.95	H(4)	3.05
H(6)	2.78	H(17)	2.99	H(10)	3.08
H(17)	2.93	H(19)	3.00	H(24)	3.08
Cs(2)	3.029	H(11)	3.12	H(21)	3.10
Cs(1)	3.163	H(6)	3.15	H(6)	3.16
H(5)	3.21	H(29)	3.23	H(25)	3.25
H(21)	3.26	H(3)	3.24		
		H(30)	3.29		

[a] Estimated standard deviations are all ±0.05 Å except O(1) to Cs(1) and to Cs(2) which are ±0.006 Å.

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The Structures of *gauche*- and *trans*-Tetrafluorohydrazine as Determined by Electron Diffraction

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The interatomic distances, bond angles, and the proportions of *gauche* and *trans* isomers present in N_2F_4 have been determined by gas-phase electron diffraction. The two rotamers are similar in structure except for the dihedral angle ($\theta_g = 67.1 \pm 0.8°$). The 47% *gauche*–53% *trans* mixture found at below room temperature indicates that the *trans* is 300–500 cal more stable than the *gauche* rotamer. The bond lengths N–N = 1.489 ± 0.007 Å and N–F = 1.375 ± 0.004 Å are the same for both species but the valence angles are slightly different ($\angle FNF_g = 105.1 \pm 1.0°$, $\angle FNF_t = 102.9 \pm 0.75°$, $\angle F_1NN_g = 100.1 \pm 1.0°$, $\angle F_2NN_g = 104.3 \pm 1.0°$, $\angle FNN_t = 100.6 \pm 0.6°$). The nonbonded mean-square amplitudes show a strong angular dependence on the equilibrium geometry due to torsional motion about the N–N bond.

Introduction

The structure of tetrafluorohydrazine has been the subject of considerable discussion in recent years. The first experimental study was made with microwaves.[1] As is typical for fluorinated molecules only a limited amount of isotopically substituted species were available. For assumed bonded distances of N–N = 1.47 Å and N–F = 1.37 Å, the valence angles were found to be ∠FNF = 108° and ∠FNN = 104°, with a dihedral angle of 65°; the estimated accuracy is 2–3°. The *trans* rotamer of N_2F_4 has C_{2h} symmetry and thus no dipole moment. The fact that the spectrum was observed indicated that a significant amount of the

[1] D. R. Lide and D. E. Mann, *J. Chem. Phys.*, **31**, 1129 (1959).