mary C≡N stretching force constants for the BF_3 adduct (f_{CN} = 18.8 mdyn/Å) with that of the free acetonitrile[31] (f_{CN} = 17.4 mdyn/Å) shows that this constant does increase upon adduct formation. The increase in f_{CN} indicates an increase in the C≡N bond strength upon coordination, which agrees with the decrease in the C≡N bond length observed in the crystal structures.[13]

The CC stretching frequency is also found to increase upon adduct formation and there is an indication that the bond length may decrease. However, the force constants for the adduct (f_{CC} = 5.32 mdyn/Å) and for free acetonitrile (f_{CC} = 5.3 mdyn/Å) agree within their limits of error. Part of the increase in ν_4 can be attributed to kinematic coupling with BN stretch since this force constant contributes to the CC stretching frequency. The increase in F_{11} and F_{99} and the decrease in F_{33} and $F_{10,10}$ agree with the shifts observed for ν_1, ν_3, ν_9, and ν_{10} upon complexation. The remaining force constants for the acetonitrile part of the molecule are similar to those of free acetonitrile.

The force constant for the donor–acceptor BN bond is of particular interest. The BN valence force constants for F_3BNH_3, $F_3BN(CH_3)_3$, and F_3BNCCH_3 are 3.97,[16] 3.53,[26] and 2.5 mdyn/Å. Thus the decrease in ν_{BN} on going from a strong to a weak adduct is matched by a decrease in f_{BN}. The weak nature of the BN bond in F_3BNCCH_3 is clear from ν_{BN}, f_{BN}, and the BN bond length (r_{BN} = 1.63 Å).[13] However, a monotonic correlation is not found between ν_{BN}, f_{BN}, or ΔH_f° and the BN bond lengths (r_{BN} = 1.60 Å for F_3BNH_3 and r_{BN} = 1.585 Å for $F_3BN(CH_3)_3$).[32]

The BF_3 stretching force constant shows the expected decrease upon coordination (f_{BF} = 4.8 mdyn/Å for F_3BNCCH_3). However, no simple monotonic correlations involving f_{BF} for adducts of this type can be found with the existing data.

Acknowledgments.—This research was supported by the National Science Foundation through Grants GP-6676 and -10117 and by the ARPA through the Northwestern Materials Research Center. We thank Professor R. C. Taylor for supplying a copy of P. Clippard's thesis and for helpful discussions. We are also grateful to Dr. G. M. Begun for a copy of Jacques Le Calve's thesis.

(31) The CN force constant of free acetonitrile used here was determined from liquid vibrational data on $H_3CC^{15}N$, H_3CCN, and D_3CCN. Comparisons with this force field minimize the errors resulting from phase differences, since the frequencies for nitriles are known to be phase dependent: B. H. Thomas and W. L. Orville-Thomas, *J. Mol. Struct.*, **3**, 161 (1969). In this force field, f_{CN} is lower than that of Duncan[24] and the difference may be attributed to the phase dependence of ν_{CN} and the change in the off-diagonal constant involving C≡N and CC bond stretch interaction.

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Boron–Nitrogen Compounds. XXXIII.[1] A Normal-Coordinate Analysis of Borazine

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Utilizing a recent reassignment of the vibrational spectrum of borazine, $(-BH-NH-)_3$, and isotopically labeled derivatives thereof, a normal-coordinate analysis on this six-membered heterocycle has been performed. The calculated valence force field was adjusted to provide a good fit for all of the available data. When the entire set of suggested assignments for the normal vibrations of $(-BH-NH-)_3$, $(-^{10}BH-NH-)_3$, $(-BH-ND-)_3$, $(-^{10}BH-ND-)_3$, $(-BD-NH-)_3$, $(-^{10}BD-NH-)_3$, and $(-BD-ND-)_3$ was utilized in a simultaneous least-squares adjustment, the average error between all of the calculated and observed frequencies was 1.01%. The calculated force constants are in agreement with recent judgments on the strength of the various bonds in the borazine molecule. The calculated potential energy distribution of the isotopically labeled derivatives indicates that the character of several BH and NH vibrations is altered substantially upon deuteration at either the boron or the nitrogen atoms. Displacements calculated for the parent borazine molecule reveal appreciable movement of the annular atoms out of the molecular plane.

Introduction

The vibrational spectrum of borazine, $(-BH-NH-)_3$, has been recently reexamined using isotopically labeled derivatives.[2] Based on the resultant data, reassignments of several fundamentals of borazine were suggested; they should have a significant bearing on the previously reported values[3-5] of a number of valence force constants of borazine. For example, a significant change in the B–N force constant was anticipated due to the reassignment of the highest B–N stretching mode of species E′ from 1605 to 1465 cm^{-1}.[2]

Also, some minor uncertainties had remained with respect to the assignment of fundamentals[2] and it

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was hoped that a normal-coordinate analysis of the data would clarify the situation and increase our understanding of the borazine molecule. The 990-cm^{-1} band had been reassigned to an E′ fundamental;[2] however, it is the only E′ mode that was observed without a Raman counterpart. Also, previous calculations by Crawford and Edsall[3] and Kubo and coworkers[6] indicated that ν_8, an A_2'' fundamental, should be found at a much higher frequency than the 917-cm^{-1} mode which was reassigned to ν_8 primarily on the basis of its band shape.[2,7]

Two previous calculations on borazine have assumed all interaction force constants to be zero.[3,6] Silberman[5] included one interaction force constant (a bend–bend interaction) in his calculations where only the in-plane modes were considered. The multiple possibilities of using data derived from isotopically labeled borazine have enabled us to obtain a least-squares-adjusted force field which includes those interaction force constants which were tested and found to be significant.

Detailed descriptions of each of the normal modes were obtained in terms of Cartesian atom displacements and potential energy distribution. The calculated atom displacements indicated that several of the out-of-plane fundamentals involve large displacements of annular atoms from the molecular plane. The potential energy distribution obtained for the normal modes indicates that the nature of the B–N and N–H vibrations is substantially altered upon deuteration of either or both the boron and the nitrogen atoms.

The Molecular Model

The molecular structure of borazine has been investigated by electron diffraction, and D_{3h} symmetry has been assigned to the molecule; all bond angles were calculated to be 120° and the BN bond length was given with a value of 1.44 Å.[8,9] The NH and BH bond distances were given with 1.02 and 1.20 Å, respectively. On this basis, the following representation can be readily determined

$$\Gamma = 4\ A_1' + 3\ A_2' + 7\ E' + 3\ E'' + 3\ A_2''$$

This term depicts the number and corresponding symmetry of the expected fundamentals of borazine.

Forty-two internal coordinates were constructed using the notation as depicted in Figure 1. The following representation was determined for the internal coordinates

$$\Gamma = 7\ A_1' + 3\ A_2' + 10\ E' + A_1'' + 3\ A_2'' + 4\ E''$$

This expression leads to a redundancy representation of

$$\Gamma = 3\ A_1' + 3\ E' + A_1'' + E''$$

The latter term was verified by the diagonalized *G* matrix. Redundancies were removed by methods discussed by Schachtschneider.[10] The use of symmetry coordinates greatly facilitated the calculation by factoring the *F* and *G* matrices in accordance with the representation generated by the internal coordinates.

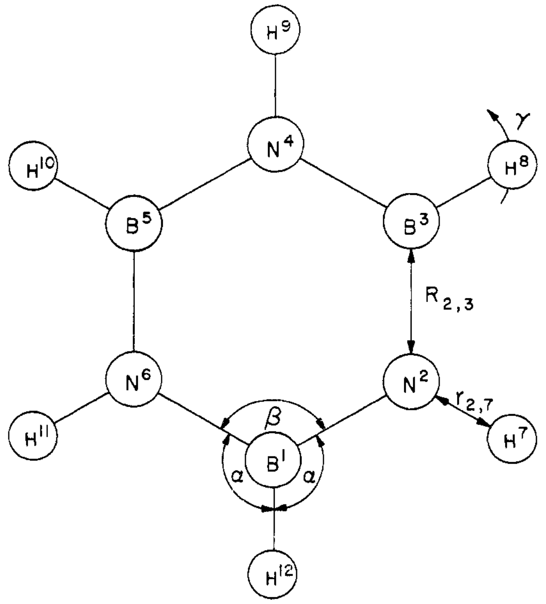

Figure 1.—Internal coordinates of borazine. (Numbering of atoms refers to the numbering used in the calculations.)

Calculations of Frequencies and Force Constants

All calculations were performed on an IBM 360-50 digital computer at the University of Kentucky Computing Center. The programs, which use the Wilson *FG* technique[11] for setting up the vibrational secular equation, were written by Schachtschneider.[10]

A number of assumptions were necessary in order to facilitate the performance of the normal-coordinate analysis. For example, although 23 interaction force constants were included, most of the off-diagonal elements in the force field were assumed to be zero; the effects of anharmonicity of NH and BH vibrations have also been ignored. An initial force field was constructed using interaction force constants judged to be significant in cyclic molecules[12] (*cf.* Table I); primarily, interaction force constants were considered for those motions involving displacements of the same atoms. Additional interaction force constants were considered, and, in all cases, a least-squares adjustment was applied in an effort to test the significance of the modifications on the force field. The final valence force field as used in the following calculations is reflected in Table I.

One of the first objectives in performing the normal-coordinate analysis of borazine was to resolve the minor uncertainties which remained in the assignment of fundamentals.[2] In pursuing this objective, the "di-

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Table I

Force Constants of Borazine[a]

No.	Description	Value[b]	Estd error
	A. Valence Force Constants		
1	BN str	5.462306	±0.152900
2	BH str	3.349860	±0.007700
3	NH str	6.667682	±0.001100
4	Planar BH bend	0.554421	±0.000000
5	Planar NH bend	0.459214	±0.001300
6	NBN ring distortion	1.344997	±0.0
7	BNB ring distortion	0.908514	±0.0
8	Nonplanar BH bend	0.517036	±0.0
9	Nonplanar NH bend	0.331620	±0.0
10	BN torsion	0.232487	±0.050000
	B. Interaction Force Constants[c]		
11	B^1N^2 str–N^2B^3 str	1.212458	±0.0
12	B^1N^2 str B^1N^6 str	0.560607	±0.100000
13	B^1N^2 str–B^3N^4 str	−0.263022	±0.050000
14	B^1N^2 str–B^4N^5 str	−0.019357	±0.010000
15	Planar B^1H bend–B^1H str	−0.181614	±0.057000
16	Planar N^2H bend–N^2H str	−0.169943	±0.016700
17	Planar B^1H bend–B^1N^2 str	0.165007	±0.140000
18	Planar N^2H bend–N^2B^3 str	0.032108	±0.020000
19	Planar B^1H bend–B^1N^6 str	−0.064749	±0.023000
20	Planar B^2H bend–N^2B^1 str	−0.054853	±0.022000
21	$N^2B^1N^6$ ring distortion–$B^1N^2B^3$ ring distortion	0.239252	±0.0
22	$N^2B^1N^6$ ring distortion–$N^2B^3N^4$ ring distortion	0.097247	±0.006300
23	$N^2B^1N^6$ ring distortion–B^1N^2 str	0.143867	±0.065000
24	$B^1N^2B^3$ ring distortion–N^2B^3 str	0.032108	±0.015400
25	Planar N^2B^1H bend–planar N^6B^1H bend	−0.008442	±0.012500
26	Planar B^1N^2H bend–planar B^3N^2H bend	0.018106	±0.010000
27	Planar N^2B^1H bend–planar B^1N^2H bend	0.020744	±0.007100
28	B^1N^2 torsion–nonplanar B^1H bend	−0.128124	±0.016800
29	B^1N^2 torsion–nonplanar N^2H bend	−0.161528	±0.005200
30	Nonplanar B^1H bend–nonplanar N^2H bend	−0.052649	±0.011000
31	B^1N^2 torsion–N^2B^3 torsion	0.001671	±0.001000
32	B^1N^2 torsion–B^3N^4 torsion	0.022024	±0.013800
33	B^1N^2 torsion–N^4B^5 torsion	−0.036196	±0.007500

[a] Calculated from data in Tables II and III. [b] Units: stretchings, mdyn/Å; bendings, mdyn Å/radian^2; stretch–bend interactions, mdyn/radian. [c] Superscripts denote numbering of atoms as depicted in Figure 1; all of the symmetrical interactions were included in the calculations though only one example of each type is depicted.

Table II

Calculated and Observed[2] Frequencies of Borazine Fundamentals (cm^{-1})[a]

Species	Obsd	Calcd	% error	$\Delta\nu$, cm^{-1}
A_1'	3452	3486	−0.986	−34
	2535	2520	0.580	15
	940	946	−0.609	−6
	852	855	−0.386	−3
E'	3486	3485	0.036	1
	2520	2519	0.061	−1
	1465	1463	0.131	2
	1406	1399	0.495	7
	1096	1105	−0.809	9
	990	987	0.344	3
	518	518	0.034	0
A_2''	917	933	−1.656	−16
	719	724	−0.661	−5
	394	379	3.776	15
E''	968	942	2.665	26
	798	770	3.505	28
	288	285	1.019	3
		Av error	1.04	10.2

[a] The per cent error presented here was obtained before the calculated frequency was rounded off to the nearest wave number.

agonal" force constants as proposed by Crawford and Edsall[3] and some estimated interaction force constants were adjusted by a least-squares perturbation technique in an effort to fit the reported[2] reassignments for the parent borazine and its isotopically labeled species. The calculated data as compared with the proposed[2] frequency assignments are listed in Tables II and III. The data compiled in these tables indicate a very good agreement between calculated and observed (assigned[2]) frequencies. Some of the resultant force constants are compared with previous calculations[3,5] and are listed in Table IV.

A complete set of force constants including interaction constants calculated for the above data was obtained after extensive perturbations; the numerical values including estimated errors are illustrated in Table I. These data appear to be consistent with values expected on the basis of the molecular model and with literature values for the type of internal displacement under consideration.[13] The value of about 5.5 mdyn/Å reflects a sizable reduction in the value of the BN force constant as compared to the value of 6.3 mdyn/Å originally proposed by Crawford and Edsall.[3] However, this difference was anticipated on the basis of the reassignment of the 1605-cm^{-1} mode from a BN ring vibration to a band belonging to the impurity, diborane.[2]

The least-squares adjustment technique used in our calculations has facilitated the calculation of estimated errors for the force constants as shown in Table I. However, in many instances little significance can be placed on these error estimates due to the random distribution of errors with respect to the frequencies. This randomness might be attributed to the anharmonicity of the B–H and N–H vibrations. Also, several of the larger estimated errors noted could be due to the fact that the corresponding force constants are not particularly sensitive to the observed data.[10]

Interaction force constants are of particular significance in the case of out-of-plane vibrations. The relatively large value of the (B–H)–torsion and (N–H)–torsion interaction force constants as shown in Table I is consistent with the data obtained in normal-coordinate calculations on the isoelectronic benzene molecule for the analogous interaction.[14] The relative positive or negative character of the internal coordinates

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TABLE III

CALCULATED AND OBSERVED FREQUENCIES (cm^{-1}) OF ISOTOPICALLY LABELED BORAZINES

Normal vib	$(^{10}BHNH)_3$		$(BDNH)_3$		$(^{10}BDNH)_3$		$(BHND)_3$		$(^{10}BHND)_3$		$(BDND)_3$	
	Obsd	Calcd	Obsd	Calcd	Obsd	Calcd	Obsd	Calcd	Obsd	Calcd	Obsd	Calcd
						A_1'						
ν_1	3452	3486	3452	3486	...	3486	2579	2572	...	2574	2567	2569
ν_2	2554	2533	1893	1910	...	1932	2521	2517	...	2529	1895	1909
ν_3	978	976	903	892	...	911	940	945	...	976	901	886
ν_4	852	856	852	847	...	851	824	822	...	823	824	818
						E'						
ν_{11}	3486	3485	3485	3485	3484	3485	2594	2568	2621	2569	2582	2568
ν_{12}	2535	2531	1897	1914	1921	1935	2519	2518	2522	2530	1895	1912
ν_{13}	1487	1500	1440	1423	1462	1462	1438	1448	1472	1484	1418	1406
ν_{14}	1408	1407	1328	1363	1392	1366	1289	1298	1304	1310	1245	1240
ν_{15}	1102	1108	1022	1008	1030	1013	1071	1060	1075	1066	797	807
ν_{16}	1005	996	813	781	816	783	786	789	796	793	766	764
ν_{17}	526	525	509	508	516	514	507	508	...	514	499	499
						A_2''						
ν_8	930	940	808	791	820	796	900	916	913	925	782	756
ν_9	725	728	716	708	723	718	546	539	551	542	540	537
ν_{10}	396	383	326	329	326	331	383	374	385	377	323	327
						E''						
ν_{18}	...	952	788	806	...	811	960	936	...	947	...	767
ν_{19}	...	771	725	737	...	747	550	583	...	583	...	581
ν_{20}	291	289	262	259	...	261	279	281	...	285	255	254
Av error												
$\Delta\nu$, cm^{-1}	8.28		14.34		12.63		10.13		13.16		8.80	
%	0.728		1.351		1.378		1.199		1.088		0.858	

TABLE IV

COMPARISON OF FORCE CONSTANTS OF BORAZINE (MDYN/Å)

No.	Description	*a*	*b*	*c*
1	BN str	6.300	6.609	5.462
2	BH str	3.423	3.428	3.350
3	NH str	6.524	6.765	6.668
4	Planar BH bend	0.35	0.778	0.554
5	Planar NH bend	0.65	0.347	0.459
6	NBN ring distortion	0.525	0.957	1.345
7	BNB ring distortion	0.525	0.957	0.909
8	Nonplanar BH bend	0.23	...	0.517
9	Nonplanar NH bend	0.42	...	0.332
10	BN torsion	0.10	...	0.232
11	BNB–NBN interaction	...	−0.05	0.239

[a] Reported by Crawford and Edsall.[3] [b] Reported by Silberman[5] (bending and interaction force constants in mdyn Å). [c] This work based on reported[2] assignments and data in Table II (bending and interaction force constants in mdyn Å/radian^2).

TABLE V

POTENTIAL ENERGY DISTRIBUTION (%) OF ν_{15} AND ν_{16} (cm^{-1}) OF BORAZINES

Borazine species	ν_{15}	ν(NB)	δ(BH)	δ(NH)	ν_{16}	ν(NB)	δ(BH)	δ(NH)	δ(NBN)	δ(BNB)
$(BHNH)_3$	1105	29	43	17	987	47	16	21	8	0
$(^{10}BHNH)_3$	1108	26	47	17	996	44	17	22	8	0
$(BHND)_3$	1060	26	51	6	790	21	2	71	6	0
$(BDNH)_3$	1008	52	7	30	780	14	74	0	1	0
$(BDND)_3$	807	12	40	42	764	21	38	29	5	0
$(^{10}BDNH)_3$	1013	51	6	31	783	13	74	0	1	0
$(^{10}BHND)_3$	1066	23	55	5	793	20	2	72	6	0

involved in this interaction must correspond with the sign of the element in the force constant matrix in order to obtain the correct contribution to the potential energy function. If this point is not taken into consideration, it will not destroy the symmetry of the calculation and hence will not be detected by improper symmetry species factoring; however, it will result in unusually high values for the frequency of ν_8. The authors are greatly indebted to Dr. J. Scherer for his extremely valuable advice concerning this matter. It may be pointed out that similar high-frequency values for ν_8 are obtained if the cited interaction force constants are deleted. As a matter of fact, all previous calculations on the borazine molecule resulted in a value of about 1200 cm^{-1} for the frequency of ν_8.[3,6] The same situation holds true for calculations of the vibrational spectra of B-trihaloborazines, $(-BX-NH-)_3$, which are presently being investigated in our laboratories.

The potential energy distributions calculated for ν_{15} and ν_{16} are presented in Table V. Kubo and coworkers[15] suggested the assignment of ν_{15} and ν_{16} to in-plane BH and NH deformations, respectively, on the basis of isotopic data obtained on $(-BH-ND-)_3$. Crawford and Edsall[3] attributed ν_{15} and ν_{16} to NH and BH deformations, respectively, based on their

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(15) H. Watanabe, T. Totani, T. Nakagawa, and M. Kubo, *Spectrochim. Acta*, **16**, 1076 (1960).

Table VI

Calculated and Observed Frequencies and Potential Energy Distribution[a] of Borazine

Planar modes	Potential energy distribution							Freq, cm^{-1}	
	NH str	BH str	BN str	BH planar bend	NH planar bend	NBN ring distortion	BNB ring distortion	Obsd	Calcd
				A_1'					
ν_1	0.99	. . .	. . .	. . .	. . .	. . .	. . .	3452	3486
ν_2	. . .	0.97	. . .	. . .	. . .	. . .	. . .	2535	2520
ν_3	. . .	0.03	0.57	0.04	0.03	0.18	0.12	940	946
ν_4	0.01	. . .	0.23	0.09	0.07	0.43	0.29	852	855
				E'					
ν_{11}	0.99	. . .	. . .	. . .	. . .	. . .	. . .	3486	3485
ν_{12}	. . .	0.96	. . .	. . .	. . .	. . .	. . .	2520	2519
ν_{13}	. . .	. . .	0.63	0.41	0.01		0.05	1465	1463
ν_{14}	0.02	. . .	0.37	0.03	0.67	0.06	. . .	1406	1400
ν_{15}	. . .	. . .	0.29	0.43	0.17	0.02	0.02	1096	1105
ν_{16}	. . .	. . .	0.47	0.16	0.21	0.08	. . .	990	987
ν_{17}	. . .	. . .	0.16	0.11	0.10	0.50	0.41	518	518

Nonplanar modes	Potential energy distribution									Freq, cm^{-1}	
							Torsion–torsion				
	BH wag	NH wag	BN torsion	NH–BH interaction	BH–torsion interaction	NH–torsion interaction	No. 31	No. 32	No. 33	Obsd	Calcd
					A_2''						
ν_8	1.10	0.30	0.21	0.29	−0.51	−0.42	. . .	0.04	−0.03	917	933
ν_9	0.29	0.52	0.15	−0.20	−0.22	−0.45	. . .	0.03	−0.02	719	724
ν_{10}	0.09	2.29	3.40	0.23	−0.59	−4.59	0.05	0.64	−0.53	394	379
					E''						
ν_{18}	1.09	0.13	0.07	0.09	−0.26	−0.14	. . .	. . .	0.01	968	942
ν_{19}	0.09	1.01	. . .	−0.08	. . .	. . .	. . .	. . .	. . .	798	770
ν_{20}	0.15	0.91	2.27	0.09	−0.53	−2.05	0.02	−0.21	0.35	288	285

[a] In some cases the PED's given for in-plane modes do not add up to 1 due to contributions of interaction constants.

normal-coordinate calculations, whereas Price, *et al.*,[16] have assigned these modes to either BH or NH bending or to a combination of both. The calculations reported in the present study seem to confirm that the specific assignment of ν_{15} and ν_{16} is dependent on the annular atoms selected for deuteration. The exact nature of the normal coordinates is subject to variation, and the interpretation of either Kubo, *et al.*,[15] or Crawford and Edsall[3] can be justified from the isotopic data. This variation in the nature of the normal vibration may interpret the spectral dissimilarities observed[2] in certain regions of the vibrational spectra of the various deuterated borazine derivatives. The potential energy distribution of all observed fundamentals of the parent borazine is depicted in Table VI.

Discussion

On the basis of the reassignments of the vibrational modes of borazine as suggested recently,[2] a normal-coordinate analysis of the molecule has been performed. The present data are clearly in consonance with the concept of delocalized electrons in the heterocycle and a BN bond order greater than 1, though the force constant for the BN stretch is significantly smaller than that previously accepted.[3]

The calculations clearly substantiate the revised[2] assignments of the borazine fundamentals and they facilitate complete descriptions of the latter in terms of potential energy distribution and Cartesian atom displacements. Also, the significance of certain interaction constants particularly for the calculation of out-of-plane fundamentals is illustrated.

After the work reported herein had been virtually completed, a reinvestigation of the structure of borazine was described.[17] The reported minor changes in the bond distance and angles will have no significant effect on the validity of the present calculations. However, the postulated[17] possibility of C_2 symmetry is in conflict with the reported spectral data[2] as well as the present normal-coordinate analysis. Assumption of C_2 symmetry would require the observation of 16 additional Raman lines all of which should have corresponding infrared absorptions. Furthermore, if the symmetry is lowered from D_{3h} to C_2, all infrared-active bands should have corresponding Raman lines. The quality of the reported spectra[2] makes it appear unlikely that such a large number of additional Raman lines should have escaped detection. On this basis, it appears unreasonable to discuss the borazine molecule with the assumption of C_2 symmetry. Indeed, Harshbarger, *et al.*,[17] discussed an alternate interpretation of their data. It was suggested[17] that the "shrinkage effects" which were observed for the C_2 model of borazine might be due to the occurrence of large out-of-plane deformations of a D_{3h} species. Hence, it is interesting to note that the equilibrium Cartesian coordinates calculated on the basis of the C_2 model of borazine[17] compare favorably with displacements for several out-of-plane vibrations calculated in the

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TABLE VII

CALCULATED OUT-OF-PLANE ATOM DISPLACEMENTS[a] AS COMPARED TO C_2 MODEL EQUILIBRIUM COORDINATES

Atom	Mass	C_2 model	ν_8	ν_9	ν_{10}	ν_{18}	ν_{19}	ν_{20}
1	10.811	0.0	0.1518	−0.1345	0.1803	−0.2258	0.0783	−0.2057
2	14.007	0.1065	−0.0801	0.0147	−0.1972	−0.0004	−0.0350	−0.0662
3	10.811	−0.1065	0.1518	−0.1345	0.1803	0.2272	−0.1071	0.2717
4	14.007	0.0	−0.0801	0.0147	−0.1972	−0.0658	−0.0950	−0.2064
5	10.811	0.1065	0.1518	−0.1345	0.1803	−0.0014	0.0288	−0.0660
6	14.007	−0.1065	−0.0801	0.0147	−0.1972	0.0662	0.1300	0.2726
7	1.008	0.7332	0.3957	1.0429	−0.1690	0.0019	0.3833	−0.0660
8	1.008	−0.8588	−0.9109	0.1949	0.6365	−1.1297	0.2838	0.7299
9	1.008	0.0	0.3957	1.0429	0.1690	0.3223	1.0418	−0.2058
10	1.008	0.8588	−0.9109	0.1949	0.6365	0.0068	−0.0763	−0.1773
11	1.008	−0.7332	0.3957	1.0429	0.1690	−0.3242	−1.4251	0.2718
12	1.008	0.0	−0.9109	0.1949	0.6365	1.1229	−0.2075	−0.5526

[a] Assuming a D_{3h} model.

present work which utilizes D_{3h} symmetry (Table VII). The vibrational mean amplitudes calculated by Harshberger, *et al.*,[17] using a D_{3h} and a C_2 model are depicted in Table VIII. The data are very similar but those obtained for the D_{3h} model are in slightly better agreement with the data obtained from the present normal-coordinate analysis. These observations tend to indicate that the borazine molecule is indeed best discussed on the basis of D_{3h} symmetry.

TABLE VIII

VIBRATIONAL MEAN AMPLITUDES

Type	D_{3h}[17]	C_2[17]	This work
B–N	0.0573	0.057 ± 0.002	0.0478734
B–H	0.0651	0.059 ± 0.012	0.0856076
N–H	0.0784	0.078 ± 0.009	0.0717101
B···B	0.0670	0.074 ± 0.003	0.0634850
N···N	0.0670	0.074 ± 0.003	0.0631891
N···B	0.0724	0.072 ± 0.003	...

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An Assignment of the Hydrogen-1 Magnetic Resonance Spectrum of Decaborane at 220 MHz

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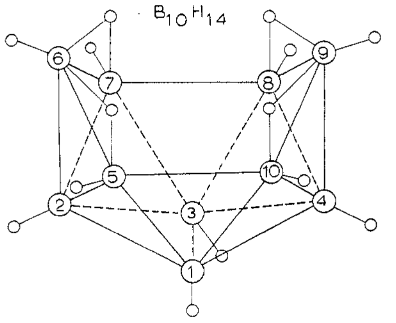
The ^{1}H nmr spectrum of $B_{10}H_{14}$ has been elucidated through the study of the 2-$BrB_{10}H_{13}$ and 1,2,3,4-$B_{10}H_{10}D_4$ derivatives. Both solvent studies and dilution studies are reported.

The structure of $B_{10}H_{14}$, given below, is well documented and can be analyzed by symmetry arguments to be composed of four potentially nonequivalent boron environments, the 1,3; 2,4; 5,7,8,10; and 6,9 positions.



The ^{11}B nmr spectrum of $B_{10}H_{14}$ consists of four sets of overlapping doublets which have been assigned[2,3] (in order of increasing field strength) to the 1,3; 6,9; 5,7,8,10; and 2,4 positions respectively.

The analysis of the ^{1}H nmr of $B_{10}H_{14}$ is complicated by the $^3/_2$ nuclear spin of the ^{11}B isotope, which results in a quartet of equal intensity lines for each non-

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