The observation that only one odd vibrational mode is necessary to explain the polarizations and intensities is very interesting. (The very weak ~17,000-cm^{-1} band, forbidden in this limit, obviously does not gain much intensity from any other vibrational mode.) Indeed, the simplicity of this vibronic coupling scheme is very unusual. In the past,[12–18] spectra of such complex nuclear systems have generally required several vibrational symmetries to be introduced, and ambiguous situations resulted.[12–15] It is not clear why similar problems do not arise in the present case. What is

known, however, is that in a five-atom model

$$\begin{matrix} S & & S \\ & \diagdown \diagup & \\ & Ni & \\ & \diagup \diagdown & \\ S & & S \end{matrix}$$
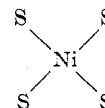
there are two b_{2u} vibrations (D_{2h}) and they are both derived from the e_u modes of D_{4h}. These latter modes have been shown to be important in vibronically induced transitions in D_{4h} (or nearly D_{4h}) systems.[16]

Further speculation about the source of the vibronic intensity is not warranted. If more information could be obtained (from vibronic spectra at low temperatures for instance), it could lead to a better understanding of the complicated problem of vibronic processes in metal chelates.

Acknowledgment.—The author wishes to thank Professor C. J. Ballhausen for numerous useful discussions on the topic of this paper and Dr. K. J. Watson for carrying out all the X-ray identifications pertinent to this study.

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Microwave Spectrum, Structure, and Dipole Moment of 2-Carbahexaborane(9), CB₅H₉[1]

By CHUN-CHUNG S. CHEUNG and ROBERT A. BEAUDET*[2,3]

The microwave spectrum of 2-carbahexaborane(9) has been studied in the region of 8–37 GHz. The rotational spectra of the normal species (all ^{11}B isotope) and seven ^{10}B-substituted species were assigned. The principal axis coordinates of the boron atoms were calculated from the moments of inertia of the normal species and of the three singly substituted ^{10}B species. The results show that the main framework is a pentagonal pyramid. The following bond lengths were accurately determined: $r_{B(3)-B(4)} = 1.759$ Å, $r_{B(4)-B(5)} = 1.830$ Å, $r_{B(1)-B(3)} = 1.782$ Å, and $r_{B(1)-B(4)} = 1.781$ Å. The Stark effect of the normal species and of two singly substituted B(10) species was measured. The molecular dipole moment was found to be 1.53 ± 0.03 D.

Introduction

The preparation of a new carborane with the empirical formula CB₅H₉ has been reported by Dunks and Hawthorne.[4] From the analysis of the ^{11}B nmr spectrum and the proton nmr spectrum the authors concluded that the molecule has two pairs of equivalent boron atoms, three bridge hydrogen atoms, and a boron atom at an apical position. The spectrum is consistent with the pentagonal pyramid shown in Figure 1.

Since a molecule with this geometry must have a nonvanishing dipole moment, the pure rotational spectrum should be observable. The microwave spectrum of a sample of naturally abundant isotopic species was investigated to determine the coordinates of the boron atoms and the dipole moment.

Experimental Section

The sample of CB₅H₉ was kindly provided by Dunks and Hawthorne. The original sample, after taking the ^{11}B nmr spectrum, had been kept in a sealed nmr tube at room temperature for several months. It was purified by fractionation before use in our microwave study. No impurity problem nor decomposition of the sample was encountered in the study of the rotational spectrum.

The microwave spectrum between 8.2 and 37.5 GHz was observed with a conventional 100-kHz Stark modulated spectrometer. Frequencies were measured by interpolating between standard frequencies with a Collins Model 51S-1 receiver. The standard frequencies were obtained by multiplying the output of a 1-MHz crystal in a Hewlett-Packard Model 5245L frequency counter with General Radio standard frequency multipliers. The uncertainties of the measured frequencies were generally less than ±0.1 MHz.

The spectrum was studied at Dry Ice temperature and at pressures between 10 and 40 μ. For better resolution, certain stronger lines were measured at pressures below 2 μ.

Dc biasing of the 100-kHz square wave was used to measure the Stark effects. The electric field calibration of the Stark cell was made with the $J = 1 \leftarrow 0$ transition of carbonyl sulfide.[5] All dipole moment measurements were performed the same day.
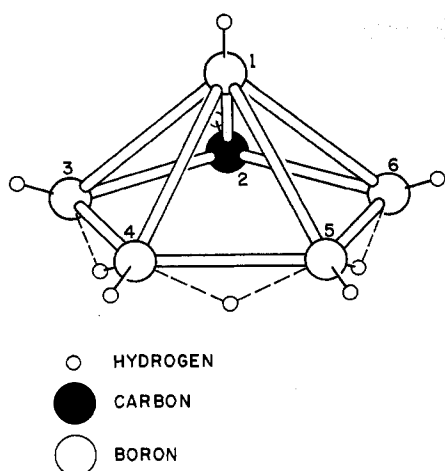
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O HYDROGEN

● CARBON

◯ BORON

Figure 1.—Geometry of CB_5H_9.

Results

Spectrum.—Since naturally abundant boron contains 81% ^{11}B and 19% ^{10}B, a variety of boron isotopic species of CB_5H_9 exist in sufficient concentrations to be observed in the spectrum. The relative abundances of the various species and our notation are given in Table I. The synthesis of this compound involves

TABLE I
THE ROTATIONAL CONSTANTS OF THE EIGHT MOST
ABUNDANT SPECIES OF CB_5H_9

Isotopic species	Natural[a] abundance, %	Rotational constants determined from the spectra,[b] MHz		
		A	B	C
Normal	35	5334.130	5296.895	3280.552
$^{10}B(3)$	16	5449.072	5303.606	3324.585
$^{10}B(4)$	16	5439.794	5317.759	3327.660
$^{10}B(1)$	8	5378.323	5340.682	3280.482
		A + B		
$^{10}B(1)$ and $^{10}B(3)$	4	10,849.10		3324.45
$^{10}B(1)$ and $^{10}B(4)$	4	10,847.80		3327.70
$^{10}B(3)$ and $^{10}B(4)$	4 ⎫	10,880.90		3371.59[c]
$^{10}B(3)$ and $^{10}B(5)$	4 ⎭	10,880.90		3373.33[c]

[a] The abundance ratio of $^{10}B:{}^{11}B$ in nature is 19:81. [b] Uncertainties are ±0.050 MHz for A, B, and C for the four major species. Uncertainties are ±0.20 MHz for $A + B$ and C for the doubly substituted species. [c] It is uncertain which constant belongs to which species.

numerous steps, many with low yields; thus synthesis of the ^{13}C-enriched species was not economically feasible at this time.

For a molecule with the geometry in Figure 1, one expects to observe c- and either a- or b-type transitions. Only two types of transitions are allowed unless isotopic substitution destroys the plane of symmetry. Strong c-type and weak a-type lines were observed for the normal species and the $^{10}B(1)$ isotopic species. Since nonzero values for all three dipole components are allowed, the spectra of the $^{10}B(3)$ and the $^{10}B(4)$ species contain all three types of transitions. However the b-type transitions of only the B(4) species were strong enough to be observed.

The spectrum of CB_5H_9 was extremely dense. Transitions have been assigned for the eight most abundant isotopic species. The relative intensities of the transitions are in good agreement with the relative abundances of the various isotopic species (Table I).

The boron nuclear quadrupole moments were found to cause some line broadening in the low J transitions, but the effects were not large enough to be a problem for the study of the four major isotopic species.

The Stark effects of the few low J transitions were clearly resolved. The single lobe of the $1(0,0) \leftarrow 0(0,0)$ transition was observed for each isotopic species listed in Table I. In the case of the c-type transitions of the three most abundant species, all the $J = 2 \leftarrow 1$ and most of the $J = 3 \leftarrow 2$ lines exhibited clear Stark lobes.

The transitions $2(1,1) \leftarrow 1(0,1)$, $2(2,1) \leftarrow 1(1,1)$, and $J = 4 \leftarrow 3$ (with $K = 4 \leftarrow 3$) were used to determine the rotational constants for the four major species. The assigned R-branch lines of these four species are listed together with the calculated values in Table II. Some of the larger discrepancies are due to the difficulty in determining the frequencies of overlapped lines.

In the case of the four "4% species," the R-branch transitions were very weak and broad. Only three were assigned for each of these species (Table III). The assignments were based on the Stark effects. The $J = 1 \leftarrow 0$ lines showed single, clear, but broad lobes, while the $J = 4 \leftarrow 3$ and the $J = 5 \leftarrow 4$ lines showed extremely fast symmetric Stark effects. Since the frequencies of these transitions were only sensitive to C and $A + B$, only two constants could be determined accurately from these R-branch transitions.

Seven Q-branch bands were found to be in the frequency range of our instrument ($K = 2 \leftarrow 3$ up to $K = 8 \leftarrow 9$). It is possible to trace up to $J = 45$ in some cases. Though there are enough transitions for a very detailed analysis, the centrifugal distortion effects are not large, and no useful information would be forthcoming from such a tedious analysis. In Table IV some transitions belonging to the $K = 2 \leftarrow 3$ band of the normal isotopic species are listed. Centrifugal distortion effects were partially corrected by including a single correction term $D_{jk}P^2\langle P_z^2 \rangle$ in the Hamiltonian. D_{jk} was found to be about 0.0020 MHz.

With the intention of determining the position of the carbon atom we have unsuccessfully searched for the transitions belonging to the ^{13}C species. Due to the rich spectrum it is likely that the weak ^{13}C lines are overshadowed by stronger lines. To avoid possible interference, one may resort to double-resonance techniques. We have examined the double-resonance signal of some low J transitions of the normal species to obtain an estimate of the order of magnitude of the intensity of the signals that can be expected for ^{13}C species. From population considerations the latter can be expected to be about 1% of the former. From the intensities of the signals for the normal species we have concluded that we cannot expect to see the double-resonance signal for the ^{13}C species in natural abundance. We feel that we could assign the spectrum of the ^{13}C species with a sample of 5% ^{13}C enrichment.

Structure of Boron Skeleton.—The Kraitchman[6] method was used to calculate the center-of-mass coordinates of the boron atoms (Table V) from the moments of inertia (Table VI). The bond lengths (Table VII) between these atoms were deduced with

(6) J. Kraitchman, *Amer. J. Phys.*, **21**, 17 (1953).

TABLE II
R-BRANCH TRANSITIONS OF THE FOUR MAJOR ISOTOPIC SPECIES OF CB$_5$H$_9$

| | Transition Frequencies[a] (MHz) | | | |
	Normal species	^{10}B(3)-species	^{10}B(4)-species	^{10}B(1)-species
c-type				
$1_{1,0}-0_{0,0}$	10631.15 (+0.12)	10752.80 (+0.12)	10757.50 (-0.05)	10719.18 (+0.17)
$2_{2,1}-1_{1,1}$[b]	21299.29 (0.00)	21650.82 (0.00)	21637.14 (0.00)	21475.65 (0.00)
$2_{1,1}-1_{0,1}$[b]	21224.82 (0.00)	21359.89 (0.00)	21393.07 (0.00)	21400.37 (0.00)
$2_{2,0}-1_{1,0}$	21262.57 (+0.01)	21513.15 (0.00)	21520.53 (-0.02)	21438.35 (-0.17)
$3_{2,2}-2_{1,2}$	31892.05 (-0.02)	32258.15 (+0.12)	32272.20 (-0.46)	32156.25 (-0.77)
$3_{1,2}-2_{0,2}$	31892.05 (+0.01)	32227.33 (+0.06)	32250.90 (-0.06)	32156.25 (+1.28)
$3_{3,1}-2_{2,1}$	31949.06 (-0.19)	32481.00 (+0.06)	32458.97 (-0.07)	32213.83 (+0.04)
$3_{2,1}-2_{1,1}$	31837.45 (-0.09)	32044.83 (+0.03)	32092.87 (-0.22)	32100.65 (-0.23)
$3_{3,0}-2_{2,0}$	31895.07 (-0.05)	32289.05 (+0.25)	32294.30 (-0.06)	32159.10 (+0.04)
a-type				
$3_{1,3}-2_{1,2}$	21718.25 (+0.30)	c	c	21761.50 (-0.10)
$3_{0,3}-2_{0,2}$	21718.25 (-0.21)	c	c	21761.50 (-0.60)
$3_{2,2}-2_{2,1}$	25732.30 (-0.04)	c	c	c
$3_{1,2}-2_{1,1}$	25841.25 (-0.24)	c	c	c
$3_{2,1}-2_{2,0}$	29745.95 (-0.27)	29766.97 (-0.15)	29853.40 (-0.08)	c
$3_{3,0}-2_{1,1}$	33986.40 (-0.04)	c	c	c
$4_{1,4}-3_{1,3}$[b]	28279.30 (0.00)	28647.25 (0.00)	28671.57 (0.00)	28322.80 (0.00)
$4_{0,4}-3_{0,3}$	28279.30 (0.00)	28647.25 (0.00)	28671.57 (0.00)	28322.80 (0.00)
$4_{2,3}-3_{2,2}$	32349.15 (+1.18)	c	c	32481.00 (+1.41)
$4_{1,3}-3_{1,2}$	32349.15 (-1.35)	c	c	32481.00 (-1.12)
$4_{3,2}-3_{3,1}$	36307.25 (-0.34)	36420.30 (-0.06)	36511.35 (-0.31)	36526.10 (-0.02)
$4_{2,2}-3_{2,1}$	36523.20 (-0.14)	37178.45 (+0.03)	c	36744.35 (+0.05)
$5_{1,5}-4_{1,4}$	34840.28 (-0.12)	35296.40 (+0.03)	35327.16 (+0.31)	34883.65 (-0.11)
$5_{0,5}-4_{0,4}$	34840.28 (-0.12)	35296.40 (+0.03)	35327.16 (+0.31)	34883.65 (-0.11)
b-type				
$4_{3,2}-3_{2,1}$	d	c	37243.63 (-0.09)	d
$4_{2,2}-3_{3,1}$	d	c	36430.60 (-0.15)	d

[a] The deviations in frequency between observed and calculated values are given in parentheses after the observed values. The lines were in general measured to an accuracy of better than 0.1 MHz. [b] Transitions used to determine the rotational constants. [c] Not observed due to extremely weak intensity or interference by stronger lines. [d] Forbidden by symmetry.

TABLE III
R-BRANCH TRANSITIONS (MHz) OF THE FOUR DOUBLY SUBSTITUTED SPECIES[a]

Transitions[b]	^{10}B(1) and ^{10}B(3)	^{10}B(1) and ^{10}B(4)	^{10}B(3) and ^{10}B(4)	^{10}B(3) and ^{10}B(5)
1(1,0)-0(0,0)	10,843.25	10,847.94	10,880.90	10,880.90
$J = 4 \leftarrow 3$ $K = 4 \leftarrow 3$	28,691.00	28,716.90	29,040.75	29,052.85
$J = 5 \leftarrow 4$ $K = 5 \leftarrow 4$	35,339.90	35,371.95	35,784.13	35,799.64

[a] In the case of the last two species, it is uncertain which set of frequencies belongs to which species. [b] The lines are in general measured to an accuracy of better than 0.1 MHz.

the aid of symmetry consideration. The listed uncertainties in the bond lengths are only based on the uncertainties in the rotational constant determination. However, the overall accuracy is probably not better

than ±0.007 Å for any bond length. The lengths of these bonds are examined and compared with similar bonds in other molecules in the Discussion. It should be pointed out that since ^{10}B(1) substitution has no appreciable effect on the rotational constant C (Table I), we have assumed that the apex boron atom is located exactly on the c axis. The actual position of this atom should not be more than 0.02 Å from the c axis.

Molecular Dipole Moment.—The molecular dipole moment was determined from the $M = 0$ lobes of the $2(1,1) \leftarrow 1(0,1)$ and $2(2,1) \leftarrow 1(1,1)$ transitions of the normal species. The symmetry of the molecule allowed only two nonvanishing dipole moment components. Since a-type and c-type transitions were observed, μ_b must be zero. The magnitude of μ_a and μ_c

TABLE IV

$K = 2 \leftarrow 3$ Q-BRANCH TRANSITIONS OF NORMAL SPECIES[a]

Transitions	Obsd freq, MHz		Transitions	Obsd freq, MHz	
$6_{4,2}-6_{4,3}$	10,148.12	$(-0.20)^{b,c}$	$6_{5,2}-6_{3,3}$	10,184.38	$(+0.07)$
$7_{5,2}-7_{5,3}$	10,127.70	(-0.13)	$7_{6,2}-7_{4,3}$	10,192.86	$(+0.19)$
$8_{6,2}-8_{6,3}$	10,097.35	(-0.01)	$8_{7,2}-8_{5,3}$	10,205.62	$(+0.18)$
$9_{7,2}-9_{7,3}$	10,054.48	(-0.09)	$9_{8,2}-9_{6,3}$	10,224.19	$(+0.19)$
$10_{8,2}-10_{8,3}$	9,996.46	$(+0.21)$	$10_{9,2}-10_{7,3}$	10,250.10	$(+0.14)$
$11_{9,2}-11_{9,3}$	9,920.70	$(+0.31)$	$11_{10,2}-11_{8,3}$	10,285.27	$(+0.10)$
$12_{10,2}-12_{10,3}$	9,824.78	$(+0.32)$	$12_{11,2}-12_{9,3}$	10,331.85	$(+0.12)$
$13_{11,2}-13_{11,3}$	9,706.92	$(+0.44)$	$13_{12,2}-13_{10,3}$	10,392.16	$(+0.12)$
$14_{12,2}-14_{12,3}$	9,565.30	$(+0.39)$	$14_{13,2}-14_{11,3}$	10,468.85	$(+0.05)$
$15_{13,2}-15_{13,3}$	9,399.22	$(+0.44)$	$15_{14,2}-15_{12,3}$	10,564.88	(-0.10)
$16_{14,2}-16_{14,3}$	9,208.14	$(+0.46)$	$16_{15,2}-16_{13,3}$	10,683.83	(-0.08)
$17_{15,2}-17_{15,3}$	8,992.12	$(+0.38)$	$17_{16,2}-17_{14,3}$	10,828.95	(-0.21)
$18_{16,2}-18_{16,3}$	8,751.92	$(+0.35)$	$18_{17,2}-18_{15,3}$	11,004.33	(-0.26)
$19_{17,2}-19_{17,3}$	8,488.43	$(+0.24)$	$19_{18,2}-19_{16,3}$	11,214.06	(-0.22)
$20_{18,2}-20_{18,3}$	8,203.13	$(+0.13)$	$20_{19,2}-20_{17,3}$	11,462.24	(-0.17)

[a] Transitions belonging to $J = 3, 4,$ and 5 were too weak to be observed. [b] The deviation in frequency between observed and calculated values are given in parentheses. The lines are in general measured to an accuracy of better than 0.1 MHz. [c] A centrifugal distortion term $D_{jk}J(J + 1)\langle P_z^2 \rangle$ has been used to correct for the energy levels, where $D_{jk} = 0.0020$ MHz.

TABLE V

ATOMIC COORDINATES FROM KRAITCHMAN EQUATIONS

Atom	Coordinates,[a] Å		
	a	b	c
B(1)	$0.000^b \pm 0.020$	$0.000^b \pm 0.020$	$+0.879_2 \pm 0.001$
B(3)	$+0.563_5 \pm 0.002$	$+1.305_6 \pm 0.001$	$-0.194_0 \pm 0.003$
B(4)	$-1.150_5 \pm 0.002$	$+0.914_9 \pm 0.001$	$-0.127_0 \pm 0.004$
B(5)	$-1.150_5 \pm 0.002$	$-0.914_9 \pm 0.001$	$-0.127_0 \pm 0.004$
B(6)	$+0.563_5 \pm 0.002$	$-1.305_6 \pm 0.001$	$-0.194_0 \pm 0.003$

[a] Signs of the coordinates are assigned to be consistent with the [11]B nmr structure. [b] Assumed to be zero.

TABLE VI

MOMENTS OF INERTIA[a] OF CB_5H_9 (AMU Å²)

Isotopic species	$I_A{}^b$	$I_B{}^b$	$I_C{}^c$
Normal	94.7729	95.4391	154.0994
[10]B(3)	92.7738	95.3184	152.0584
[10]B(4)	92.9320	95.0647	151.9179
[10]B(1)	93.9942	94.6566	154.1027

[a] Using the conversion factor of 5.05531×10^5 MHz amu Å². [b] Uncertainties of 0.0009 amu Å². [c] Uncertainties of 0.0023 amu Å².

TABLE VII

BOND LENGTHS IN CB_5H_9

| Bond	Length,[a] Å	Bond	Length,[a] Å
B(3)–B(4)	1.759 ± 0.007	B(1)–B(3)	1.782 ± 0.004
B(4)–B(5)	1.830 ± 0.010	B(1)–B(4)	1.781 ± 0.005

[a] Uncertainties are based on only the uncertainties in the rotational constants of the four major species. However, the overall accuracy is probably not better than ± 0.007 Å for any bond length.

were determined to be 0.65 and 1.38 D, respectively. Making an angle of 25° with the c axis, the total dipole moment of the molecule was determined to be 1.53 ± 0.03 D.

The molecule has almost a symmetric oblate top. [10]B(3) or [10]B(4) substitution could be expected to cause a large rotation of the principal axis system along the c axis. While μ_c should not be appreciably affected by such a rotation, μ_a and μ_b can be greatly changed. From the $M = 0$ Stark lobes of the transitions $2(1,1) \leftarrow 1(0,1)$ and $2(2,1) \leftarrow 1(1,1)$, μ_a and μ_b were determined to be 0.61 and 0.22 D for the [10]B(3) species (a rotation of 20°) and 0.49 and 0.43 D for the [10]B(4) species (a rotation of 42°).

Discussion

The geometry of 2-carbahexaborane(9) as proposed by Dunks and Hawthorne (Figure 1) is strongly supported by our results. First, such a geometry would be a nearly symmetric rotor. Our rotational constants (5334, 5297, and 3081 MHz) are indeed those of a nearly symmetric oblate rotor. Second, our results verify the existence of a plane of symmetry with two pairs of equivalent boron atoms. Third, a boron atom of the proposed pentagonal pyramid would be located very near the unique axis, and we have found the apex boron to be within 0.02 Å from the c axis. Fourth, the boron skeleton (Figure 2) does appear to be a part
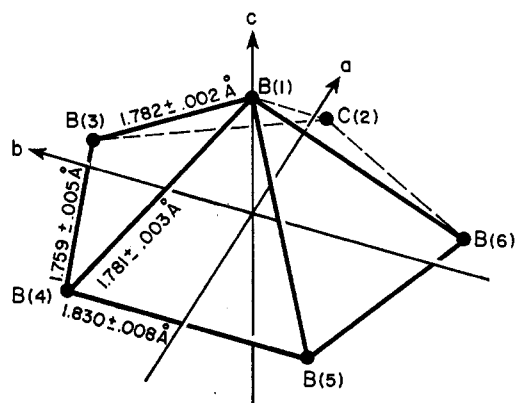
Figure 2.—Skeletal structure of CB_5H_9.

of a pentagonal pyramid. One may note the large separation of 2.30_1 Å between B(3) and B(6). The lone carbon, if bonded to B(3) and B(6), would form a comfortable near-planar five-membered ring with the four basal borons. Examination of the bond lengths lends additional support as discussed in the next paragraph.

If the complete geometry of this molecule (including the hydrogen atoms) is as proposed by Dunks and Hawthorne, the B–B bond lengths determined by us should be comparable to similar bonds in other carboranes. In Figure 3 the structure of this molecule is compared with those of hexaborane[7] (X-ray de-

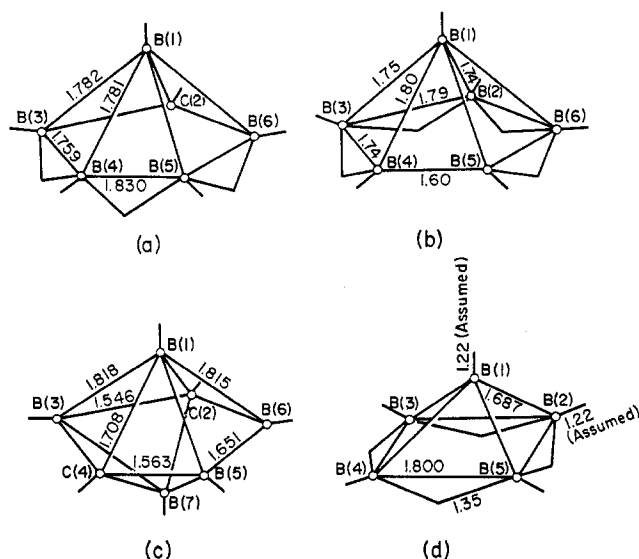(7) F. L. Hirshfeld, K. Zriks, R. E. Dickerson, E. L. Lippert, Jr., and W. N. Lipscomb, J. Chem. Phys., 28, 56 (1958).

Figure 3.—Structures of (a) 2-carbahexaborane(9), (b) hexa-borane,[7] (c) 2,4-$C_2B_5H_7$,[8] and (d) pentaborane.[9]

termination), 2,4-$C_2B_5H_7$[8] (microwave determination), and pentaborane[9] (microwave determination). First, we may compare the apex to base B–B bonds. The bonds in 2-carbahexaborane(9) are 1.78$_2$ and 1.78$_1$ Å as comparable with those in hexaborane (1.75, 1.74, and 1.80 Å) and 2,4-$C_2B_4H_7$ (1.81$_8$ and 1.81$_5$ Å) but much longer than the apex to base bond in pentaborane (1.68$_7$ Å). We feel justified to conclude that the apical boron in 2-carbahexaborane(9) is hexacoordinated as in hexaborane and 2,4-$C_2B_5H_7$ rather than pentacoordinated as in pentaborane. This set of data is consistent with a pentagonal pyramid. Second, the B(4)–B(5) bond (1.83 Å) is only slightly longer than similar bonds in hexaborane (B(2)–B(3), 1.79 Å) and penta-borane (base B–B bond, 1.80 Å). Meanwhile, the shorter B(3)–B(4) bond (1.75$_9$ Å) in 2-carbahexa-borane(9) is very slightly longer than the analogous B(2)–B(3) bond (1.74 Å) in hexaborane. In each comparison, the B–B bonds are in a very similar bonding environment.

CNDO/2 molecular orbital theory[10] has been used

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(9) H. J. Hrostowski and R. J. Myers, *ibid.*, **22**, 262 (1954).
(10) G. A. Segal and J. A. Pople, *ibid.*, **44**, 3289 (1966).

in the structural calculation for several carboranes.[11] The calculated bond lengths of the boron–carbon skeletons are very close to the corresponding experimental values. It would be interesting to speculate on the location of the carbon in this molecule now that the orientation of the borons has been completely determined. After certain reasonable assumptions[12] about the orientations of the hydrogen were made, the parameters $r_{CB(1)}$, $r_{CB(3)}$, and $\angle HCB(1)$ were varied in the CNDO/2 calculation until the molecular energy minimum was attained. At such an energy minimum, $r_{CB(1)} = 1.71_3$ Å, $r_{CB(3)} = 1.53_0$ Å, and $\angle HCB(1) = 130°$. The carbon atom is located slightly above the base boron plane (0.006 Å). Such a geometry would yield a set of rotational constants $A = 5277$ MHz, $B = 5267$ MHz, and $C = 3222$ MHz (with B(1) located very close to the c axis), in good agreement with the experimental values. The CNDO results are not sensitive to reasonable variations in the hydrogen positions.

With the positions of the boron atoms already determined from isotopic substitutions one may be tempted to extract directly the position of the carbon atom by fitting the carbon coordinates to the observed moments of inertia. This again requires assumptions about the positions of the hydrogen atoms. However, small changes in the hydrogen bond angles severely affect the fitted carbon out-of-plane position. Hence, we do not feel that such a fit is meaningful.

(11) C. S. Cheung, G. A. Segal, and R. A. Beaudet, *J. Amer. Chem. Soc.*, **92**, 4158 (1970).
(12) The assumptions were $r_{CH} = 1.10$ Å, all $r_{BH(t)} = 1.20$ Å, all $r_{BH(b)} = 1.34$ Å, the apex H is on the c axis, B(3)H(t) and B(4)H(t) are on the plane of the base B atoms, $\angle B(3)B(4)H(t) = \angle B(5)B(4)H(t) = \angle B(4)B(3)H(t) = 128.6°$, and all three B–H(b)–B bonds are bent down below the base by 57°. H(t) and H(b) refer to terminal hydrogens and bridged hydrogens, respectively. These arbitrary assumptions were partially based on the BH bonds determined for pentaborane[9] in which the base BH(T)'s were found to bend up by 3° above the base while the bridge H's were found to bend down by 57°