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SYNTHESIS, CHARACTERIZATION AND VIBRATIONAL INVESTIGATION OF DIVINYLBORINIC ANHYDRIDE

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Summary

The new molecule divinylborinic anhydride $[(\text{CH}_2=\text{CH})_2\text{B}]_2\text{O}$ has been prepared by the limited hydrolysis of divinylchloroborane. Characterization of the compound has included the preparation of 1 : 1 adducts with trimethylphosphine, dimethylphosphine and trimethylamine. Boron-11 and carbon-13 NMR spectra have been obtained and have been interpreted in terms of mesomeric interactions between the empty boron $p\pi$ orbital and unshared pairs of electrons on oxygen as well as the π electron system of the vinyl moiety. The Raman spectra ($3500\text{--}20\text{ cm}^{-1}$) of liquid and solid $[(\text{C}_2\text{H}_3)_2\text{B}]_2\text{O}$ and the infrared spectra ($3500\text{--}200\text{ cm}^{-1}$) of gaseous and solid $[(\text{C}_2\text{H}_3)_2\text{B}]_2\text{O}^*$ have been investigated for both the ^{16}O and ^{18}O isotopic species. The vibrational data indicate that the molecule possesses C_1 symmetry and a linear B—O—B angle.

Introduction

In a recent report from this laboratory [1], the vibrational spectra of dimethylborinic anhydride $(\text{CH}_3)_2\text{BOB}(\text{CH}_3)_2$ were presented and interpreted in terms of C_2 molecular symmetry in the fluid phases. A bent B—O—B skeleton with the $\text{B}(\text{CH}_3)_2$ groups twisted was implied. In the solid phase, however,

* $\text{C}_2\text{H}_3 = \text{CH}_2=\text{CH}$.

the B—O—B skeleton was found to be linear and the spectra were interpreted in terms of D_{2h} molecular symmetry.

The C_2 molecular structure of $(CH_3)_2BOB(CH_3)_2$ was first postulated by Lanthier and Graham [2] based on the temperature dependence of the 1H NMR spectrum of the molecule. A bent B—O—B skeleton with the $B(CH_3)_2$ groups twisted was suggested. This conformation would maximize a $p\pi-p\pi$ interaction between the sp^3 hybridized lone pairs of oxygen with the two boron atoms.

The C_2 molecular structure was subsequently confirmed by an electron diffraction study [3]. In this study, a B—O—B angle of $144.4 \pm 2.7^\circ$ and a dihedral angle of $72.1 \pm 6.8^\circ$ between the BC_2 planes was reported. A question remains, however, as to the importance of the postulated B—O pi interaction in determining the molecular geometry of dimethylborinic anhydride.

Since we have previously presented evidence which suggests a pi interaction occurs between the vinyl substituents and the boron atom in vinylhaloboranes [4,5] and trivinylborane [5,6], we felt that a study of the unknown divinylborinic anhydride molecule might help assess the importance of the B—O pi interaction in determining the molecular structure of dimethylborinic anhydride. Any pi delocalization within the $B(C_2H_3)_2$ groups should reduce the Lewis acidity of the boron atoms with a concomitant reduction in any B—O pi interaction which might also exist. If a B—O pi interaction is important in determining molecular geometry, as was suggested for dimethylborinic anhydride, we anticipated that the molecular structure of divinylborinic anhydride would be substantially altered as a result of competition between the vinyl groups and oxygen for the boron $p\pi$ orbital. Thus, in order to more fully understand the factors which influence the structure of molecules containing a B—O—B linkage, we have undertaken the synthesis, characterization and vibrational investigation of the new molecule divinylborinic anhydride.

Experimental

All preparative work was carried out in a standard high vacuum system employing greaseless stopcocks. Divinylchloroborane was synthesized from tetravinyltin (M and T Chemicals Inc.) and BCl_3 (Stauffer) by condensing 57 mmoles BCl_3 into an all glass reaction vessel containing 10 ml (≈ 56 mmoles) degassed tetravinyltin. The 500 ml all glass reaction vessel was isolated from the vacuum line and warmed to room temperature. When both reactants began to melt, a vigorous exothermic reaction occurred. The rate of reaction was moderated by cooling the reaction vessel in liquid nitrogen. After several freeze-thaw cycles, the contents of the bulb were separated on a low temperature vacuum fractionation column. Products include $ClB(C_2H_3)_2$ along with smaller quantities of $Cl_2BC_2H_3$ and $B(C_2H_3)_3$.

Preparation of $(C_2H_3)_4B_2O$ and $(C_2H_3)_4B_2^{18}O$

Degassed, distilled H_2O (5.1 mmoles) or $H_2^{18}O$ (99 atom % ^{18}O , Stohler) and 10.9 mmoles $(C_2H_3)_2BCl$ were condensed into a 250 ml all-glass reaction vessel. The liquid nitrogen dewar was removed and the reaction vessel warmed to room temperature. As the compounds began to melt, vigorous effervescence

was observed for approximately one minute. No further reaction was observed even when the bulb was repeatedly frozen to -196°C and thawed. The contents of the vessel were vacuum fractionated yielding: 9.7 mmoles HCl; 1.5 mmoles of a mixture of $(\text{C}_2\text{H}_3)_2\text{BCl}$ and $(\text{C}_2\text{H}_3)_3\text{B}$; and 4.7 mmoles $(\text{C}_2\text{H}_3)_4\text{B}_2\text{O}$. Identity of known products was established by infrared and/or vapor pressure measurement.

Characterization

Divinylborinic anhydride is a relatively nonvolatile liquid with a vapor pressure of 8 Torr at 25.0°C and is spontaneously flammable on contact with air. The compound is thermally unstable and slowly decomposes at room temperature to $\text{B}(\text{C}_2\text{H}_3)_3$ $\{\delta(^{11}\text{B}) = +56.7 \text{ ppm}\}$ and $(\text{C}_2\text{H}_3\text{BO})_3$ $\{\delta(^{11}\text{B}) = +28.0 \text{ ppm}\}$. The latter formulation was inferred by the similarity of the ^{11}B chemical shift to that of several similar derivatives [7]. A pure sample of divinylborinic anhydride exhibited a melting point of -131°C (Stock plunger apparatus).

Spectroscopic studies

NMR spectra were acquired on a Varian Associates XL-100-15 spectrometer. A neat sample of $(\text{C}_2\text{H}_3)_4\text{B}_2\text{O}$ exhibited a single ^{11}B resonance 39.0 ppm deshielded with respect to external $\text{BF}_3 \cdot \text{O}(\text{C}_2\text{H}_5)_2$. The ^1H decoupled ^{13}C spectrum exhibited a broad singlet at $\delta(^{13}\text{C}) = +135.4 \text{ ppm}$ assigned to C_α and a sharp singlet at $\delta(^{13}\text{C}) = +137.0 \text{ ppm}$ assigned to C_β . The ^{13}C chemical shifts were referenced to external TMS.

Mass spectra were acquired on a Perkin-Elmer RMU-6 spectrometer. The mass spectrum of $(\text{C}_2\text{H}_3)_4\text{B}_2\text{O}$ is complex and no molecular ion was observed. Several ions observed which are consistent with the molecular formula include: $\text{C}_2\text{H}_3\text{BOH}^+$ $m/e = 55, 100\%$; $\text{C}_2\text{H}_3\text{BOB}^+$ $m/e = 65, 40\%$; $(\text{C}_2\text{H}_3)_2\text{BOH}^+$, $m/e = 82, 60\%$; $(\text{C}_2\text{H}_3)\text{BOB}(\text{C}_2\text{H}_2^+)$, $m/e = 91, 60\%$; $(\text{C}_2\text{H}_3)_2\text{BOB}(\text{C}_2\text{H}_2)^+$ $m/e = 118, 8\%$; $(\text{C}_2\text{H}_3)_2\text{BOB}(\text{C}_2\text{H}_3)^+$ $m/e = 119, 5\%$.

Additionally, an exact mass was determined for the $P - 1$ ion using an AEI MS 902 spectrometer: calculated for $^{12}\text{C}_8\text{H}_{11}\text{B}_2\text{O}$ 145.0996; found 145.0998.

Adduct formation

Trimethylphosphine, dimethylphosphine and trimethylamine adducts of divinylborinic anhydride were prepared by condensing a 1:2 mole ratio of $(\text{C}_2\text{H}_3)_4\text{B}_2\text{O}$ and the base into a reaction vessel equipped with a greaseless stopcock. The contents of the reaction vessel were slowly warmed to 0°C and held at that temperature for 15 minutes. The vessel was cooled to $\sim -35^{\circ}\text{C}$ and subjected to dynamic vacuum for several hours. The stoichiometry of the adducts was determined to be 1.0 to 1.0 after accounting for the $(\text{CH}_3)_3\text{P}$, $(\text{CH}_3)_2\text{PH}$ and $(\text{CH}_3)_3\text{N}$ recovered. ^{11}B NMR spectra of the 1 : 1 adducts were obtained. The trimethylamine adduct exhibited a single resonance ($\delta(^{11}\text{B}) = 20.4 \text{ ppm}$) with a half height line width of 130 Hz. The trimethylphosphine adduct also consisted of a single resonance ($\delta(^{11}\text{B}) = 18.3 \text{ ppm}$, $\Delta\nu_{1/2} = 110 \text{ Hz}$). The spectrum of the dimethylphosphine adduct consisted of three major resonances at $\delta(^{11}\text{B}) = 40.2 \text{ ppm}$ ($\Delta\nu_{1/2} = 70 \text{ Hz}$), 29.7 ppm (170 Hz) and -16.4 ppm (40 Hz). The ^{31}P NMR spectrum of the trimethylphosphine adduct of divinylborinic anhydride exhibited a single resonance at $\delta(^{31}\text{P}) = -45.0 \text{ ppm}$ ($\Delta\nu_{1/2} = 30 \text{ Hz}$) (referenced to 85% o- H_3PO_4).

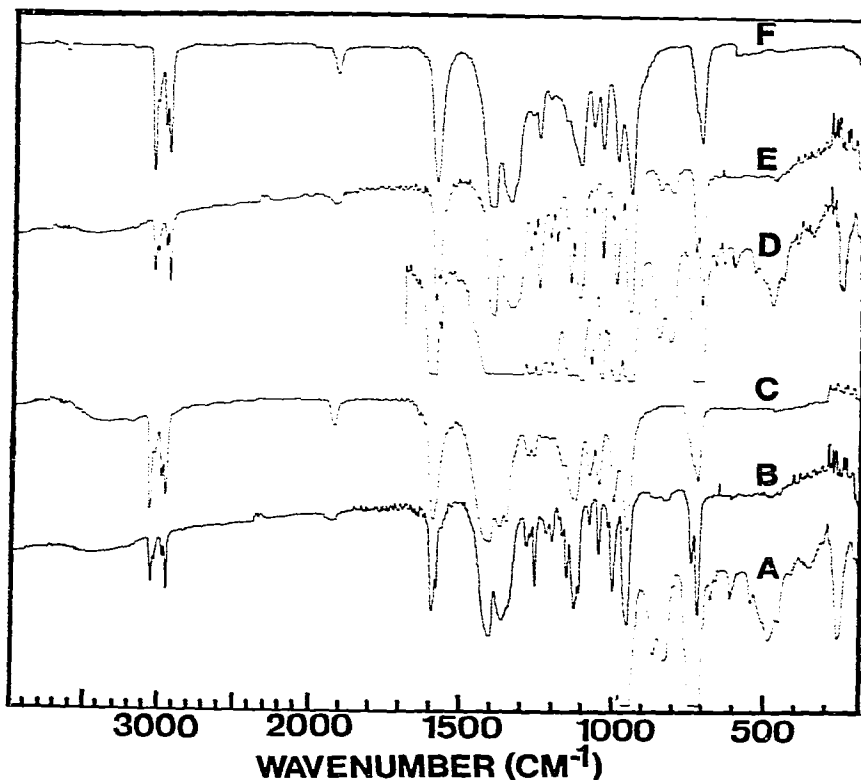


Fig. 1. Infrared spectra of solid (A and B) and gaseous (C) divinyborinic anhydride- ^{16}O . Infrared spectra of solid (D and E) and gaseous (F) divinyborinic anhydride- ^{18}O .

Vibrational studies

A Perkin-Elmer Model 621 infrared spectrophotometer was used for recording mid-infrared spectra from 4000 to 200 cm^{-1} . A 10 cm cell with cesium iodide windows was used to obtain the spectrum of the gas phase; sample pressure in the cell was 5 mmHg . A low-temperature cell equipped with cesium iodide windows was employed to record the spectra of the solid samples. Conventional vacuum deposition techniques were used to obtain the solid film on the cesium iodide substrate. The substrate was held at approximately 77 K during deposition and then the solid films were annealed until there was no change in the spectrum. Additional spectra were obtained using a closed cycle helium refrigerator at approximately 20 K . However, no additional information was obtained. Typical spectra are shown in Figure 1.

The Raman spectra were recorded on a Cary Model 82 Raman spectrophotometer equipped with a Spectra Physics Model 171 Argon ion laser with a frequency of 514.5 nm for excitation. The Raman spectra of liquid divinyborinic anhydride were obtained using a Harney-Miller [8] type cell cooled with the vapors of boiling nitrogen. Spectra were recorded at approximately -100°C . The Raman spectra of the solids were obtained using a cold cell similar to that employed for the mid-infrared, except the sample holder consists of a solid

brass plate at an angle of 75° from the normal. Deposition and annealing procedures are similar to those used for the mid-infrared studies. Spectra obtained using a closed cycle helium refrigerator at approximately 20 K yielded no additional information.

Results

The infrared and Raman spectra appear relatively simple for a molecule with 63 normal vibrations; however numerous accidental degeneracies, particularly among the vinyl motions, are expected. For this reason useful information concerning the molecular symmetry of divinylborinic anhydride should come from the vibrations associated with the heavy atom skeleton.

Molecular symmetries to consider for divinylborinic anhydride should include the possibility of either a bent or linear B—O—B central skeleton. A non-symmetric C_1 structure is indicated by the absence of depolarized lines in the Raman spectra of the liquid. For C_1 symmetry, all 63 fundamentals are polarized except for an accidentally depolarized band at 3062 cm^{-1} .

The observed frequencies for divinylborinic anhydride are listed in Table 1. The Raman line occurring at 620 cm^{-1} can confidently be assigned to the B—O—B symmetric stretch by comparison to dimethylborinic anhydride [1] and other compounds containing X—O—X linkages [9]. Raman spectra are shown in Fig. 2. A shift to lower frequency of this line in the spectrum of the ^{18}O substituted compound would be indicative of a bent B—O—B skeleton since the B—O—B symmetric stretch involves no movement of the oxygen if the skeleton is linear. No appreciable shift of the B—O—B symmetric stretch is observed upon solidification or isotopic substitution, clearly indicating a linear B—O—B angle in all phases.

Vibrational assignment

As previously stated, the molecule contains a linear B—O—B skeleton and has C_1 symmetry. Therefore all 63 modes are both infrared and Raman active and all Raman bands are expected to be polarized. Local symmetry may effect the polarization ratios resulting in some "accidentally depolarized" bands. This is the case with the band corresponding to the CH_2 asymmetric stretches at 3062 cm^{-1} . Numerous degeneracies, particularly among the vinyl modes, are expected.

The majority of the information about the structure will come from the vibrations associated with the heavy atom skeleton. Therefore, only these skeletal vibrations will be discussed. The assignment appears in Table 1.

The B—O—B asymmetric stretch occurs at 1374 cm^{-1} in the ^{16}O compound and at 1366 cm^{-1} in the ^{18}O compound. The B—O—B symmetric stretch occurs at approximately 620 cm^{-1} in both the ^{16}O and ^{18}O compounds. This frequency varies less than 5 cm^{-1} upon solidification. A B—O—B angle of 180° is clearly indicated.

The modes associated with the alpha carbons (C_α) and the boron atom fall within the regions suggested in divinylmethylborane [10] and trivinylborane [6]. The B—C asymmetric stretching modes should fall in the region from 1100 to 1200 cm^{-1} . Two prominent bands are visible in the infrared spectrum of the

TABLE 1
INFRARED AND RAMAN SPECTRA (CM⁻¹) AND ASSIGNMENTS FOR DIVINYLBORNIC ANHYDRIDE [(CH₂=CH)₂B]₂O^a

¹⁶ O			¹⁸ O			Assignment
Infrared	Raman		Infrared	Raman		
gas	solid	liquid	gas	solid	liquid	solid
3073s	3062m	3062dp, m	3072s	3062m	3064dp, m	3063m
3044w	3040w		3046w	3041w		
2995m	2985w	2990p, vs	2995m	2984w	2987p, vs	2986s
2969s	2959m	2960p, w	2969s	2959s	2959m	2958m
1938w	1936w		1940w	1938w		
1612s	1612s	1600p, s	1610vs	1612s	1612p?, m	1613m
				1598vs	1600p, vs	1600vs
				1584m		1582w
1430vs(br)	1420vs(br)	1418p, m	1424vs(br)	1422vs(br)	1420p, m	1418m
1374vs	1384s(br)		1366vs(br)	1356vs(br)		
1296w	1300w		1296vw	1300w		
	1286w			1285w(eh)		
1278w	1272m	1285p, m	1274m	1269s	1287p, m	1299m
				1180w		
1175(eh)	1166m			1165s		1166vw
1146m	1140s	1135vw(br)	1140s	1138s	1132p, vw	1131vw
	1126s	1123w		1126s		

asymmetric C-H stretches (accidentally depolarized)

symmetric C-H stretches 'in-phase'

symmetric C-H stretches 'out-of-phase'

2 X 970

C=C stretches

CH₂ deformation

B-O-B asymmetric stretch

C-H 'in-plane' bends

B-C asymmetric stretches

1094m	1094w	1094m	1092w	1092w							
1074m	1061w	1064m	1061m	1061m							CH ₂ twists
	1032w		1030(sh)	1030(sh)							combination
1015m	1016m	1034vw	1033vw	1015m	1015s	1015s	1015m	1015m	1011vw		CH ₂ rocks
969m	970s		1012vw	969vs	972w	972w	970s	970p, w	970w		CH ₂ wags
	882vw		972w				876vw				
	848w						838w				
753(sh)	755m		756vw		756vw	756vw	754m				
738m	735s		736vw		737s	736vw	734s		787vw		B-C symmetric stretches
	690vw										
	675vw										
	625vw						686vw				
	558vw	620p, vw	623w				687vw	662p, w	621w		B-O-B symmetric stretch
	490w						622vw				
	470vw		525vw(br)				554vw				
		450p(br)vw	497vw(br)						528vw		
	360vw						496w				
	276w	275p, w	370vw				462w	450p(br)vw	458vw		B-C ₂ wag
			337vw(br)						416vw(br)		(B-O in-plane)
			273w						370vw		B-C ₂ scissors
									388vw		
									272w		B-C ₂ rock
											(B-O out-of-plane)
											B-C=C bends
									201w		

^a Abbreviations used: s, strong; m, medium; w, weak; v, very; br, broad; sh, shoulder; p, polarized; dp, depolarized.

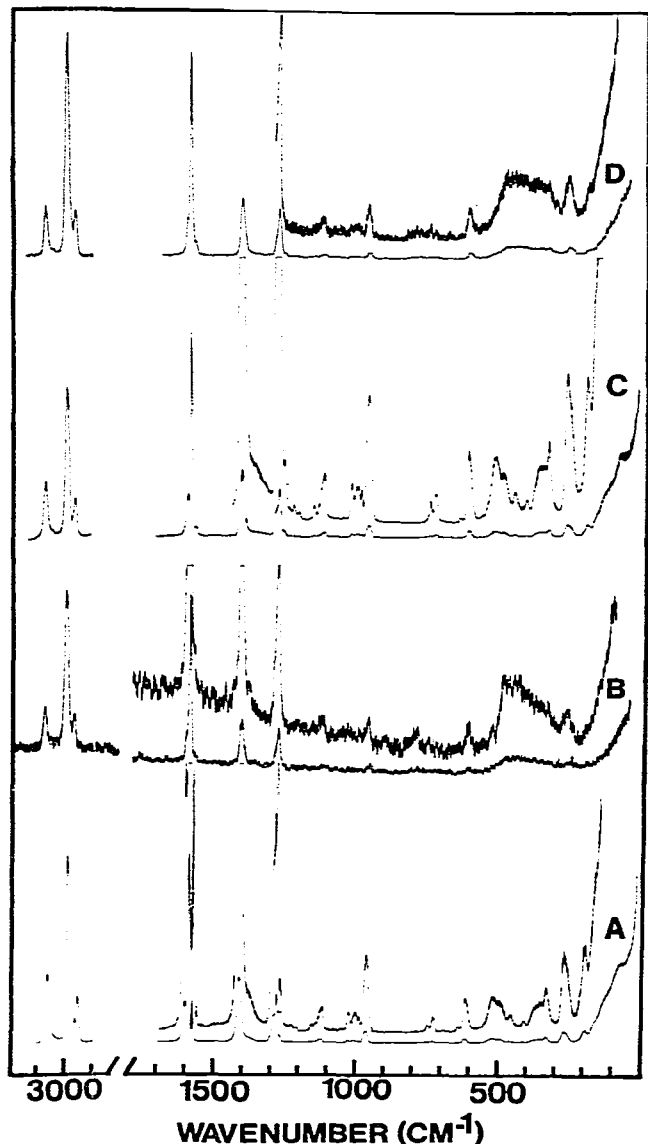


Fig. 2. Raman spectra of solid (A) and liquid (B) divinylborinic anhydride- ^{16}O . Raman spectra of solid (C) and liquid (D) divinylborinic anhydride- ^{18}O .

solid within this region (see Fig. 1). The out-of-phase asymmetric stretch occurs at 1166 cm^{-1} and the in-phase asymmetric stretch occurs at 1140 cm^{-1} . The B—C symmetric stretching modes occur at 755 and 735 cm^{-1} for the out-of-phase and in-phase modes, respectively. The B—C wagging modes (B—O in plane bend) appear as a broad band centered around 470 cm^{-1} . The BC_2 rocking modes (B—O out of plane bend) occur at approximately 275 cm^{-1} . The BC_2 scissoring modes occur at 370 cm^{-1} for the out of phase motion and at 337 cm^{-1} for the in phase motion. The torsions of the BC_2 groups were not observed.

The C=C stretching modes appear as three bands in the Raman spectrum of the solid at 1612, 1598 and 1584 cm^{-1} . The B=C bending modes appear as a weak band in the Raman spectrum of the solid at 201 cm^{-1} (see Fig. 2).

Discussion

Divinylborinic anhydride is easily prepared by the limited hydrolysis of divinylchloroborane in much the same manner as dimethylborinic anhydride is prepared [2]. Interestingly, the thermal stability of the vinyl compound is significantly less than that of the corresponding methyl compound since $(\text{C}_2\text{H}_3)_4\text{-B}_2\text{O}$ decomposes readily at room temperature to yield trivinylborane and a cyclic boron-oxygen compound.

A considerable amount of experimental data indicates that the electron deficiency of tricoordinate boron is compensated by $p\pi-p\pi$ interactions between boron and π -donor groups, such as $-\text{NR}_2$, $-\text{OR}$ and unsaturated organic moieties [5,11,12]. One of the interesting features of divinylborinic anhydride is that there are two different π -donor groups which can interact with the empty boron $p\pi$ orbital. A comparison of nuclear magnetic resonance parameters of this molecule with closely related molecules reveals that it is very likely that both groups are mesomerically interacting to some extent with the boron orbital. The ^{11}B chemical shift of $(\text{C}_2\text{H}_3)_2\text{BOB}(\text{C}_2\text{H}_3)_2$ is deshielded by 39 ppm from $\text{BF}_3 \cdot \text{O}(\text{C}_2\text{H}_5)_2$ and can be compared to the ^{11}B chemical shifts of $(\text{CH}_3)_2\text{-BOB}(\text{CH}_3)_2$ (+52 ppm [13]), $(\text{C}_2\text{H}_5)_2\text{BOB}(\text{C}_2\text{H}_5)_2$ (+52.6 ppm [14]) and $(\text{C}_6\text{H}_5)_2\text{BOB}(\text{C}_6\text{H}_5)_2$ (46 ppm [7]). Thus $(\text{C}_2\text{H}_3)_2\text{BOB}(\text{C}_2\text{H}_3)_2$ appears to represent the most shielded resonance reported for a diorganylborinic anhydride molecule. Although the interpretation of ^{11}B chemical shifts is not always straightforward due to various influences (both inductive and mesomeric) exerted by all substituents, one can usually obtain a good idea of the influence of $p\pi-p\pi$ interactions upon the ^{11}B chemical shift by examining the shifts of closely related compounds.

A study of magnetically active nuclei in the substituent can also be instructive with regard to the π -donor properties of the groups which may be involved in π -bonding to boron. In this regard ^{13}C NMR has been especially valuable in studying vinylboranes [5], phenylboranes [12], and boron-substituted aromatic heterocycles [12]. Treatment of vinylboranes as monosubstituted ethylene derivatives and a determination of the ^{13}C chemical shifts of the terminal vinyl carbons has demonstrated that ^{13}C NMR may be the most sensitive technique in studying delocalization of π electron density from the vinyl group into the empty boron $p\pi$ orbital. The C_β chemical shift of $(\text{C}_2\text{H}_3)_2\text{BOB}(\text{C}_2\text{H}_3)_2$ is deshielded by 14.2 ppm from the ^{13}C chemical shift of C_2H_4^* which is similar to the value found for trivinylborane [5] and certainly implies some delocalization of the vinyl π electron density. Thus all NMR parameters indicate some electron delocalization in this molecule.

With regard to the Lewis acidity of divinylborinic anhydride, the molecule contains two trigonal boron atoms and, as such, is capable of reacting with a

* The ^{13}C chemical shift of C_2H_4 is 122.8 ppm deshielded from TMS.

Lewis base such as $(\text{CH}_3)_3\text{P}$, $(\text{CH}_3)_2\text{PH}$ and $(\text{CH}_3)_3\text{N}$ to form complexes with a stoichiometry of 1 : 1, 1 : 2 and/or a mixture of both complexes. Based upon our experimental results for each of these reactions, only the 1 : 1 adduct is formed. Identification of the 1 : 1 adduct by ^{11}B NMR should indicate two nonequivalent boron atoms, i.e., one resonance representing a three-coordinate boron atom and a second resonance for a four-coordinate boron atom. The ^{11}B NMR spectra for the $(\text{CH}_3)_3\text{P}$ ($\delta(^{11}\text{B}) = 18.3$ ppm) and $(\text{CH}_3)_3\text{N}$ ($\delta(^{11}\text{B}) = 20.4$ ppm) adducts consist of a single resonance shielded with respect to divinylborinic anhydride. The increased shielding of 20.7 ppm for the $(\text{CH}_3)_3\text{P}$ adduct and 18.6 ppm for the $(\text{CH}_3)_3\text{N}$ adduct arises from electron donation by the base to the boron atoms. Since only a single resonance is observed for the 1 : 1 adduct, the structure of the adduct must be one in which the two boron atoms are magnetically equivalent. This structure can be viewed as a four membered ring, BOBP , in which the phosphorus atom is donating equally to both boron atoms or as a rapid exchange of the base between the two boron atoms. This exchange would be rapid with respect to the ^{11}B NMR time scale such that the observed resonance would be an average between the two states. The exchange process would be expected to show temperature dependence, i.e., as the temperature is lowered this motion would at some point begin to slow and the line should broaden. The low temperature ^{11}B NMR spectrum of the $(\text{CH}_3)_3\text{P}$ adduct clearly shows a temperature dependence. At ambient temperature the resonance has a half height linewidth of 110 Hz. As the temperature is lowered to -68°C , the linewidth increases to approximately 1500 Hz and at -105°C the resonance has nearly disappeared. At temperatures lower than -105°C solubility problems with the adduct prevent further acquisition of data. This line broadening, however, may not arise from the slowing of the exchange process. An increase in the viscosity of the solution as the temperature is lowered will change the correlation time for the molecules. This will affect the transverse relaxation time, T_2 , and hence the linewidth. Thus the data do not allow a definite conclusion to be made regarding the structure of the 1 : 1 adducts. The origin of three resonances in the ^{11}B NMR spectrum of the dimethylphosphine adduct is not understood at this time because the stoichiometry of the reaction was 1 : 1. Clearly, further work on these adducts is needed.

The infrared and Raman data clearly indicate that divinylborinic anhydride possesses C_1 symmetry. In view of the results obtained for trivinylborane [6] and divinylmethylborane [10], it is not surprising that similar steric effects exist in divinylborinic anhydride. The linear B—O—B angle may be explained in terms of a $p\pi-p\pi$ overlap between the vacant $2p_z$ orbital on the boron atoms and the lone pairs of the oxygen atom. Thus, the overlap between the vinyl groups and the boron atom is minimal, resulting in a non-planar divinylboryl moiety. The twisting of the vinyl groups resulting in C_1 symmetry would conceivably make crystal packing difficult. Obtaining spectra which contain lattice modes characteristic of a crystal was impossible even using very low temperatures. Unfortunately, no torsional data could be obtained due to the instability of divinylborinic anhydride at room temperature.

In conclusion, the new molecule divinylborinic anhydride has been prepared and characterized by spectroscopic methods. Carbon-13 NMR indicates some π interaction between the vinyl group and the empty boron orbital while infrared

and Raman data clearly demonstrate that the molecule has a linear B—O—B skeleton and that the vinyl groups are twisted out of the plane, leading to C_1 symmetry. As was the case for the vinyl difluoroborane molecule [4], ^{13}C NMR may be a more sensitive technique for the detection of relatively minimal delocalization of π electron density between unsaturated organic groups and trigonal boron atoms. Work is continuing in our laboratories to verify this conclusion.

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