15 (1)° respectively. Since small distortions from the trigonal-bipyramid configuration may produce a tetragonal pyramid (Cotton & Wilkinson, 1972), we tested the possibility of this second configuration by looking for a planar square base. The 'most planar' arrangement was that of atoms N(2), O(1), O(3), O(5*W*) for which the r.m.s. deviation from the best least-squares plane through them was 0·42 (2) Å These figures and the comparison of actual angles with the theoretical values for the two models (Table 3) show that the observed five-coordination polyhedron is much closer to the ideal trigonal-bipyramid (C_{3h}) configuration than to that of the tetragonal pyramid (C_{4v}). We conclude that the distortions from the ideal O_h configuration imposed by the bites of the bidentate α-Aib groups raise the energy of the resulting six-coordination polyhedron to a value similar to that of the trigonal-bipyramid configuration, therefore making possible the simultaneous occurrence of five- and six-coordination.

All water molecules are involved in hydrogen bonding to carboxylate groups or to other water molecules. Table 3 is a list of these hydrogen bonds and some intermolecular short contacts.

The support of the organizations FAPESP, CAPES, CNPq and BID-FINEP is gratefully acknowledged.

Table 3. *Hydrogen bonds and short intermolecular distances (distances in Å, angles in °)*

a	*b*	*c*	*ab*	*ac*	*bc*	∠*abc*
N(1)	H(N1)	O(7^{i})	0·83 (4)	3·055 (4)	2·28 (4)	155 (1)
N(1)	H'(N1)	O(7^{ii})	0·72 (5)	2·977 (4)	2·27 (5)	168 (1)
N(2)	H(N2)	O(7^{i})	0·92 (4)	3·030 (4)	2·16 (4)	158 (1)
N(2)	H'(N2)	O(4^{iii})	0·96 (4)	2·951 (5)	2·01 (4)	165 (1)
N(3)	H(N3)	O(1^{iii})	0·86 (5)	3·218 (4)	2·45 (5)	149 (1)
N(3)	H'(N3)	O(2^{iv})	0·89 (5)	3·121 (4)	2·24 (5)	171 (1)
O(5*W*)	H(5*W*)	O(3^{iii})	0·65 (6)	2·711 (5)	2·11 (6)	155 (1)
O(5*W*)	H'(5*W*)	O(8*W*^{ii})	1·01 (6)	2·757 (4)	1·80 (6)	155 (1)
O(8*W*)	H(8*W*)	O(2^{v})	0·75 (4)	2·661 (4)	1·94 (4)	161 (1)
O(8*W*)	H'(8*W*)	O(1^{ii})	0·96 (4)	2·764 (4)	1·83 (4)	163 (1)

Symmetry code: (i) $\frac{1}{2}-x, \frac{1}{2}-y, 1-z$; (ii) x, y, z; (iii) $x, -y, z-\frac{1}{2}$; (iv) $-x, y, \frac{1}{2}-z$; (v) $-x, -y, 1-z$.

References

CASTELLANO, E. E., OLIVA, G., ZUKERMAN-SCHPECTOR, J. & CALVO, R. (1986). *Acta Cryst.* C**42**, 16–19.

COTTON, F. A. & WILKINSON, G. (1972). *Advanced Inorganic Chemistry*. New York: John Wiley.

CROMER, D. T. & LIBERMAN, D. (1970). *J. Chem. Phys.* **53**, 1891–1898.

CROMER, D. T. & MANN, J. B. (1968). *Acta Cryst.* A**24**, 321–324.

FREEMAN, H. C. (1967). *Adv. Protein Chem.* **22**, 257–424.

HAMILTON, W. C. (1959). *Acta Cryst.* **12**, 609–610.

JOHNSON, C. K. (1965). *ORTEP*. Report ORNL-3794. Oak Ridge National Laboratory, Tennessee.

OLIVA, G., CASTELLANO, E. E., ZUKERMAN-SCHPECTOR, J. & CALVO, R. (1986). *Acta Cryst.* C**42**, 19–21.

SHELDRICK, G. M. (1976). *SHELX76*. Program for crystal structure determination. Univ. of Cambridge, England.

STEWART, R. F., DAVIDSON, E. R. & SIMPSON, W. T. (1965). *J. Chem. Phys.* **42**, 3175–3187.

Acta Cryst. (1986). C**42**, 24–27

Structure of Caesium 3,3'-*commo*-Bis(8,9,12-tribromooctahydro-1,2-dicarba-3-cobalta-*closo*-dodecaborate)(1−)

BY PETER SIVÝ

Faculty of Chemical Technology, Slovak Technical University, Department of Chemical and Technical Physics and Nuclear Technique, Jánska 1, 812 37 *Bratislava, Czechoslovakia*

ANTON PREISINGER AND OSWALD BAUMGARTNER

Institute of Mineralogy, Crystallography and Structural Chemistry, Technical University, Getreidemarkt 9, *A*-1060 *Vienna, Austria*

FEDOR VALACH AND BRANISLAV KOREŇ

Faculty of Chemical Technology, Slovak Technical University, Department of Chemical and Technical Physics and Nuclear Technique, Jánska 1, 812 37 *Bratislava, Czechoslovakia*

AND ĽUBOMÍR MÁTEL

Department of Nuclear Chemistry, Comenius University, 842 15 *Bratislava, Czechoslovakia*

(*Received* 19 *February* 1985; *accepted* 27 *August* 1985)

Abstract. $Cs[Co(C_2H_8B_9Br_3)_2]$, $M_r = 930{\cdot}0$, monoclinic, $C2/c$, $a = 15{\cdot}145$ (2), $b = 14{\cdot}953$ (2), $c = 11{\cdot}855$ (1) Å, $\beta = 113{\cdot}850$ (9)°, $V = 2455{\cdot}5$ Å^3, $Z = 4$, $D_m = 2{\cdot}51$, $D_x = 2{\cdot}52$ Mg m^{-3}, λ(Mo $K\alpha$) = 0·71069 Å, $\mu = 11{\cdot}63$ mm^{-1}, $F(000) = 1688$, $T = 293$ K. Final $R = 0{\cdot}044$ for 1736 observed reflections.

0108-2701/86/010024-04$01.50

The π-sandwich complex consists of two icosahedra with Co forming the common apex. All Br atoms are bonded to B with an average distance of $1\cdot96 \pm 0\cdot01$ Å. The Co atom is situated at a centre of symmetry. This work substantiates the relationship between metal d-electron configuration of two-cage carbametallaboranes and slip distortion proposed by Wing [*J. Am. Chem. Soc.* (1968), **90**, 4828–4834].

Introduction. The title compound was synthesized by Mátel, Macášek, Rajec, Heřmánek & Plešek (1982). The substitution reactions of the cage atoms are of interest in relation to the stability of the coordination polyhedron in a radioactive environment. The title compound is applicable for the extraction separation of univalent and bivalent cations from nitric- and hydrochloric-acid media (Macášek, Mátel & Kyrš, 1978; Mátel, 1982).

Wing (1968, 1970) pointed out the relationship between d-electron configuration and slip distortion for d^8 and d^9 complexes while those with d^7 or less d electrons are symmetric π-sandwich complexes.

Experimental. Dark-red tetragonal-bipyramidal crystals, D_m by flotation in $CHBr_3/CCl_4$; Weissenberg photographs (Cu $K\alpha$ radiation) indicated the monoclinic system, space group $C2/c$ (No. 15) or Cc (No. 9); crystal size $0\cdot15 \times 0\cdot18 \times 0\cdot21$ mm; Philips X-ray diffractometer, graphite monochromator, $\theta/2\theta$ scan, $2\theta_{max} = 55°$, $0\cdot0333°\ s^{-1}$ scan speed, time per reflection approx. 60 s, 15 s each for left and right background; three standard reflections, variation 4·1%; 33 reflections with $5\cdot4 < 2\theta < 10\cdot8°$ used for refinement of lattice parameters; absorption correction applied, maximum and minimum transmission factors: 0·3832, 0·2386; index range $-19 \le h \le 18$, $0 \le k \le 19$, $0 \le l \le 15$; 3087 reflections measured, 2839 unique, $R_{int} = 0\cdot04$, 1736 $[I > 2\sigma(I)]$ considered observed. Co, Cs and Br atoms located by direct methods with *MULTAN*80 (Main *et al.*, 1980). A Fourier synthesis determined all atom positions except those of H. The occurrence of neighbouring atoms of C in the five-membered ring bonded to the Co atom as in $[(C_2B_9H_{11})_2Co]Cs$ (Zalkin, Hopkins & Templeton, 1967) was assumed. All calculations performed with *XRAY*72 (Stewart, Kruger, Ammon, Dickinson & Hall, 1972); scattering factors and f', f'' (for heavy atoms) from *Internatonal Tables for X-ray Crystallography* (1962); refinement by full-matrix least squares, F values. In first cycles heavy atoms refined anisotropically and all other atoms isotropically as B. Two atoms with the lowest value of the isotropic temperature parameter ($U = 0\cdot023$ Å^2) chosen as C, B atoms had U in range $0\cdot026$–$0\cdot041$ Å^2; H atoms located by difference Fourier synthesis; final difference map had maximum and minimum heights 0·8 and $-0\cdot7$ e Å^{-3}; non-H atoms refined anisotropically; H isotropically; final $R = 0\cdot044$, $wR = 0\cdot040$, $w = 0\cdot947/[\sigma^2(F_o) + 0\cdot0003F_o^2]$; $(\Delta/\sigma)_{max}$ in final refinement cycle 0·019 (H atom). Calculations performed using the CYBER74 computer, Technical University, Vienna, Austria, and the M4030-1, Slovak Technical University, Bratislava, Czechoslovakia.

Discussion. Atom coordinates and equivalent isotropic thermal parameters are shown in Table 1.* In Fig. 1 the $[(C_2B_9H_8Br_3)_2Co]^-$ anion is depicted. Fig. 2 shows the arrangement of the anion complexes and cations in the unit cell. Co is situated at the common apex of two icosahedra. Table 2 gives bond distances, bond angles involving the Br atoms and selected average values. The C(1)—C(2) distance [1·59 (1) Å] is significantly shorter than the analogous average distance $1\cdot70 \pm 0\cdot03$ Å in $[(C_2B_9H_{11})_2Co]Cs$ (Zalkin *et al.*, 1967).

Thermal oscillations of all atoms of the $(C_2B_9)Co$ cage are lower in the present structure than in $[(C_2B_9H_{11})_2Co]Cs$. The fact that the C atoms are not disordered is due to the presence of the three Br atoms bonded directly to the icosahedron. The Cs^+ cation is 'ion-bonded' to the complex anion. The closest contacts between the anion and Cs^+ involve H(7) [3·08 (9) Å] and Br(3) [3·650 (9) Å]. The closest intermolecular contacts of each principal type are Br···H = 2·91 (6), C···H = 3·16 (7), B···H = 3·01 (7), and H···H = 2·70 (13) Å.

The distances of corresponding pairs of atoms which are on opposite sides of the least-squares plane defined by Co, B(6), B(8) and B(10) show – within the standard deviations – the m (C_s) symmetry of an icosahedron; this includes the Br atoms and thus the symmetry of the anion complex is $2/m$ (C_{2h}).

Wing (1968) defined electron-rich metalloaromatics. In Table 3, data for two-cage carbametallaboranes of the type $(C_2B_9)_2M$ ($M = Cu^{II}$, Cu^{III}, Au^{III}, Ni^{III}, Ni^{IV}, Co^{III}, and Cr^{III}) are listed according to their d^n-electron configuration.† The second column in Table 3 shows the symmetry of the metal position and the third column its d^n-electron configuration (in formal valence state). Application of standard statistical procedures shows that the means of the M—C and M—B bond distances differ significantly at the 95% probability level in the case of the distorted π-allylic complexes for each symmetrically independent icosahedron (fourth and fifth columns). The fact that in the case of the symmetric π-sandwich complexes the question of

* Lists of structure amplitudes, anisotropic thermal parameters, H-atom parameters and the results of least-squares-planes' calculations have been deposited with the British Library Lending Division as Supplementary Publication No. SUP 42463 (21 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

† Obtained by means of a search of the Cambridge Structural Database (1984).

Table 1. *Fractional atomic coordinates and equivalent isotropic thermal parameters with e.s.d.'s in parentheses*

$$U_{eq} = \tfrac{1}{3}\textstyle\sum_i\sum_j U_{ij}a_i^*a_j^*\mathbf{a}_i.\mathbf{a}_j.$$

	x	y	z	U_{eq}(Å^2)
Co	0·25	0·75	0·5	0·0225 (5)
C(1)	0·2800 (5)	0·6174 (5)	0·5290 (6)	0·031 (3)
C(2)	0·3678 (6)	0·6768 (5)	0·5307 (8)	0·035 (3)
B(4)	0·1785 (5)	0·6362 (5)	0·3981 (7)	0·028 (3)
B(5)	0·2517 (7)	0·5367 (5)	0·4211 (8)	0·037 (4)
B(6)	0·3721 (7)	0·5632 (6)	0·5091 (8)	0·039 (4)
B(7)	0·3416 (6)	0·7414 (5)	0·4045 (7)	0·029 (3)
B(8)	0·2171 (6)	0·7134 (5)	0·3122 (7)	0·028 (3)
B(9)	0·2141 (6)	0·5944 (5)	0·2808 (7)	0·032 (3)
B(10)	0·3309 (6)	0·5522 (5)	0·3462 (8)	0·037 (3)
B(11)	0·4114 (6)	0·6407 (6)	0·4269 (8)	0·037 (3)
B(12)	0·3136 (6)	0·6616 (6)	0·2828 (8)	0·032 (3)
Br(1)	0·1300 (1)	0·7899 (1)	0·1796 (1)	0·0460 (4)
Br(2)	0·1169 (1)	0·5442 (1)	0·1274 (1)	0·0506 (4)
Br(3)	0·3354 (1)	0·6863 (1)	0·1354 (1)	0·0517 (4)
Cs	0·0	0·3755 (1)	0·25	0·1027 (7)

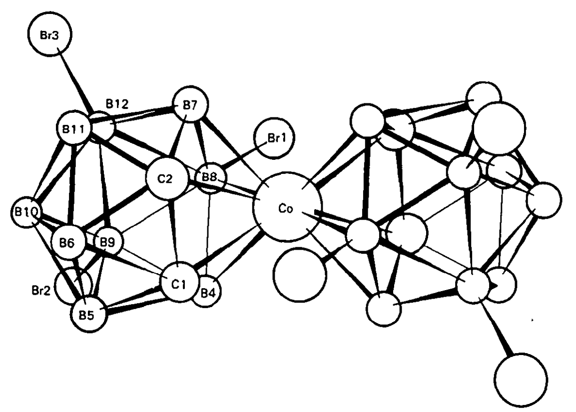

Fig. 1. Structure of the $[(C_2B_9H_8Br_3)_2Co]^-$ anion. (H atoms have been omitted.)

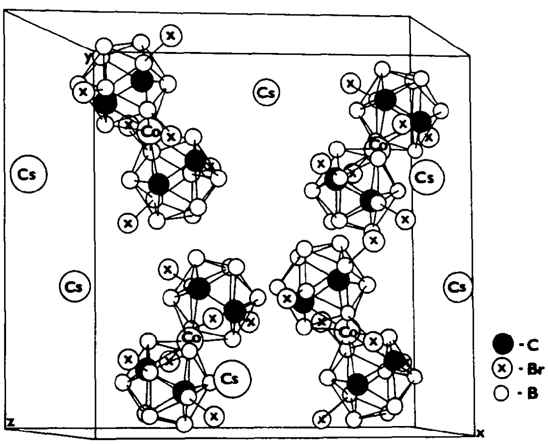

Fig. 2. General view of the structure.

Table 2. *Interatomic distances* (Å), *selected angles* (°) *and averaged values with e.s.d.'s in parentheses*

Co–C(1)	2·032 (7)	B(6)–B(10)	1·78 (1)
–C(2)	1·997 (9)	–B(11)	1·77 (2)
–B(4)	2·114 (9)	B(7)–B(8)	1·81 (2)
–B(7)	2·120 (12)	–B(11)	1·80 (1)
–B(8)	2·146 (9)	–B(12)	1·79 (1)
C(1)–C(2)	1·59 (1)	B(8)–B(9)	1·82 (1)
–B(4)	1·71 (2)	–B(12)	1·81 (1)
–B(5)	1·68 (1)	B(10)–B(9)	1·74 (1)
–B(6)	1·71 (1)	–B(11)	1·79 (1)
C(2)–B(6)	1·72 (1)	–B(12)	1·78 (1)
–B(7)	1·69 (1)	B(12)–B(9)	1·80 (1)
–B(11)	1·70 (2)	–B(11)	1·78 (2)
B(4)–B(5)	1·81 (1)	Br(1)–B(8)	1·960 (12)
–B(8)	1·79 (1)	Br(2)–B(9)	1·968 (14)
–B(9)	1·80 (1)	Br(3)–B(12)	1·940 (11)
B(5)–B(6)	1·74 (2)		
–B(9)	1·75 (1)		
–B(10)	1·77 (2)		
H(1)–C(1)	0·93 (9)		
H(2)–C(2)	0·69 (7)		
H(4)–B(4)	1·35 (6)		
H(5)–B(5)	1·17 (8)		
H(6)–B(6)	1·01 (6)		
H(7)–B(7)	1·19 (7)		
H(10)–B(10)	1·25 (9)		
H(11)–B(11)	1·16 (8)		
Co–B(8)–Br(1)	118·8 (4)		
B(4)–B(8)–Br(1)	124·4 (5)		
B(7)–B(8)–Br(1)	123·4 (5)		
B(9)–B(8)–Br(1)	117·1 (4)		
B(12)–B(8)–Br(1)	115·5 (5)		
B(4)–B(9)–Br(2)	120·1 (5)		
B(5)–B(9)–Br(2)	121·6 (5)		
B(8)–B(9)–Br(2)	120·7 (4)		
B(10)–B(9)–Br(2)	121·3 (5)		
B(12)–B(9)–Br(2)	122·3 (6)		
B(7)–B(12)–Br(3)	121·9 (6)		
B(8)–B(12)–Br(3)	122·5 (5)		
B(9)–B(12)–Br(3)	122·7 (5)		
B(10)–B(12)–Br(3)	120·5 (6)		
B(11)–B(12)–Br(3)	121·3 (6)		

Averaged distances and angles

No. averaged		Av. (Å,°)
2	Co–C	2·015 ±0·024[a]
3	Co–B	2·127 ±0·017
1	C–C	1·59 (1)
6	C–B	1·702 ±0·015
18	B–B	1·783 ±0·023
3	B–Br	1·956 ±0·014
2	H–C	0·805 ±0·170
6	H–B	1·187 ±0·109
30	B–B–B	60·0 ±0·9[a]
4	B–C–B	63·0 ±1·4
8	C–B–B	58·5 ±0·9
1	C(1)–B(6)–C(2)	55·3 (5)
2	B–C–C	62·4 ±0·6
1	C(1)–Co–C(2)	46·5 (3)
2	C–Co–B	48·5 ±0·2
2	B–Co–B	49·9 ±0·2
2	Co–C–C	66·7 ±1·6
2	Co–C–B	68·9 ±1·0
2	Co–B–C	62·7 ±0·8
4	Co–B–B	65·1 ±1·0
2	H–C–Co	116·7 ±0·3
2	H–B–Co	119·8 ±2·3
2	H–C–C	121·3 ±1·3
2	H–C–B(4,7)	123·0 ±0·5
4	H–C–B(5,6,11)	106·1 ±2·1
6	H–B–C	124·8 ±3·8
22	H–B–B	121·1 ±7·0

(*a*) E.s.d.'s of average values are calculated *via* the expression $\sigma = [\sum_{i=1}^{n}(x_i - \bar{x})^2/(n-)]^{1/2}$, where x_i is the *i*th value and $\bar{x}$ is the mean of *n* equivalent measurements.

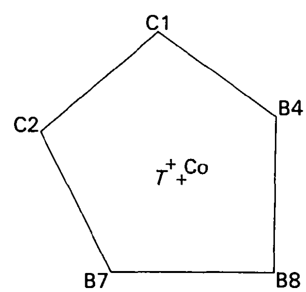

Fig. 3. Projection of Co onto the least-squares plane of atoms C(1), C(2), B(4), B(7), B(8). *T* denotes the centroid of the five atoms defining the plane.

Table 3. *Distribution of carbametallaboranes with* $(C_2B_9H_{11})_2^{4-}$ *π-ligands according to the d-electron configuration of the transition metal*

	Crystallographic symmetry of metal atom	d^n	$\bar{x}_{M-C}$ (Å)		$\bar{x}_{M-B}$ (Å)	σ^2_{M-L} (Å^2)	Slip* (Å)	
$[(C_2B_9H_{11})_2Cu^{II}][Et_4N]_2^a$	$\bar{1}$	d^9	2·578 (9)	≠	2·198 (58)	0·045	0·492 (4)	Distorted π-allylic complexes
$[(C_2B_9H_{11})_2Cu^{III}][(C_6H_5)_3PCH_3]^b$	$\bar{1}$	d^8	2·505 (7)	≠	2·123 (64)	0·046	0·416 (11)	
	$\bar{1}$	d^8	2·530 (42)	≠	2·110 (70)	0·056	0·508 (12)	
$[(C_2B_9H_{11})_2Au^{III}][(Et_2NCS_2)_2Au]^c$	$\bar{1}$	d^8	2·767 (10)	≠	2·244 (36)	0·083	0·633 (4)	
$[(C_2B_9H_{11})_2Ni^{III}][(CH_3)_4N]^d$	$\bar{1}$	d^7	2·146 (1)	=	2·125 (30)	0·00058	0·047 (3)	Symmetric π-sandwich complexes
$[(C_2B_9H_{11})_2Ni^{IV}]^e$	1	d^6	2·071 (8)	=	2·104 (17)	0·00048	0·034 (1)	
	1	d^6	2·072 (1)	=	2·101 (15)	0·00038	0·032 (1)	
$[(C_2B_9H_8Br_3)_2Co^{III}][(CH_3)_4N]^f$	$\bar{1}$	d^6	2·015 (35)	=	2·103 (61)	0·00452	0·063 (12)	
	$\bar{1}$	d^6	2·025 (7)	≠	2·133 (35)	0·00415	0·073 (9)	
	$\bar{1}$	d^6	1·990 (14)	≠	2·137 (15)	0·00662	0·088 (11)	
	$\bar{1}$	d^6	2·070 (28)	≠	2·150 (26)	0·00247	0·050 (11)	
$[(C_2B_9H_{11})_2Co^{III}]Cs^g$	$\bar{1}$	d^6	2·068 (7)	=	2·072 (15)	0·00400	0·015 (26)	
$[(C_2B_9H_8Br_3)_2Co^{III}]Cs^h$	$\bar{1}$	d^6	2·015 (24)	≠	2·127 (17)	0·00403	0·057 (3)	
$[(C_2B_9H_{10}I)_2Co^{III}]Cs^i$	$\bar{1}$	d^6	2·029 (2)	≠	2·129 (22)	0·00329	0·061 (2)	
$[(C_2B_9H_{10}I)Co^{III}(C_2B_9H_{11})]Cs^j$	1	d^6	2·041 (13)	=	2·108 (31)	0·00185	0·047 (4)	
	1	d^6	2·042 (25)	=	2·107 (24)	0·00172	0·027 (4)	
$[\{C_2B_9H_9(CH_3)_2\}_2Cr^{III}]^k$	2	d^3	2·267 (7)	=	2·258 (8)	0·00007	0·044 (3)	

References: (*a*) Wing (1967) (Et = ethyl); (*b*) Wing (1968); (*c*) Colquhoun, Greenhough & Wallbridge (1977); (*d*) Hansen, Hazell, Hyatt & Stucky (1973); (*e*) St Clair, Zalkin & Templeton (1970); (*f*) De Boer, Zalkin & Templeton (1968); (*g*) Zalkin *et al.* (1967); (*h*) present work; (*i*) Sivý, Preisinger, Baumgartner, Valach, Koreň & Mátel (1986*a*); (*j*) Sivý *et al.* (1986*b*); (*k*) St Clair, Zalkin & Templeton (1971).

* Distance between projection of metal onto least-squares plane through atoms bonded directly to the metal, and the centroid of the plane (see text and Fig. 3).

equality of means is not of such significance is evident from the sixth column of Table 3. It gives the estimate of variance calculated for all ten bonds of the central atom with ligand atoms; this is smaller by approximately one order of magnitude than that of the electron-rich (d^8 and d^9) carbametallaboranes. The last column in Table 3 lists distances between the unweighted centroid of the five atoms of the icosahedron which are directly bonded to the metal atom and the orthogonal projection of the metal onto the least-squares plane defined by these atoms. It is evident that these distances are several tenths of an Å in the case of the electron-rich carbametallaboranes and decrease by as much as one order of magnitude in complexes in which the metal has d^7 and lower electron configurations.

Fig. 3 illustrates this in the case of the present structure. The distance Co—centroid(T) is 0·057 (3) Å. It is thus classified as a symmetric π-sandwich complex with Co^{III} having d^6 formal valence electron configuration.

References

Cambridge Structural Database (1984). Univ. Chemical Laboratory, Lensfield Road, Cambridge CB2 1EW, England.

Colquhoun, H. M., Greenhough, T. J. & Wallbridge, M. G. H. (1977). *Acta Cryst.* B**33**, 3604–3607.

De Boer, B. G., Zalkin, A. & Templeton, D. H. (1968). *Inorg. Chem.* **7**, 2288–2294.

Hansen, F. V., Hazell, R. G., Hyatt, C. & Stucky, G. D. (1973). *Acta Chem. Scand.* **27**, 1210–1218.

International Tables for X-ray Crystallography (1962). Vol. III, pp. 202, 215. Birmingham: Kynoch Press. (Present distributor D. Reidel, Dordrecht.)

Macášek, F., Mátel, Ľ. & Kyrš, M. (1978). *Radiochem. Radioanal. Lett.* **35**, 247–254.

Main, P., Fiske, S. J., Hull, S. E., Lessinger, L., Germain, G., Declercq, J.-P. & Woolfson, M. M. (1980). *MULTAN*80. *A System of Computer Programs for the Automatic Solution of Crystal Structures from X-ray Diffraction Data.* Univs. of York, England, and Louvain, Belgium.

Mátel, Ľ. (1982). *The Radiated-Chemical Reactions of Dicarbollyls in Polar Solvents.* PhD Thesis, Comenius Univ., Bratislava, Czechoslovakia.

Mátel, Ľ., Macášek, F., Rajec, P., Heřmánek, S. & Plešek, J. (1982). *Polyhedron*, **1**, 511–519.

St Clair, D., Zalkin, A. & Templeton, D. H. (1970). *J. Am. Chem. Soc.* **92**, 1173–1179.

St Clair, D., Zalkin, A. & Templeton, D. H. (1971). *Inorg. Chem.* **10**, 2587–2591.

Sivý, P., Preisinger, A., Baumgartner, O., Valach, F., Koreň, B. & Mátel, Ľ. (1986*a*). *Acta Cryst.* C**42**, 28–30.

Sivy, P., Preisinger, A., Baumgartner, O., Valach, F., Koreň, B. & Mátel, Ľ. (1986*b*). *Acta Cryst.* C**42**, 30–33.

Stewart, J. M., Kruger, G. J., Ammon, H. L., Dickinson, C. W. & Hall, S. R. (1972). The *XRAY*72 system–version of June 1972. Tech. Rep. TR-192. Computer Science Center, Univ. of Maryland, College Park, Maryland.

Wing, R. M. (1967). *J. Am. Chem. Soc.* **89**, 5599–5604.

Wing, R. M. (1968). *J. Am. Chem. Soc.* **90**, 4828–4834.

Wing, R. M. (1970). *J. Am. Chem. Soc.* **92**, 1187–1190.

Zalkin, A., Hopkins, E. T. & Templeton, D. H. (1967). *Inorg. Chem.* **6**, 1911–1915.