Journal of Organometallic Chemistry, 192 (1980) 421—429

SYNTHESIS AND CRYSTAL STRUCTURE OF CYCLOPENTADIENYL(1,4-DIMETHYL-1,4-DIBORA-2,5-CYCLOHEXADIENE)COBALT

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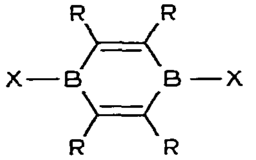
(Received December 11th, 1979)

Summary

The synthesis of the organometallic derivative cyclopentadienyl(1,4-dimethyl-1,4-diboracyclohexa-2,5-diene)cobalt is described. This complex, $[(CH_3BC_4H_4BCH_3)Co(\eta\text{-}C_5H_5)]$, forms red-orange monoclinic crystals, space group $P2_1/a$ with $Z = 4$ in a unit cell of dimensions a 11.362(7), b 7.467(7), c 13.290(12) Å, β 103.76(6)°. The structure has been elucidated by heavy-atom methods from 1732 reflections ($I > 2\sigma(I)$) measured on a Syntex $P2_1$ four-circle diffractometer and refined to $R = 0.055$. In the coordination complex all six atoms of the cyclohexadiene ring are within bonding distance of the metal atom, but the two boron atoms bend away from the metal atom, and the ring elongates slightly in the B---B direction. As a standard of comparison the known geometry of the free ligand [1,4-difluoro-1,4-dibora-2,3,5,6-tetramethylcyclohexa-2,5-diene] is used. The terminal methyl groups on the boron atoms, by contrast, bend slightly back towards the metal atom. The cyclopentadienyl ring remains planar but is positionally disordered.

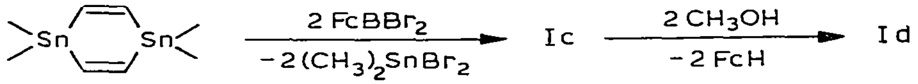
Introduction

Two routes to the chemistry of 1,4-diboracyclohexa-2,5-dienes (I) are known. Timms has shown that boron monohalides (BF and BCl) react with acetylenes (C_2H_2, CH_3C_2H and $C_2(CH_3)_2$) on cocondensation to form 1,4-diboracyclohexa-2,5-dienes such as Ia and Ib [1—3]. Five transition metal complexes of the ligand L = Ib have been prepared [4] and the structures of the compounds NiL_2 [4] and $LNi(CO)_2 \cdot L$ [5] have been determined by X-ray crystallography.



(Ia: R = H, X = F;
Ib: R = CH_3, X = F;
Ic: R = H, X = $(C_5H_5)Fe(C_5H_4)$ = Fc;
Id: R = H, X = CH_3O;
Ie: R = H, X = CH_3)

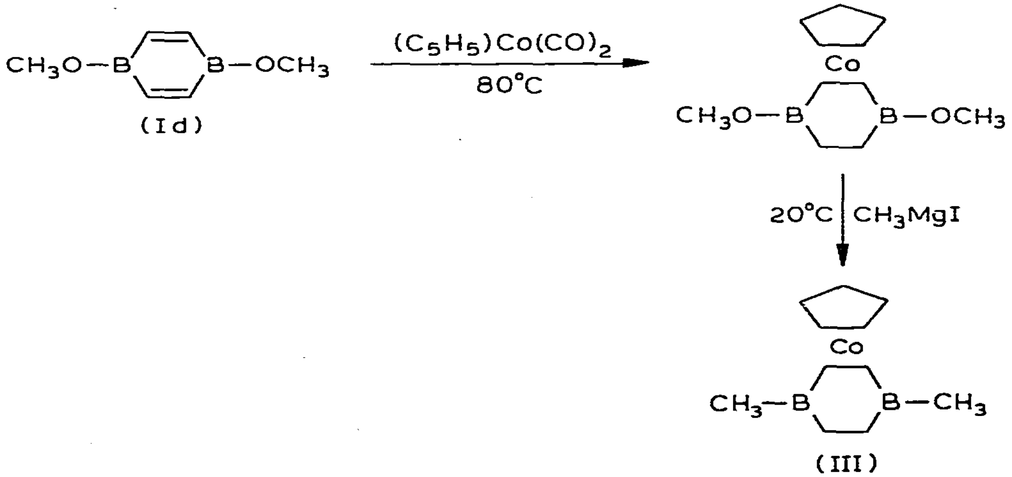
Recently an alternative and conventional approach to 1,4-diboracyclohexa-2,5-dienes (I) has been developed. Treatment of 1,1,4,4-tetramethyl-1,4-distannacyclohexa-2,5-diene (II) [6] with ferrocenyldibromoborane [7] leads to the 1,4-diferrocenyl derivative Ic [8] which on controlled methanolysis affords the 1,4-dimethoxy derivative Id [8].



The present work was undertaken to study the influence of the substituent at boron on the structural features of transition metal complexes of type I ligands. Cyclopentadienyl(1,4-dimethyl-1,4-diboracyclohexa-2,5-diene)cobalt (III) was chosen as a model compound since the possible π-interaction between the p_z-orbital at boron and the lone pair at fluorine in complexes of the ligand Ib is eliminated in complexes of Ie.

Preparative results

The new complex III was obtained by heating Id [8] with $(C_5H_5)Co(CO)_2$ and subsequent treatment with an excess of CH_3MgI. Isolation of the intermediate dimethoxy complex $(C_5H_5)CoL$ with L = Id presented difficulties and in fact was unnecessary for the present purpose.



(Id)

(III)

The new complex III is air-stable and thermally stable up to at least 300°C. Cyclic voltammetry in acetonitrile with $[(n\text{-}C_4H_9)_4N]\text{-}PF_6$ as supporting electrolyte reveals an irreversible oxidation with an anodic peak potential of +1.52 V vs. SCE. Under the same conditions a quasi-reversible reduction is found with peak potentials at −1.66 V and −1.34 V vs. SCE for reduction and reoxidation respectively. These observations demonstrate that the ligand Ie acts as a very strong acceptor in binding to the metal.

X-Ray diffraction results

The molecular structure of complex III is illustrated in Figure 1 which also shows the crystallographic atom-numbering sequence. The atomic fractional co-ordinates are listed in Table 1, the bond lengths and inter-bond angles in Table 2. The cyclopentadienyl ring atoms are disordered in the plane of the ring to give two sets of five atoms, each defining a regular pentagon but staggered unsymmetrically with respect to one another. The site occupation factor is close to 0.5 and in the final cycles of refinement the value was fixed at 0.5. The mean Co—C(cyclopentadienyl) distance is 2.04 Å, (Table 2), very close to values reported for other cobalt-cyclopentadienyl complexes, such as 2.06(4) Å in $[(\eta\text{-}C_5H_5)(CO)_2CoHgCl_2]$, [9], 2.08(3) Å in $[(\eta\text{-}C_5H_5)Co(C_5H_5Ph)]$, [10], 2.08(3) Å in $[(\eta\text{-}C_5H_5)Co(C_5(CF_3)_4O)]$ [11], and 2.09(1) Å in $[\{(\eta\text{-}C_5H_5)(CO)Co(SnMe_2)\}_2]$, [12]. Interest centres, however, on the diboracyclohexadiene ring. Here all six atoms are within bonding distance of the cobalt atom [Co—C = 2.094 Å (mean), Co—B = 2.225 Å (mean)] but, as in previously-determined structures of this type, [4,5], the ring bends slightly

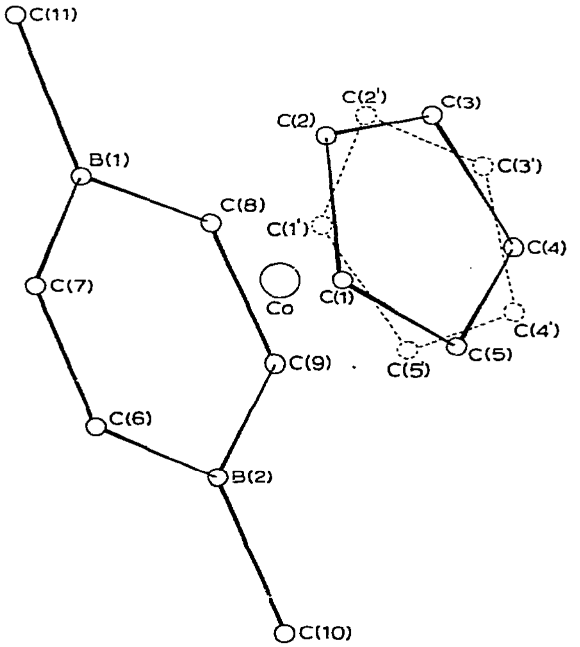


Fig. 1. The molecular structure of $[(CH_3BC_4H_4BCH_3)Co(\eta\text{-}C_5H_5)]$.

TABLE 1

ATOMIC POSITIONAL PARAMETERS (FRACTIONAL CO-ORDINATES) AND TEMPERATURE FACTORS FOR COMPLEX III WITH ESTIMATED STANDARD DEVIATIONS IN PARENTHESES

Atom	n[a]	x	y	z
Co	1.0	0.4983 (1)	0.4654 (1)	0.2504 (1)
1,4-Dimethyl-1,4-diboracyclohexa-2,5-diene ligand				
B(1)	1.0	0.5032 (6)	0.2356 (10)	0.3572 (6)
B(2)	1.0	0.3142 (6)	0.3736 (9)	0.1669 (5)
C(6)	1.0	0.4179 (6)	0.2466 (8)	0.1606 (5)
H(6)	1.0	0.4256	0.2011	0.0853
C(7)	1.0	0.5047 (8)	0.1859 (7)	0.2499 (8)
H(7)	1.0	0.5760	0.0982	0.2384
C(8)	1.0	0.4119 (5)	0.3794 (9)	0.3645 (5)
H(8)	1.0	0.4130	0.4353	0.4397
C(9)	1.0	0.3249 (5)	0.4443 (8)	0.2774 (5)
H(9)	1.0	0.2633	0.5480	0.2893
C(10)	1.0	0.2198 (5)	0.4491 (10)	0.0680 (5)
C(11)	1.0	0.6066 (6)	0.1716 (9)	0.4541 (5)
(Methyl hydrogen atoms not located)				
Cyclopentadienyl ligand (disordered)				
C(1)	0.5	0.625 (1)	0.548 (3)	0.176 (1)
H(1)	0.5	0.655	0.472	0.117
C(2)	0.5	0.679 (1)	0.542 (2)	0.287 (1)
H(2)	0.5	0.756	0.464	0.326
C(3)	0.5	0.609 (1)	0.661 (2)	0.335 (1)
H(3)	0.5	0.624	0.688	0.416
C(4)	0.5	0.519 (1)	0.737 (2)	0.257 (1)
H(4)	0.5	0.453	0.832	0.271
C(5)	0.5	0.524 (2)	0.675 (2)	0.158 (1)
H(5)	0.5	0.465	0.712	0.085
C(1′)	0.5	0.661 (2)	0.533 (3)	0.226 (2)
H(1′)	0.5	0.729	0.439	0.214
C(2′)	0.5	0.646 (2)	0.604 (3)	0.318 (2)
H(2′)	0.5	0.703	0.574	0.394
C(3′)	0.5	0.557 (2)	0.712 (3)	0.301 (2)
H(3′)	0.5	0.527	0.783	0.362
C(4′)	0.5	0.503 (1)	0.729 (2)	0.201 (2)
H(4′)	0.5	0.428	0.818	0.170
C(5′)	0.5	0.555 (2)	0.619 (3)	0.146 (2)
H(5′)	0.5	0.530	0.596	0.062

Anisotropic temperature factors in the form $\exp -2\pi^2 (U_{11}a^{*2}h^2 + U_{22}b^{*2}k^2 + U_{33}c^{*2}l^2 + 2U_{12}a^*b^*hk + 2U_{13}a^*c^*hl + 2U_{23}b^*c^*kl)$

Atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23} (Å^2)
Co	0.021 (0)	0.024 (0)	0.039 (0)	−0.006 (1)	0.006 (0)	−0.001 (1)
B(1)	0.019 (3)	0.038 (4)	0.045 (5)	−0.007 (3)	0.004 (3)	0.008 (4)
B(2)	0.026 (3)	0.028 (4)	0.042 (4)	−0.008 (3)	0.006 (3)	−0.003 (3)
C(6)	0.032 (3)	0.029 (3)	0.036 (4)	−0.009 (3)	0.010 (3)	−0.009 (3)
C(7)	0.024 (3)	0.023 (3)	0.054 (4)	−0.002 (4)	0.008 (2)	−0.014 (6)
C(8)	0.026 (3)	0.041 (4)	0.032 (3)	−0.001 (3)	0.004 (3)	−0.001 (3)
C(9)	0.023 (3)	0.031 (4)	0.056 (4)	0.001 (3)	0.019 (3)	−0.003 (3)
C(10)	0.030 (3)	0.061 (4)	0.048 (4)	0.003 (3)	0.001 (3)	0.006 (4)
C(11)	0.036 (4)	0.059 (5)	0.048 (4)	0.004 (3)	0.007 (3)	0.014 (4)

Isotropic temperature factors (non-hydrogen atoms)

Atom	U_{iso} (Å^2)	Atom	U_{iso} (Å^2)
C(1)	0.022 (3)	C(1′)	0.052 (4)
C(2)	0.022 (2)	C(2′)	0.060 (5)
C(3)	0.029 (3)	C(3′)	0.068 (6)
C(4)	0.025 (3)	C(4′)	0.038 (3)
C(5)	0.036 (3)	C(5′)	0.054 (5)

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[a] Fixed population parameter.

TABLE 2

INTERATOMIC DISTANCES (Å) AND BOND ANGLES (°) FOR COMPLEX III

(a) Distances			
1,4-Dimethyl-1,4-diboracyclohexa-2,5-diene ligand			
Co—C(6)	2.100 (6)	B(1)—C(7)	1.473 (12)
Co—C(7)	2.088 (5)	B(1)—C(8)	1.513 (10)
Co—C(8)	2.094 (6)	B(2)—C(6)	1.529 (10)
Co—C(9)	2.092 (5)	B(2)—C(9)	1.540 (9)
Co—B(1)	2.219 (7)	C(6)—C(7)	1.429 (11)
Co—B(2)	2.230 (6)	C(8)—C(9)	1.416 (8)
Co—C(6,7) [a]	1.968 (6)	B(1)—C(11)	1.596 (9)
Co—C(8,9) [a]	1.970 (6)	B(2)—C(10)	1.589 (9)
Disordered cyclopentadienyl ligand			
Co—C(1)	2.034 (17)	Co—C(1′)	2.006 (17)
Co—C(2)	2.076 (11)	Co—C(2′)	1.994 (18)
Co—C(3)	2.074 (14)	Co—C(3′)	2.023 (21)
Co—C(4)	2.038 (12)	Co—C(4′)	2.074 (16)
Co—C(5)	2.046 (17)	Co—C(5′)	2.036 (20)
(Mean Co—C	2.054)	(Mean Co—C	2.026)
C(1)—C(2)	1.465 (21)	C(1′)—C(2′)	1.382 (26)
C(2)—C(3)	1.431 (20)	C(2′)—C(3′)	1.278 (29)
C(3)—C(4)	1.386 (20)	C(3′)—C(4′)	1.325 (27)
C(4)—C(5)	1.405 (26)	C(4′)—C(5′)	1.345 (26)
C(5)—C(1)	1.470 (27)	C(5′)—C(1′)	1.550 (24)
(Mean C—C	1.43)	Mean C—C	1.38)
C(1)—C(1′)	0.714 (24)	C(1′)—C(2)	0.793 (17)
(b) Angles			
1,4-Dimethyl-1,4-diboracyclohexa-2,5-diene ligand			
B(1)—C(7)—C(6)	124.1 (7)	C(8)—B(1)—C(7)	114.0 (6)
C(7)—C(6)—B(2)	122.6 (6)	C(11)—B(1)—C(7)	121.8 (7)
C(6)—B(2)—C(9)	112.2 (6)	C(11)—B(1)—C(8)	123.1 (6)
B(2)—C(9)—C(8)	123.0 (5)	C(10)—B(2)—C(6)	123.6 (6)
C(9)—C(8)—B(1)	123.1 (6)	C(10)—B(2)—C(9)	123.4 (6)
Disordered cyclopentadienyl ligand			
C(1)—C(2)—C(3)	106.5 (12)	C(1′)—C(2′)—C(3′)	110.2 (19)
C(2)—C(3)—C(4)	108.6 (12)	C(2′)—C(3′)—C(4′)	113.2 (20)
C(3)—C(4)—C(5)	112.1 (13)	C(3′)—C(4′)—C(5′)	110.7 (17)
C(4)—C(5)—C(1)	105.8 (14)	C(4′)—C(5′)—C(1′)	103.2 (15)
C(5)—C(1)—C(2)	107.0 (15)	C(5′)—C(1′)—C(2′)	102.6 (16)

[a] C(*m*,*n*) is the midpoint of the line joining C(*m*) to C(*n*).

along the C(7)—C(8) and C(6)—C(9) directions away from the metal atom at a dihedral angle of some $6\frac{1}{2}$° (Table 3), suggesting, as also do the bond lengths within the ring (see below), that the interactions between the two C=C olefinic bonds and the cobalt atom are more pronounced than those between the boron and cobalt atoms. In any case the ring must be regarded as a four-electron donor. Furthermore, the exocyclic methyl group shows a second bend, this time towards the metal atom, thereby increasing the overlap between the p_z-orbital of the boron atom and the metal orbitals. The angle between the exocyclic B—C bond and the adjacent BC_2 plane of the ring is 9.0°.

It is interesting to study changes in geometry which occur when ligands undergo complexation with a metal, and for purposes of comparison use may be made of the known structures of bis(1,4-difluoro-2,3,5,6-tetramethyl-1,4-diboracyclohexa-2,5-diene)nickel(0), [4], and of dicarbonyl(1,4-difluoro-

TABLE 3

EQUATIONS OF SOME LEAST-SQUARES PLANES [a] AND LINES; DISTANCES (Å) OF RELEVANT ATOMS FROM THESE PLANES ARE GIVEN IN SQUARE BRACKETS

Plane(1)	C(1), C(2), C(3), C(4), C(5) $7.451x + 5.598y - 3.221z = 7.164$ [Co 1.653].
Plane(2)	C(6), C(7), C(8), C(9) $7.479x + 5.569y - 3.406z = 3.956$ [Co. 1.510].
Plane(3)	B(1), C(7), C(8) $8.079x + 5.250y - 2.318z = 4.475$
Plane(4)	B(2), C(6), C(9) $6.830x + 5.794y - 4.366z = 3.582$
Line(5)	B(2), C(10) Direction cosines: −0.6557, 0.3547, −0.6666
Line(6)	Direction cosines: 0.7148, −0.2993, 0.6321

Angles (°) between planes and lines:

(1)—(2)	0.8	(4)—(5)	81.9
(2)—(3)	6.3	(3)—(6)	80.1
(2)—(4)	6.8	(2)—(5)	88.2
		(2)—(6)	86.9

[a] x, y, z are fractional crystal co-ordinates.

2,3,5,6-tetramethyl-1,4-diboracyclohexa-2,5-diene)nickel(0), [5]. By a felicitous chance, crystals of the dicarbonyl-complex also contained molecules of the free ligand, so that for these systems we have information about the geometry of the free ligand as well as that of the complexes. Some comparative figures are given in Table 4. In all cases complexation lengthens C=C and shortens B—C, and in the cobalt complex III the effect is greater than in either of the nickel complexes. For the $FB(CMe)_4BF$ ligand also complexation lengthens the B—F bond. Exactly analogous changes have been observed in the formally similar duroquinone, when it is involved in formation of the complexes bis(duroquinone)nickel(0), [13], and (cycloocta-1,5-diene)(duroquinone)nickel(0), [14]. A qualitative view of the bonding would suggest that the ring olefinic C=C bonds donate electrons to the metal, while vacant orbitals around the boron atoms accept electrons from filled *d*-orbitals on the metal. In complex III, where the ligand has F replaced by Me, the situation is simpler in that no

TABLE 4

CHARACTERISTIC PARAMETERS OF SOME DIBORACYCLOHEXADIENE RINGS ($XB(CR)_4BX = L$)

Compound	C = C	B—C	B—X	C—$\hat{B}$—C	α *
L (X = F, R = Me)	1.339	1.567	1.305	123°	—
L_2Ni (X = F, R = Me)	1.392	1.531	1.359	123°	5.6°
$LNi(CO)_2$ (X = F, R = Me)	1.395	1.527	1.386	118°	8.5°
(η-C_5H_5)CoL (X = Me, R = H)	1.423	1.514	1.593	113°	6.5°

* α is the mean dihedral angle between the plane defined by the four carbon atoms of the ring and the planes defined by each boron atom and its two neighbouring ring carbon atoms.

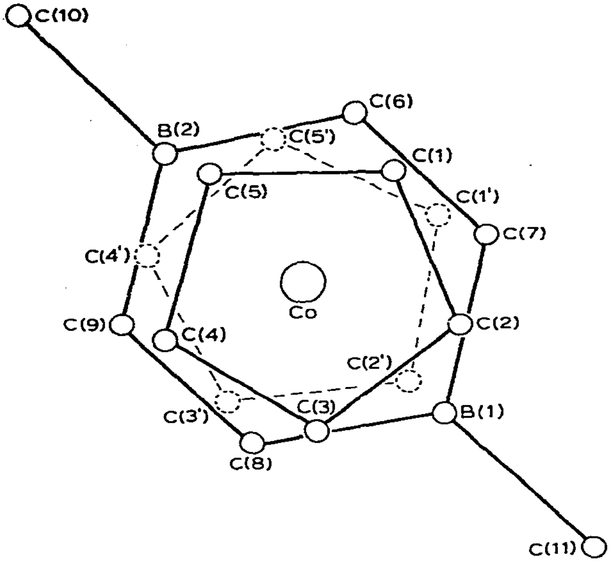

Fig. 2. Molecular structure of III seen in projection perpendicular to the plane of the cyclopentadienyl ring.

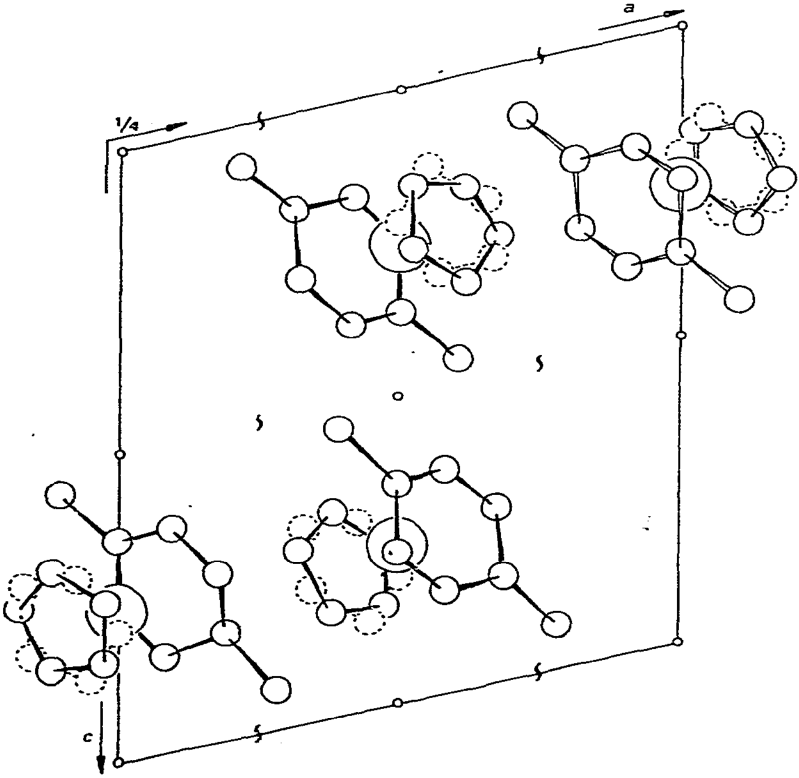

Fig. 3. Contents of the monoclinic unit cell of III seen in projection down *b* looking towards the origin.

π-interaction can occur between the boron atom and the exocyclic moiety. The effects are correspondingly more pronounced. A molecular orbital model for bis(duroquinone)nickel(0), [15], suggests that back-donation of *d*-electrons from the metal atom to the C_4B_2 ring will be mainly into a molecular orbital which is bonding with respect to the B—C bonds and antibonding with respect to the olefinic C=C and exocyclic B—X (X = F or Me) bonds. Hence, the more effective the back-donation, the greater the effect on the bond length changes; and on this basis ($CH_3BC_4H_4BCH_3$) would appear to be a much better acceptor than (FBC_4Me_4BF).

Figure 2 shows a projection of the molecule normal to the mean ring planes to show their relative orientation, while in Figure 3 the packing of the molecules within the monoclinic unit cell is displayed.

Experimental

Cyclopentadienyl(1,4-dimethyl-1,4-diboracyclohexa-2,5-diene)cobalt (III)

0.93 g (2.66 mmol) 1,1,4,4-tetramethyl-1,4-distannacyclohexa-2,5-diene (II) [6] are treated as described previously [8] with $(C_5H_5)Fe(C_5H_4BBr_2)$ [7] in CS_2 and subsequently with CH_3OH in toluene. To the resulting solution of Id and $Fe(C_5H_5)_2$ in toluene 0.5 ml (3.6 mmol) $(C_5H_5)Co(CO)_2$ were added and the mixture was heated to 80°C for 1 h. Evolution of CO sets in at 60°C (!). Chromatography on Al_2O_3 (neutral, 7% H_2O) with CH_2Cl_2 as eluent affords a band of $Fe(C_5H_5)_2$ and unreacted $(C_5H_5)Co(CO)_2$. Further elution with CH_2Cl_2/CH_3OH (98/2) gives a reddish brown band. The solvent is carefully removed in vacuo. The oily dark red residue (0.39 g) is then redissolved in 10 ml ether. 5 mmol CH_3MgI in 20 ml ether are added at room temperature. Magnesium salts precipitate instantly and stirring is continued for 1 h. Hydrolysis with moist Al_2O_3 at —80°C, solvent removal in vacuo, and chromatography on Al_2O_3 (neutral, 7% H_2O; column 30 cm long, 2 cm wide) in pentane produces a red band. Concentration of the eluate and slow cooling to —80°C affords 126 mg (0.55 mmol; 21% based on II) red, air-stable platelets of complex III, m.p. 122°C, no dec. <300°C. Found: C, 58.24; H, 6.66. $C_{11}H_{15}B_2Co$ calcd.: C, 58.00; H, 6.64%. ^1H NMR (τ, rel. to internal TMS, in CS_2): 5.18s ($C_4H_4B_2$), 5.30s (C_5H_5), 9.42s (2 CH_3) ppm. ^{11}B NMR (δ, rel. to external $BF_3 \cdot O(C_2H_5)_2$, in CS_2): 24 ppm. Mass spectrum (70 eV): m/e ($I_{rel.}$ (>10%)) 228 (100; M^+), 213 (62; $M^+ - CH_3$), 200 (10; $M^+ - C_2H_4$), 188 (19; $M^+ - C_2H_5B$), 124 (35; $Co(C_5H_5)^+$), 114 (3; M^{2+}), 59 (12; Co^+).

Crystal Structure Determination of [$(CH_3BC_4H_4BCH_3)Co(\eta\text{-}C_5H_5)$]

The plate-like orange-red crystals of the original sample were too large for intensity measurement, so a piece of approximate linear dimensions 0.3 mm was cut off and mounted in a Lindemann capillary tube under nitrogen. Intensities were collected at 200 K to $2\theta = 60°$ on a Syntex $P2_1$ four-circle diffractometer, with Mo-K_α X-radiation, at a scan rate which varied from 0.04 to 0.48° s^{-1}, the slowest rate for the weakest reflections, monitored in a preliminary 2 s count. Two check reflections (2 0 $\bar{2}$ and $\bar{1}$ 1 0) were measured every 50 reflections but no significant decay was observed. The data contained an unusually high proportion of very weak reflections; in fact all reflections for which $h + k + l \neq 2n$ were systematically weak, suggesting pseudo-body-centring in the position of the cobalt atom (see below). The peak profiles were also undesirably broad. As a result, reflections for which $I < 2.0\sigma(I)$ were regarded as unobserved and were not included in either the solution or the refinement of the structure. Of the total 3371 independent reflections, 1732 were observed.

Results

Crystal Data. $C_{11}H_{15}B_2Co$, $M = 227.8$, Monoclinic, a 11.362(7), b 7.467(7), c 13.290(12) Å, β 103.76(6)° at 200 K, $U = 1068$ Å^3, $D_m = 1.33$ g cm^{-3}, $Z = 4$, $D_c = 1.38$ g cm^{-3}, $F(000) = 472$, space group $P2_1/a$ (No. 14), Mo-K_α X-radiation (graphite monochromator), $\bar{\lambda} = 0.71069$ Å, μ(Mo-K_α) = 14.5 cm^{-1}.

The structure was solved by heavy-atom methods and refined by blocked-matrix least squares. Hydrogen atoms were incorporated at calculated positions (C—H 1.08 Å) and were not refined. All other atoms were ascribed anisotropic thermal parameters except those of the cyclopentadienyl ring (because of positional disorder). Refinement converged at $R = 0.0495$ ($R' = 0.0399$) with a mean shift-to-error ratio in the last cycle of 0.2. A weighting scheme of the form $\omega = 1/\sigma^2(F_0)$, where $\sigma(F_0)$ is the estimated error in the observed structure factor based on counting statistics only, gave a satisfactory weight analysis. The data were not corrected for the effects of X-ray absorption (μ(Mo-K_α) = 14.5 cm^{-1}). Atomic scattering factors were those of ref. 16 for non-hydrogen atoms and of ref. 17 for hydrogen. All computational work was carried out on the South-West Computer Network with the "SHEL-X" system of programs [18]. Tables of observed and calculated structure factors and of all thermal parameters are available from the British Lending Library as Publication No SUP 90044.

Acknowledgement

We thank Dr. U. Koelle for the electrochemical measurements and Mr. P. Watkins for technical assistance. This work was in part supported by Deutsche Forschungsgemeinschaft and by Fonds der Chemischen Industrie; also in part by the Science Research Council of Great Britain.

References

1 P.L. Timms, J. Amer. Chem. Soc., 90 (1968) 4585.
2 P.L. Timms, Advan. Inorg. Chem. Radiochem., 14 (1972) 121.
3 P.L. Timms, Acc. Chem. Res., 6 (1973) 118.
4 P.S. Maddren, A. Modinos, P.L. Timms and P. Woodward, J. Chem. Soc. Dalton Trans., (1975) 1272.
5 J.A.K. Howard, I.W. Kerr and P. Woodward, J. Chem. Soc. Dalton Trans., (1975) 2466.
6 G.E. Herberich and B. Hessner, Z. Naturforsch. B, 33 (1978) 180.
7 T. Renk, W. Ruf and W. Siebert, J. Organometal. Chem., 120 (1976) 1.
8 G.E. Herberich and B. Hessner, J. Organometal. Chem., 161 (1978) C36.
9 I.W. Nowell and D.R. Russell, J. Chem. Soc. Dalton, (1972) 2393.
10 M.R. Churchill and R. Mason, Proc. Roy. Soc. (A), 279 (1964) 191.
11 M. Gerloch and R. Mason, Proc. Roy. Soc. (A), 279 (1964) 170.
12 J. Weaver and P. Woodward, J. Chem. Soc. Dalton, (1973) 1060.
13 G.G. Aleksandrov and Yu.T. Struchkov, J. Struct. Chem., (1974) 1001.
14 M.D. Glick and L.F. Dahl, J. Organometallic Chem., 3 (1965) 200.
15 G.N. Schrauzer and H. Thyret, Z. Naturforsch., 16б (1961) 353; Theor. Chim. Acta, 1 (1963) 172.
16 D.T. Cromer and J.B. Mann, Acta Cryst. A, 24 (1965) 321.
17 R.F. Stewart, E.R. Davidson and W.T. Simpson, J. Chem. Phys., 42 (1965) 3175.
18 G.M. Sheldrick, "SHEL-X", Cambridge, 1975.