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THE CRYSTAL STRUCTURE OF Cs2(B9C2H11)Co(B8C2H10) Co(B9C2H11)*H2O, A SALT OF A THREE-ICOSAHEDRAL- FRAGMENT METALLOCARBORANE

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David St. Clair, Allan Zalkin, and David H. Templeton

April 1969

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UNIVERSITY OF CALIFORNIA

Lawrence Radiation Laboratory
Berkeley, California 94720

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CONTRIBUTION FROM THE LAWRENCE RADIATION LABORATORY AND DEPARTMENT OF CHEMISTRY, UNIVERSITY OF CALIFORNIA, BERKELEY, CALIFORNIA 94720

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]

By David St. Clair, Allan Zalkin, and David H. Templeton

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

The crystal structure of the monohydrate of the 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 Å., b = 19.240 Å., c = 20.682 Å., β = 98.00°. The calculated density is ρ = 1.871 g/cc. 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 ten light atom icosahedron are occupied by cobalts each of which is common to another icosahedron containing eleven 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

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(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 reference 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.

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consisted of two of the previously known eleven atom icosahedral fragments each having a cobalt atom bonded to the open face with the cobalts linked together via a new ten 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

The dark red crystals were received from Professor Hawthorne of the University of California, Riverside. One was cut to the dimensions 0.11 x 0.12 x 0.23 mm and was glued to a glass fiber with its b axis coincident with the rotation axis of the fiber.

The space group and approximate cell dimensions were determined from oscillation, Weissenberg and precession photographs. Using a manual General Electric XRD-5 diffractometer, space group absences were checked and accurate unit cell dimensions were obtained from measurements of the h00, 0k0, and 00ℓ reflections with the b axis of the crystal parallel to the φ axis of the goniostat. Intensity data were measured with this manually operated diffractometer using a quarter circle, Eulerian cradle goniostat, and a scintillation counter equipped with a pulse height discriminator for detection of the diffracted beam. Molybdenum Kα X-rays were used (Mo $K\alpha_1$; $\lambda = 0.70926$ Å.) after the Kβ radiation was filtered out by a 0.003 inch thick Zr filter placed in front of the receiving slit. One complete set of independent reflections (including space group absences) with $2\theta \leq 45^\circ$ ($\sin\theta/\lambda = 0.995$) was measured using the stationary crystal, stationary counter technique by taking ten second counts at the maximum intensity settings. Excluding space group extinctions, there were 3649 independent reflections of which 344 had intensities less than their estimated standard deviations.

The absorption coefficient is $\mu = 38$ cm^{-1}. Absorption effects on the data were neglected. It is estimated that the scale factors which would be applied to the intensity data would very by less than 12 %.

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 done 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, $\sigma(I) = [I + 2I_b + (0.05I)^2]^{\frac{1}{2}}$, 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

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

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atoms whose scattering factors are those of Stewart, Davidson and Simpson[5].

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(5) R. F. Stewart, E. R. Davidson and W. T. Simpson, Table II, J. Chem. Phys., 42, 3175(1965).

Cromer's corrections for anomalous dispersion[6] applied to the scattering

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

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factors of the Cs and Co are $\Delta f' = -0.5$ and $\Delta f'' = +2.6$ electrons and $\Delta f' = +0.4$ and $\Delta f'' = +1.0$ electrons, respectively. The anisotropic temperature factors were of the form $\exp(-\beta_{11}h^2-\beta_{22}k^2-\beta_{33}\ell^2-2\beta_{12}hk-2\beta_{13}h\ell-2\beta_{23}k\ell)$.

Crystal Data

The crystals were found to be monoclinic with unit cell dimensions, measured at room temperature (~22°), $\underline{a}$ = 7.089 ± 0.004 Å., $\underline{b}$ = 19.240 ± 0.014 Å., $\underline{c}$ = 20.682 ± 0.004 Å., $\underline{\beta}$ = 98.00 ± 0.06 degrees. There are four formula units, $Cs_2Co_2B_{26}C_6OH_{34}$, per unit cell. The density is calculated to be $\underline{\rho}$ = 1.87 g/cc. No density measurement was made because the sample was lost.

The observed extinction rules, $\underline{h0\ell}$, $\underline{\ell}$ = $\underline{2n}$ and $\underline{0k0}$, $\underline{k}$ = $\underline{2n}$, correspond to space group $P2_1/c$. All atoms lie on the general symmetry related positions, ± ($\underline{x,y,z}$ and $\underline{x,\frac{1}{2}-y,\frac{1}{2}+z}$).

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 was synthesized from which the coordinates of the thirty two boron and carbon atoms were found. Since a water of crystallization was not expected, the oxygen atom which appeared in this Fourier was disregarded. When the positions and thermal parameters of these thirty two light atoms, all with the scattering power of boron, were incorporated into the refinement, the R value dropped to 0.105. Inspection of the bond distances and thermal parameters allowed location of five of the six carbon atoms and gave indications that the sixth carbon was disordered between only two atomic positions in one of the icosahedral cages. So in all further refinements, five of these atoms were given the scattering power of carbon and two were given the scattering power of half carbon and half boron. Following another series of refinements in which the Cs and Co atoms were given anisotropic thermal parameters, another difference Fourier was prepared in which again appeared the oxygen atom as well as thirty two of the thirty four hydrogen atoms. The two hydrogens in the water molecule did not appear. After some blunders in the intensity data were corrected, a final series of full matrix least squares refinement was carried out in which 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 sixty nine atoms, six anisotropic temperature parameters for each Cs and Co atom, individual isotropic temperature parameters for the thirty three light

atoms excluding hydrogens, and an average temperature parameter for all thirty two hydrogens were refined. The conventional R value for all non-zero-weighted data reached R = 0.034 for 3305 data, the weighted R value was R_2 = 0.039 and the conventional R value calculated with all 3649 data was R = 0.041. The standard deviation of observation of unit weight was 1.2 and the r.m.s. values of $(|F_o| - |F_c|)/\sigma(F_o)$ averaged over small intensity intervals approximated this value over the entire intensity range. No parameter in the final refinement differed from that of the previous refinement by an amount greater than one tenth of its estimated 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, 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 eleven-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 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 number 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

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.

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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,b,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 $\underline{B} = 2.6 \pm 0.2$ Å^2.

(c) Standard deviations for $\underline{x}$, $\underline{y}$, and $\underline{z}$ are ±0.007, ±0.003, and ±0.003, respectively.

TABLE IV

Observed and Calculated Structure Factors

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

OBSERVED AND CALCULATED STRUCTURE FACTORS

FCA(0,0,0) = 2960

L	FOB	FCA
H,K= -1, -6	3	88
21	0	8*
H,K= -1, -5	4	401
21	5	94
21	62	65
H,K= -1, -4	7	137
21	106	110
H,K= -1, -3	9	84
21	0	1*
22	0	13*
H,K= -1, -2	12	67
21	33	130
22	93	100
H,K= -1, -1	15	101
21	80	79
22	17	19*
H,K= 0, 0	2	2777
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	8	115
1	78	69
3	84	76
5	365	356
7	201	196
9	88	85
11	210	208
13	295	291
15	325	320
17	73	77
19	46	42
21	68	68
23	39	37
H,K= 0, 2	1	252
2	253	248
3	217	241
4	93	95
5	71	70
6	194	206
7	41	30
8	123	127
9	147	150
10	176	174
11	56	56
12	264	262
13	67	68
14	269	270
15	64	69
16	174	173
17	30	29
18	21	20
19	219	215
20	12	12*
21	0	12*
H,K= 0, 3	1	192
2	296	291
3	307	296
4	572	575
5	8	6*
6	120	116
7	247	243
8	670	673
9	46	36
10	76	77
11	152	152
12	85	85
13	79	82
14	194	193
15	0	73*
16	126	125
17	70	70
18	78	77
19	60	63
20	114	117
21	0	21*
H,K= 0, 4	1	188
2	694	708
3	418	402
4	260	247
5	44	44
6	128	121
7	70	72
8	78	77
9	276	272
10	124	120
11	78	77
12	37	32
13	188	182
14	0	35
15	133	138
16	74	73
17	10	10*
18	76	73
19	157	157
H,K= 0, 5	1	303
2	26	24
3	320	418
4	159	160
5	73	78
6	12	14*
7	154	151
8	124	120
9	276	272
10	27	27
11	152	156
12	32	22
13	188	182
14	0	48
15	133	138
16	74	73
17	10	10*
18	76	73
19	157	157
H,K= 0, 6	1	303
2	26	24
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H,K= 0, 14	1	303
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H,K= 0, 16	1	303
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7	154	151
8	124	120
9	276	272
10	27	27
11	152	156
12	32	22
13	188	182
14	0	48
15	133	138
16	74	73
17	10	10*
18	76	73
19	157	157
H,K= 0, 17	1	303
2	26	24
3	320	418
4	159	160
5	73	78
6	12	14*
7	154	151
8	124	120
9	276	272
10	27	27
11	152	156
12	32	22
13	188	182
14	0	48
15	133	138
16	74	73
17	10	10*
18	76	73
19	157	157
H,K= 0, 18	1	303
2	26	24
3	320	418
4	159	160
5	73	78
6	12	14*
7	154	151
8	124	120
9	276	272
10	27	27
11	152	156
12	32	22
13	188	182
14	0	48
15	133	138
16	74	73
17	10	10*
18	76	73
19	157	157
H,K= 0, 19	1	303
2	26	24
3	320	418
4	159	160
5	73	78
6	12	14*
7	154	151
8	124	120
9	276	272
10	27	27
11	152	156
12	32	22
13	188	182
14	0	48
15	133	138
16	74	73
17	10	10*
18	76	73
19	157	157
H,K= 0, 20	1	303
2	26	24
3	320	418
4	159	160
5	73	78
6	12	14*
7	154	151
8	124	120
9	276	272
10	27	27
11	152	156
12	32	22
13	188	182
14	0	48
15	133	138
16	74	73
17	10	10*
18	76	73
19	157	157
H,K= 0, 21	1	303
2	26	24
3	320	418
4	159	160
5	73	78
6	12	14*
7	154	151
8	124	120
9	276	272
10	27	27
11	152	156
12	32	22
13	188	182
14	0	48
15	133	138
16	74	73
17	10	10*
18	76	73
19	157	157
H,K= 0, 22	1	303
2	26	24
3	320	418
4	159	160
5	73	78
6	12	14*
7	154	151
8	124	120
9	276	272
10	27	27
11	152	156
12	32	22
13	188	182
14	0	48
15	133	138
16	74	73
17	10	10*
18	76	73
19	157	157
H,K= 0, 23	1	303
2	26	24
3	320	418
4	159	160
5	73	78
6	12	14*
7	154	151
8	124	120
9	276	272
10	27	27
11	152	156
12	32	22
13	188	182
14	0	48
15	133	138
16	74	73
17	10	10*
18	76	73
19	157	157
H,K= 0, 24	1	303
2	26	24
3	320	418
4	159	160
5	73	78
6	12	14*
7	154	151
8	124	120
9	276	272
10	27	27
11	152	156
12	32	22
13	188	182
14	0	48
15	133	138
16	74	73
17	10	10*
18	76	73
19	157	157
H,K= 1, 0	2	277
2	88	84
4	401	403
6	94	95
8	62	65
10	37	37
12	137	137
14	106	110
16	150	156
18	116	124
20	52	53
22	42	42
H,K= 1, 1	2	199
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= 1, 2	1	252
2	253	248
3	217	241
4	93	95
5	71	70
6	194	206
7	41	30
8	123	127
9	147	150
10	176	174
11	56	56
12	264	262
13	67	68
14	269	270
15	64	69
16	174	173
17	30	29
18	21	20
19	219	215
20	12	12*
21	0	12*
H,K= 1, 3	1	192
2	296	291
3	307	296
4	572	575
5	8	6*
6	120	116
7	247	243
8	670	673
9	46	36
10	76	77
11	152	152
12	85	85
13	79	82
14	194	193
15	0	73*
16	126	125
17	70	70
18	78	77
19	60	63
20	114	117
21	0	21*
H,K= 1, 4	1	188
2	694	708
3	418	402
4	260	247
5	44	44
6	128	121
7	70	72
8	78	77
9	276	272
10	124	120
11	78	77
12	37	32
13	188	182
14	0	48
15	133	138
16	74	73
17	10	10*
18	76	73
19	157	157
H,K= 1, 5	1	303
2	26	24
3	320	418
4	159	160
5	73	78
6	12	14*
7	154	151
8	124	120
9	276	272
10	27	27
11	152	156
12	32	22
13	188	182
14	0	48
15	133	138
16	74	73
17	10	10*
18	76	73
19	157	157
H,K= 1, 6	1	303
2	26	24
3	320	418
4	159	160
5	73	78
6	12	14*
7	154	151
8	124	120
9	276	272
10	27	27
11	152	156
12	32	22
13	188	182
14	0	48
15	133	138
16	74	73
17	10	10*
18	76	73
19	157	157
H,K= 1, 7	1	303
2	26	24
3	320	418
4	159	160
5	73	78
6	12	14*
7	154	151
8	124	120
9	276	272
10	27	27
11	152	156
12	32	22
13	188	182
14	0	48
15	133	138
16	74	73
17	10	10*
18	76	73
19	157	157
H,K= 1, 8	1	303
2	26	24
3	320	418
4	159	160
5	73	78
6	12	14*
7	154	151
8	124	120
9	276	272
10	27	27
11	152	156
12	32	22
13	188	182
14	0	48
15	133	138
16	74	73
17	10	10*
18	76	73
19	157	157
H,K= 1, 9	1	303
2	26	24
3	320	418
4	159	160
5	73	78
6	12	14*
7	154	151
8	124	120
9	276	272
10	27	27
11	152	156
12	32	22
13	188	182
14	0	48
15	133	138
16	74	73
17	10	10*
18	76	73
19	157	157
H,K= 1, 10	1	303
2	26	24
3	320	418
4	159	160
5	73	78
6	12	14*
7	154	151
8	124	120
9	276	272
10	27	27
11	152	156
12	32	22
13	188	182
14	0	48
15	133	138
16	74	73
17	10	10*
18	76	73
19	157	157
H,K= 1, 11	1	303
2	26	24
3	320	418
4	159	160
5	73	78
6	12	14*
7	154	151
8	124	120
9	276	272
10	27	27
11	152	156
12	32	22
13	188	182
14	0	48
15	133	138
16	74	73
17	10	10*
18	76	73
19	157	157
H,K= 1, 12	1	303
2	26	24
3	320	418
4	159	160
5	73	78
6	12	14*
7	154	151
8	124	120
9	276	272
10	27	27
11	152	156
12	32	22
13	188	182
14	0	48
15	133	138
16	74	73
17	10	10*
18	76	73
19	157	157
H,K= 1, 13	1	303
2	26	24
3	320	418
4	159	160
5	73	78
6	12	14*
7	154	151
8	124	120
9	276	272
10	27	27
11	152	156
12	32	22
13	188	182
14	0	48
15	133	138
16	74	73
17	10	10*
18	76	73
19	157	157
H,K= 1, 14	1	303
2	26	24
3	320	418
4	159	160
5	73	78
6	12	14*
7	154	151
8	124	120
9	276	272
10	27	27
11	152	156
12	32	22
13	188	182
14	0	48
15	133	138
16	74	73
17	10	10*
18	76	73
19	157	157
H,K= 1, 15	1	303
2	26	24
3	320	418
4	159	160
5	73	78
6	12	14*
7	154	151
8	124	120
9	276	272
10	27	27
11	152	156
12	32	22
13	188	182
14	0	48
15	133	138
16	74	73
17	10	10*
18	76	73
19	157	157
H,K= 1, 16	1	303
2	26	24
3	320	418
4	159	160
5	73	78
6	12	14*
7	154	151
8	124	120
9	276	272
10	27	27
11	152	156
12	32	22
13	188	182
14	0	48
15	133	138
16	74	73
17	10	10*
18	76	73
19	157	157
H,K= 1, 17	1	303
2	26	24
3	320	418
4	159	160
5	73	78
6	12	14*
7	154	151
8	124	120
9	276	272
10	27	27
11	152	156
12	32	22
13	188	182
14	0	48
15	133	138
16	74	73
17	10	10*
18	76	73
19	157	157
H,K= 1, 18	1	303
2	26	24
3	320	418
4	159	160
5	73	78
6	12	14*
7	154	151
8	124	120
9	276	272
10	27	27
11	152	156
12	32	22
13	188	182
14	0	48
15	133	138
16	74	73
17	10	10*
18	76	73
19	157	157
H,K= 1, 19	1	303
2	26	24
3	320	418
4	159	160
5	73	78
6	12	14*
7	154	151
8	124	120
9	276	272
10	27	27
11	152	156
12	32	22
13	188	182
14	0	48
15	133	138
16	74	73
17	10	10*
18	76	73
19	157	157
H,K= 1, 20	1	303
2	26	24
3	320	418
4	159	160
5	73	78
6	12	14*
7	154	151
8	124	120
9	276	272
10	27	27
11	152	156
12	32	22
13	188	182
14	0	48
15	133	138
16	74	73
17	10	10*
18	76	73
19	157	157
H,K= 1, 21	1	303
2	26	24
3	320	418
4	159	160
5	73	78
6	12	14*
7	154	151
8	124	120
9	276	272
10	27	27
11	152	156
12	32	22
13	188	182
14	0	48
15	133	138
16	74	73
17	10	10*
18	76	73
19	157	157
H,K= 1, 22	1	303
2	26	24
3	320	418
4	159	160
5	73	78
6	12	14*
7	154	151
8	124	120
9	276	272
10	27	27
11	152	156
12	32	22
13	188	182
14	0	48
15	133	138
16	74	73
17	10	10*
18	76	73
19	157	157
H,K= 1, 23	1	303
2	26	24
3	320	418
4	159	160
5	73	78
6	12	14*
7	154	151
8	124	120
9	276	272
10	27	27
11	152	156
12	32	22
13	188	182
14	0	48
15	133	138
16	74	73
17	10	10*
18	76	73
19	157	157
H,K= 1, 24	1	303
2	26	24
3	320	418
4	159	160
5	73	78
6	12	14*
7	154	151
8	124	120
9	276	272
10	27	27
11	152	156
12	32	22
13	188	182
14	0	48
15	133	138
16	74	73
17	10	10*
18	76	73
19	157	157
H,K= 2, 0	1	137
2	118	113
4	1137	1134
6	1118	1113
8	1137	1134
10	1118	1113
12	1137	1134
14	1118	1113
16	1137	1134
18	1118	1113
20	1137	1134
22	1118	1113
H,K= 2, 1	2	277
4	401	403
6	94	95
8	62	65
10	37	37
12	137	137
14	106	110
16	150	156
18	116	124
20	52	53
22	42	42
H,K= 2, 2	2	277
4	401	403
6	94	95
8	62	65
10	37	37
12	137	137
14	106	110
16	150	156
18	116	124
20	52	53
22	42	42
H,K= 2, 3	1	192
2	296	291
3	307	296
4	572	575
5	8	6*
6	120	116
7	247	243
8	670	673
9	46	36
10	76	77
11	152	152
12	85	85
13	79	82
14	194	193
15	0	73*
16	126	125
17	70	70
18	78	77
19	60	63
20	114	117
21	0	21*
H,K= 2, 4	1	188
2	694	708
3	418	402
4	260	247
5	44	44
6	128	121
7	70	72
8	78	77
9	276	272
10	124	120
11	78	77
12	37	32
13	188	182
14	0	48
15	133	138
16	74	73
17	10	10*
18	76	73
19	157	157
H,K= 2, 5	1	303
2	26	24
3	320	418
4	159	160
5	73	78
6	12	14*
7	154	151
8	124	120
9	276	272
10	27	27
11	152	156
12	32	22
13	188	182
14	0	48
15	133	138
16	74	73
17	10	10*
18	76	73
19	157	157
H,K= 2, 6	1	303
2	26	24
3	320	418
4	159	160
5	73	78
6	12	14*
7	154	151
8	124	120
9	276	272
10	27	27
11	152	156
12	32	22
13	188	182
14	0	48
15	133	138
16	74	73
17	10	10*
18	76	73
19	157	157
H,K= 2, 7	1	303
2	26	24
3	320	418
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5	73	78
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8	124	120
9	276	272
10	27	27
11	152	156
12	32	22
13	188	182
14	0	48
15	133	138
16	74	73
17	10	10*
18	76	73
19	157	157
H,K= 2, 8	1	303
2	26	24
3	320	418
4	159	160
5	73	78
6	12	14*
7	154	151
8	124	120
9	276	272
10	27	27
11	152	156
12	32	22
13	188	182
14	0	48
15	133	138
16	74	73
17	10	10*
18	76	73
19	157	157
H,K= 2, 9	1	303
2	26	24
3	320	418
4	159	160
5	73

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the first one and bisects the bonds between atoms 12 to 13 and 18 to 19. The 2-fold 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) to B(1), makes an angle of 117° with the axis of cage III, Co(2) to B(32). The cages are arranged such that all 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 eleven-atom icosahedral fragments[7], only the angles involving the

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

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ten-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 contents of the unit cell seen from a view along the a axis. This drawing together with the distances given in Table IX reveals a series of interactions between the cesium ions, the oxygens of the water molecules and the hydrogen atoms attached to the anion. The cesium ions

TABLE V

Bond Distances

Atom 1	Atom 2	Distance (Å)	Atom 1	Atom 2	Distance (Å)
Co(1)	C(8)	2.051 ± .006	C(7)	B(2)	1.702 ± .009
Co(1)	C(7)	2.051 ± .006	B(11)	B(10)	1.815 ± .009
Co(1)	B(11)	2.094 ± .007	B(11)	B(2)	1.787 ± .009
Co(1)	B(10)	2.113 ± .007	B(11)	B(6)	1.772 ± .009
Co(1)	B(9)	2.081 ± .007	B(10)	B(9)	1.797 ± .009
Co(1)	C(12)	2.070 ± .005	B(10)	B(6)	1.775 ± .009
Co(1)	C(13)	2.061 ± .005	B(10)	B(5)	1.774 ± .009
Co(1)	B(14)	2.070 ± .006	B(9)	B(5)	1.776 ± .009
Co(1)	B(15)	2.100 ± .007	B(9)	B(4)	1.792 ± .009
Co(1)	B(16)	2.072 ± .006	B(3)	B(2)	1.762 ± .010
Co(2)	C(12)	2.065 ± .005	B(3)	B(4)	1.754 ± .009
Co(2)	C(13)	2.065 ± .005	B(2)	B(6)	1.759 ± .009
Co(2)	B(17)	2.053 ± .007	B(6)	B(5)	1.772 ± .009
Co(2)	B(20)	2.072 ± .006	B(5)	B(4)	1.776 ± .009
Co(2)	B(21)	2.101 ± .007	B(1)	B(3)	1.759 ± .010
Co(2)	C(22)	2.043 ± .006	B(1)	B(2)	1.775 ± .010
Co(2)	BC(23)	2.080 ± .006	B(1)	B(6)	1.779 ± .009
Co(2)	B(24)	2.087 ± .007	B(1)	B(5)	1.774 ± .009
Co(2)	B(25)	2.105 ± .007	B(1)	B(4)	1.754 ± .010
Co(2)	BC(26)	2.055 ± .006	C(12)	C(13)	1.561 ± .007
C(8)	C(7)	1.613 ± .008	C(12)	B(16)	1.719 ± .008
C(8)	B(9)	1.700 ± .008	C(12)	B(20)	1.713 ± .008
C(8)	B(3)	1.734 ± .009	C(13)	B(14)	1.695 ± .008
C(8)	B(4)	1.688 ± .009	C(13)	B(17)	1.720 ± .008
C(7)	B(11)	1.682 ± .008	B(14)	B(15)	1.808 ± .009

C(7)	B(3)	1.727 ± .009	B(14)	B(17)	1.823 ± .009
B(14)	B(18)	1.783 ± .009	BC(23)	B(28)	1.728 ± .009
B(15)	B(16)	1.791 ± .009	B(24)	B(25)	1.801 ± .009
B(15)	B(18)	1.791 ± .009	B(24)	B(28)	1.797 ± .009
B(15)	B(19)	1.768 ± .009	B(24)	B(29)	1.804 ± .009
B(16)	B(19)	1.783 ± .009	B(25)	BC(26)	1.729 ± .009
B(16)	B(20)	1.824 ± .009	B(25)	B(29)	1.790 ± .009
B(17)	B(18)	1.790 ± .009	B(25)	B(30)	1.814 ± .009
B(18)	B(19)	1.786 ± .009	BC(26)	B(30)	1.715 ± .009
B(19)	B(20)	1.786 ± .009	BC(26)	B(31)	1.747 ± .009
B(21)	B(17)	1.792 ± .009	B(27)	B(28)	1.772 ± .010
B(21)	B(18)	1.800 ± .009	B(27)	B(31)	1.748 ± .010
B(21)	B(19)	1.783 ± .009	B(28)	B(29)	1.764 ± .009
B(21)	B(20)	1.786 ± .009	B(29)	B(30)	1.787 ± .009
C(22)	BC(23)	1.643 ± .008	B(30)	B(31)	1.749 ± .010
C(22)	BC(26)	1.636 ± .008	B(32)	B(27)	1.764 ± .010
C(22)	B(27)	1.702 ± .009	B(32)	B(28)	1.775 ± .010
C(22)	B(31)	1.706 ± .009	B(32)	B(29)	1.784 ± .009
BC(23)	B(24)	1.729 ± .009	B(32)	B(30)	1.782 ± .009
BC(23)	B(27)	1.752 ± .009	B(32)	B(31)	1.750 ± .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	Number	Average	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 is there are 5 or more values to include in the calculation of that average.

(b) The root-mean-square deviation from the average is given by $\sigma = [\Sigma\Delta^2/(n - 1)]^{\frac{1}{2}}$, 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 ± .2	Co(1)	B(16)	B(15)	65.4 ± .3
C(12)	Co(2)	C(13)	44.4 ± .2	Co(2)	B(17)	B(21)	65.9 ± .3
C(12)	Co(1)	B(16)	49.0 ± .2	Co(2)	B(21)	B(17)	63.1 ± .3
C(13)	Co(1)	B(14)	48.5 ± .2	Co(2)	B(21)	B(20)	63.8 ± .3
C(12)	Co(2)	B(20)	48.9 ± .2	Co(2)	B(20)	B(21)	65.5 ± .3
C(13)	Co(2)	B(17)	49.4 ± .2	C(12)	C(13)	B(14)	112.9 ± .4
B(14)	Co(1)	B(15)	51.4 ± .2	C(12)	C(13)	B(17)	112.0 ± .4
B(15)	Co(1)	B(16)	50.8 ± .2	C(13)	C(12)	B(16)	112.0 ± .4
B(17)	Co(2)	B(21)	51.1 ± .2	C(13)	C(12)	B(20)	112.1 ± .4
B(20)	Co(2)	B(21)	50.7 ± .2	B(14)	C(13)	B(17)	64.5 ± .4
Co(1)	C(12)	C(13)	67.5 ± .2	B(16)	C(12)	B(20)	64.2 ± .4
Co(1)	C(13)	C(12)	68.1 ± .2	C(13)	B(14)	B(17)	58.4 ±..3
Co(2)	C(12)	C(13)	67.8 ± .2	C(13)	B(17)	B(14)	57.1 ± .3
Co(2)	C(13)	C(12)	67.8 ± .2	C(12)	B(16)	B(20)	57.7 ± .3
Co(1)	C(12)	B(16)	65.5 ± .3	C(12)	B(20)	B(16)	58.1 ± .3
Co(1)	C(13)	B(14)	66.1 ± .3	C(13)	B(14)	B(15)	104.7 ± .4
Co(2)	C(12)	B(20)	65.8 ± .3	C(12)	B(16)	B(15)	104.7 ± .4
Co(2)	C(13)	B(17)	64.9 ± .3	C(13)	B(17)	B(21)	104.9 ± .4
Co(1)	B(14)	C(13)	65.5 ± .3	C(12)	B(20)	B(21)	105.3 ± .4
Co(1)	B(16)	C(12)	65.4 ± .3	B(14)	B(15)	B(16)	105.5 ± .4
Co(2)	B(17)	C(13)	65.7 ± .3	B(17)	B(21)	B(20)	105.5 ± .4
Co(2)	B(20)	C(12)	65.3 ± .2	C(13)	B(14)	B(18)	103.9 ± .4
Co(1)	B(14)	B(15)	65.2 ± .3	C(13)	B(17)	B(18)	102.5 ± .4
Co(1)	B(15)	B(14)	63.5 ± .3	C(12)	B(16)	B(19)	102.7 ± .4
Co(1)	B(15)	B(16)	63.8 ± .3	C(12)	B(20)	B(19)	102.8 ± .4

B(15)	B(14)	B(18)	59.8 ± .4	B(16)	B(19)	B(21)	110.3 ± .4
B(21)	B(17)	B(18)	60.3 ± .4	B(18)	B(19)	B(20)	107.9 ± .5
B(15)	B(16)	B(19)	59.3 ± .4	Co(1)	C(13)	B(17)	125.1 ± .3
B(21)	B(20)	B(19)	59.9 ± .4	Co(1)	B(14)	B(17)	119.1 ± .3
B(14)	B(15)	B(18)	59.4 ± .4	Co(1)	B(14)	B(18)	118.5 ± .4
B(17)	B(21)	B(18)	59.8 ± .4	Co(1)	B(15)	B(18)	116.6 ± .3
B(16)	B(15)	B(19)	60.1 ± .4	Co(1)	B(15)	B(19)	116.9 ± .3
B(20)	B(21)	B(19)	60.0 ± .4	Co(1)	B(16)	B(19)	117.6 ± .3
B(14)	B(17)	B(18)	59.1 ± .4	Co(1)	B(16)	B(20)	118.4 ± .3
B(17)	B(14)	B(18)	59.5 ± .4	Co(1)	C(12)	B(20)	124.3 ± .3
B(16)	B(20)	B(19)	59.2 ± .4	Co(2)	C(12)	B(16)	124.7 ± .3
B(20)	B(16)	B(19)	59.3 ± .4	Co(2)	B(20)	B(16)	118.8 ± .3
B(17)	B(18)	B(15)	110.0 ± .5	Co(2)	B(20)	B(19)	118.0 ± .3
B(17)	B(18)	B(19)	106.7 ± .5	Co(2)	B(21)	B(19)	116.7 ± .3
B(14)	B(18)	B(19)	106.9 ± .5	Co(2)	B(21)	B(18)	116.2 ± .3
B(14)	B(18)	B(21)	109.3 ± .5	Co(2)	B(17)	B(18)	119.1 ± .3
B(15)	B(18)	B(21)	109.0 ± .5	Co(2)	B(17)	B(14)	118.4 ± .3
B(15)	B(19)	B(21)	110.9 ± .5	Co(2)	C(13)	B(14)	124.4 ± .3
B(15)	B(19)	B(20)	110.3 ± .5	Co(1)	C(12)	Co(2)	134.1 ± .2
B(16)	B(19)	B(18)	108.3 ± .5	Co(1)	C(13)	Co(2)	134.7 ± .2

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.

Acknowledgment

We wish to thank J. N. Francis and M. F. Hawthorne of the University of California, Riverside, for providing us with the crystals used in this work.

Figure Captions

Figure 1: Drawing of the $(Co_2B_{26}C_6H_{32})^{-2}$ anion (hydrogen atoms not shown).

Figure 2: Framework drawing of the projection of the unit cell contents down the a axis.

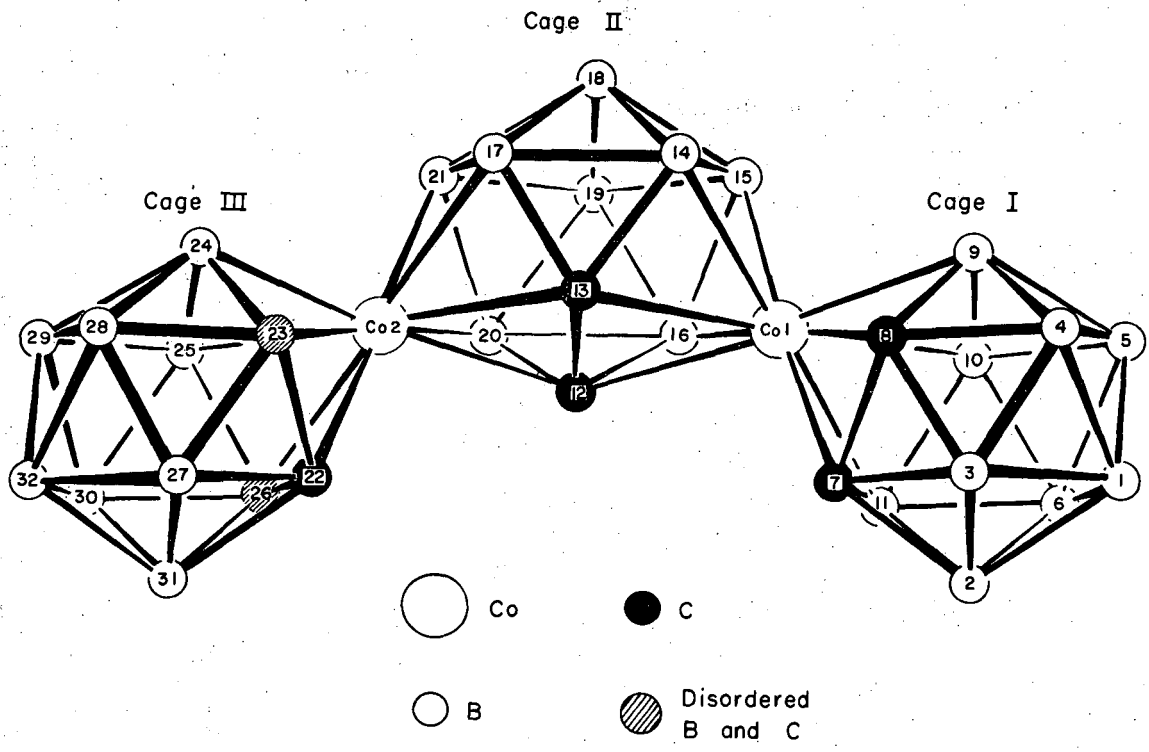
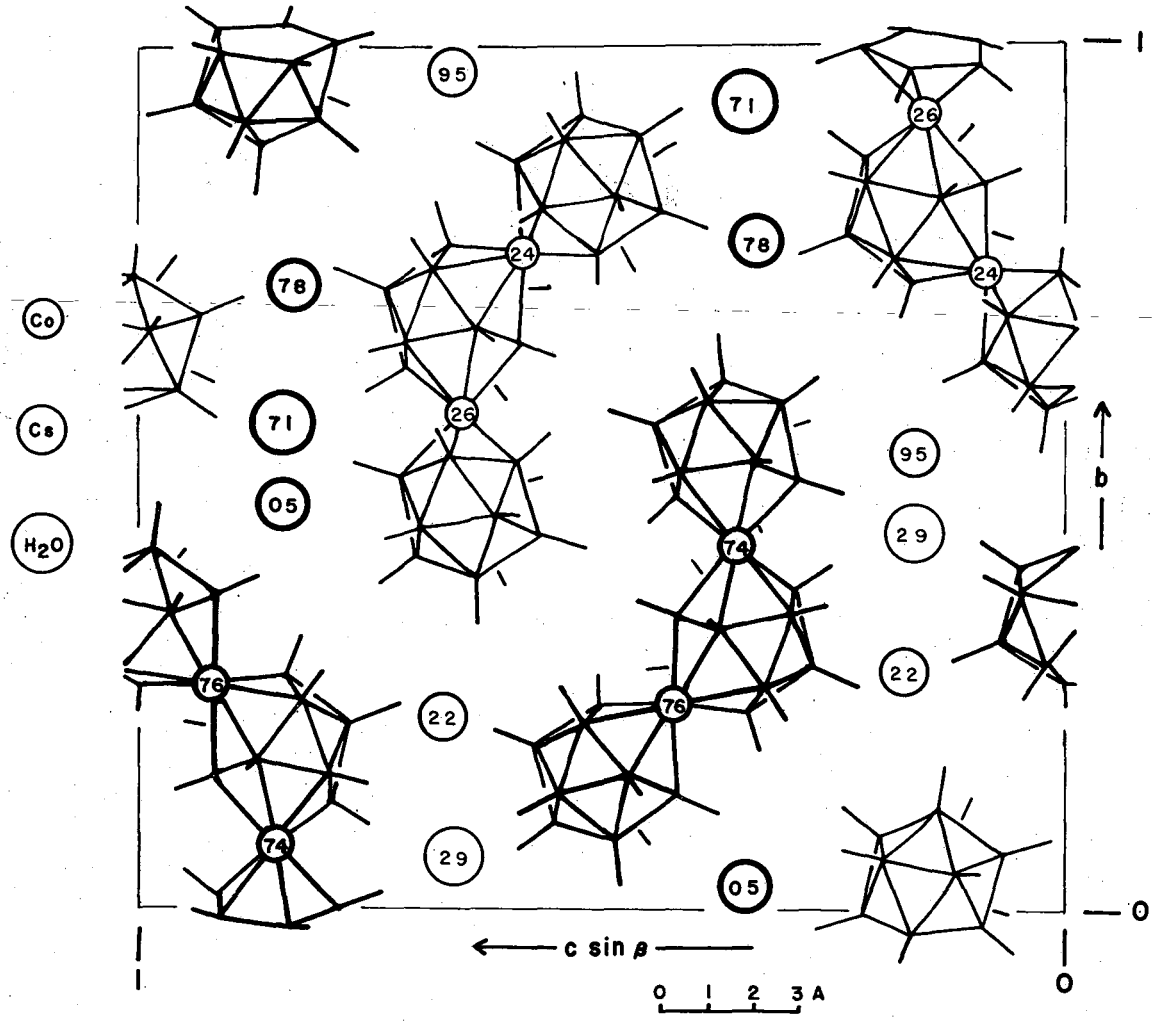


Figure I

XBL6810-6853


95
71
26
78
24
78
24
Co
Cs
71
26
95
b
05
29
H_2O
74
76
22
76
22
74
29
05
1
0
c sin β
0 1 2 3 A
1
0

XBL 681-83

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