

The slip-distortion value (Wing, 1968), the distance between the centroid of the least-squares plane defined by atoms C(1), C(2), B(4), B(7), and B(8) (Fig. 1) and the projection of the Co atom onto this plane, is 0.061 (2) Å. The title compound thus belongs to the class of symmetric π -sandwich complexes.

Two-cage carbametallaboranes, not combined with a bond, with two neighbouring C atoms in each cage directly bonded to the metal were investigated with respect to the ligand pseudosymmetry. Let d be the distance between the atom in the structure and its projection onto the selected plane, and $\sigma(d)$ the corresponding estimated standard deviation. The two atoms on the opposite sides of this plane are mirror images (on statistical significance level of 0.05) if $||d_1| - |d_2|| \leq 1.96\sqrt{\sigma^2(d_1) + \sigma^2(d_2)}$. The chosen least-squares plane is defined by the atoms Co, B(8), B(6), and B(10) (Fig. 1). If for all four pairs of atoms [B(4), B(7); B(5), B(11); B(9), B(12); C(1), C(2)] the corresponding distances satisfy this condition, the

selected plane can be considered a mirror plane m (C_s) of the icosahedron. Carrying out this test for ligand pseudosymmetry on the two-cage carbametallaboranes listed by Sivý *et al.* (1986) shows that there is no correlation between the results of the test and the magnitudes of the slip distortion.

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Structure of Caesium 8-Iodo-3,3'-*commo*-bis(decahydro-1,2-dicarba-3-cobalta-*closo*-dodecaborate)(1-)*

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Abstract. Cs[Co(C₂H₁₁B₉)(C₂H₁₀B₉I)], $M_r = 582.53$, monoclinic, $P2_1/n$, $a = 20.721$ (4), $b = 13.167$ (1), $c = 7.462$ (1) Å, $\beta = 95.00$ (1)°, $V = 2028.1$ Å³, $Z = 4$, $D_m = 1.91$, $D_x = 1.91$ Mg m⁻³, $\lambda(\text{Mo } K\alpha) =$

0.71069 Å, $\mu = 3.89$ mm⁻¹, $F(000) = 1080$, $T = 293$ K. Final $R = 0.045$ for 2579 observed reflections. The molecule of *closo*-carbacobaltaborane consists of two icosahedra around the Co atom, creating a π -sandwich conformation. The two neighbouring C atoms of the icosahedral fragments were distinguished unambiguously from the B atoms. In the structure there are two enantiomorphous rotational isomers.

* Alternative name: caesium (η -undecahydrido-7,8-dicarba-*nido*-undecaborato)(η -decahydrido-10-iodo-7,8-dicarba-*nido*-undecaborato)cobaltate(1-).

Introduction. Following earlier structural studies of $[(C_2B_9H_8Br_3)_2Co]Cs$ (Sivý, Preisinger, Baumgartner, Valach, Koreň & Mátel, 1986a) and $[(C_2B_9H_{10}I)_2Co]Cs$ (Sivý *et al.*, 1986b), we now report the structure of the title compound (Mátel, Macášek, Rajec, Heřmánek & Plešek, 1982).

This work is part of a more extensive research of caesium salts of carbametallaboranes with halide substituents as materials suitable for the separation of caesium (Macášek, Mátel & Kyrš, 1978; Mátel, 1982).

Experimental. Orange tetragonal-prismatic crystal, $0.07 \times 0.08 \times 0.39$ mm, D_m by flotation in $CHBr_3/CCl_4$; space group $P2_1/n$ (No. 14) indicated from preliminary Weissenberg photographs [$\lambda(Cu K\alpha) = 1.5405$ Å]; intensity data measured with computer-controlled Philips PW 1100 diffractometer, Mo $K\alpha$ radiation, graphite monochromator, $2\theta_{max} = 55^\circ$, $\theta/2\theta$ scan, $0.0333^\circ s^{-1}$ scan speed, each peak being scanned *ca* 30 s plus 15 s left and right background; three standard reflections, variation 6.4%; index range $-26 \leq h \leq 26$, $0 \leq k \leq 17$, $0 \leq l \leq 9$; 5271 reflections measured, 4690 unique, $R_{int} = 0.029$, 2111 considered unobserved [$I < 2.5\sigma(I)$]; lattice parameters determined from 18 reflections with $3.94 < 2\theta < 14.97^\circ$; absorption corrections applied, maximum and minimum transmission factors: 0.8140, 0.7537; positions of three heavy atoms (Cs, I, Co) determined by direct methods with *MULTAN80* (Main *et al.*, 1980); further calculations with *SHELX76* (Sheldrick, 1976); atom scattering factors and f' , f'' from *International Tables for X-ray Crystallography* (1974); positions of remaining non-H atoms located from a Fourier synthesis. The problem of differentiating C atoms from B atoms was solved as follows: Cs, I and Co were refined anisotropically, the remaining atoms isotropically as B. After five cycles of full-matrix least squares based on F ($R = 0.056$) the two neighbouring atoms in each icosahedron with the lowest temperature parameters, $U = 0.021-0.025$ Å², were chosen as C. Other atoms refined as B had $U = 0.027-0.047$ Å². Following anisotropic refinement of all non-H atoms, a difference Fourier synthesis located all 21 H atoms; H atoms refined isotropically; $w = 1.0187/[\sigma^2(F_o) + 0.000387F_o^2]$: final $R = 0.045$, $wR = 0.041$; maximum and minimum values of electron density in a final difference map 0.8 and $-0.7 e \text{ \AA}^{-3}$; $(\Delta/\sigma)_{max} 0.044$ (H atom). Calculations performed using the CYBER74 computer, Technical University, Vienna, Austria, and the M4030-1, Slovak Technical University, Bratislava, Czechoslovakia.

Discussion. Fig. 1 shows the molecule with the atom numbering. Fig. 2 illustrates the arrangement of the molecules in the unit cell, viewed along the c axis. These units are mutually separated by normal van der Waals distances. The closest intermolecular contacts of each

principal type are $I \cdots H = 3.13$ (7), $C \cdots H = 3.14$ (8), $B \cdots H = 2.96$ (8) and $H \cdots H = 2.25$ (10) Å.

Atomic parameters are in Table 1.* Table 2 gives bond distances and bond angles at the central Co atom, angles involving I and selected mean bond angles. In Table 3 are shown details of least-squares-planes' calculations.

In contrast to the parent compound, $[(C_2B_9H_{11})_2Co]Cs$ (Zalkin, Hopkins & Templeton, 1967), and compounds with an even number of halide substituents in the icosahedra, $[(C_2B_9H_8Br_3)_2Co][N(CH_3)_4]$ (De Boer, Zalkin & Templeton, 1968), $[(C_2B_9H_8Br_3)_2Co]Cs$ (Sivý *et al.*, 1986a) and $[(C_2B_9H_{10}I)_2Co]Cs$ (Sivý *et al.*, 1986b), in which Co is always situated at a symmetry centre, in the present structure Co is situated in a general position, I being substituted

* Lists of structure amplitudes, anisotropic thermal parameters, H-atom parameters and bond lengths involving H atoms have been deposited with the British Library Lending Division as Supplementary Publication No. SUP 42464 (33 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

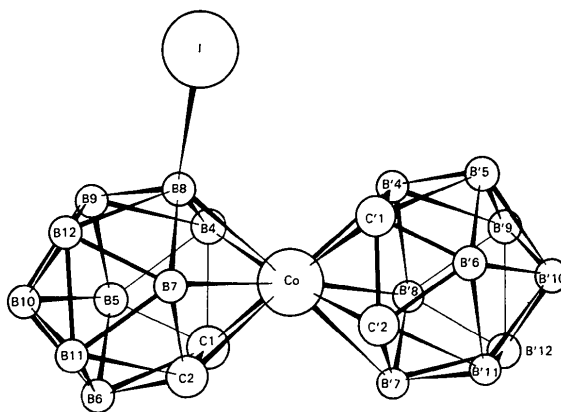


Fig. 1. The $[(C_2B_9H_{10}I)Co(C_2B_9H_{11})]^-$ anion showing the atom numbering. (H atoms are omitted.)

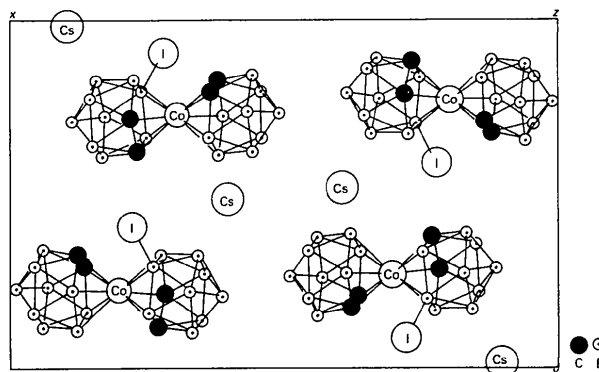


Fig. 2. Projection of the crystal structure onto (001).

Table 1. Atomic coordinates and equivalent isotropic temperature factors (Å²) with e.s.d.'s in parentheses
$$U_{eq} = \frac{1}{3} \sum_i \sum_j U_{ij} a_i^* a_j^* a_i a_j$$

	x	y	z	U _{eq}
Cs	0.3962 (1)	0.4825 (1)	0.2371 (1)	0.0428 (2)
I	0.7217 (1)	0.0923 (1)	-0.1633 (1)	0.0437 (2)
Co	0.6972 (1)	0.2737 (1)	0.2167 (1)	0.0261 (3)
C(1)	0.7689 (4)	0.3792 (6)	0.2471 (11)	0.033 (3)
C(2)	0.7814 (4)	0.2860 (7)	0.3810 (11)	0.031 (3)
B(4)	0.7520 (4)	0.3372 (7)	0.0259 (12)	0.030 (3)
B(5)	0.8298 (5)	0.3910 (9)	0.1075 (15)	0.044 (4)
B(6)	0.8478 (5)	0.3593 (8)	0.3374 (16)	0.045 (4)
B(7)	0.7754 (5)	0.1723 (7)	0.2747 (13)	0.031 (3)
B(8)	0.7604 (4)	0.2027 (7)	0.0433 (11)	0.028 (3)
B(9)	0.8260 (5)	0.2772 (8)	-0.0212 (14)	0.040 (3)
B(10)	0.8842 (5)	0.2912 (9)	0.1724 (15)	0.041 (4)
B(11)	0.8522 (5)	0.2268 (8)	0.3519 (14)	0.039 (3)
B(12)	0.8411 (5)	0.1745 (8)	0.1330 (13)	0.037 (3)
C'(1)	0.6210 (4)	0.1763 (6)	0.1777 (12)	0.034 (3)
C'(2)	0.6357 (4)	0.2086 (7)	0.3864 (11)	0.034 (3)
B'(4)	0.6143 (4)	0.2765 (7)	0.0376 (13)	0.030 (3)
B'(5)	0.5458 (5)	0.2051 (8)	0.0952 (14)	0.037 (3)
B'(6)	0.5604 (5)	0.1601 (9)	0.3184 (16)	0.046 (4)
B'(7)	0.6397 (5)	0.3359 (9)	0.4089 (13)	0.040 (4)
B'(8)	0.6230 (5)	0.3857 (8)	0.1834 (13)	0.036 (3)
B'(9)	0.5444 (5)	0.3398 (8)	0.1047 (14)	0.037 (3)
B'(10)	0.5124 (5)	0.2687 (9)	0.2753 (14)	0.045 (4)
B'(11)	0.5705 (5)	0.2627 (9)	0.4648 (15)	0.047 (4)
B'(12)	0.5596 (5)	0.3769 (9)	0.3352 (14)	0.042 (4)

in only one of the two fragments. The magnitude of the slip distortion (Wing, 1967) is 0.047 (4) and 0.027 (4) Å for planes 1 and 4 (Table 3) (mean value: 0.037 ± 0.014 Å), which corresponds, according to the classification of Sivý *et al.* (1986a), to a symmetric π -sandwich complex. (Variance of distances of all ten bonds of Co^{III} with the nearest ligand atoms is $\sigma^2 = 0.0016 \text{ \AA}^2$; the mean Co—C and Co—B bond distances are shown in Table 2.) The atoms defining each of the planes 1–6 (Table 3) are, however, not exactly coplanar (χ^2 test). The I—B(8) bond length is 2.217(10) Å. The I atom is at a distance of 0.520 (1) Å from plane 1 and is situated on the same side as Co. The mean C—C distance 1.61 ± 0.02 Å is shorter in the present structure than the analogous mean distance 1.70 ± 0.03 Å in [(C₂B₉H₁₁)₂Co]Cs (Zalkin *et al.*, 1967). It is of interest that corresponding distances in the two icosahedra are equal within the limits of experimental error except for only one case, C(1)—B(4), 1.75 (1) Å, and C'(1)—B'(4), 1.68 (1) Å. The [(C₂B₉H₁₀I)Co^{III}(C₂B₉H₁₁)]⁻ anion has a structure similar to that of the parent anion [(C₂B₉H₁₁)₂Co^{III}]⁻. However, the I atom now eliminates the possibility of disorder (found in the parent anion) (Zalkin *et al.*, 1967). The icosahedral ligands in the present structure take up a staggered conformation. This is illustrated by the interannular angles through the central atom from the atoms of plane 1 to the atoms of plane 4, *i.e.* C(1)—Co—C'(1) = 175.9 (5), C(2)—Co—B'(4) = 173.7 (5), B(4)—Co—C'(2) = 174.4 (4), B(7)—Co—B'(8) = 173.5 (4) and B(8)—Co—B'(7) = 174.4 (4)°.

The mean distances of Co from the B atoms of planes 2 and 5 are 3.34 ± 0.02 and 3.33 ± 0.02 Å.

The atom of the anion closest to Cs⁺ is H'(8) at 2.87 (8) Å, and of the non-H atoms it is B'(8) at a distance of 3.58 (1) Å.

Table 2. Bond lengths (Å) and selected angles (°) with e.s.d.'s in parentheses

Co—C(1)	2.032 (8)	Co—C'(1)	2.024 (9)
—C(2)	2.050 (13)	—C'(2)	2.060 (12)
—B(4)	2.073 (12)	—B'(4)	2.083 (14)
—B(7)	2.115 (10)	—B'(7)	2.108 (13)
—B(8)	2.135 (12)	—B'(8)	2.129 (11)
C(1)—C(2)	1.59 (1)	C'(1)—C'(2)	1.62 (1)
—B(4)	1.75 (1)	—B'(4)	1.68 (1)
—B(5)	1.71 (2)	—B'(5)	1.68 (1)
—B(6)	1.73 (2)	—B'(6)	1.73 (2)
C(2)—B(6)	1.73 (1)	C'(2)—B'(6)	1.72 (1)
—B(7)	1.69 (1)	—B'(7)	1.69 (2)
—B(11)	1.69 (1)	—B'(11)	1.68 (2)
B(4)—B(5)	1.82 (1)	B'(4)—B'(5)	1.79 (1)
—B(8)	1.78 (1)	—B'(8)	1.80 (1)
—B(9)	1.79 (1)	—B'(9)	1.78 (1)
B(5)—B(6)	1.77 (2)	B'(5)—B'(6)	1.77 (2)
—B(9)	1.78 (2)	—B'(9)	1.78 (2)
B(6)—B(11)	1.75 (2)	B'(6)—B'(11)	1.74 (2)
B(7)—B(8)	1.77 (1)	B'(7)—B'(8)	1.81 (1)
—B(11)	1.79 (2)	—B'(11)	1.81 (2)
—B(12)	1.80 (2)	—B'(12)	1.79 (2)
B(8)—B(9)	1.78 (1)	B'(8)—B'(9)	1.79 (2)
—B(12)	1.79 (1)	—B'(12)	1.81 (2)
—I	2.217 (10)		
B(9)—B(12)	1.79 (2)	B'(9)—B'(12)	1.79 (2)
B(10)—B(5)	1.77 (2)	B'(10)—B'(5)	1.77 (2)
—B(6)	1.75 (2)	—B'(6)	1.76 (2)
—B(9)	1.81 (2)	—B'(9)	1.76 (2)
—B(11)	1.76 (2)	—B'(11)	1.78 (2)
—B(12)	1.79 (2)	—B'(12)	1.76 (2)
B(11)—B(12)	1.77 (1)	B'(11)—B'(12)	1.79 (2)

Averaged distances and angles

	No. averaged		Av. (Å, °)
C(1)—Co—C(2)	45.8 (3)	Co—C	2.041 ± 0.017
C(2)—Co—B(7)	48.0 (4)	Co—B	2.107 ± 0.025
B(7)—Co—B(8)	49.3 (4)	C—C	1.61 ± 0.02
B(8)—Co—B(4)	50.1 (4)	C—B	1.71 ± 0.02
B(4)—Co—C(1)	50.4 (4)	B—B	1.78 ± 0.02
		C—H	0.91 ± 0.11
C'(1)—Co—C'(2)	46.6 (4)	B—H	1.11 ± 0.08
C'(2)—Co—B'(7)	47.7 (4)		
B'(7)—Co—B'(8)	50.6 (4)	C—Co—C	46.2 ± 0.6
B'(8)—Co—B'(4)	50.7 (4)	C—Co—B	48.6 ± 1.2
B'(4)—Co—C'(1)	48.3 (4)	B—Co—B	50.2 ± 0.6
		Co—C—C	66.9 ± 1.1
C(1)—Co—C'(1)	175.9 (5)	Co—C—B	67.4 ± 0.9
C(2)—Co—C'(2)	101.8 (3)	Co—B—C	64.1 ± 0.4
B(7)—Co—B'(7)	125.1 (4)	Co—B—B	64.9 ± 1.3
B(8)—Co—B'(8)	135.0 (4)	C—C—B	112.0 ± 1.1
B(4)—Co—B'(4)	91.3 (4)	C—B—C	55.2 ± 1.0
		B—C—B	63.0 ± 1.3
I—B(8)—Co	120.3 (4)	C—B—B	58.5 ± 1.1
—B(4)	125.0 (5)	B—B—B	60.0 ± 0.6
—B(7)	123.4 (6)		
—B(9)	114.4 (5)		
—B(12)	113.2 (6)		

Table 3. Deviations of atoms (Å) from specified least-squares planes

Plane 1: C(1),C(2),B(4) B(7),B(8)		Plane 2: B(5),B(6),B(9) B(11),B(12)		Plane 3: Co,B(8),B(6), B(10)	
C(1)	0.012 (8)	B(5)	-0.010 (10)	Co	0.009 (1)
C(2)	0.009 (8)	B(6)	0.018 (10)	B(8)	-0.010 (9)
B(4)	-0.028 (8)	B(9)	-0.001 (10)	B(6)	-0.010 (11)
B(7)	-0.027 (10)	B(11)	-0.019 (8)	B(10)	0.012 (11)
B(8)	0.033 (8)	B(12)	0.012 (10)		
Co	-1.482 (1)	B(10)	0.940 (10)	C(1)	0.773 (8)
I	-0.520 (1)	I	-2.101 (1)	C(2)	-0.814 (9)
				B(4)	1.432 (9)
				B(7)	-1.436 (9)
				B(5)	1.425 (11)
				B(11)	-1.413 (11)
				B(9)	0.904 (11)
				B(12)	-0.880 (10)
Plane 4: C'(1),C'(2), B'(4),B'(7),B'(8)		Plane 5: B'(5),B'(6), B'(9),B'(11),B'(12)		Plane 6: Co,B'(8),B'(6), B'(10)	
C'(1)	-0.005 (8)	B'(5)	0.009 (8)	Co	0.005 (1)
C'(2)	-0.009 (8)	B'(6)	-0.013 (10)	B'(8)	-0.006 (10)
B'(4)	0.017 (8)	B'(9)	-0.002 (10)	B'(6)	-0.006 (11)
B'(7)	0.020 (10)	B'(11)	0.011 (10)	B'(10)	0.007 (11)
B'(8)	-0.022 (8)	B'(12)	-0.005 (10)		
Co	1.480 (1)	B'(10)	-0.917 (10)	C'(1)	0.793 (9)
				C'(2)	-0.822 (8)
				B'(4)	1.434 (9)
				B'(7)	-1.449 (10)
				B'(5)	1.433 (10)
				B'(11)	-1.429 (11)
				B'(9)	0.881 (10)
				B'(12)	-0.906 (10)

The two icosahedral cages are rotated with respect to one another through an angle of $108(1)^\circ$ from the orientation in which the C atoms would overlap (Fig. 1). In the unit cell there are two (–) and two (+)-enantiomorphic rotational isomers. The angle B(10)–Co–B'(10) is $177.1(4)^\circ$ and thus the molecule as a whole is slightly bent.

Using the general nomenclature which has been described by Janoušek, Plešek, Heřmánek, Baše, Todd & Wright (1981) for rotation of non-bridged $(C_2B_9H_{11})_2^{2-}$ sandwiches, the staggered conformation (*s*-1,4',2,1') is 'frozen' in the present structure. This conformation corresponds to a transition state inter-

mediate between (*s*-1,8',2,4') *trans*-antiprismatic and (*s*-1,1',2,2') *cis*-antiprismatic. The reason for the occurrence of this conformation may lie in the steric effect of the halide substituent and repulsion between δ^+ partially charged C atoms present in opposite planes. Thus rotation into one of the non-symmetric conformations will be prevented. A different situation was found in the crystal structure of $(C_2B_9H_{11})_2Ni$ (St Clair, Zalkin & Templeton, 1970). Here the enantiomorphic rotational isomers have cages mutually turned through an angle of 36° . The vectors B(10) to Ni of the first cage and Ni to B(10) of the second cage are parallel. In this case, the structure is 'frozen' in the (*s*-1,1',2,2') *cis*-antiprismatic conformation.

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Structure of Bis(5-chloro-8-quinolinolato-*N,O*)bis(pyridine)nickel(II)–Pyridine Dihydrate

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Abstract. $[Ni(C_9H_5ClNO)_2(C_5H_5N)_2] \cdot C_5H_5N \cdot 2H_2O$, $M_r = 689.2$, triclinic, $P\bar{1}$, $a = 15.729(5)$, $b = 11.065(5)$, $c = 9.497(7)$ Å, $\alpha = 95.89(2)$, $\beta =$

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$105.20(2)$, $\gamma = 90.37(2)^\circ$, $V = 1586 \cdot (1) \text{Å}^3$, $Z = 2$, $D_m = 1.44$, $D_x = 1.44 \text{ g cm}^{-3}$, $\lambda(\text{Mo K}\alpha) = 0.71069 \text{ Å}$, $\mu = 8.3 \text{ cm}^{-1}$, $F(000) = 712$, $T = 298 \text{ K}$, final $R =$

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