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Microwave Spectrum, Structure, and Dipole Moment of 1,7-Dicarba-*closo*-octaborane(8), $C_2B_6H_8$

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The microwave spectrum of 1,7-dicarba-*closo*-octaborane(8), $C_2B_6H_8$, has been observed and the rotational spectra of nine isotopic species have been assigned. Coordinates of all boron atoms were accurately located and boron–boron bond lengths were determined. The results support those of earlier x-ray diffraction studies and confirm that the slightly distorted D_{2d} geometry of the C_2B_6 unit exists in the gas phase. The bond distances are $B_2–B_3$ = 1.813 Å, $B_2–B_5$ = 1.843 Å, $B_2–B_6$ = 1.685 Å, $B_3–B_4$ = 1.886 Å, $B_3–B_6$ = 1.880 Å, and $B_5–B_6$ = 1.949 Å. The molecular dipole was measured to be μ = 1.40 + 0.01 D.

Introduction

The structure of the carborane 1,7-$C_2B_6H_8$ has been the topic of much discussion. Williams and Gerhart proposed a dodecahedral structure similar to that of B_8Cl_8[1] based on the mass spectrum and ^{11}B NMR data.[2] More recently, proton NMR and ^{11}B NMR analyses of the *C,C′*-dimethyl derivative have indicated the equivalence of the methyl groups and their adjacent carbon atoms.[3] These data are consistent with a square-antiprismatic structure. Single-crystal x-ray diffraction studies have shown the structure to consist of a dodecahedron which is distorted toward a square antiprism.[4] These results indicate a molecule with C_2 symmetry which exhibits chirality. To confirm that this molecule retains its distorted chiral structure in the gas phase the microwave spectrum was investigated and the structure of the boron atoms was determined. The dipole moment was also obtained.

Experimental Section

Previously, the carborane 1,7-$C_2B_6H_8$ had been prepared by the pyrolysis of 1,3-dicarbanidononaborane(13), $C_2B_7H_{13}$, in diphenyl ether. By using an improved synthesis described by Dunks and Hawthorne,[5] the yield of 1,7-$C_2B_6H_8$ has been doubled. A 60% yield is obtained by slow, low-pressure pyrolysis of $C_2B_7H_{13}$. The original sample of $C_2B_6H_8$ was kindly provided by T. Onak. The sample was stored in a Pyrex tube in liquid nitrogen without further purification. No problems involving impurity or decomposition were encountered. The microwave spectrum between 8 and 40 GHz was observed at dry ice temperature and at pressures between 10 and 50 mTorr. A standard 100-kHz Stark-modulated spectrometer was used in this investigation. Frequency measurements were calibrated by using a General Radio Co. standard frequency multiplier, Type 1112-A, with a Hewlett-Packard HP5245L electronic counter. Stark effects were studied by D.C. biasing the 100-kHz square wave. The effective waveguide spacing was determined by measuring the Stark shifts of the $J = 1 \leftarrow 0$ transitions of carbonyl sulfide.

Spectra

Initial predictions of the rotational constants were made using the skeletal structural parameters of 1,7-$B_6H_8C_2(CH_3)_2$.[4] Such predictions indicated that $C_2B_6H_8$ is a near-prolate symmetric rotor with the principal axes directed as shown in Figure 1. The point symmetry of the molecule is C_2; the C_2 axis is coincident with the inertial *c* axis and passes through the midpoints of the B(3)–B(4) bond and the B(5)–B(6) bond. The dipole moment of the parent species lies only along the *c*-axis direction, however small *a* and *b* dipole components are present in certain species when the axes are rotated upon isotopic substitution. Nevertheless, only *c*-type transitions were observable for all boron isotopic species.

Table I. Rotational Constants[a] of the Isotopic Species of 1,7-$C_2B_6H_8$

Isotopic species	Rel intens[b]	*A*, MHz	*B*, MHz	*C*, MHz
Normal	1	3885.03	3124.79	3091.11
2-^{10}B	0.47	3902.60	3168.02	3129.77
3-^{10}B	0.47	3932.73	3148.87	3102.46
5-^{10}B	0.47	3936.42	3148.20	3102.41
2,4-^{10}B	0.11	3950.88	3195.05	3137.75
2,5-^{10}B	0.11	3954.51	3187.74	3145.86
2,6-^{10}B	0.11	3954.40	3195.58	3138.62
3,5-^{10}B	0.11	3984.03	3178.81	3107.45
3,6-^{10}B	0.11	3985.41	3159.25	3126.70

[a] Uncertainties are 0.04 MHz or less. [b] The natural abundance ratio of ^{10}B:^{11}B is 19:81.

Most of the boron isotopic species exist in sufficient concentrations to be observed in natural abundance. Assignment of a value of 1 to the intensity of the normal species gives relative intensities of various substituted boron isotopes as listed in Table I. Most species were assigned on the basis of Stark effects and relative intensities. The relative intensity pattern for the isotopic species is consistent with the relative abundance of the isotopes of a molecule belonging to a C_2 point group. In principle, the variation in intensities due to nuclear spin statistics can also be used; however calculations reveal the differences are too small to be useful. Four doubly substituted species and the ^{13}C species were too weak to be observed.

Table II. R-Branch Transitions[a] of the Four Major Isotopic Species of 1,7-$C_2B_6H_8$ (MHz)

Transitions	Normal		$2\text{-}^{10}B$		$3\text{-}^{10}B$		$5\text{-}^{10}B$	
	ν_{obsd}	Δ	ν_{obsd}	Δ	ν_{obsd}	Δ	ν_{obsd}	Δ
$1_{11} \rightarrow 2_{21}$	14 479.78	−0.10						
$1_{01} \rightarrow 2_{11}$	13 259.27	−0.13						
$1_{10} \rightarrow 2_{20}$	14 747.19	−0.11						
$2_{12} \rightarrow 3_{22}$	21 029.41	−0.05	21 212.17	+0.31	21.244.49	−0.34	21 253.79	−0.06
$2_{21} \rightarrow 3_{31}$	22 533.70	−0.08	22 622.85	+0.05	22 790.70	+0.14	22 808.20	−0.40
$2_{20} \rightarrow 3_{30}$	22 532.64	−0.07			22 788.86	+0.24	22 806.18	−0.53
$2_{02} \rightarrow 3_{12}$	19 526.35	+0.13	19 762.60	+0.26	19 700.67	−0.37	19 700.67	−0.33
$2_{11} \rightarrow 3_{21}$	20 933.95	+0.05	21 104.72	+0.44	21 115.67	+0.11		
$3_{31} \rightarrow 4_{41}$	30 303.39	+0.05	30 466.21	−1.14	30 655.38	+0.24	30 680.25	−0.32
$3_{13} \rightarrow 4_{23}$	27 295.70	*b*	27 566.78	*b*	27 565.45	*b*	27 572.82	*b*
$3_{22} \rightarrow 4_{32}$	28 751.79	−0.02	28 963.73	+0.34	29 045.58	−0.16	29 062.52	−0.41
$3_{21} \rightarrow 4_{31}$	28 746.50	*b*	28 956.38	*b*	29 036.14	*b*	29 053.62	*b*
$3_{03} \rightarrow 4_{13}$	25 811.5	−0.5						
$3_{30} \rightarrow 4_{40}$	30 303.39	+0.27	30 466.21	−1.14	30 655.38	+0.29	30 680.25	−0.27
$3_{12} \rightarrow 4_{22}$	27 110.01	*b*	27 359.02	*b*	27 316.78	*b*	27 326.97	*b*
$3_{12} \rightarrow 4_{04}$	23 969.99	+0.11	24 302.04	+0.09	24 030.31	−0.23	24 027.01	−0.68
$3_{21} \rightarrow 4_{13}$	22 693.86	+1.52						
$3_{22} \rightarrow 4_{14}$	22 361.35	+0.13						
$3_{31} \rightarrow 4_{23}$	20 975.27	−1.44						
$4_{32} \rightarrow 5_{42}$	36 519.66	+0.10	36 765.59	+0.02	36 907.32	+0.24	36 931.46	−0.30
$4_{14} \rightarrow 5_{24}$	33 578.81	+0.16	33 940.94	+0.30	33 908.46	−0.55	33 913.80	−0.62
$4_{41} \rightarrow 5_{51}$	38 073.36	−0.04	38 272.21	−0.34	38 520.66	+0.06	38 552.71	−0.70
$4_{23} \rightarrow 5_{33}$	34 971.69	−0.31	35 266.83	−0.14	35 304.81	−0.15	35 320.96	−0.21
$4_{40} \rightarrow 5_{50}$	38 073.36	+0.23	38 272.21	−0.34	38 520.66	+0.06	38 552.71	−0.69
$4_{22} \rightarrow 5_{32}$	34 955.59	−0.79	35 246.13	−0.12	35 276.64	−0.06	35 293.40	−0.37
$4_{04} \rightarrow 5_{14}$	32 117.66	+0.14	32 541.14	+0.64	32 426.33	−0.50	32 421.49	−0.60
$4_{31} \rightarrow 5_{41}$	28 977.63	+0.24	36 765.59	+0.26	36 907.32	+0.61	36 931.46	+0.05
$4_{13} \rightarrow 5_{23}$	33 279.91	−0.02	33 608.63	+0.05	33 513.59	−0.34	33 523.56	+0.10
$4_{31} \rightarrow 5_{23}$	27 226.79	+1.02						
$4_{13} \rightarrow 5_{05}$	30 099.09	−0.06	30 497.57	−0.21	30 153.43	−0.84	30 147.77	−3.88
$4_{22} \rightarrow 5_{14}$	28 977.63	+0.24	29 484.28	+0.84	29 139.70	−0.89	29 120.97	−0.48
$4_{23} \rightarrow 5_{15}$	28 489.32	+0.09						
$4_{32} \rightarrow 5_{24}$	27 187.70	−0.36						
$5_{15} \rightarrow 6_{25}$	39 878.27	−0.11						
$5_{05} \rightarrow 6_{15}$	38 446.50	−0.10						
$5_{32} \rightarrow 6_{24}$	33 470.02	+0.20						
$5_{14} \rightarrow 6_{06}$	36 198.59	−0.13						
$5_{41} \rightarrow 6_{33}$	31 866.77	+0.57						
$5_{23} \rightarrow 6_{15}$	35 266.93	+1.10						
$5_{42} \rightarrow 6_{34}$	31 864.65	+0.31						
$5_{24} \rightarrow 6_{16}$	34 598.47	+0.07						
$5_{33} \rightarrow 6_{25}$	33 395.74	+0.23						

[a] $\Delta = \nu_{obsd} - \nu_{calcd}$. [b] Used to calculate rotational constants.

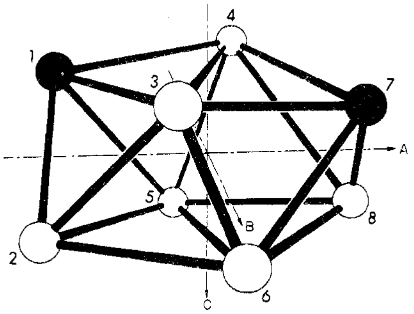

Figure 1. Molecular structure of $C_2B_6H_8$.

High-*J* Q-branch lines cluttered much of the spectrum and R-branch lines for several isotopic species overlapped, preventing resolution of Stark lobes for the weaker transitions.

In the initial microwave search, observation of several strong transitions with resolvable Stark effects led to the assignment of the normal species. Subsequently, predictions for the rotational spectra of the singly substituted species were made. Stark effects were observable in most cases and assignments were made with little difficulty. Calculated spectra were obtained by assuming a rigid-rotor model with no centrifugal distortion. A minimum of three transitions is required to define a unique set of rotational constants. In practice, each of these transitions should be sensitive to at least one of the rotational constants. With this consideration, rotational constants for the four major species were determined by using the transitions $4_{23} \leftarrow 3_{13}$, $4_{31} \leftarrow 3_{21}$, and $4_{22} \leftarrow 3_{12}$. By using the same transitions to fit these four isotopic species, small errors due to centrifugal distortion tend to cancel each other, since only differences in rotational constants are used to calculate the structure. Observed and calculated values of the frequencies for R-branch transitions belonging to these species agree quite closely and are listed in Table II.

Five doubly substituted boron isotopic species were also assigned. Accurate predictions of the spectra were possible after a determination of the structure involving the normal and singly substituted species. Pressure broadening and line broadening due to boron nuclear quadrupole splitting became a significant problem for the weaker lines; hence, assignments were considerably more difficult. Few lines belonging to the 2,3-^{10}B species were observed and no reasonable rigid-rotor frequency fit could be obtained. The frequencies of observed transitions for all assigned doubly substituted boron isotopic species are listed in Table III. Rotational constants of all assigned species are given in Table I.

Stark Effect and Dipole Moment

The dipole moment was determined from the $M = |1|$ and $M = |2|$ lobes of the $4_{2,3} \leftarrow 3_{1,3}$ transition of the normal species. Electric field calibration of the Stark cell was made by using OCS whose dipole moment was taken as 0.715 21 D.[6] The

Table III. R-Branch Transitions[a] of the Doubly Substituted Species of 1,7-$C_2B_6H_8$ (MHz)

	2,4-^{10}B		2,5-^{10}B		2,6-^{10}B		3,5-^{10}B		3,6-^{10}B	
Transition	ν_{obsd}	Δ	ν_{obsd}	Δ	ν_{obsd}	Δ	ν_{obsd}	Δ	ν_{obsd}	Δ
$2_{21} \rightarrow 3_{31}$			22 940.35	−0.04	22 940.86	−0.12				
$2_{20} \rightarrow 3_{30}$			22 938.75	−0.02	22 938.08	+0.08				
$2_{11} \rightarrow 3_{21}$					21 295.1	+0.66				
$3_{31} \rightarrow 4_{41}$	30 823.63	+0.54			30 848.9	+0.48	31 032.15	+0.03	31 040.76	−0.28
$3_{22} \rightarrow 4_{32}$	29 262.11	+0.63	29 276.77	−0.43	29 281.17	+0.12				
$3_{21} \rightarrow 4_{31}$	29 247.24	+0.63	29 269.03	−0.14	29 266.02	−0.39				
$3_{30} \rightarrow 4_{40}$	30 823.63	+0.64	30 848.0	−0.63	30 848.9	+0.58	31 032.15	+0.20	31 040.76	−0.26
$4_{31} \rightarrow 5_{41}$							37 319.91	+1.21	37 327.25	+0.12
$4_{32} \rightarrow 5_{42}$	37 156.90	*b*	37 182.76	*b*	37 183.61	*b*	37 319.91	*b*	37 327.25	*b*
$4_{14} \rightarrow 5_{24}$	34 302.94	+0.50	34 239.68	−0.06	34 316.25	+0.09	34 308.8	+0.3	34 119.67	+0.27
$4_{41} \rightarrow 5_{51}$	38 725.58	+0.76	38 757.05	−0.64	38 757.05	−0.14	39 000.19	+0.06	39 011.50	−0.36
$4_{23} \rightarrow 5_{33}$	35 607.19	+0.77	35 617.27	−0.14	35 627.15	−0.06	35 664.64	+0.21	35 648.06	−0.12
$4_{40} \rightarrow 5_{50}$	38 725.58	+0.76	38 757.05	−0.64	38 757.05	−0.14	39 000.19	+0.07	39 011.50	−0.36
$4_{22} \rightarrow 5_{32}$	35 562.15	−0.83	35 593.56	−0.15	35 584.47	+0.06	35 603.00	+0.40	35 633.7	+0.1
$4_{04} \rightarrow 5_{14}$	32 902.14	+0.92	32 782.12	−0.23	32 908.47	+0.42	32 840.8	+0.9	32 523.83	+0.27
$4_{13} \rightarrow 5_{23}$	33 836.62	*b*	33 878.71	*b*	33 852.21	*b*	33 748.62	*b*	33 826.77	*b*
$5_{05} \rightarrow 6_{15}$	39 437.84	*b*	39 256.64	*b*	39 444.58	*b*	39 384.45	*b*	38 917.73	*b*

[a] $\Delta = \nu_{\text{obsd}} - \nu_{\text{calcd}}$. [b] Used to calculate rotational constants.

Table IV. Second-Order Stark Effect in 1,7-$C_2B_6H_8$

Transitions	ν/E^2, MHz (cm/V)^2	μ, D
$3_{13} \leftarrow 4_{23}$, $\lvert M\rvert = 1$	-2.60×10^{-5}	1.406
$3_{13} \leftarrow 4_{23}$, $\lvert M\rvert = 2$	-1.08×10^{-4}	1.401
	Av	1.40 ± 0.01

frequency shifts for the second-order Stark effects of these lobes were measured and are summarized in Table IV. A plot of frequency shift vs. the square of the applied electric field gave a linear relationship with fields up to several hundred volts per centimeter in both cases. A value of 1.40 ± 0.01 D for μ was obtained from a least-squares fit of the data.

Molecular Structure

The coordinates of all the boron atoms were determined by using the Kraitchman method.[7] With this method the coordinates of a particular atom can be calculated from changes in the moments of inertia when an isotopic substitution is made at that atom. Costain has shown that if zero-point vibrational effects are identical in both reference and isotopic species, they should cancel each other and structural errors are minimized.[8] The rigid-cage structure of $C_2B_6H_8$ should be well suited for an accurate structural determination. With the normal species as the reference, coordinates of the boron atoms were calculated by using the singly substituted species. Since several doubly substituted species were assigned, coordinates were also calculated using each of the singly substituted species as the reference and appropriate doubly substituted species. Coordinates of the boron atoms obtained in this manner are listed in Table V. Typically, isotopic substitutions rotate the principal axes and shift the center of mass. Therefore coordinates obtained in this manner are relative to the principal-axis system of the reference species and direct comparisons are not possible. Consequently, the coordinates were transformed back into the normal-species frame and averaged.

Inherent with the Kraitchman method is the ambiguity in signs of coordinates, since only squares of coordinates are determined. With knowledge of the molecular geometry, the signs can be guessed with reasonable certainty. Furthermore, moments calculated from these coordinates must agree with the observed moments of inertia. At this point the assignments of the 3-^{10}B and 5-^{10}B species were questioned, since the absolute values of the B(3) and B(5) coordinates are relatively close. However, interchanging the B(3) and B(5) coordinates with appropriate sign changes resulted in large discrepancies between coordinates when transformed back into the principal-axis system of the normal species. Signs of all other coordinates were obvious from the predicted geometry of the molecule. With the reasonable assumption of C_2 symmetry, three symmetry-related pairs of coordinates were obtained.

Table V. Coordinates[a] of 1,7-$C_2B_6H_8$ in Principal-Axis Systems

Atom	Coordinate	Normal	2-^{10}B	3-^{10}B	5-^{10}B
2	*a*	−1.3568 (0.0008)			−1.3592 (0.0008)
	b	0.4768 (0.0026)			0.6510 (0.0016)
	c	0.5675 (0.0020)			0.3563 (0.0026)
8	*a*	1.3568 (0.0008)		1.3414 (0.0008)	1.3626 (0.0008)
	b	−0.4768 (0.0026)		−0.2428 (0.0052)	−0.2185 (0.0058)
	c	0.5675 (0.0020)		0.7049 (0.0017)	0.7078 (0.0017)
3	*a*	−0.3660 (0.0032)			−0.3783 (0.0031)
	b	0.8699 (0.0019)			0.4463 (0.0039)
	c	−0.8969 (0.0016)			−1.1483 (0.0014)
4	*a*	0.3660 (0.0032)	0.3046 (0.0038)		0.3600 (0.0032)
	b	−0.8699 (0.0019)	−0.7244 (0.0024)		−1.1565 (0.0009)
	c	−0.8969 (0.0016)	−1.0211 (0.0015)		−0.4736 (0.0016)
5	*a*	−0.2285 (0.0052)	−0.2432 (0.0048)	−0.2485 (0.0047)	
	b	−0.9461 (0.0018)	−1.0616 (0.0013)	−0.5674 (0.0030)	
	c	0.8885 (0.0016)	0.7473 (0.0014)	1.1484 (0.0014)	
6	*a*	0.2285 (0.0052)	0.2657 (0.0044)	0.2188 (0.0054)	
	b	0.9461 (0.0018)	0.8016 (0.0021)	1.2039 (0.0009)	
	c	0.8885 (0.0016)	1.0193 (0.0014)	0.4853 (0.0015)	

[a] Errors based on a 0.04-MHz uncertainty in the rotational constants are given in parentheses.

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

Atom	Coordinate	Normal	$2\text{-}^{10}B$	$3\text{-}^{10}B$	$5\text{-}^{10}B$	Av[b]
2	*a*	−1.3568 (0.0008)			−1.3572 (0.0008)	−1.3569 (0.0008)
	b	0.4768 (0.0026)			0.4803 (0.0018)	0.4757 (0.0037)
	c	0.5675 (0.0020)			0.5640 (0.0024)	0.5673 (0.0024)
8	*a*	1.3568 (0.0008)		1.3551 (0.0008)	1.3585 (0.0008)	1.3569 (0.0008)
	b	−0.4768 (0.0026)		−0.4705 (0.0050)	−0.4753 (0.0054)	−0.4757 (0.0037)
	c	0.5675 (0.0020)		0.5714 (0.0024)	0.5663 (0.0028)	0.5673 (0.0024)
3	*a*	−0.3660 (0.0032)			−0.3652 (0.0031)	−0.3629 (0.0034)
	b	0.8699 (0.0020)			0.8691 (0.0036)	0.8702 (0.0022)
	c	−0.8969 (0.0016)			−0.8964 (0.0020)	−0.8962 (0.0016)
4	*a*	0.3660 (0.0032)	0.3587 (0.0038)		0.3617 (0.0034)	0.3629 (0.0034)
	b	−0.8699 (0.0020)	−0.8670 (0.0024)		−0.8747 (0.0010)	−0.8702 (0.0022)
	c	−0.8969 (0.0016)	−0.8992 (0.0015)		−0.8923 (0.0015)	−0.8962 (0.0016)
5	*a*	−0.2285 (0.0052)	−0.2307 (0.0048)	−0.2274 (0.0047)		−0.2292 (0.0049)
	b	−0.9461 (0.0018)	−0.9479 (0.0013)	−0.9454 (0.0029)		−0.9471 (0.0018)
	c	0.8885 (0.0016)	0.8861 (0.0014)	0.8879 (0.0017)		0.8868 (0.0015)
6	*a*	0.2285 (0.0052)	0.2378 (0.0044)	0.2216 (0.0054)		0.2292 (0.0049)
	b	0.9461 (0.0018)	0.9455 (0.0021)	0.9504 (0.0010)		0.9471 (0.0018)
	c	0.8885 (0.0016)	0.8879 (0.0015)	0.8838 (0.0014)		0.8868 (0.0015)

[a] Errors based on a 0.04-MHz uncertainty in the rotational constants are given in parentheses. [b] Averages are based on absolute coordinates of all symmetrically equivalent atoms assuming C_2 symmetry.

Table VII. Bond Distances and Bond Angles for $1,7\text{-}C_2B_6H_8$

Atoms	Distance, Å: This work[a]	Distance, Å: Ref 4
B_2-B_3	1.813 ± 0.007	1.772 ± 0.008
B_2-B_5	1.843 ± 0.008	1.806 ± 0.007
B_2-B_6	1.685 ± 0.008	1.696 ± 0.009
B_3-B_4	1.886 ± 0.007	1.894 ± 0.007
B_3-B_6	1.880 ± 0.006	1.842 ± 0.007
B_5-B_6	1.949 ± 0.006	1.902 ± 0.007

Atoms	Angle, deg: This work[a]	Angle, deg: Ref 4
B_2-B_5-B_6	52.7 ± 0.5	54.4 ± 0.3
B_5-B_2-B_6	66.9 ± 0.6	65.7 ± 0.3
B_2-B_6-B_5	60.4 ± 0.6	59.9 ± 0.3
B_2-B_3-B_6	54.3 ± 0.5	55.9 ± 0.3
B_2-B_6-B_3	60.8 ± 0.5	59.9 ± 0.3
B_3-B_2-B_6	64.9 ± 0.5	64.1 ± 0.3

[a] The quoted errors are obtained from the errors given in Table VI and by estimating zero-point vibrational errors.

Coordinates for all of the boron atoms with errors are listed in Table VI. The final bond distances and bond angles were calculated from the average values of the coordinates and are compared to those determined by x-ray diffraction techniques in Table VII. Uncertainties in the bond distances are based on estimated errors in the rotational constants of 0.04 MHz.

Discussion

Although the ^{13}C and ^{2}H species were not studied, a meaningful boron skeletal structure was obtained. With the exception of a few minor deviations, our results support the distorted skeletal structure of $B_6H_6C_2(CH_3)_2$ as determined by Hart and Lipscomb.[4] The C_2B_6 framework is essentially a dodecahedron which is distorted toward a square antiprism. This geometry is quite similar to that of the isoelectronic species $B_8H_8^{2-}$ [9] and B_8Cl_8.[1] Bond distances follow the same general trend and are longest between atoms with high coordination number. The electron-deficient boron atoms B(3) and B(4) have a rather long bond distance of 1.886 Å which is comparable to the B–B distance in $C_4B_2H_6$ having similar electron deficiency.[10] The unusually long B(5)–B(6) distance of 1.949 Å also contributes to the distortion toward a square shape. Furthermore, the ratio of the bond distances B(2)–B(8) to B(5)–B(6) of 1.48 is slightly less than that obtained from x-ray data and is significantly smaller than the 1.62 value for an ideal polyhedron. It has been suggested that the carbon–carbon nuclear charge repulsions are partly responsible for these distortions.[11] It is interesting to note that except for a slight decrease in the B(2)–B(6) and B(3)–B(4) distances a general expansion of the molecule is apparent. This suggests that crystal packing forces, not present in gas phase, may compress the molecule.

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Registry No. $1,7\text{-}C_2B_6H_8$, 23732-90-3; $2\text{-}^{10}B\text{-}1,7\text{-}C_2B_6H_8$, 59110-01-9; $3\text{-}^{10}B\text{-}1,7\text{-}C_2B_6H_8$, 59110-02-0; $5\text{-}^{10}B\text{-}1,7\text{-}C_2B_6H_8$, 59110-03-1; $2,4\text{-}^{10}B\text{-}1,7\text{-}C_2B_6H_8$, 59110-04-2; $2,5\text{-}^{10}B\text{-}1,7\text{-}C_2B_6H_8$, 59110-05-3; $2,6\text{-}^{10}B\text{-}1,7\text{-}C_2B_6H_8$, 59110-06-4; $3,5\text{-}^{10}B\text{-}1,7\text{-}C_2B_6H_8$, 59123-37-4; $3,6\text{-}^{10}B\text{-}1,7\text{-}C_2B_6H_8$, 59110-07-5.

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