-0.092 (18) and 0.094 (21) Å, respectively. The Pt—N(1) bond, 2.015 (15) Å, is slightly longer than Pt—N(2), 1.961 (15) Å, reflecting the different hybridization of the donor atoms. The 'bite' angle of the chelating ligand is 89.0 (7)°. In square-planar platinum(II) complexes the bite angle of the chelate ring takes up the theoretical value of 90° only in the case of seven-membered metallacycles (Maresca, Natile, Intini, Gasparrini, Tiripicchio & Tiripicchio Camellini, 1986), while much smaller values are found for five- and six-membered rings (Geue & Snow, 1971; Gollogly & Hawkins, 1972; Corey & Bailar, 1959; Fanizzi, Maresca, Natile, Lanfranchi, Manotti Lanfredi & Tiripicchio, 1988). This indicates that increasing the ring size decreases the steric strain within it and therefore the low occurrence of hepta-atomic rings is due to thermodynamic rather than steric factors.

The rather short N(3)—C(3) bond, 1.38 (3) Å, and the rough planarity of the aminic group at N(3) suggest extensive electron delocalization within the amidine moiety. Consequently, the N(2)C(3)N(3)C(2) torsion angle is only 26 (4)° although this causes some steric repulsion between the adjacent phenyl and tert-butyl groups. This situation is quite comparable to that found in (2), in which the ligand is monodentate, and in [Pt(NH=CPhNBu^{t}CH$_2$CH$_2$NHBu$'$)Cl(NHCOPh)], in which the ligand participates in a chelate ring (Maresca, Natile, Intini, Gasparrini, Tiripicchio & Tiripicchio Camellini, 1986).

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Structure of Benzyltrimethylammonium 7,7,7-Tricarbonyldodecahydro-7-cobalta-*nido*-undecaborate(1 −)

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Abstract. [PhCH$_2$NMe$_3$][7,7,7-(CO)$_3$-7-CoB$_{10}$H$_{12}$], C$_{10}$H$_{16}$N$^+$.B$_{10}$C$_3$CoH$_{12}$O$_3^-$, $M_r = 413.39$, monoclinic, $P2_1/c$, $a = 10.634$ (5), $b = 14.118$ (5), $c = 14.168$ (4) Å, $\beta = 91.81$ (3)°, $V = 2126.0$ Å^3, $Z = 4$, $D_x = 1.291$ Mg m^{-3}, Mo $K\alpha$, $\lambda = 0.71069$ Å, $\mu = 0.82$ mm^{-1}, $F(000) = 856$, $T = 185$ (1) K, $R = 0.0985$ for 1967 independent observed reflections. The anion has effective C_s molecular symmetry, with one carbonyl ligand lying *endo* to the open face of the cage. R.m.s. misfit calculations suggest that the B$_{10}$H$_{12}$ moiety is better described as the *arachno* fragment {B$_{10}$H$_{12}$}$^{4-}$, and hence that the formal metal oxidation state is $+3$, the overall geometry of
the cobaltaborane approximating to that of the *nido* fragment of an icosahedron.

Introduction. At their simplest level metallaboranes and metallahetereoboranes can be viewed in two ways, either as complexes between a metal and a (hetero)borane ligand, or as heteroboranes in which the metal atom occupies a polyhedral vertex. In many cases these two views are entirely complementary and semantical.

Recent studies (Wynd, Welch & Parish, 1989; Wynd, 1988) from this laboratory, however, suggest that in some systems a distinction can be made

Table 1. Coordinates and equivalent isotropic displacement parameters of refined atoms with e.s.d.'s in parentheses

	x	y	z	$U_{eq}*(Å^2)$
Co(7)	0·24060 (16)	0·09793 (13)	0·02488 (11)	0·0272 (8)
C(A)	0·1186 (12)	0·0919 (10)	0·1115 (8)	0·035 (7)
O(A)	0·0437 (9)	0·0923 (8)	0·1666 (7)	0·052 (6)
C(B)	0·2480 (13)	−0·0270 (11)	0·0047 (10)	0·046 (9)
O(B)	0·2585 (12)	−0·1056 (7)	−0·0096 (8)	0·067 (8)
C(C)	0·3785 (12)	0·1193 (7)	0·0940 (7)	0·025 (6)
O(C)	0·4700 (9)	0·1334 (8)	0·1393 (7)	0·054 (7)
B(1)	0·1382 (13)	0·2187 (12)	−0·1682 (10)	0·032 (8)
B(2)	0·1912 (12)	0·1041 (11)	−0·1239 (9)	0·030 (7)
B(3)	0·1065 (15)	0·1871 (12)	−0·0546 (11)	0·038 (9)
B(4)	0·1554 (13)	0·3037 (11)	−0·0803 (10)	0·031 (8)
B(5)	0·2699 (14)	0·2938 (10)	−0·1690 (9)	0·029 (8)
B(6)	0·2903 (14)	0·1716 (12)	−0·1970 (9)	0·033 (8)
B(8)	0·2139 (14)	0·2538 (10)	0·0256 (10)	0·031 (8)
B(9)	0·3189 (13)	0·3225 (10)	−0·0528 (10)	0·028 (8)
B(10)	0·4066 (15)	0·2341 (11)	−0·1304 (10)	0·034 (8)
B(11)	0·3587 (13)	0·1120 (9)	−0·1022 (9)	0·029 (7)
C(2)	0·6362	0·3520	0·0755	0·033 (3)
C(3)	0·6220	0·3772	0·1697	0·041 (3)
C(4)	0·7269	0·4028	0·2255	0·044 (3)
C(5)	0·8461	0·4033	0·1871	0·040 (3)
C(6)	0·8603	0·3781	0·0928	0·034 (3)
C(1)	0·7554	0·3524	0·0370	0·027 (3)
C(7)	0·7716 (11)	0·3232 (9)	−0·0646 (8)	0·027 (3)
N(1)	0·7568 (8)	0·4026 (7)	−0·1370 (6)	0·026 (5)
C(8)	0·7726 (14)	0·3593 (11)	−0·2326 (9)	0·045 (9)
C(9)	0·8522 (12)	0·4808 (8)	−0·1203 (10)	0·039 (8)
C(10)	0·6257 (11)	0·4476 (9)	−0·1355 (9)	0·034 (7)

$$*U_{eq} = (1/3)\Sigma_i\Sigma_j U_{ij} a_i^* a_j^* \mathbf{a}_i.\mathbf{a}_j.$$

Table 2. Internuclear distances (Å) and selected interbond angles (°) with e.s.d.'s in parentheses

Co(7)—C(A)	1·816 (13)	B(4)—B(8)	1·754 (21)
Co(7)—C(B)	1·788 (15)	B(4)—B(9)	1·789 (20)
Co(7)—C(C)	1·763 (11)	B(5)—B(6)	1·785 (21)
Co(7)—B(2)	2·158 (14)	B(5)—B(9)	1·758 (20)
Co(7)—B(3)	2·187 (16)	B(5)—B(10)	1·753 (21)
Co(7)—B(8)	2·219 (15)	B(6)—B(10)	1·768 (21)
Co(7)—B(11)	2·237 (14)	B(6)—B(11)	1·726 (20)
C(A)—O(A)	1·133 (16)	B(8)—B(9)	1·871 (20)
C(B)—O(B)	1·135 (19)	B(9)—B(10)	1·924 (21)
C(C)—O(C)	1·165 (15)	B(10)—B(11)	1·845 (21)
B(1)—B(2)	1·818 (20)		
B(1)—B(3)	1·714 (22)		
B(1)—B(4)	1·735 (21)		
B(1)—B(5)	1·756 (21)		
B(1)—B(6)	1·807 (21)		
B(2)—B(3)	1·790 (21)		
B(2)—B(6)	1·778 (20)	C(1)—C(7)	1·512 (14)
B(2)—B(11)	1·801 (20)	C(7)—N(1)	1·525 (15)
B(3)—B(4)	1·768 (22)	N(1)—C(8)	1·500 (17)
B(3)—B(8)	1·844 (21)	N(1)—C(9)	1·513 (16)
B(4)—B(5)	1·783 (20)	N(1)—C(10)	1·533 (16)
C(A)—Co(7)—C(B)	95·6 (6)	B(1)—B(5)—B(6)	61·4 (8)
C(A)—Co(7)—C(C)	103·4 (6)	B(4)—B(5)—B(9)	60·7 (8)
C(B)—Co(7)—C(C)	102·6 (6)	B(6)—B(5)—B(10)	60·0 (8)
B(2)—Co(7)—B(3)	48·7 (6)	B(9)—B(5)—B(10)	66·5 (8)
B(2)—Co(7)—B(11)	48·3 (5)	B(1)—B(6)—B(2)	61·0 (8)
B(3)—Co(7)—B(8)	49·5 (6)	B(1)—B(6)—B(5)	58·5 (8)
Co(7)—C(A)—O(A)	176·8 (12)	B(2)—B(6)—B(11)	61·8 (8)
Co(7)—C(B)—O(B)	176·6 (13)	B(5)—B(6)—B(10)	59·1 (8)
Co(7)—C(C)—O(C)	179·6 (10)	B(10)—B(6)—B(11)	63·7 (9)
B(2)—B(1)—B(3)	60·8 (8)	Co(7)—B(8)—B(3)	64·4 (7)
B(2)—B(1)—B(6)	58·7 (8)	B(3)—B(8)—B(4)	58·8 (8)
B(3)—B(1)—B(4)	61·7 (9)	B(4)—B(8)—B(9)	59·0 (8)
B(4)—B(1)—B(5)	61·4 (8)	B(4)—B(9)—B(5)	60·3 (8)
B(5)—B(1)—B(6)	61·1 (8)	B(4)—B(9)—B(8)	57·2 (8)
Co(7)—B(2)—B(3)	66·5 (7)	B(5)—B(9)—B(10)	56·7 (8)
Co(7)—B(2)—B(11)	68·1 (6)	B(5)—B(10)—B(6)	60·9 (8)
B(1)—B(2)—B(3)	56·7 (8)	B(5)—B(10)—B(9)	56·9 (8)
B(1)—B(2)—B(6)	60·3 (8)	B(6)—B(10)—B(11)	57·0 (8)
B(6)—B(2)—B(11)	57·7 (8)	Co(7)—B(11)—B(2)	63·5 (6)
Co(7)—B(3)—B(2)	64·8 (7)	B(2)—B(11)—B(6)	60·5 (8)
Co(7)—B(3)—B(8)	66·2 (7)	B(6)—B(11)—B(10)	59·2 (8)
B(1)—B(3)—B(2)	62·5 (9)	C(2)—C(1)—C(7)	120·2 (7)
B(1)—B(3)—B(4)	59·8 (9)	C(6)—C(1)—C(7)	119·8 (7)
B(4)—B(3)—B(8)	58·1 (8)	C(1)—C(7)—N(1)	115·3 (9)
B(1)—B(4)—B(3)	58·6 (8)	C(7)—N(1)—C(8)	107·2 (9)
B(1)—B(4)—B(5)	59·9 (8)	C(7)—N(1)—C(9)	112·1 (9)
B(3)—B(4)—B(8)	63·1 (9)	C(7)—N(1)—C(10)	111·7 (9)
B(5)—B(4)—B(9)	59·0 (8)	C(8)—N(1)—C(9)	110·3 (9)
B(8)—B(4)—B(9)	63·8 (8)	C(8)—N(1)—C(10)	108·1 (9)
B(1)—B(5)—B(4)	58·7 (8)	C(9)—N(1)—C(10)	107·5 (9)

between the formalisms of metal–ligand complex and heteroborane, in that all metallaboranes and metalla-heteroboranes are metal–ligand complexes, but not all are *properly* described as heteroboranes. The distinction relies on assessment of the 'verticity' of the metal atom – the extent to which it acts as a true cluster vertex and not simply a bridge between several B atoms. Analysis of structural data on $MB_{10}H_{12}$ metallaboranes reveals subtle trends in verticity that, *inter alia*, appear to be a function of the position of M in the Periodic Table (Wynd, Macgregor, Yellowlees & Welch, 1990).

Unfortunately, limited data are available for cases where M is a 'typical' transition metal, in spite of the fact that many such species are known (Kennedy, 1986). The only representative compound to have been crystallographically characterized is [7-(CO)-1,7,7-(PPh₃)₃-7-IrB₁₀H₁₁] (Crook, 1982), a derivative of the $MB_{10}H_{12}$ cluster type, which awaits full publication. Therefore, to understand fully the emerging patterns in verticity amongst $MB_{10}H_{12}$ metallaboranes, we have resynthesized [7,7,7-(CO)₃-7-CoB₁₀H₁₂]⁻ (Klanberg, Wegner, Parshall & Muetterties, 1968), using cobalt, a 'typical' transition metal, for the purpose of the crystallographic study reported herein. Suitable crystals were afforded as the [PhCH₂NMe₃]⁺ salt.

Experimental. Compound prepared as [NMe₄]⁺ salt, converted to Na⁺ salt by ion exchange chromatography, and precipitated from aqueous solution as [PhCH₂NMe₃]⁺ salt by addition of an aqueous solution of benzyltrimethylammonium bromide; purity checked by IR spectroscopy (CH₂Cl₂ solution, ν_{B-H} 2505, ν_{C-O} 2065, 2020, and 2000 cm⁻¹) and microanalysis (found: C, 37·7; H, 6·92; N, 3·48%. $C_{13}H_{28}B_{10}CoNO_3$ requires: C, 37·8; H, 6·83; N, 3·39%); small yellow plates grown by slow cooling of a CH₂Cl₂ solution containing hexane; crystal, 0·5 × 0·27 × 0·05 mm, mounted on an Enraf–Nonius CAD-4 diffractometer (Mo $K\alpha$ X-radiation, graphite monochromator, ULT-1 low-temperature attachment); cell parameters and orientation matrix from least-squares refinement of the setting angles ($7 < \theta < 13°$) of 25 centred reflections; data collection by ω–2θ scans in 96 steps with ω scan width (0·8 + 0·34tanθ)°; data (h: 0 to 12, k: 0 to 16, l: −16 to 16) measured for $1 \le \theta \le 25°$ over 110 X-ray hours; corrections for Lorentz and polarization effects applied (Gould & Smith, 1986); 4128 independent reflections measured, of which 2199 [$F \ge 2·0\sigma(F)$]

retained; structure solution *via* Patterson synthesis (Co) and iterative full-matrix least-squares refinement (on F)/ΔF syntheses (C, O, B, N) (Sheldrick, 1976); analysis of variance revealed anomalously poor agreement for $hk0$ reflections, and analysis of the intensities of two check reflections as functions of time suggested fluctuations in beam power during the period over which these data were measured. Consequently all $hk0$ reflections omitted from data set; empirical absorption correction (Walker & Stuart, 1983) applied to remaining 1967 reflections (correction factors 0·782–1·141); all non-H atoms except benzyl C atoms refined with anisotropic thermal parameters; phenyl C atoms treated as regular planar hexagon (C—C = 1·395 Å); cage H and benzyl H atoms set in idealized positions, the former assigned an (invariant) isotropic thermal parameter (U_{cage-H} = 0·08 Å^2), and the latter a (refined) group thermal parameter [$U_{benzyl-H}$ = 0·062 (17) Å^2 at convergence]; methyl H atoms not included in calculations; unit weights assigned throughout; 207 variables, data:variable ratio > 9·5:1; max. shift/e.s.d. in final cycle < 0·02; R = 0·0985, attributed to size and quality of crystal; max. and min. residues in final difference Fourier synthesis 0·76 and −0·69 e Å^{-3} respectively; scattering factors for C, H, B, N and O inlaid in *SHELX*76. Those for Co from *International Tables for X-ray Crystallography* (1974); Fig. 1 drawn using *EASYORTEP* (Mallinson & Muir, 1985); molecular geometry calculations *via CALC* (Gould & Taylor, 1986).

Discussion. The anion has effective, non-crystallographically imposed, C_s molecular symmetry about the plane containing Co(7), B(5), and B(1). Table 1* lists the coordinates of refined atoms and equivalent isotropic thermal parameters, whilst Table 2 collates internuclear distances and selected interbond angles determined. A perspective view of the anion is presented in Fig. 1.

A recent study of [Cy$_3$PAu(B$_{10}$H$_{12}$)]$^-$ (Cy = cyclo-C$_6$H$_{11}$) (Wynd, Welch & Parish, 1989) and analysis of the structures of several MB$_{10}$H$_{12}$ congeners already in the literature (Wynd, 1988; Wynd, Macgregor, Yellowlees & Welch, 1990) have shown that the {B$_{10}$} portions of a number of these species are geometrically more similar to the {B$_{10}$} fragment of B$_{10}$H$_{14}$ (Brill, Dietrich & Dierks, 1971) than to the corresponding {B$_{10}$} fragment of [B$_{11}$H$_{13}$]$^{2-}$ (Fritchie, 1967), *i.e.* that the {B$_{10}$} unit is better described as {B$_{10}$H$_{12}$}$^{2-}$, a *nido* fragment of an octa-

decahedron, than {B$_{10}$H$_{12}$}$^{4-}$, an *arachno* fragment of an icosahedron.

This analysis has been based on the results of 'r.m.s. misfit' calculations (Gould & Taylor, 1986). Application of the same analysis to the {B$_{10}$} fragment of the present compound affords r.m.s. misfit values of 0·147 Å *versus* B$_{10}$H$_{14}$ and 0·070 Å *versus* [B$_{11}$H$_{13}$]$^{2-}$, on the basis of which the {B$_{10}$H$_{12}$} unit in this species appears to be formally present as {B$_{10}$H$_{12}$}$^{4-}$, *i.e.* [(CO)$_3$CoB$_{10}$H$_{12}$]$^-$ appears to be better described as a true *nido*-icosahedral species, in which the metal atom is formally in the +3 oxidation state. Current studies are directed towards independent measurement of the oxidation state of Co in the compound. The 'verticity' of the metal atom (Wynd, 1988; Wynd, Macgregor, Yellowlees & Welch, 1990) is calculated to be 69·1%. We are currently assessing the utility of a number of structural parameters for polyhedral classification, and for the present compound these include: B(2)—B(3) 1·790 (21); B(9)—B(10) 1·924 (21); B(8)···B(11) 3·136 (20) Å; and displacement of the Co atom from the least-squares plane through the B(8)B(9)B(10)-B(11) sequence 0·321 (15) Å.

The Co(CO)$_3$ unit is orientated such that it conforms to the effective mirror plane through the cage, and the C(C)O(C) carbonyl ligand is *endo* to the open polyhedral face. C—Co—C angles are not equal. Those involving C(C) average 103·0 (8)°, whilst C(A)—Co—C(B) is 95·6 (6)°. Moreover, the Co—C(C) bond is the shortest of its type and the C(C)—O(C) bond the longest of its type, but unfortunately the general lack of high precision in the model is such that the differences involved are
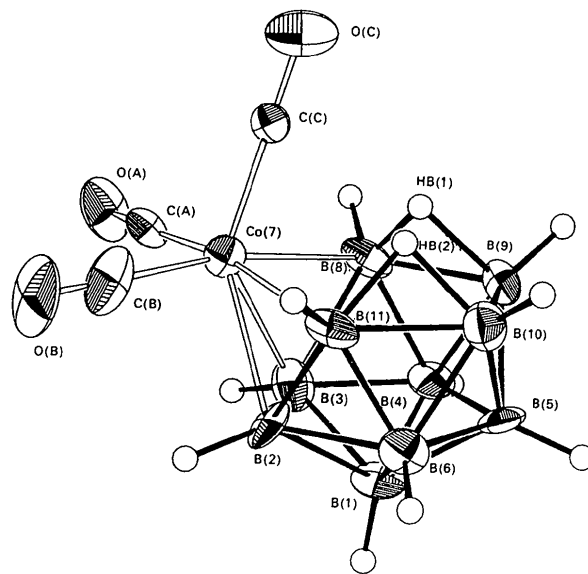
Fig. 1. Perspective view of [7,7,7-(CO)$_3$-7-CoB$_{10}$H$_{12}$]$^-$ (50% thermal ellipsoids, except for the H atoms which have an artificial radius of 0·1 Å for clarity).

not strictly statistically significant. Nevertheless, taken together these results are not inconsistent with the conclusion that there is more π back bonding from Co to C(C)O(C) than to the other carbonyl ligands. This point is one of several that we are currently addressing through extended Hückel molecular orbital calculations on $[(CO)_3CoB_{10}H_{12}]^-$ and related species.

Distances and angles within the $[PhCH_2NMe_3]^+$ cation are unexceptional and fully consistent with those determined in recent studies in this department (Mitchell & Welch, 1987; Wynd & Welch, 1989).

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Three Chromium(III) Complexes with Mixed Amino Acid Ligands: (L-Cysteinato)-(L-histidinato)chromium(III) 3·5-Hydrate, (L-Aspartato)(L-histidinato)chromium(III) 1·5-Hydrate and Bis(DL-histidinato)chromium(III) Chloride 4·2-Hydrate

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Abstract. [Cr(L-Cys)(L-His)].3·5H₂O (I): [Cr(C₆H₈-N₃O₂)(C₃H₅NO₂S)].3·5H₂O, $M_r = 388·4$, orthorhombic, $P2_12_12_1$, $a = 13·808$ (2), $b = 20·228$ (3), $c = 23·367$ (5) Å, $V = 6526·6$ Å³, $Z = 16$, $D_x = 1·581$ g cm⁻³, Mo $K\alpha$, $\lambda = 0·71069$ Å, $\mu = 8·12$ cm⁻¹, $F(000) = 3232$, $T = 294$ K, final $R = 0·037$ for 4668 reflections. [Cr(L-Asp)(L-His)].1·5H₂O (II): [Cr(C₄H₅NO₄)(C₆H₈N₃O₂)].1·5H₂O, $M_r = 364·2$, orthorhombic, $P2_122_1$, $a = 6·135$ (1), $b = 11·398$ (1), $c = 20·191$ (1) Å, $V = 1411·9$ Å³, $Z = 4$, $D_x = 1·713$ g cm⁻³, Mo $K\alpha$, $\lambda = 0·71069$ Å, $\mu = 7·99$ cm⁻¹, $F(000) = 752$, $T = 294$ K, final $R = 0·037$ for 1253 observed reflections. [Cr(DL-His)₂]Cl.4·2-H₂O (III): [Cr(C₆H₈N₃O₂)₂]Cl.4·2H₂O, $M_r = 471·4$, orthorhombic, $Ccca$, $a = 15·334$ (3), $b = 32·038$ (8), c = 16·635 (2) Å, $V = 8172·3$ Å³, $Z = 16$, $D_x = 1·532$, Mo $K\alpha$, $\lambda = 0·71069$ Å, $\mu = 7·00$ cm⁻¹, $F(000) = 3920$, $T = 294$ K, final $R = 0·056$ for 1789 reflections. The ligands in all three complexes are tridentate. In (I) (four complexes per asymmetric unit) and (II) the arrangement of the ligands is *fac-cis*-N(amino), *cis*-O(carboxyl). In (III) two isomers, *fac-trans*-N(imidazole) and *fac-trans*-N(amino), cocrystallize. Metal–ligand bond lengths are: Cr—N(amino) 2·043 (5)–2·068 (5) Å, Cr—O(carboxyl) 1·963 (3)–1·998 (4) Å, Cr—S(thiol) 2·371 (2)–2·397 (2) Å, Cr—N(imidazole) 2·037 (4)–2·078 (5) Å. There is evidence that Cr—S(thiol) bonds exert a structural *trans* effect, and that their lengths in turn are influenced by the softness of the ligand in the *trans* position.

Introduction. Few structure analyses of amino acid complexes of Cr have been reported. Among these

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