Table 3. H-*bond distances* (Å) *and angles* (°)

O—H···O	O···O	O—H	H···O	O—H···O
O(11)—H(19)···O(6$^{\rm i}$)	2·877 (5)	0·88 (4)	2·00 (4)	171 (4)
O(12)—H(20)···O(6)	2·689 (5)	0·88 (3)	1·88 (4)	152 (4)
O(13)—H(21)···O(1$^{\rm ii}$)	2·697 (6)	0·89 (4)	2·01 (5)	133 (4)
O(13)—H(21)···O(2$^{\rm ii}$)	2·908 (6)	0·89 (4)	2·21 (5)	134 (4)
O(14)—H(34)···O(1$^{\rm ii}$)	2·662 (5)	1·05 (5)	1·63 (5)	167 (4)
O(15)—H(35)···O(6)	2·681 (4)	0·77 (5)	1·92 (5)	171 (6)
O(16)—H(36)···O(11$^{\rm iii}$)	2·934 (4)	0·88 (3)	2·18 (5)	144 (4)

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

The tea ligands have an extended conformation which is also encountered in $(\text{tea})_2\text{Sr}(\text{NO}_3)_2$ (Voegele, Fischer & Weiss, 1974*b*), $(\text{tea})_3\text{NaI}$ (Voegele, Fischer & Weiss, 1974*a*) and in $(\text{tea})_2\text{Ba}(\text{CH}_3\text{COO}^-)_2$ (Voegele, Thierry & Weiss, 1974). This requires three nearly planar C—N—C—C fragments for each tea and a *gauche* conformation of the terminal OH groups with respect to the C—N bonds. The geometries of both tea's show a good mutual correspondence; the maximal differences in bond lengths and angles are 0·02 Å and 1·2° respectively and they compare well with the geometries observed in the Sr, Na and Ba complexes. The six N—C—C—O torsion angles range from 52·0 (8) to 64·3 (7)°, compared with an overall range of 46·8 (4) to 67·4 (4)° in the three complexes mentioned above.

All six tea hydroxyl groups, within the coordination sphere of Ba, take part in hydrogen bonds; one of the OH groups is a double donor (Table 3). The phenolic O atoms are strong acceptors as O(1) of dnp1 accepts two and O(6) of dnp2 three hydrogen bonds. The two remaining acceptors are a nitro-group O next to phenolic O in dnp1 and an O atom of a tea ligand. Each Ba cluster is connected by donor and acceptor hydrogen bonds to four other Ba clusters, thus forming a strong two-dimensional network parallel with the *ab* plane. Two of the hydrogen bonds which link tea O atoms to phenolic O of dnp2 are within the Ba cluster. Although dnp2 is not involved in the coordination to Ba, it effectively contributes to the interaction energy by its participation in three acceptor bonds of phenolic O.

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9,9-Bis(triphenylphosphine)-7,8-dicarba-9-rhoda-*nido*-undecaborane(11), $\mathbf{C_{38}H_{41}B_8P_2Rh}$, an *endo-nido*-Carbarhodaborane Complex Containing an Acidic Bridging Hydrogen

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Abstract. $M_r = 749{\cdot}2$, monoclinic, $P2_1/n$, $a = 18{\cdot}950\,(6)$, $b = 12{\cdot}057\,(3)$, $c = 15{\cdot}585\,(5)$ Å, $\beta = 97{\cdot}80\,(3)°$, $V = 3527{\cdot}9$ Å^3, $Z = 4$, $D_x = 1{\cdot}41$ g cm^{-3}, $\lambda(\text{Mo } K\alpha) = 0{\cdot}7107$ Å, $\mu = 5{\cdot}93$ cm^{-1}, $F(000) = 1536$, $T = 117$ K, final $R = 0{\cdot}038$ for 5021 unique observed reflections. Rh can be considered to possess a pseudo square-planar coordination with $C_2B_8H_{11}$ as a bidentate ligand. Distances to Rh within the icosahedral fragment are Rh—C = 2·198 (4), Rh—B = 2·132 (4), 2·181 (4) and 2·238 (4) Å. An acidic hydrogen bridges B(10) and B(11) at distances of 1·25 (5) and 1·29 (5) Å, B—H—B = 95 (3)°.

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Table 1. *Positional and vibrational parameters*

$$B_{\text{eq}} = \tfrac{8}{3}\pi^2 \textstyle\sum_i \sum_j U_{ij} a_i^* a_j^* \mathbf{a}_i . \mathbf{a}_j.$$

	x	y	z	B_{eq}/ B_{iso}(Å^2)
Rh(9)	0·78311 (1)	−0·15097 (2)	−0·00541 (2)	0·9
P(1)	0·70370 (5)	−0·24977 (8)	0·06367 (6)	1·1
P(2)	0·88217 (5)	−0·27643 (8)	0·01102 (6)	1·1
B(1)	0·73648 (23)	0·10088 (36)	−0·09992 (28)	1·3
B(2)	0·76267 (23)	0·05722 (36)	−0·19951 (28)	1·4
B(3)	0·82858 (24)	0·08739 (35)	−0·11120 (29)	1·5
B(4)	0·79630 (23)	0·02772 (36)	−0·01782 (29)	1·4
B(5)	0·70468 (22)	−0·01650 (37)	−0·04790 (27)	1·3
B(6)	0·68688 (24)	−0·00216 (37)	−0·16344 (27)	1·4
B(10)	0·70383 (22)	−0·13737 (37)	−0·11584 (27)	1·3
B(11)	0·75041 (24)	−0·09043 (36)	−0·20808 (28)	1·5
C(7)	0·83000 (20)	−0·03258 (31)	−0·16956 (24)	1·4
C(8)	0·84967 (20)	−0·04019 (31)	−0·07260 (24)	1·3
H(1)	0·7155 (28)	0·1750 (43)	−0·0927 (34)	
H(2)	0·7605 (27)	0·1067 (43)	−0·2607 (33)	
H(3)	0·8714 (28)	0·1504 (41)	−0·1083 (33)	
H(4)	0·8170 (27)	0·0671 (42)	0·0432 (34)	
H(5)	0·6658 (28)	0·0007 (43)	−0·0106 (33)	
H(6)	0·6333 (27)	0·0140 (42)	−0·1986 (33)	
H(7)	0·8658 (28)	−0·0348 (42)	−0·2040 (34)	
H(8)	0·8957 (28)	−0·0443 (44)	−0·0544 (34)	
H(10)	0·6629 (27)	−0·1995 (43)	−0·1262 (33)	
H(11)	0·7446 (27)	−0·1261 (43)	−0·2748 (34)	
H(*Br*)	0·7480 (27)	−0·1762 (41)	−0·1640 (33)	
C(11)	0·6207 (2)	−0·1793 (3)	0·0801 (2)	1·37 (6)
C(12)	0·6191 (2)	−0·1078 (3)	0·1503 (2)	1·64 (7)
C(13)	0·5567 (2)	−0·0516 (4)	0·1613 (3)	2·21 (7)
C(14)	0·4958 (2)	−0·0673 (4)	0·1033 (3)	2·33 (8)
C(15)	0·4964 (2)	−0·1370 (4)	0·0330 (3)	2·26 (8)
C(16)	0·5587 (2)	−0·1931 (3)	0·0211 (3)	1·67 (7)
C(21)	0·6687 (2)	−0·3834 (3)	0·0220 (2)	1·20 (6)
C(22)	0·6942 (2)	−0·4318 (3)	−0·0495 (2)	1·46 (6)
C(23)	0·6672 (2)	−0·5324 (3)	−0·0828 (3)	1·88 (7)
C(24)	0·6139 (2)	−0·5865 (3)	−0·0451 (3)	1·94 (7)
C(25)	0·5874 (2)	−0·5388 (3)	0·0249 (3)	1·79 (7)
C(26)	0·6141 (2)	−0·4381 (3)	0·0582 (2)	1·55 (7)
C(31)	0·7445 (2)	−0·2733 (3)	0·1758 (2)	1·25 (6)
C(32)	0·7935 (2)	−0·1931 (3)	0·2108 (2)	1·60 (7)
C(33)	0·8273 (2)	−0·2021 (3)	0·2957 (3)	1·99 (7)
C(34)	0·8128 (2)	−0·2908 (4)	0·3462 (3)	2·15 (7)
C(35)	0·7648 (2)	−0·3722 (3)	0·3117 (3)	2·05 (7)
C(36)	0·7307 (2)	−0·3632 (3)	0·2275 (3)	1·74 (7)
C(41)	0·8695 (2)	−0·4260 (3)	0·0199 (2)	1·24 (6)
C(42)	0·8464 (2)	−0·4676 (3)	0·0962 (2)	1·49 (6)
C(43)	0·8259 (2)	−0·5778 (3)	0·1001 (2)	1·70 (7)
C(44)	0·8274 (2)	−0·6482 (3)	0·0304 (3)	1·89 (7)
C(45)	0·8520 (2)	−0·6086 (3)	−0·0439 (3)	1·87 (7)
C(46)	0·8733 (2)	−0·4991 (3)	−0·0491 (2)	1·65 (7)
C(51)	0·9320 (2)	−0·2612 (3)	−0·0810 (2)	1·23 (6)
C(52)	0·8968 (2)	−0·2796 (3)	−0·1647 (2)	1·38 (6)
C(53)	0·9309 (2)	−0·2626 (3)	−0·2365 (2)	1·60 (7)
C(54)	1·0005 (2)	−0·2239 (3)	−0·2275 (3)	1·77 (7)
C(55)	1·0359 (2)	−0·2042 (3)	−0·1443 (3)	1·89 (7)
C(56)	1·0026 (2)	−0·2227 (3)	−0·0716 (2)	1·51 (6)
C(61)	0·9454 (2)	−0·2409 (3)	0·1067 (2)	1·30 (6)
C(62)	0·9896 (2)	−0·3187 (3)	0·1524 (3)	1·71 (7)
C(63)	1·0351 (2)	−0·2891 (3)	0·2266 (3)	1·89 (7)
C(64)	1·0373 (2)	−0·1799 (3)	0·2552 (3)	1·90 (7)
C(65)	0·9943 (2)	−0·1000 (3)	0·2093 (3)	1·81 (7)
C(66)	0·9491 (2)	−0·1307 (3)	0·1355 (2)	1·53 (6)

Units of each e.s.d., in parentheses, are those of the least significant digit of the corresponding parameter.
If B has no e.s.d., it is the equivalent isotropic B for an atom refined anisotropically. B was set at 2·0 Å^2 for all H atoms.

Introduction. Although *exo-nido* species of the formulation MC_2B_9, $M =$ Rh, Ir, have been structurally characterized (Doi, Teller & Hawthorne, 1980; Marder, 1981; Knobler, Marder, Mizusawa, Teller, Long, Behnken & Hawthorne, 1984), the *endo-nido* complexes formulated as $\mathrm{RhC_2B_8}$ have not. The *closo-* and *exo-nido*-$\mathrm{RhC_2B_9}$ species have been shown to be catalytically active. As part of our continuing investigation of the catalytic activity of icosahedral carbarhodaboranes, a new species formulated as *endo-nido*-$\mathrm{RhC_2B_8H_{11}}$ has been studied.

Table 2. *Interatomic distances* (Å) *and intramolecular angles* (°)

Rh(9)–B(10)	2·132 (4)
Rh(9)–B(4)	2·181 (4)
Rh(9)–C(8)	2·198 (4)
Rh(9)–B(5)	2·238 (4)
Rh(9)–P(1)	2·298 (1)
Rh(9)–P(2)	2·397 (1)
P(1)–C(21)	1·828 (4)
P(1)–C(31)	1·835 (4)
P(1)–C(11)	1·835 (4)
P(2)–C(41)	1·827 (4)
P(2)–C(51)	1·831 (4)
P(2)–C(61)	1·832 (4)
B(1)–H(1)	0·99 (5)
B(1)–B(2)	1·772 (6)
B(1)–B(6)	1·776 (6)
B(1)–B(5)	1·777 (6)
B(1)–B(3)	1·785 (6)
B(1)–B(4)	1·818 (6)
B(2)–H(2)	1·12 (5)
B(2)–C(7)	1·690 (6)
B(2)–B(6)	1·764 (6)
B(2)–B(3)	1·766 (6)
B(2)–B(11)	1·798 (6)
B(3)–H(3)	1·11 (5)
B(3)–C(8)	1·680 (5)
B(3)–C(7)	1·711 (6)
B(3)–B(4)	1·803 (6)
B(4)–H(4)	1·09 (5)
B(4)–C(8)	1·630 (6)
B(4)–B(5)	1·816 (6)
B(5)–H(5)	1·02 (5)
B(5)–B(6)	1·795 (6)
B(5)–B(10)	1·800 (6)
B(6)–H(6)	1·10 (5)
B(6)–B(10)	1·802 (6)
B(6)–B(11)	1·815 (6)
B(10)–H(10)	1·07 (5)
B(10)–H(*Br*)	1·29 (5)
B(10)–B(11)	1·874 (6)
B(11)–H(11)	1·12 (5)
B(11)–H(*Br*)	1·25 (5)
B(11)–C(7)	1·696 (6)
C(7)–H(7)	0·92 (5)
C(7)–C(8)	1·509 (5)
C(8)–H(8)	0·88 (5)

B(10)–Rh(9)–B(4)	85·94 (17)
B(10)–Rh(9)–C(8)	87·46 (15)
B(10)–Rh(9)–B(5)	48·58 (16)
B(10)–Rh(9)–P(1)	89·06 (12)
B(10)–Rh(9)–P(2)	126·20 (12)
B(4)–Rh(9)–C(8)	43·71 (15)
B(4)–Rh(9)–B(5)	48·51 (16)
B(4)–Rh(9)–P(1)	130·08 (12)
B(4)–Rh(9)–P(2)	122·37 (12)
C(8)–Rh(9)–B(5)	79·62 (15)
C(8)–Rh(9)–P(1)	173·12 (10)
C(8)–Rh(9)–P(2)	86·71 (10)
B(5)–Rh(9)–P(1)	93·63 (11)
B(5)–Rh(9)–P(2)	165·38 (11)
P(1)–Rh(9)–P(2)	100·13 (4)
B(2)–B(1)–B(6)	59·60 (24)
B(2)–B(1)–B(5)	108·40 (30)
B(2)–B(1)–B(3)	59·54 (24)
B(2)–B(1)–B(4)	104·49 (29)
B(6)–B(1)–B(5)	60·69 (24)
B(6)–B(1)–B(3)	109·39 (30)
B(6)–B(1)–B(4)	106·57 (29)
B(5)–B(1)–B(3)	111·66 (30)
B(5)–B(1)–B(4)	60·67 (23)
B(3)–B(1)–B(4)	60·04 (24)
C(7)–B(2)–B(6)	105·60 (29)
C(7)–B(2)–B(3)	59·28 (23)
C(7)–B(2)–B(1)	103·83 (29)
C(7)–B(2)–B(11)	58·08 (24)
B(6)–B(2)–B(3)	110·83 (30)
B(6)–B(2)–B(1)	60·30 (24)
B(6)–B(2)–B(11)	61·26 (25)
B(3)–B(2)–B(1)	60·59 (24)
B(3)–B(2)–B(11)	109·41 (30)
B(1)–B(2)–B(11)	108·09 (30)
C(8)–B(3)–C(7)	52·85 (22)
C(8)–B(3)–B(2)	101·48 (29)
C(8)–B(3)–B(1)	103·68 (30)
C(8)–B(3)–B(4)	55·67 (23)
C(7)–B(3)–B(2)	58·13 (24)
C(7)–B(3)–B(1)	102·44 (30)
C(7)–B(3)–B(4)	97·08 (28)
B(2)–B(3)–B(1)	59·87 (24)
B(2)–B(3)–B(4)	105·38 (30)
B(1)–B(3)–B(4)	60·90 (24)
C(8)–B(4)–B(3)	58·34 (23)
C(8)–B(4)–B(5)	110·90 (30)
C(8)–B(4)–B(1)	104·30 (30)
C(8)–B(4)–Rh(9)	68·70 (20)
B(3)–B(4)–B(5)	109·03 (30)
B(3)–B(4)–B(1)	59·06 (23)
B(3)–B(4)–Rh(9)	121·42 (26)
B(5)–B(4)–B(1)	58·53 (23)
B(5)–B(4)–Rh(9)	67·40 (19)
B(1)–B(4)–Rh(9)	118·27 (26)
B(1)–B(5)–B(6)	59·64 (24)
B(1)–B(5)–B(10)	110·67 (30)
B(1)–B(5)–B(4)	60·80 (24)
B(1)–B(5)–Rh(9)	117·34 (25)
B(6)–B(5)–B(10)	60·16 (24)
B(6)–B(5)–B(4)	105·88 (29)
B(6)–B(5)–Rh(9)	113·17 (25)
B(10)–B(5)–B(4)	108·75 (29)
B(10)–B(5)–Rh(9)	62·62 (19)
B(4)–B(5)–Rh(9)	64·09 (19)
B(2)–B(6)–B(1)	60·09 (24)
B(2)–B(6)–B(5)	107·98 (30)
B(2)–B(6)–B(10)	113·02 (30)
B(2)–B(6)–B(11)	60·30 (24)
B(1)–B(6)–B(5)	59·67 (24)
B(1)–B(6)–B(10)	110·62 (29)
B(1)–B(6)–B(11)	107·18 (30)
B(5)–B(6)–B(10)	60·07 (23)
B(5)–B(6)–B(11)	106·50 (29)
B(10)–B(6)–B(11)	62·40 (24)
H(10)–B(10)–H(*Br*)	99·92 (336)
H(*Br*)–B(10)–B(5)	133·13 (231)
H(*Br*)–B(10)–B(6)	100·55 (229)
H(*Br*)–B(10)–B(11)	41·46 (226)
H(*Br*)–B(10)–Rh(9)	90·00 (232)
B(5)–B(10)–B(6)	59·77 (23)
B(5)–B(10)–B(11)	103·84 (29)
B(5)–B(10)–Rh(9)	68·80 (19)
B(6)–B(10)–B(11)	59·14 (23)
B(6)–B(10)–Rh(9)	117·95 (26)
B(11)–B(10)–Rh(9)	106·79 (24)
H(*Br*)–B(11)–C(7)	104·11 (241)
H(*Br*)–B(11)–B(2)	142·68 (239)
H(*Br*)–B(11)–B(6)	101·53 (236)
H(*Br*)–B(11)–B(10)	43·12 (234)
C(7)–B(11)–B(2)	57·77 (23)
C(7)–B(11)–B(6)	103·15 (29)
C(7)–B(11)–B(10)	109·98 (30)
B(2)–B(11)–B(6)	58·44 (24)
B(2)–B(11)–B(10)	108·16 (30)
B(6)–B(11)–B(10)	58·46 (23)
C(8)–C(7)–B(2)	112·96 (31)
C(8)–C(7)–B(11)	114·60 (31)
C(8)–C(7)–B(3)	62·53 (24)
B(2)–C(7)–B(11)	64·14 (25)
B(2)–C(7)–B(3)	62·58 (25)
B(11)–C(7)–B(3)	117·30 (31)
C(7)–C(8)–B(4)	114·04 (32)
C(7)–C(8)–B(3)	64·62 (25)
C(7)–C(8)–Rh(9)	115·74 (25)
B(4)–C(8)–B(3)	66·00 (25)
B(4)–C(8)–Rh(9)	67·59 (20)
B(3)–C(8)–Rh(9)	127·09 (25)
C(12)–C(11)–C(16)	118·78 (34)
C(12)–C(11)–P(1)	120·36 (28)
C(16)–C(11)–P(1)	120·83 (28)
B(11)–H(*Br*)–B(10)	95·42 (338)

Experimental. Deep-red crystals prepared by the reaction of $RhCl(PPh_3)_3$ and *nido*-$C_2B_8H_{12}$ in ethanol (Jung & Hawthorne, 1980). Parallelepiped 0·2 × 0·2 × 0·4 mm, random orientation on a Syntex $P\bar{1}$ diffractometer, orientation matrix and unit-cell dimensions from 15 carefully centered reflections with $2\theta < 22°$; intensities measured for $2\theta < 50°$ (h_{max}22, k_{max}14, $|l_{max}|$18); intensities of three standard reflections measured every 97 reflections showed no significant change during data collection; total of 6695 independent reflections, 5021 independent reflections with $I > 3\sigma(I)$ used in structure solution and refinement; absorption corrections made (range of transmission factors 0·935–0·958, av. 0·946), no correction for extinction; structure determined by heavy-atom methods and refined by least squares on F (Busing, Martin & Levy, 1962), scattering factors and anomalous-dispersion terms from *International Tables for X-ray Crystallography* (1974); a difference electron density map, after refinement with isotropic thermal parameters of all non-H atoms, contained no peaks greater than 1 e Å^{-3}; all H atoms located at peak heights of *ca* 0·5–0·8 e Å^{-3}, including the bridging B—H—B (at 0·7 e Å^{-3}), terminal B—H, and all H's on phenyl groups; refinement completed with anisotropic temperature factors for non-H non-phenyl atoms, isotropic temperature factors for phenyl atoms and H atoms, H atoms included in fixed located positions with the exception of the 11 H atoms associated with the RhC_2B_8 icosahedral fragment; for the latter, positional parameters refined; for all H atoms B set at 2 Å^2. A total of 295 parameters were refined, $R = 0·038$, $R_w = 0·049$, weights $1/\sigma^2(F_o)$, g.o.f. = 1·502; largest positional-parameter and vibrational-parameter shifts in final cycle of refinement for non-H atoms 0·03 and 0·04, respectively, largest peak in difference map 0·8 e Å^{-3} (near phenyl group 3). All calculations performed on a UCLA Departmental DEC VAX 11/780 using the *UCLA Crystallographic Package* [locally edited versions of *CARESS, PROFILE, MULTAN*78 (Main, Hull, Lessinger, Germain, Declercq & Woolfson, 1978), *ORFLS, ORFFE, ABSORB* and *ORTEP*].

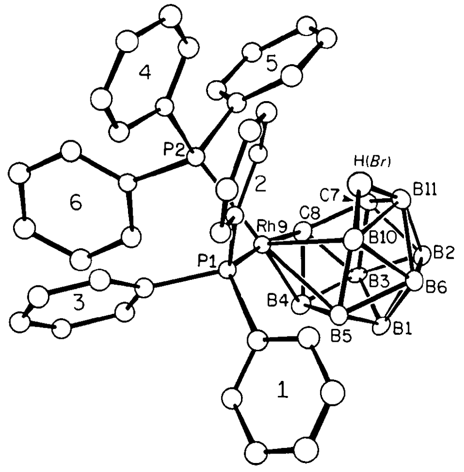

Fig. 1. A perspective view of the molecule.

Discussion. Final atomic parameters for all refined atoms are given in Table 1.* The atom-numbering scheme is illustrated in Fig. 1 (Johnson, 1965). Selected bond distances and angles and their e.s.d.'s (Busing, Martin & Levy, 1964) are given in Table 2. A similar molecular structure has been previously postulated for $(CH_3)_2MB_{10}H_{12}$ (M = Ge, Sn) (Loffredo & Norman, 1971). The methyl groups on the Group IV element are thought to lie on a plane of symmetry in positions *exo* and *endo* relative to the open face of the *nido* 11-atom fragment. In the title compound an approximate plane of symmetry relates C(7) and C(8) to B(11) and B(10), respectively; however, the P atoms of the two phosphine groups are not within 1·2 Å of this plane. The C_2B_8 fragment occupies ten vertices of a nearly regular icosahedron. Rh occupies a vertex 0·56 Å from the least-squares plane through the other atoms of the open face, C(7), C(8), B(10) and B(11).

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* Lists of structure factors, final H-atom positions for H not bonded to B, anisotropic temperature factors and a complete listing of bond lengths and angles have been deposited with the British Library Lending Division as Supplementary Publication No. SUP 39484 (33 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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