(11) Z. T. Wakefield, S. E. Allen, J. F. McCullough, R. C. Sheridan, and J. J. Kohler, *J. Agric. Food Chem.*, **19**, 99 (1971).
(12) Unpublished TVA data.
(13) M. C. Miller and R. A. Shaw, *J. Chem. Soc.*, 3233 (1963).
(14) E. Steger, *Chem. Ber.*, **94**, 266 (1961).
(15) L. F. Audrieth and D. B. Sowerby, *Chem. Ber.*, **94**, 2670 (1961).
(16) The sublimation pressures of amorphous red phosphorus were taken from T. D. Farr, "Phosphorus, Properties of the Element and Some of Its Compounds", Chemical Engineering Report No 8, Tennessee Valley Authority, Muscle Shoals, Ala., 1950.
(17) C. Hugot, *Ann. Chim. Phys.*, **21**, 5 (1900).
(18) A Stock and H, Gruneberg, *Ber. Dtsch. Chem. Ges.*, **40**, 2573 (1907).
(19) D. R. Stull and H. Prophet, *Natl. Stand. Ref. Data Ser., Natl. Bur. Stand.*, No. **37** (1971).
(20) C. C. Stephenson, R. L. Potter, T. G. Maple, and J. C. Morrow, *J. Chem. Thermodyn.* **1**, 59 (1969).
(21) W. L. Roth, T. W. DeWitt, and A. J. Smith, *J. Am. Chem. Soc.*, **69**, 2881 (1947).
(22) The entropy of PN_2H may be estimated to be S_{759} = 36.5 eu from the expression $s = {}^3/_2R \ln A + C$, where s is the entropy contribution of each atomic species in the solid and A is the atomic weight; the constant C is first evaluated with polymeric amorphous red phosphorus[16] as the reference solid: W. M. Latimer, *J. Am. Chem. Soc.*, **43**, 818 (1921).
(23) Yu. V. Azhikina, M. Ya. Koroleva, B. M. Maslennikov, and L. Ya. Kulikova, *Izv. Akad. Nauk SSSR, Neorg. Mater.*, **4**, 1711 (1968).
(24) Experimental results confirm the equilibrium of eq 8. This equilibrium is easily established from the amide side of the reaction. However, the reaction of ammonia with phospham generally proceeds only to a slight extent and ceases long before equilibrium is established. Recent results indicate that small quantities of ammonium chloride may be an effective catalyst for promoting reaction 8. These results will be discussed in a subsequent publication.

Contribution from the Chemistry Department,
University of Southern California, Los Angeles, California 90007

Microwave Spectrum, Structure, and Dipole Moment of 1,6-Dicarbanonaborane(9)

KAR-KUEN LAU and ROBERT A. BEAUDET*

Received October 31, 1975 AIC50783R

The microwave spectra of six isotopic species of 1,6-$C_2B_7H_9$ have been assigned. This compound is the largest carborane whose structure has been determined by microwave rotational spectroscopy. The bond distances are B_8–B_9 = 1.712 Å, B_5–B_9 = 1.995 Å, B_3–B_4 = 1.976 Å, B_7–B_9 = 1.784 Å, and B_2–B_3 = 1.805 Å. The most interesting results of this study are correlations of the B–B bond lengths with the simple inductive rule. A molecular dipole moment of 2.14 ± 0.17 D was determined from the Stark effect.

Introduction

The molecular structures of small carboranes, 2,4-$C_2B_5H_7$,[1,2] 1,2-$C_2B_4H_6$,[3] CB_5H_9,[4] 2-Cl-1,6-$C_2B_4H_6$,[5] 2,3,-4,5-$C_4B_2H_6$,[6] CB_5H_7,[7] have been determined in this laboratory by microwave rotational spectroscopy, whereas the molecular structures of large carboranes have been determined by x-ray diffraction. Recently we have extended our efforts of structural determinations to a few intermediate carboranes. These carboranes are interesting because both the microwave and x-ray methods which are equally applicable can be compared. These findings are useful to correlate structural parameters between small and large carboranes.

During our studies of intermediate carboranes, two compounds appeared to have rotational spectra amenable to microwave analysis. One of these compounds, 1,6-dicarbaoctaborane(8), 1,6-$C_2B_6H_8$, is reported elsewhere.[8] Our results of the structural determination of 1,6-dicarbanonaborane(9), 1,6-$C_2B_7H_9$, are reported here. To the best of our knowledge, this is the largest molecule where structure has been determinated by microwave rotational spectroscopy.

The synthesis and reaction of 1,6-$C_2B_7H_9$ were recently review by Dunks and Hawthorne.[9] Early proton and boron NMR measurements on 1,6-$C_2B_7H_9$[10] have shown that it has three types of borons—a five-coordinated apical boron, four six-coordinated equatorial borons bonded to one carbon each, and two six-coordinated borons each bonded to two carbons. The x-ray diffraction study of the *C,C*-dimethyl derivative[11] of this compound has been completed. Since there are two molecules per unit cell and no molecular symmetry imposed by the space group, two independent determinations of all bond distances and angles were obtained. Comparison of these two independent determinations indicates that the equivalent bond length differs by as much as 0.07 Å. These deviations are substantially larger than the typical errors for structural parameters.

Our investigation of the rotational spectra of six isotopic species in the gas phase has permitted an accurate structural determination with standard deviations an order of magnitude better than the x-ray work. Furthermore the molecule is slightly distorted in the solid state. Though the gross agreement between the microwave and x-ray results is within the reported standard deviations of the x-ray work, disagreement exists in the relative magnitudes of the bond lengths B_2–B_3 and B_4–B_5.

Experimental Section

The sample of 1,6-$C_2B_7H_9$ used in this work was kindly provided by Professor M. F. Hawthorne at the University of California at Los Angeles. The identity of the sample was confirmed by boron-11 NMR. Though a colorless solid at room temperature, it remained vaporized in the gold-plated Stark cell even when cooled to dry ice temperatures. On the other hand, the sample did condense in an ordinary cooled copper Stark cell.

The spectra were measured between 8 and 40 GHz with a 100-kHz Stark-modulated microwave spectrometer. For the less abundant isotopes, double-resonance experiments aided greatly in the successful assignments. Since these experiments depend upon the existence of an energy level common to two transitions of a particular isotope, the technique was found to be a powerful tool for selecting the transitions belonging to the same isotopic species. Standard microwave search techniques were subsequently employed to assign additional transitions. This double-resonance technique has been previously described.[12]

Spectra

The molecule 1,6-$C_2B_7H_9$ is an oblate top with presumably C_{2v} symmetry. Boron has two naturally occurring isotopes. Boron-11, with spin $^3/_2$, is 81% abundant, and boron-10, with spin 3, is 19% abundant. Assuming C_{2v} symmetry, the six most abundant isotopic species differing in the number and location of ^{10}B atoms incorporated in the molecule will be in the ratio of 1:1:0.5:0.25:0.25:0.25, where the normal species is included. The observed spectrum was extremely dense and intense. However the a-type transitions $J\ (K, J) \leftarrow J-1\ (K, J-1)$ where $K = 0$ or 1 were very strong and were readily assigned

Table I. Frequencies of Assigned Transitions in 1,6-$B_7C_2H_9$ (MHz)[a]

	Normal ^{11}B		4-^{10}B		3-^{10}B		8-^{10}B	
Transitions	ν_{obsd}	Δ^b	ν_{obsd}	Δ^b	ν_{obsd}	Δ^b	ν_{obsd}	Δ^b
$5_{41} \leftarrow 4_{40}$	27 400.27	−0.05	27 510.69	0.09	27 795.52	0.16	27 975.75	−0.08
$5_{33} \leftarrow 4_{22}$	26 057.23	−0.04	26 263.92	0.11				
$5_{05} \leftarrow 4_{04}$	24 133.30	−0.05	24 286.41	0.04			24 426.61	−0.01
$5_{32} \leftarrow 4_{31}$	27 074.68	0.02	27 273.20	0.21	27 285.36	0.29		
$5_{14} \leftarrow 4_{13}$	25 074.67	−0.09	25 247.02	0.06	25 245.05	−0.61	25 350.65	−0.56
$5_{33} \leftarrow 4_{32}$	25 980.93	−0.03	26 156.61	0.08				
$5_{15} \leftarrow 4_{14}$	24 133.30	−0.03	24 286.41	0.07			24 426.61	0.01
$5_{42} \leftarrow 4_{41}$	26 654.98	0.05	26 797.87	0.13				
$5_{24} \leftarrow 4_{23}$	25 072.28	−0.02	25 242.80	0.00	25 245.05	0.08	25 350.65	−0.57
$6_{42} \leftarrow 5_{41}$	32 733.07	−0.02	32 950.47	−0.04	33 025.62	−0.03	33 015.93	*c*
$6_{24} \leftarrow 5_{23}$	30 752.23	−0.38	30 975.27	−0.04	30 968.39	0.03	31 066.88	−0.02
$6_{06} \leftarrow 5_{05}$	28 866.10	0.06	29 047.88	−0.04	29 046.93	0.21	29 220.16	0.56
$6_{51} \leftarrow 5_{50}$	32 842.67	−0.14	32 946.73	−0.13	33 365.74	0.13	33 629.62	*c*
$6_{33} \leftarrow 5_{32}$	31 780.33	*c*	32 048.00	*c*	31 974.82	*c*	32 000.83	0.80
$6_{15} \leftarrow 5_{14}$	29 805.77	−0.14	30 006.05	0.07	30 006.05	−0.06	30 143.07	0.00
$6_{52} \leftarrow 5_{51}$	32 179.51	−0.14	32 338.75	0.61	32 578.67	−0.02	32 773.62	−0.02
$6_{34} \leftarrow 5_{33}$	30 743.21	−0.10	30 959.30	0.02	30 965.63	0.16	31 066.88	−0.28
$6_{16} \leftarrow 5_{15}$	28 866.10	0.06	29 047.88	0.04	29 046.93	0.21	29 220.16	0.56
$6_{43} \leftarrow 5_{42}$	31 618.15	*c*	31 826.41	*c*	31 893.10	*c*	31 982.81	0.14
$6_{25} \leftarrow 5_{24}$	29 805.77	0.02	30 006.05	0.40	30 006.05	−0.23	30 143.07	0.00
$7_{25} \leftarrow 6_{24}$			35 727.24	−0.04	35 727.24	−0.23	35 859.03	−0.44
$7_{07} \leftarrow 6_{06}$	33 598.75	0.00	33 809.34	0.00	33 807.88	−0.01	34 012.58	*c*
$7_{34} \leftarrow 6_{33}$	36 438.83	0.09	36 717.05	0.00	36 694.15	−0.01	36 784.52	0.41
$7_{16} \leftarrow 6_{15}$	34 538.30	0.10	34 767.52	0.40	34 767.52	0.12	34 936.24	0.21
$7_{53} \leftarrow 6_{52}$	37 236.30	0.54	37 470.59	0.63	37 586.31	0.06	37 692.66	0.06
$7_{35} \leftarrow 6_{34}$	35 478.62	−0.11	35 725.58	−0.06	35 727.24	−0.07	35 859.03	0.45
$7_{17} \leftarrow 6_{16}$	33 598.75	*c*	33 809.34	*c*	33 807.88	*c*	34 012.58	0.00
$7_{44} \leftarrow 6_{43}$	36 412.20	0.07	36 671.28	0.19	36 685.60	−0.04	36 782.7	0.5
$7_{26} \leftarrow 6_{25}$	34 538.30	−0.04	34 767.52	0.40	34 767.52	0.12	34 936.24	0.21

[a] Experimental errors are ±0.1 MHz unless otherwise noted. [b] $\Delta = \nu_{obsd} - \nu_{calcd}$. [c] Used to calculate rotational constants

Table II. Frequencies of Assigned Transitions of the Doubly Isotopic ^{10}B Species of 1,6-$B_7C_2H_9$[a]

	3,4-^{10}B		4,8-^{10}B	
Transitions	ν_{obsd}	Δ^b	ν_{obsd}	Δ^b
$5_{41} \leftarrow 4_{40}$	27 904.61	−0.73	28 077.01	−0.16
$5_{05} \leftarrow 4_{04}$	24 442.59	0.34	24 585.8	−0.12
$5_{14} \leftarrow 4_{13}$			25 527.39	−0.34
$5_{15} \leftarrow 4_{14}$	24 442.59	0.35	24 585.8	0.22
$6_{42} \leftarrow 5_{41}$	33 273.5	0.1	33 312.37	0.31
$6_{24} \leftarrow 5_{23}$	31 193.5	−0.3		
$6_{06} \leftarrow 5_{05}$	29 233.3	0.4	29 408.74	0.09
$6_{51} \leftarrow 5_{50}$	33 465.15	*c*	33 717.15	*c*
$6_{33} \leftarrow 5_{32}$	32 247.26	*c*	32 270.69	*c*
$6_{18} \leftarrow 5_{19}$	30 211.21	0.40	30 350.37	0.01
$6_{52} \leftarrow 5_{51}$			32 916.04	−0.30
$6_{34} \leftarrow 5_{33}$	31 187.71	0.60	31 291.89	−0.01
$6_{16} \leftarrow 5_{15}$	29 233.3	0.4	29 408.74	−0.09
$6_{43} \leftarrow 5_{42}$	32 110.81	−0.16	32 209.71	−0.14
$6_{25} \leftarrow 5_{24}$	30 211.21	0.34	30 350.37	0.03
$7_{25} \leftarrow 6_{24}$	35 979.98	0.18	36 115.23	−0.08
$7_{07} \leftarrow 6_{06}$	34 023.61	*c*	34 231.63	*c*
$7_{34} \leftarrow 6_{33}$	36 972.55	−0.21	37 062.01	−0.25
$7_{16} \leftarrow 6_{15}$	35 001.66	0.32	35 173.27	−0.01
$7_{35} \leftarrow 6_{34}$	35 979.98	−0.69	36 115.23	0.00
$7_{17} \leftarrow 6_{16}$	34 023.61	0.00	34 231.63	0.00
$7_{44} \leftarrow 6_{43}$	36 953.25	−0.09	37 056.54	0.16
$7_{26} \leftarrow 6_{25}$	35 001.66	0.33	35 173.27	−0.01

[a] Experimental errors are ±0.1 MHz unless otherwise noted. [b] $\Delta = \nu_{obsd} - \nu_{calcd}$. [c] Used to calculate rotational constants.

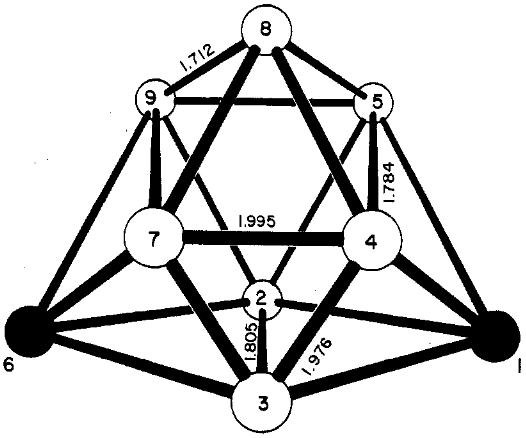

Figure 1. Structure of 1,6-$C_2B_7H_9$.

on the basis of partially resolvable Stark effects and a fit to the data.

The structure of 1,6-$C_2B_7H_9$ is shown in Figure 1. The C_2 symmetry axis coincides with the principal *a* axis which passes through the apex boron and the center of the $B_4B_5B_7B_9$ unit and which bisects the B_2–B_3 bond. Due to the molecular symmetry, the molecular dipole lies along the *a* axis. When the symmetry is broken by the unsymmetrical ^{10}B substitution, none of the principal axes rotates far enough to provide ob-

Table III. Rotational Constants and Moments of Inertia of the Isotopic Species of 1,6-$B_7C_2H_9$[a]

Isotopic species	*A*, MHz	*B*, MHz	*C*, MHz	I_a, amu Å^2	I_b, amu Å^2	I_c, amu Å^2
Normal ^{11}B	2867.79	2806.37	2366.36	176.2789	180.1369	213.6323
4-^{10}B	2898.63	2823.30	2380.76	174.4034	179.0567	212.3401
3-^{10}B	2881.58	2839.91	2380.58	175.4353	178.0095	212.3562
8-^{10}B	2867.70	2848.90	2396.49	176.2844	177.4477	210.9464
4,8-^{10}B	2900.17	2865.04	2411.49	174.3108	176.4481	201.6342
3,4-^{10}B	2913.05	2856.81	2395.34	173.5401	176.9564	211.0477

[a] Estimated errors in the rotational constants are $\Delta A = \Delta B = \pm 0.03$ MHz and $\Delta C = \pm\ 0.01$ MHz. The conversion factor to convert MHz to amu Å^2 was 5.05376×10^5 MHz amu Å^2.

Table IV. Stark Effect in $1,6\text{-}C_2B_7H_9$

Transition	$10^5\Delta\nu/E^2$, MHz (cm/V)^2	μ_a, D
$6_{33} \leftarrow 5_{32}$, $\lvert M\rvert = 2$	0.752	2.06
$6_{33} \leftarrow 5_{32}$, $\lvert M\rvert = 1$	0.211	2.06
$6_{43} \leftarrow 5_{42}$, $\lvert M\rvert = 2$	3.233	2.21
$6_{43} \leftarrow 5_{42}$, $\lvert M\rvert = 1$	0.891	2.25
		Av 2.14 ± 0.17

Table V. Coordinates[a] of Atoms in Principal Axis Systems of Isotopic Species[b]

	Normal	3-^{10}B	8-^{10}B	4-^{10}B
B_2[c]	−1.1403 (0.0016)			
	0 (0.0079)			
	−0.9021 (0.0020)			
B_3	−1.1403 (0.0016)			−1.1370 (0.0016)
	0 (0.0079)			0.1435 (0.0091)
	0.9021 (0.0020)			0.8957 (0.0019)
B_4	0.5664 (0.0040)	0.5796 (0.0040)	0.5841 (0.0060)	
	−0.9975 (0.0018)	−0.9977 (0.0018)	−0.9977 (0.0023)	
	0.8921 (0.0020)	0.8858 (0.0020)	0.8909 (0.0019)	
B_5[c]	0.5664 (0.0040)			
	−0.9975 (0.0018)			
	−0.8921 (0.0020)			
B_7[c]	0.5664 (0.0040)			
	0.9975 (0.0018)			
	0.8921 (0.0020)			
B_9[c]	0.5664 (0.0040)			
	0.9975 (0.0018)			
	−0.8921 (0.0020)			
B_8	1.6345 (0.0013)			1.6275 (0.0013)
	0 (0.0000)			−0.2035 (0.0038)
	0 (0.0329)			0 (0.0229)

[a] Errors based on 0.04-MHz uncertainty in the rotational constants are given in parentheses. [b] These coordinates were determined by Kraitchman's monosubstitution method. [c] Determined assuming C_{2v} symmetry.

servable b- or c-type transitions. We observed only transitions of a-type selection rules for all the isotopic species. The transitions $J\ (K, J) \leftarrow J-1\ (K, J-1)$ where $K = 0$ or 1 of the different isotope species form clusters of strong signals. We predicted that the prominent signals in each cluster from low to high frequency would be in an intensity ratio of 1:1:0.5 corresponding to normal, 4-^{10}B, and 3-^{10}B species, respectively. The first attempt to assign the normal species was complicated because the relative intensities of the strong signals in each cluster did not agree with the predicted intensity pattern. Instead we observed four strong signals in each cluster with intensity ratio 1:1.5:0.5. This observation contradicted our predictions. As more data were collected, it became clear that the C rotational constants of the 4-^{10}B and 3-^{10}B carbon species were so close that their $J\ (K, J) \leftarrow J-1\ (K, J-1)$ transitions overlapped when $K = 0$ or 1. Therefore, their combined intensity was stronger than those of the normal species. In order to fit the observed rotational spectrum, transitions sensitive to the A and B constants were necessary. These transitions did not form easily recognized clusters and were scattered in the spectrum. Also they did not overlap accidentally. The relative intensities of these observed transitions for the normal, 4-^{10}B, and 3-^{10}B species followed closely that predicted for C_{2v} symmetry for this compound. The weakest two transitions in the low-frequency end of each cluster have not been assigned. Since they gave almost identical substitution parameters for the base borons (4, 5, 7, or 9) as those from the ground-state data, they probably belong to an excited skeletal vibrational mode of the normal and 4-^{10}B species.

It was more difficult to assign transitions for the 8-^{10}B and the weaker doubly substituted species 3,4-^{10}B, 3,5-^{10}B, and 4,8-^{10}B because of their weaker intensities. As mentioned in the Experimental Section, double-resonance techniques were useful to assign the transitions of these three species. The frequencies of the assigned transitions are cited in Tables I and II. The rotational constants and moments of inertia for all assigned isotopic species are given in Table III.

Dipole Moment

Stark effect measurements were made on the $|M| = 1, 2$ lobes of the $6_{43} \leftarrow 5_{42}$ and $|M| = 1, 2$ lobes of the $4_{22} \leftarrow 3_{21}$ transitions. The observed stark coefficients are given in Table IV. The cell spacing was determined[13] by using the $2 \leftarrow 1$ transition of OCS. The dipole moment was determined to be 2.14 ± 0.17 D.

Molecular Structure

The coordinates in Table V were determined from the Kraitchman substitution method[14] by using four isotopic species as the reference molecules. In order to incorporate all

Table VI. Coordinates[a] of Atoms in Principal Axis System of the Normal Species

	Normal	Carbon ^{10}B	Apex ^{10}B	Base ^{10}B	Average
B_2[b]	−1.1403 (0.0016)			−1.1387 (0.0019)	−1.1395 (0.0018)
	0 (0.0079)			−0.0095 (0.0090)	0.0[b]
	−0.9021 (0.0020)			−0.9031 (0.0019)	−0.9026 (0.0019)
B_3	−1.1403 (0.0016)			−1.1387 (0.0019)	−1.1395 (0.0018)
	0 (0.0079)			0.0095 (0.0090)	0[b]
	0.9021 (0.0020)			0.9031 (0.0019)	0.9026 (0.0019)
B_4	0.5664 (0.0040)	0.5650 (0.0040)	0.5692 (0.0060)		0.5669 (0.0047)
	−0.9975 (0.0018)	−0.9977 (0.0018)	−0.9977 (0.0023)		−0.9976 (0.0020)
	0.8921 (0.0020)	0.8935 (0.0020)	0.8909 (0.0019)		0.8922 (0.0020)
B_5[b]	0.5664 (0.0040)	0.5650 (0.0040)	0.5692 (0.0060)		0.5669 (0.0047)
	−0.9975 (0.0018)	−0.9977 (0.0018)	−0.9977 (0.0023)		−0.9976 (0.0020)
	−0.8921 (0.0020)	−0.8935 (0.0020)	−0.8909 (0.0019)		−0.8922 (0.0020)
B_7[b]	0.5664 (0.0040)	0.5650 (0.0040)	0.5692 (0.0060)		0.5669 (0.0047)
	0.9975 (0.0018)	0.9977 (0.0018)	0.9977 (0.0023)		0.9976 (0.0020)
	0.8921 (0.0020)	0.8935 (0.0020)	0.8909 (0.0019)		0.8922 (0.0020)
B_9[b]	0.5664 (0.0040)	0.5650 (0.0040)	0.5692 (0.0060)		0.5669 (0.0047)
	0.9975 (0.0018)	0.9977 (0.0018)	0.9977 (0.0023)		0.9976 (0.0020)
	−0.8921 (0.0020)	−0.8935 (0.0020)	−0.8909 (0.0019)		−0.8922 (0.0020)
B_8	1.6345 (0.0013)			1.6348 (0.0013)	1.6346 (0.0013)
	0 (0.0000)			−0.0030 (0.0038)	0[b]
	0 (0.0329)			−0.0310 (0.0229)	0[b]

[a] Errors based on 0.04-MHz uncertainty in the rotational constants are given in parentheses. [b] Assuming C_{2v} symmetry.

Table VII. Structure of 1,6-$C_2B_7H_9$

	Distances, Å	
	1,6-$C_2B_7H_9$[a]	C,C-Me_2-1,6-$C_2B_7H_9$[b]
B_8-B_9	1.712 ± 0.006	1.698 ± 0.026
B_5-B_9	1.995 ± 0.004	1.984 ± 0.031
B_3-B_4	1.976 ± 0.007	1.969 ± 0.021
B_7-B_9	1.784 ± 0.004	1.772 ± 0.046
B_2-B_3	1.805 ± 0.004	1.764 ± 0.049

[a] This work. The quoted errors are obtained from the errors given in Table VI. [b] Reference 11.

of the data from different reference molecules, we transformed all coordinates into the principal axis system of the normal species. This not only gives a direct comparison of all the coordinates but also serves to confirm the correct sign assignment for the coordinates.

The transformations which we used to obtain Table V were carried out in two steps. First we calculated the 3 × 3 transformation matrices, which were needed to rotate the axes of each isotopic species to axes parallel to the principal axes of the normal species by using the observed moments of inertia of the normal species, and the substitution coordinates of an atom in the normal species frame. The moment of inertia is written in the principal axes of the normal species for the isotopic species. The transforming matrix (T) that diagonalizes the moment of inertia matrix is readily obtained. The inverse transformation ($\mathbf{T}^{-1}$), which is simply the transpose of **T**, is the 3 × 3 transformation matrix to rotate the axes back to the principal axes of the normal species. After each appropriate rotation, we corrected for the shift of center of mass coordinates from each reference species to the normal species by means of the center of mass equations. The final results after the transformations are presented in Table VI. The average coordinates and errors were calculated by assuming C_{2v} symmetry which was indeed confirmed by the observed relative intensity ratio of the different isotopic species. From these coordinates the final structure given in Table VII, was calculated.

Discussion

The molecular structure of 1,6-$C_2B_7H_9$ is a tricapped trigonal prism as shown in the figure. X-ray data have been found for the *C,C*-dimethyl derivative of the 1,6-$C_2B_7H_9$. Hence comparisons are made in Table VII between the microwave structure of the parent compound 1,6-$B_7C_2H_9$ and the x-ray structure of its *C,C*-dimethyl derivative. In accordance with the x-ray work, we found the shortest B–B distances to be those involving the apical borons (B_4–B_8, etc.). Similarly we did not observe abnormal lengthening of the B_2–B_3 distance between B atoms joined to two C atoms. This distance is 1.804 Å, as compared to 1.887 Å in the related compound, 1,6-$C_2B_6H_8$.[8]

The bond lengths B_2–B_3, B_4–B_5, and B_7–B_9 are identical for the isoelectronic species $B_9H_9^{2-}$.[15] The introduction of two C atoms will make B_2–B_3 unequal to the other two bonds. In the x-ray work, the bond length B_2–B_3 is shorter than the bond length B_4–B_5. However the microwave work indicates the opposite. The bonds B_2–B_3, B_4–B_5, and B_7–B_9 are of the same type. Therefore one may argue that increasing the charge of the B atoms will strengthen the bond and consequently the bond length is shorter. It is interesting to note that the present observation of a B_2–B_3 bond longer than B_4–B_5 is in fact in good agreement with the simple inductive rule.[16] The rule states that B atoms increase charge as they become bonded to more C atoms. It is quite clear that this molecule is distorted in the solid state. This distortion leads to a slight contraction of the molecular parameters. The microwave results agree to within the reported standard deviations in the x-ray work. However disagreement exists when one looks at the relative magnitudes of the bond lengths B_2–B_3 and B_4–B_5.

Acknowledgment. We wish to thank Professor Frederick Hawthorne for the sample of 1,6-$C_2B_7H_9$. We also gratefully acknowledge the support of the National Science Foundation under Grants GP-42694 and MPS74-01364 A01. We also thank the University of Southern California University Computer Center for making available computer time to carry out the necessary calculations.

Registry No. 1,6-$B_7C_2H_9$, 26894-16-6; 1,6-$B_7C_2H_9$(4-^{10}B), 58150-52-0; 1,6-$B_7C_2H_9$(3-^{10}B), 58150-53-1; 1,6-$B_7C_2H_9$(8-^{10}B), 58150-54-2; 1,6-$B_7C_2H_9$(3,4-^{10}B), 58150-55-3; 1,6-$B_7C_2H_9$(4,8-^{10}B), 58150-56-4.

References and Notes

(1) R. A. Beaudet and R. L. Poynter, *J. Chem. Phys.*, **43**, 2166 (1965).
(2) T. Onak, G. B. Dunks, R. A. Beaudet, and R. L. Poynter, *J. Am. Chem. Soc.*, **88**, 4622 (1966).
(3) R. A. Beaudet and R. L. Poynter, *J. Chem. Phys.*, **53**, 1899 (1970).
(4) C. C. Cheung and R. A. Beaudet, *Inorg. Chem.*, **10**, 1144 (1971).
(5) G. L. McKown and R. A. Beaudet, *Inorg. Chem.*, **10**, 1350 (1971).
(6) J. P. Pasinski and R. A. Beaudet, *J. Chem. Phys.*, **61**, 683 (1974).
(7) G. L. McKown, B. P. Don, P. J. Vergamini, L. H. Jones, and R. A. Beaudet, *J. Chem. Soc., Chem. Commun.*, 775 (1974).
(8) K. K. Lau, H. Rogers, and R. A. Beaudet, paper presented at the Symposium on Molecular Structure and Spectroscopy, Columbus, Ohio, June 1974.
(9) G. B. Dunks and M. F. Hawthorne, *Acc. Chem. Res.*, **6**, (1973).
(10) F. N. Tebbs, P. M. Garrett, D. C. Young, and M. F. Hawthorne, *J. Am. Chem. Soc.*, **88**, 609 (1966).
(11) T. F. Koetzle, F. E. Scarbrough, and W. N. Lipscomb, *Inorg. Chem.*, **7**, 1076 (1968).
(12) R. G. Ford and R. A. Beaudet, *J. Chem. Phys.*, **55**, 3110 (1971).
(13) J. S. Muenter, *J. Chem. Phys.*, **48**, 4544 (1968).
(14) J. Kraitchman, *Am. J. Phys.*, **21**, 17 (1953).
(15) F. Keanberg and E. L. Muetterties, *Inorg. Chem.*, **5**, 1955 (1966).
(16) F. P. Boer, J. A. Potenza, and W. N. Lipscomb, *Inorg. Chem.*, **5**, 1301 (1966).