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RESEARCH MEMORANDUM

CALCULATED HEATS OF FORMATION AND COMBUSTION OF BORON COMPOUNDS (BORON, HYDROGEN, CARBON, SILICON)

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NATIONAL ADVISORY COMMITTEE FOR AERONAUTICS

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CALCULATED HEATS OF FORMATION AND COMBUSTION OF BORON COMPOUNDS (BORON, HYDROGEN, CARBON, SILICON)

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SUMMARY

The heats of formation and combustion have been calculated for liquid and gaseous alkyl- and silyl-substituted boron compounds by a semitheoretical method. Alkylation and more especially silylation (substitution of a SiH_3 group) reduce the heat of combustion. As the molecular weight of the parent boron hydride increases, the reduction in the heats of combustion resulting from the substitution of a given number of alkyl or silyl groups decreases. As many as three carbon atoms can be substituted on boron hydrides with five or more boron atoms without reducing the heat of combustion below 25,000 Btu per pound. The substitution of one silicon atom reduces the heat of combustion as much as do three carbon atoms. Alkyl-substituted higher-molecular-weight boron hydrides may prove to be satisfactory high-energy fuels.

INTRODUCTION

Considerable effort has been put into the synthesis and investigation of the physical, thermodynamic, and kinetic properties of liquid and solid fuels containing boron and hydrogen, or boron, hydrogen, and carbon (refs. 1 to 15). These boron-containing fuels have heats of combustion as much as 70 percent higher than JP fuels (ref. 7 and this report), high flame speeds (ref. 8), and high specific impulses (ref. 9); consequently, they afford high thrust and improved range for ram-jet and rocket applications.

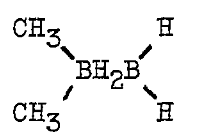
Experimental determinations of the heats of combustion of boron-containing compounds are complicated by the incompleteness of combustion of the boron and carbon (refs. 10 and 11 and unpublished Lewis data). Furthermore, it is very difficult to prepare boron hydrides or alkylated boron hydrides of high purity and maintain such purities over appreciable periods of time (unpublished Lewis data). However, the experimentally known heats of formation available for several boron hydrides and trialkylboranes can be used along with the appropriate bond energies to calculate the heats of formation of many alkyl- and silyl-(SiH_3) substituted boron hydrides. These heats of formation can then be combined with the heats of formation of the combustion products to obtain the heats of combustion of the reactants.

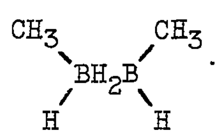
The heats of combustion of the ethyldiboranes have been calculated previously (ref. 7) from bond-energy data by a method considerably different in its details from the method used in the present report. The emphasis in reference 7 was on obtaining an approximate empirical equation which could be used to estimate roughly the heats of combustion of 3714 boron-carbon-hydrogen fuels of unknown structure. In a recent National Bureau of Standards report (ref. 12), the heats of formation of the methyl and ethyldiboranes were calculated by a method very similar to the method used in the present report. Heats of combustion (in kcal/g) for a number of boron-containing fuels have been reported without any details of the method of calculation in a report concerned particularly with solid propellants for rocket applications (ref. 14).

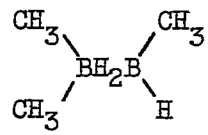
The heats of formation and combustion are calculated in this report for a large number of alkyl- and silyl-substituted boron hydrides. The depression in the heat of combustion resulting from increasing alkylation or silylation is considered. The effects on the heats of combustion of substitution of equal numbers of alkyl or silyl groups on different boron hydrides also are discussed. In addition, the lowering of the heat of combustion of a given boron hydride resulting from alkylation is compared with that resulting from silylation.

NOMENCLATURE

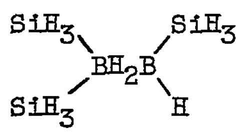
The nomenclature for boron compounds suggested in reference 16 is used in part in the present report. For simplicity, B_2H_6, B_5H_9, and $B_{10}H_{14}$ will be referred to in this report as diborane, pentaborane, and decaborane rather than diborane-6, pentaborane-9, and decaborane-14, as suggested in reference 16. The substituted compounds R_3B will be called trialkylboranes (R, alkyl radical). Substituted alkyldiboranes and silyldiboranes will be named as suggested in reference 16 and illustrated in the following list:


1,1-Dimethyldiborane


1,2-Dimethyldiborane



1,1,2-Trimethyldiborane



1,1,2-Trisilyldiborane

The name boryl for the BH_2- radical suggested in reference 16 is adopted as are the names methylboryl and dimethylboryl for $(CH_3)BH$- and $(CH_3)_2B$-, respectively. Compounds of the types $R_2BCH_2BR_2$ and $R_2BC_2H_4BR_2$ will be named in the following way:

$H_2BCH_2BH_2$	Diborylmethane
$H_2BCH_2CH_2BH_2$	1,2-Diborylethane
$H_2BCH_2BHCH_3$	Borylmethylborylmethane
$CH_3HBCH_2BHCH_3$	Bis-methylborylmethane
$H_2BCH_2CH_2BHCH_3$	1-Boryl-2-methylborylethane
$(CH_3)_2BCH_2CH_2B(CH_3)_2$	1,2-Bis(dimethylboryl)ethane

The radicals formed by removal of a hydrogen atom from the boron hydrides other than borane will be given the anyl ending. Thus, the radicals B_5H_8 and $B_{10}H_{13}$ will be referred to in the present report as the pentaboranyl and decaboranyl radicals. Consequently, alkylated and silylated derivatives of pentaborane and decaborane may be named as substituted hydrocarbons and silanes, but more common usage calls for naming these compounds as alkyl and silyl derivatives of the various boron hydrides. When two radicals are joined, as in $B_5H_8B_5H_8$, the bi prefex will be used as in biphenyl $C_6H_5C_6H_5$. Since the thermochemical information is insufficient to differentiate thermally between nonequivalent boron atoms in pentaborane and decaborane, the numbering of the skeletal boron atoms will not be used. To illustrate,

$B_5H_8CH_3$	Methylpentaborane, or pentaboranylmethane
$B_5H_8SiH_3$	Silylpentaborane, or pentaboranylsilane

$B_5H_8C_2H_5$	Ethylpentaborane, or pentaboranylethane
$B_5H_8B_5H_8$	Bipentaboranyl
$B_5H_8CH_2B_5H_8$	Dipentaboranylmethane
$B_5H_8CH_2CH_2B_5H_8$	1,2-Dipentaboranylethane
$B_{10}H_{13}CH_3$	Methyldecaborane, or decaboranylmethane
$B_{10}H_{13}B_{10}H_{13}$	Bidecaboranyl
$B_{10}H_{13}CH_2CH_2B_{10}H_{13}$	1,2-Didecaboranylethane

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HEATS OF FORMATION OF BORON HYDRIDES, TRIALKYLBORANES, ALKYL AND SILYL RADICALS, AND GASEOUS BORON AND CARBON

The heats of formation of diborane B_2H_6, pentaborane B_5H_9, and decaborane $B_{10}H_{14}$ have been determined at the National Bureau of Standards (ref. 6) from the thermal decomposition of the hydrides to boron and hydrogen. These values are listed in table I. The heat of formation of borane BH_3 listed in table II was calculated from the heat of reaction of 28 kcal per mole for the reaction $B_2H_6 \rightarrow 2BH_3$ (ref. 13) and the heat of formation of diborane. The heats of formation of B_2H_5, B_2H_4, B_2H_3, B_2H_2, B_5H_8, and $B_{10}H_{13}$ in table II have been estimated by assuming that the bond dissociation energy for breaking the first boron-to-hydrogen bond so as to form B_2H_5, B_5H_8, and $B_{10}H_{13}$ and the average boron-hydrogen bond energy in forming B_2H_4, B_2H_3, and B_2H_2 may be approximated by the average boron-to-hydrogen bond energy in borane. This assumption will be discussed in more detail in the following section on bond energies.

The heats of combustion of the trimethyl-, triethyl-, tri-n-propyl-, and tri-n-butylboranes have been determined (refs. 6, 10, and 15). Complete combustion of boron-containing compounds (refs. 10 and 15) is difficult to obtain. Residues of both boron and carbon and possibly partially oxidized products also often remain after combustion. Although the residues may be partially corrected for by analysis (unpublished Lewis data), the uncertainties in the experimental heats of combustion at present range from ±1 to ±2 percent. As a consequence, the heats of formation of the trialkylboranes are uncertain from ±5 to ±15 kcal per mole.

The heats of formation of alkyl free radicals, for example, CH_3, CH_3CH_2, and $CH_3CH_2CH_2$, may be obtained from the heats of formation of the parent hydrocarbons and the bond dissociation energies of the radical-to-hydrogen bonds of these hydrocarbons. The bond dissociation energies for the radical-hydrogen bonds are obtained from electron impact measurements in the mass spectrograph (ref. 17), from studies of the kinetics of bromination of hydrocarbons (refs. 18 and 19), and from kinetics of pyrolysis
3714 (ref. 20). The values for the radical-hydrogen bond dissociation energies from electron impact measurements agree within the experimental errors with the results from kinetics of bromination. The heats of formation of the methyl and ethyl radicals are uncertain to ±1 kcal per mole, while the heat of formation of the n-propyl radical is uncertain to ±2 kcal per mole. The most probable values for the heats of formation of the alkyl free radicals are listed in table II. The use of dissociation processes involving alkyl free radicals, where possible, avoids entirely the uncertainty as to the heat of sublimation of carbon. Actually, the calculated heats of formation are independent of the choice of the heat of sublimation of carbon as long as the appropriate carbon-hydrogen and boron-carbon bond energies are used with a given choice of the heat of sublimation of carbon.

The heat of formation of the silyl free radical SiH_3 in table II is estimated from the heat of formation of silane SiH_4 (ref. 21) and the average silicon-hydrogen bond energy (see following section).

The higher heat of sublimation of carbon is listed in table I. The heat of sublimation of boron given is that reported in reference 6.

BOND ENERGIES

The experimental average Y-Z bond energies $\overline{D}_{exp}(Y\text{-}Z)$ may be obtained from dissociation processes such as

$$YZ_n(g) \rightarrow Y(g) + nZ(g)$$

by using the expression

$$\overline{D}_{exp}(Y\text{-}Z) = \Delta H_a/n$$

where ΔH_a is the heat of atomization and n is the number of Y-Z bonds broken in the dissociation process. The experimental average bond energies for the boron-hydrogen and boron-carbon bonds may be calculated from the dissociation processes

$$BH_3(g) \rightarrow B(g) + 3H(g)$$

and

$$BR_3(g) \rightarrow B(g) + 3R(g)$$

where R is alkyl radical. Similarly, the experimental average bond energies may be obtained for the carbon-hydrogen and silicon-hydrogen bonds from the dissociation processes

$$CH_4(g) \rightarrow C(g) + 4H(g)$$

and

$$SiH_4(g) \rightarrow Si(g) + 4H(g)$$

Another method of obtaining average bond energies uses Pauling's equations (ref. 22) involving the arithmetic and geometric means of the nonpolar bond energies. The equation involving the geometric mean is more satisfactory to use and has therefore been employed to calculate the average bond energy for the boron-silicon bond for which no experimental data are available. This equation is

$$\overline{D}_{gm}(Y\text{-}Z) = \sqrt{D(Y\text{-}Y)D(Z\text{-}Z)} + 23.06\left[x_Y - x_Z\right]^2$$

Where D(Y-Y) and D(Z-Z) are nonpolar bond energies, that is, D(C-C), D(Cl-Cl), and so forth; x_Y and x_Z are the electronegativities of atoms Y and Z (ref. 22). The D(B-B) and x_B have been obtained by solving simultaneous (Pauling) equations using data for the boron compounds BH_3, BBr_3, and BR_3, where the heats of formation, D(H-H), D(Br-Br), D(C-C), x_H, x_{Br}, and x_C, are known. The value of D(B-B) also has been determined by solving the simultaneous equations involved in the decomposition reactions for BH_3, B_2H_6, B_5H_9, and $B_{10}H_{14}$. The numbers of the various types of bonds (B-H, B-B, BHB, BBB) are taken from reference 23. The average values obtained for D(B-B) and x_B are 80 kcal per mole and 2.0 units, respectively. (Pauling (ref. 22) previously obtained an x_B of 1.95 using more limited data.) These values may then be substituted back into Pauling's equation to obtain such bond energies as $\overline{D}_{gm}$(Si-B). All the pertinent average bond energies obtained experimentally or from Pauling's equation are listed in table III.

Actually bond dissociation energies such as (B_5H_8)-H are desired, not average energies. For example, by use of the average bond energy $\overline{D}$(B-H) in pentaborane, the assumption is made implicitly that all boron-hydrogen bonds have equal energies. Furthermore, it is assumed that the apex boron in B_5H_9 is the same as the base boron atom (ref. 3). Similarly, the four different types of boron atom in decaborane (ref. 3) are assumed to have equal D(B-H) values. Unfortunately, no bond-dissociation-energy data for specific dissociations $B_nH_{n'}$-H are available for boron hydrides. When more detailed information on bond energies and bond dissociation energies of boron hydrides does become available, it may become possible to estimate the differences in boron-hydrogen bond energies among nonequivalent boron atoms in the higher boron hydrides.

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METHODS OF CALCULATION

Heats of Formation

The heats of formation of boron-containing molecules for which there are no experimental data from heats of combustion, heats of decomposition, and so forth, can now be computed. The method to be used involves atomization or dissociation reactions. For example, methylpentaborane (or pentaboranylmethane) $B_5H_8CH_3$ may be (1) atomized into gaseous atoms or (2) dissociated by breaking a single boron-carbon bond as follows:

$$B_5H_8CH_3(g) \rightarrow 5B(g) + C(g) + 11\ H(g) \tag{1}$$

$$B_5H_8CH_3(g) \rightarrow B_5H_8^{\cdot}(g) + CH_3(g) \tag{2}$$

Where possible, the molecules of interest will be dissociated (eq. (2)) into boron hydride fragments such as gaseous pentaborane and alkyl or silyl radicals. For the alkylated diborylmethanes, dipentaboranylmethane, and didecaboranylmethanes, decompositions to gaseous carbon also are involved. In such cases care was taken to use the appropriate values for average carbon-hydrogen and boron-carbon bond energies (table III).

The heats of these dissociation reactions are taken as the sums of the bond energies for the bonds broken in formation of the fragments. Thus, in the dissociation reaction for $B_5H_8CH_3(g)$ given in equation (2), one boron-carbon bond is broken; therefore, the heat of dissociation is just 89 kcal per mole.

In general, the heat of formation ΔH_f^o will be given by

$$\Delta H_f^o = \Sigma\Delta H_{f(products)}^o - \Delta H_{(dissociation)}$$

or by

$$\Delta H_f^o = \Sigma \Delta H_f^o(\text{products}) - \Sigma \overline{D}(Y-Z)$$

The approximate nature of the bond energies used means that the heats of formation (table II) calculated from them are uncertain to perhaps ±5 to ±15 kcal per mole, although some errors may cancel each other out in the calculation. Fortunately, the contributions of the heats of formation of the alkylated and silylated boron hydrides are rarely greater than 5 percent of the heats of combustion. Hence, the uncertainties in the heats of formation result in uncertainties in the heats of combustion of only 1 to 2 percent. 3714

Heats of Vaporization

The heats of formation of the gaseous molecules have been obtained by the procedure of the preceding section. Since the heats of formation of the liquids are also needed, the heats of vaporization of the liquids must be estimated. But, because most of the molecules considered have not been synthesized, neither heats of vaporization ΔH_{vap} nor boiling points are generally available.

The present investigation shows that the extremely simple expression

$$\Delta H_{vap} = 2 + \Sigma n(\text{C, B, Si atoms})$$

will give ΔH_{vap} values with an average deviation of 1 kcal per mole and less from the experimental heats of vaporization at the boiling point of the boron hydrides, trialkylboranes, alkyldiboranes, and alkylsilanes. This comparison is given in table IV. From these calculated heats of vaporization, the heats of formation of the liquids have been calculated from the heats of formation of the gases.

The heats of formation (gas phase and liquid phase) of the alkylated and silylated boron hydrides are listed in table V.

Heats of Combustion

The heats of combustion ΔH_c of the gaseous and liquid alkylated and silylated boron hydrides can now be calculated.

The heats of formation of the products of combustion considered are listed in the following table:

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CN-2

Oxide	Heat of formation (at 25° C), ΔH_f^o, kcal/mole
H_2O(g)	-57.80
B_2O_3(crystalline)	-305.4
B_2O_3(amorphous)	-301.0
CO_2(g)	-94.05
SiO_2(amorphous)	-208.1

The heats of formation of water vapor and of carbon dioxide are accurately known (ref. 21). The heats of formation of crystalline and amorphous boric oxide (ref. 6) probably still are uncertain to ±1 kcal per mole. The heat of formation of amorphous silica is used (refs. 24 and 25) because X-ray analysis shows that the silica resulting from bomb calorimetry of silanes is amorphous (ref. 26).

Heats of formation and combustion appear in table V for substances in the liquid, solid, or gaseous state. Heats of combustion were calculated for reactions yielding both amorphous and crystalline boric oxide as products. These values have uncertainties of ±200 to ±500 Btu per pound.

The heats of combustion of the various series of boron compounds are plotted in figure 1. Only the heats of combustion of the liquid boron compounds oxidized to B_2O_3(amorphous) are plotted in these figures. However, as can be seen from table V, the heats of combustion for the gaseous compound are only 100 to 300 Btu per pound higher than those for the same substance in the liquid state. The values plotted represent the lowest heats of combustion of those listed in table V. The most favorable heat-of-combustion values, which are for the boron compounds in the gaseous state oxidized to B_2O_3(crystalline), are 100 to 700 Btu per pound higher.

DISCUSSION OF RESULTS

The heats of combustion listed in table V and plotted in figure 1 provide data from which a number of interesting conclusions can be drawn. The effects of alkylation or silylation of a given boron hydride and on different boron hydrides now may be examined in detail.

Trialkyl- and Trisilylboranes

Alkylation and silylation have a common detrimental effect on the heats of combustion of the parent boron hydrides. Alkylation of borane to form R_3B compounds reduces the heat of combustion to a range of values only 10 to 20 percent higher than those for JP fuels (ΔH_c for JP fuels, from 18,000 to 19,000 Btu/lb). Silylation to form $B(SiH_3)_3$ reduces the heat of combustion below that of most hydrocarbons (see table V and fig. 1(a)).

Alkyl- and Silyldiboranes

While diborane has a heat of combustion of more than 31,000 Btu per pound, the heat of combustion of monomethyldiborane is 4700 Btu per pound lower. Further alkylation lowers the heats of combustion to between 20,000 and 24,000 Btu per pound. The monoalkyldiboranes are unstable with respect to rearrangement to di- or trialkyldiboranes.

Silylation of diborane, even monosilylation, drastically depresses the heat of combustion. The heat of combustion of monosilyldiborane is as low as that of trimethyldiborane and the heats of combustion of tri- and tetrasilyldiborane are no better than those of JP fuels (table V and fig. 1(b)).

Alkyl- and Silyltetraboranes

The heat of combustion of tetraborane itself is only 600 Btu per pound less than that of diborane and is about 1400 Btu per pound higher than that of pentaborane. Although the heats of combustion fall off more rapidly with alkylation and silylation of tetraborane than pentaborane, the higher initial heat of combustion of the parent compound tetraborane results in a higher heat of combustion for all the alkylated and silylated tetraboranes considered when compared with the corresponding alkylated or silylated pentaboranes (see following section). Although tetraborane itself is rather unstable, the alkylated or silylated derivatives might possibly be appreciably more stable (table V and fig. 1(c)).

Alkyl- and Silylpentaboranes

Alkylation of the heavier pentaborane molecule has less-drastic consequences on the heat of combustion than alkylation does for diborane. The methylpentaborane (or pentaboranylmethane) has a heat of combustion only about 2100 Btu per pound lower than does pentaborane itself. Even propylpentaborane (or pentaboranylpropane) has a heat of combustion of about 25,000 Btu per pound, which is quite an appreciable gain over JP fuels. Silylation again causes a much larger depression in the heats of combustion than does alkylation. Silylpentaborane (or pentaboranylsilane) with only one silicon atom has a heat of combustion about the same as that of propylpentaborane with three carbon atoms (table V and fig. 1(d)).

Alkyl- and Silyldecaboranes

When the even heavier molecule decaborane is considered, it can be seen (table V and fig. 1(e)) that alkylation has a very small effect on the heat of combustion. Methyldecaborane (or decaboranylmethane) has a heat of combustion only 1000 Btu per pound less than does decaborane. Of even more interest is the fact that methyldecaborane, ethyldecaborane, and propyldecaborane all have heats of combustion larger than the corresponding alkylpentaboranes despite the higher heat of combustion of pentaborane compared with decaborane. Also, the silyldecaborane has a heat of combustion over 1000 Btu per pound higher than that of silylpentaborane. Again, as with diborane and pentaborane, the heat of combustion is depressed about as much by one silyl group as by one propyl group substituted on decaborane.

Diborylmethane, Diborylethane, and Their Alkyl Derivatives

Diborylmethane $H_2BCH_2BH_2$, 1,2-diborylethane $H_2BC_2H_4BH_2$, and their alkyl derivatives show no outstanding advantages in their heats of combustion compared with the previously discussed boron hydride derivatives. Although diborylmethane has a high heat of combustion (26,000 to 27,000 Btu per pound), alkylation rapidly depressed the heat of combustion to values only 10 to 20 percent higher than those of JP fuels (table V and fig. 1(f)). The compound 1,2-diborylethane has a heat of combustion of only about 25,000 Btu per pound and alkylation depresses the heat of combustion into the range from 21,000 to 22,000 Btu per pound (table V and fig. 1(f)).

Bipentaboranyl and Bidecaboranyl

Bipentaboranyl $B_5H_8B_5H_8$ and bidecaboranyl $B_{10}H_{13}B_{10}H_{13}$ would be formed by the combination of two pentaboranyl or decaboranyl radicals. Their heats of combustion (table V and fig. 1(g)) appear to be only slightly lower than those of the respective parent hydrides, pentaborane and decaborane; consequently, these compounds or their alkylated derivatives should be very good high-energy fuels.

Dipentaboranyl- and Didecaboranylalkanes

The heats of combustion of dipentaboranylmethane $B_5H_8CH_2B_5H_8$, 1,2-dipentaboranylethane $B_5H_8C_2H_4B_5H_8$, didecaboranylmethane $B_{10}H_{13}CH_2B_{10}H_{13}$, and 1,2-didecaboranylethane $B_{10}H_{13}C_2H_4B_{10}H_{13}$ also have been calculated. The heats of combustion of these compounds are in the range from 26,000 to 28,000 Btu per pound (table V and fig. 1(g)). Their heats of combustion appear to be slightly higher than the methyl and ethyl derivatives of pentaborane and decaborane. The didecaboranylalkanes have heats of combustion as high or higher than the dipentaboranylalkanes with the same number of carbon atoms. If the liquid dipentaboranyl- and didecaboranylalkanes could be prepared, they might be very satisfactory high-energy fuels. Even higher dipentaboranyl- and didecaboranylalkanes, such as 1,2-didecaboranylbutane, should have quite high heats of combustion in the range of 25,000 to 26,000 Btu per pound (estimated by extrapolation) and may have very satisfactory liquid ranges, low volatilities, and fairly high densities.

Heats of Combustion of Isomers

It should be noted that many of the compounds mentioned in this report can have a number of isomers. For example, the alkyl group in an alkylpentaborane could be attached to either the apex or the base boron atom in pentaborane. Again, in dipentaboranylmethane, the two pentaboranyl radicals could be joined by the methylene group apex to apex, apex to base, or base to base. Quite probably these isomers have somewhat different heats of combustion. The present status of thermochemical knowledge of boron compounds does not justify the refinement of estimating the differences in the heats of formation of isomers, and consequently, in their heats of combustion.

CONCLUDING REMARKS

The present calculations of the heats of combustion of alkylated and silylated boron hydrides indicate that alkylated derivatives of pentaborane and higher boron hydrides should be among the best high-energy fuels. The higher the boron content, the less alkylation will affect the heat of combustion of the boron hydride. However, it is also possible that considerable alkylation would be necessary to obtain a liquid fuel from a compound such as bidecaboranyl. The preparation of compounds such as $B_5H_8(CH_2)_nB_5H_8$ and $B_{10}H_{13}(CH_2)_nB_{10}H_{13}$ might result in very satisfactory liquid fuels. However, further synthetic work is necessary before the exact nature of the best or several best boron-containing high-energy fuels can be specified.

As more accurate and extensive thermochemical data become available for boron hydrides and alkylated boron hydrides, calculations of the type made here also can become more accurate and extensive. In view of the experimental difficulties involved in the thermochemistry of boron compounds, the procedure of using a small amount of experimental data as a base from which to make extensive semitheoretical calculations will probably be of value for some time to come.

It also must be remembered that most of the compounds for which calculations are made in this report have never been prepared. Furthermore, many of these compounds may be very unstable and undergo decomposition, rearrangement, or polymerization reactions. The answers to such questions of stability await further synthesis work and physical measurements.

The value of a given compound as a fuel is determined by a number of other considerations besides its heat of combustion. A compound may have
3714 a desirable heat of combustion but an unsatisfactory liquid range. A loss in heat of combustion through alkylation may result in a fuel which has a wide liquid range and also better handling characteristics. Furthermore, a higher combustion efficiency, obtained by alkylation or possibly silylation, may compensate or more than compensate for the loss in heat of combustion.

Obviously, all the factors mentioned and perhaps others must be balanced against each other in obtaining the most desirable fuel. A boron-containing fuel is probably undesirable if it has a heat of combustion no higher or very little higher than those of JP fuels. The exception might be a boron fuel which is being used for its high flame velocity and high thrust rather than its high heat content. However, most of the boron fuels with high heat contents also probably have high flame velocities and thrust; thus it appears that use of a low-heat-content boron fuel would rarely be advantageous.

SUMMARY OF RESULTS

Estimation of the heats of combustion of several families of alkyl- and silyl-substituted boron hydrides shows that

1. Alkylation and especially silylation (substitution of SiH_3 groups) of boron hydrides decrease considerably the heats of combustion.

2. As the molecular weight of the parent boron hydride increases from borane to decaborane and then to bidecaboranyl, the depression in the heats of combustion resulting from the substitution of a given number of carbon or silicon atoms decreases.

3. The heats of combustion of borane and diborane are rapidly reduced by alkylation to values only 10 to 20 percent higher than those of JP fuels.

4. The heats of combustion of borane and diborane are even more rapidly reduced by substitution of silyl groups. The tri- and tetrasilyldiboranes have heats of combustion very near those of JP fuels (about 19,000 Btu/lb).

5. The heat of combustion of tetraborane is calculated to be much closer to the heat of combustion of diborane than that of pentaborane. The heats of combustion of all of the alkyl (e.g., CH_3, C_2H_5, C_3H_7) and silyl (SiH_3) derivatives of tetraborane considered were higher than those of the corresponding pentaborane derivatives (see the following result).

6. The heats of combustion of the alkylpentaboranes B_5H_8R and the alkyldecaboranes $B_{10}H_{13}R$ with R = CH_3, C_2H_5, and C_3H_7 are equal to or greater than 25,000 Btu per pound. The heats of combustion of $B_5H_8SiH_3$ and $B_{10}H_{13}SiH_3$ are about the same as those of the alkylated derivatives with $R = C_3H_7$.

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7. The heats of combustion of the alkylated diborylmethanes and ethanes are even lower than those of the alkylated diboranes.

8. The heats of combustion of bipentaboranyl and bidecaboranyl are only slightly lower than those of pentaborane and decaborane. However, the heats of combustion of the dipentaboranylalkanes and the didecaboranylalkanes are somewhat higher (up to 500 Btu/lb) than those of the alkylpentaboranes and alkyldecaboranes with the same number of carbon atoms.

9. The heats of vaporization for the large proportion of the compounds considered for which there are no experimental values were estimated by the simple empirical formula $\Delta H_{vap} = 2 + \Sigma n(B, C, Si \text{ atoms})$. Experimental heats of vaporization for boron hydrides, alkyldiboranes, trialkylboranes, and alkylsilanes can be reproduced within 1 kcal per mole with this empirical equation.

Lewis Flight Propulsion Laboratory
National Advisory Committee for Aeronautics
Cleveland, Ohio, July 29, 1955

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TABLE I. - EXPERIMENTAL HEATS OF FORMATION OF BORON HYDRIDES, TRIALKYLBORANES, AND GASEOUS CARBON AND BORON ATOMS

[Temperature, 25° C]

Substance	Heat of formation, ΔH_f^o kcal/mole		Reference
	Liquid	Gas	
B_2H_6	---	7.53	6
B_5H_9	7.8	15.0	6
$B_{10}H_{14}$	8(crystalline)	26	6
$(CH_3)_3B$	-34.5 ± 3.5	-29.3 ± 3.5	[a,b]6
$(C_2H_5)_3B$	-46.8 ± 4.7	-38.0 ± 4.7	[a]6
	-23 ± 8	-14 ± 8	(c)
$(\underline{n}\text{-}C_3H_7)_3B$	-65	-54	[d]6
	-40 ± 8	-29 ± 8	(c)
$(\underline{n}\text{-}C_4H_9)_3B$	-83.9 ± 4.2	-70.8 ± 4.2	[a]6
	-94	-81	15
C	0(graphite)	171.7	21
B	0(crystalline)	141 ± 5	6
Si	0(crystalline)	100 ± 10	(e)

[a]Private communication from W. H. Johnson and E. J. Prosen, Nat. Bur. Standards.

[b]Values of $\Delta H_f^o(l)$ and $\Delta H_f^o(g)$ calculated from data in refs. 10 and 6 are essentially the same as Nat. Bur. Standards values.

[c]Unpublished Lewis data.

[d]Interpolated from experimental data on $(C_2H_5)_3B$ and $(\underline{n}\text{-}C_4H_9)_3B$.

[e]Average value from data of ref. 27.

TABLE II. - CALCULATED HEATS OF FORMATION OF ALKYL AND SILYL RADICALS AND UNSTABLE SPECIES OF BORON HYDRIDES AND ALKYLATED BORON HYDRIDES

[Temperature, 25° C]

Substance (gas)	Heat of formation, ΔH_f^o, kcal/mole	Calculated from data in refs. -
CH_3	32	17,18
C_2H_5	25	17,19
$\underline{n}$-C_3H_7	22	17,20
SiH_3	14	21
BH_3	18	6,14 (see tables I and III)
B_2H_5	48	
B_2H_4	89	
B_2H_3	130	
B_2H_2	171	
B_4H_{10}	19	
B_4H_9	60	
B_5H_8	56	
$B_{10}H_{13}$	67	
$B(CH_3)_2CH_2$	19	6,21 (see tables I and III)
$B(CH_3)_2$	28	
$B(CH_3)_2H$	-15	
$B(CH_3)(CH_2)H$	33	
$B(CH_3)$	85	
$B(CH_3)H_2$	2	
$B(CH_2)H_2$	50	
$B_5H_8CH_2$	49	6,21 (see tables I and III)
$B_{10}H_{13}CH_2$	60	6,21 (see tables I and III)

TABLE III. - AVERAGE BOND ENERGIES

Bond	Average bond energy, $\bar{D}$, kcal/mole	Source
C-H	99.5	[a]CH_4
Si-H	81 ± 2	[a]SiH_4
B-H	93 ± 2	[b]BH_3
B-(CH_3)	89 ± 2	[c]$B(CH_3)_3$
B-(C_2H_5)	81 ± 4	[c]$B(C_2H_5)_3$
B-(n-C_3H_7)	83 ± 4	[c]B(n-$C_3H_7)_3$
B-Si	63 ± 5	Pauling equation[d]
B-B	80 ± 5	Pauling equation and dissociation reactions of boron hydrides
(B-H-B)	107 ± 5	Dissociation reactions of boron hydrides
(B-B-B)	96 ± 3	Dissociation reactions of boron hydrides and heat of sublimation and crystal structure of crystalline boron

[a]Calculated from data in ref. 21.

[b]Calculated from data in refs. 6 and 13.

[c]Calculated from average values of $\Delta H_f^o(g)$ for BR_3 compounds (see table I).

[d]Taking D(Si-Si) as 50 kcal/mole (see table I).

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TABLE IV. - ESTIMATION OF HEATS OF VAPORIZATION BY THE RELATION

$$\Delta H = 2 + \Sigma n(C,B,Si)$$

Compound	Heat of vaporization, ΔH_{vap}, kcal/mole		Difference, kcal/mole	Average deviation	Ref.
	Experimental	Calculated			
B_2H_6	3.45	4	+0.5		21
B_4H_{10}	6.47	6	-0.5		21
B_5H_9	[a]7.2	7	-0.2		6
$B_{10}H_{14}$	12.13	12	-0.1	0.3	(b)
$B(CH_3)_3$	[a]5.2	6	+0.8		(c)
$B(C_2H_5)_3$	[a]8.8	9	+0.2		6
$B(\underline{n}\text{-}C_3H_7)_3$	[a]11.0	12	+1.0		6
$B(\underline{n}\text{-}C_4H_9)_3$	[a]13.1	15	+1.9	1.0	6
$(CH_3)_2B_2H_4$,(1,1)	5.5	6	+0.5		21
$(CH_3)_3B_2H_3$	7.0	7	0		21
$(CH_3)_4B_2H_2$	7.3	8	+0.7		21
$(C_2H_5)_2B_2H_4$,(1,1)	8.1	8	-0.1	0.3	21
CH_3SiH_3	4.39	4	-0.4		26
$(CH_3)_2SiH_2$	5.10	5	-0.1		26
$(CH_3)_3SiH$	5.82	6	+0.2		26
$(CH_3)_4Si$	6.25	7	+0.7		26
$C_2H_5SiH_3$	5.33	5	-0.3		26
$(C_2H_5)_2SiH_2$	7.18	7	-0.2		26
$(CH_2{=}CH)SiH_3$	5.12	5	-0.1		26
$(\underline{n}\text{-}C_4H_9)SiH_3$	7.37	7	-0.4		26
$(\underline{i}\text{-}C_4H_9)SiH_3$	7.05	7	0	0.3	26

[a]Experimental data on ΔH_{vap} at 25° C.

[b]Data from ref. 28.

[c]Private communication from W. H. Johnson and E. J. Prosen, Nat. Bur. Standards.

TABLE V. - HEATS OF FORMATION AND COMBUSTION OF BORON COMPOUNDS (B,H,C,Si)

Compound	Heat of formation (at 25° C), ΔH_f^0, kcal/mole		Heat of combustion, ΔH_c, Btu/lb			
			To B_2O_3(amorphous)		To B_2O_3(crystalline)	
	Solid or liquid	Gas	Solid or liquid	Gas	Solid or liquid	Gas
B	0(s)	[a]141.9	25,000(s)	48,500	25,400(s)	48,900
BH_3	15(l)	18	32,800(l)	33,200	33,100(l)	33,500
$B(CH_3)_3$	[a,b]-35(l)	[a,b]-29	21,200(l)	21,400	21,300(l)	21,400
$B(C_2H_5)_3$	[a,b]-47,-23(l)	[a,b]-38,-14	[c]20,500(l)	[c]20,600	[c]20,500(l)	[c]20,600
$B(\underline{n}\text{-}C_3H_7)_3$	[a,b]-65,-40(l)	[a,b]-54,-29	[c]19,900(l)	[c]20,100	[c]20,000(l)	[c]20,100
$B(\underline{n}\text{-}C_4H_9)_3$	[a,b]-84,-94(l)	[a,b]-71,-81	[c]19,500(l)	[c]19,600	[c]19,500(l)	[c]19,600
$B(SiH_3)_3$	-12(l)	-6	17,700(l)	17,800	17,700(l)	17,800
B_2H_6	4(l)	[a]7.5	31,100(l)	31,300	31,400(l)	31,600
$B_2H_5CH_3$	-14(l)	-9	26,400(l)	26,600	26,600(l)	26,800
$B_2H_4(CH_3)_2$	-31(l)	-25	24,100(l)	24,300	24,300(l)	24,500
$B_2H_3(CH_3)_3$	-48(l)	-41	22,800(l)	22,900	22,900(l)	23,000
$B_2H_2(CH_3)_4$	-65(l)	-57	21,800(l)	22,000	21,900(l)	22,100
$B_2H_5C_2H_5$	-14(l)	-8	24,700(l)	24,900	24,800(l)	25,000
$B_2H_4(C_2H_5)_2$	-31(l)	-23	22,600(l)	22,700	22,700(l)	22,800
$B_2H_3(C_2H_5)_3$	-48(l)	-38	21,500(l)	21,700	21,600(l)	21,800
$B_2H_2(C_2H_5)_4$	-65(l)	-53	20,900(l)	21,100	21,000(l)	21,100

[a]Experimental value.

[b]Two different experimental values reported (see table I).

[c]Average values.

[redacted]

TABLE V. - Continued. HEATS OF FORMATION AND COMBUSTION OF BORON COMPOUNDS (B,H,C,Si)

Compound	Heat of formation (at 25° C), ΔH_f^o, kcal/mole		Heat of combustion, ΔH_c, Btu/lb			
			To B_2O_3(amorphous)		To B_2O_3(crystalline)	
	Solid or liquid	Gas	Solid or liquid	Gas	Solid or liquid	Gas
$B_2H_5SiH_3$	-6(l)	-1	22,800(l)	23,000	23,000(l)	23,200
$B_2H_4(SiH_3)_2$	-15(l)	-9	20,300(l)	20,400	20,400(l)	20,500
$B_2H_3(SiH_3)_3$	-24(l)	-17	19,000(l)	19,100	19,100(l)	19,200
$B_2H_2(SiH_3)_4$	-33(l)	-25	18,300(l)	18,400	18,300(l)	18,400
B_4H_{10}	13(l)	19	30,500(l)	30,700	30,800(l)	31,000
$B_4H_9CH_3$	-2(l)	5	27,800(l)	28,000	28,000(l)	28,200
$B_4H_9C_2H_5$	-10(l)	-2	26,200(l)	26,400	26,400(l)	26,600
$B_4H_9C_3H_7$	-14(l)	-5	25,100(l)	25,300	25,300(l)	25,500
$B_4H_9SiH_3$	4(l)	11	25,000(l)	25,200	25,200(l)	25,400
B_5H_9	[a]7.8(l)	[a]15.0	29,100(l)	29,300	29,400(l)	29,600
$B_5H_8CH_3$	-7(l)	1	27,000(l)	27,200	27,200(l)	27,400
$B_5H_8C_2H_5$	-15(l)	-6	25,700(l)	25,900	25,900(l)	26,100
$B_5H_8C_3H_7$	-19(l)	-9	24,800(l)	25,000	25,000(l)	25,100
$B_5H_8SiH_3$	-1(l)	7	24,600(l)	24,800	24,800(l)	25,000
$B_{10}H_{14}$	[a]8(s)	[a]26	28,200(s)	28,500	28,500(s)	28,800
$B_{10}H_{13}CH_3$	-1(l)	12	27,200(l)	27,400	27,300(l)	27,700
$B_{10}H_{13}C_2H_5$	-9(l)	5	26,400(l)	26,600	26,700(l)	26,800
$B_{10}H_{13}C_3H_7$	-13(l)	2	25,800(l)	25,900	26,000(l)	26,200
$B_{10}H_{13}SiH_3$	5(l)	18	25,800(l)	25,900	26,000(l)	26,200

[a]Experimental value.

[redacted]

TABLE V. - Concluded. HEATS OF FORMATION AND COMBUSTION OF BORON COMPOUNDS (B,H,C,Si)

Compound	Heat of formation (at 25° C), ΔH_f^o, kcal/mole		Heat of combustion, ΔH_c, Btu/lb			
			To B_2O_3(amorphous)		To B_2O_3(crystalline)	
	Solid or liquid	Gas	Solid or liquid	Gas	Solid or liquid	Gas
$H_2BCH_2BH_2$	12(l)	17	26,300(l)	26,500	26,500(l)	26,800
$H_2BCH_2BH(CH_3)$	-7(l)	-1	23,900(l)	24,100	24,100(l)	24,300
$H_2BCH_2B(CH_3)_2$	-27(l)	-20	22,500(l)	22,600	22,600(l)	22,800
$(CH_3)HBCH_2BH(CH_3)$	-27(l)	-20	22,500(l)	22,600	22,600(l)	22,800
$(CH_3)HBCH_2B(CH_3)_2$	-47(l)	-39	21,500(l)	21,700	21,600(l)	21,800
$(CH_3)_2BCH_2B(CH_3)_2$	-66(l)	-57	20,800(l)	21,000	20,900(l)	21,100
$H_2BC_2H_4BH_2$	10(l)	16	24,500(l)	24,700	24,600(l)	24,800
$H_2BC_2H_4BH(CH_3)$	-8(l)	-1	23,000(l)	23,100	23,100(l)	23,300
$H_2BC_2H_4B(CH_3)_2$	-23(l)	-15	22,000(l)	22,200	22,100(l)	22,300
$(CH_3)HBC_2H_4BH(CH_3)$	-26(l)	-18	22,000(l)	22,100	22,100(l)	22,200
$(CH_3)HBC_2H_4B(CH_3)_2$	-41(l)	-32	21,300(l)	21,500	21,400(l)	21,600
$(CH_3)_2BC_2H_4B(CH_3)_2$	-56(l)	-46	20,800(l)	21,000	20,900(l)	21,100
$B_5H_8B_5H_8$	20(l)	32	28,800(l)	29,000	29,100(l)	29,300
$B_5H_8CH_2B_5H_8$	2(l)	15	27,600(l)	27,700	27,900(l)	28,000
$B_5H_8C_2H_4B_5H_8$	-6(l)	8	26,700(l)	26,900	27,000(l)	27,200
$B_{10}H_{13}B_{10}H_{13}$	32(l)	54	28,200(l)	28,300	28,500(l)	28,600
$B_{10}H_{13}CH_2B_{10}H_{13}$	14(l)	37	27,600(l)	27,700	27,900(l)	28,000
$B_{10}H_{13}C_2H_4B_{10}H_{13}$	12(l)	36	27,100(l)	27,300	27,400(l)	27,600

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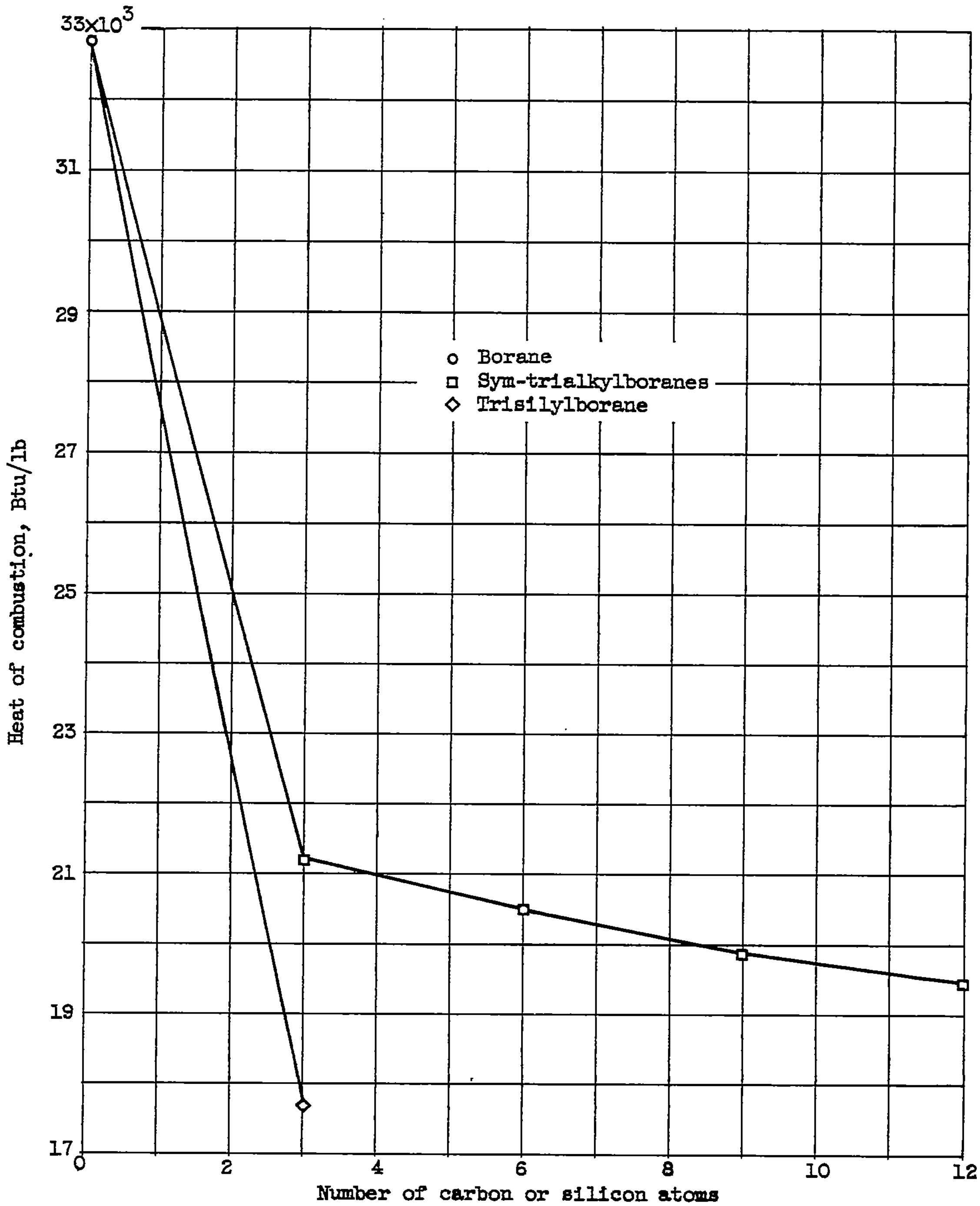
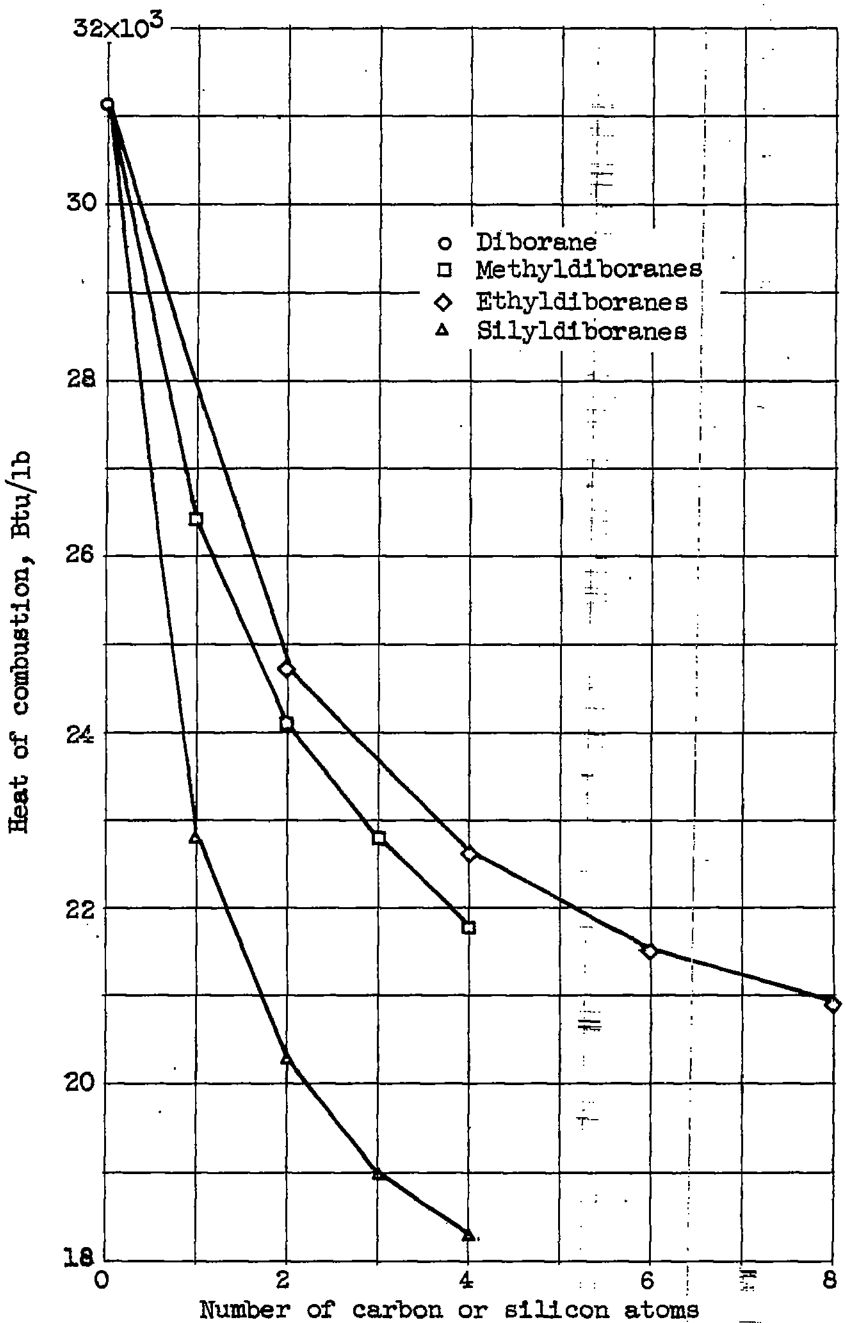


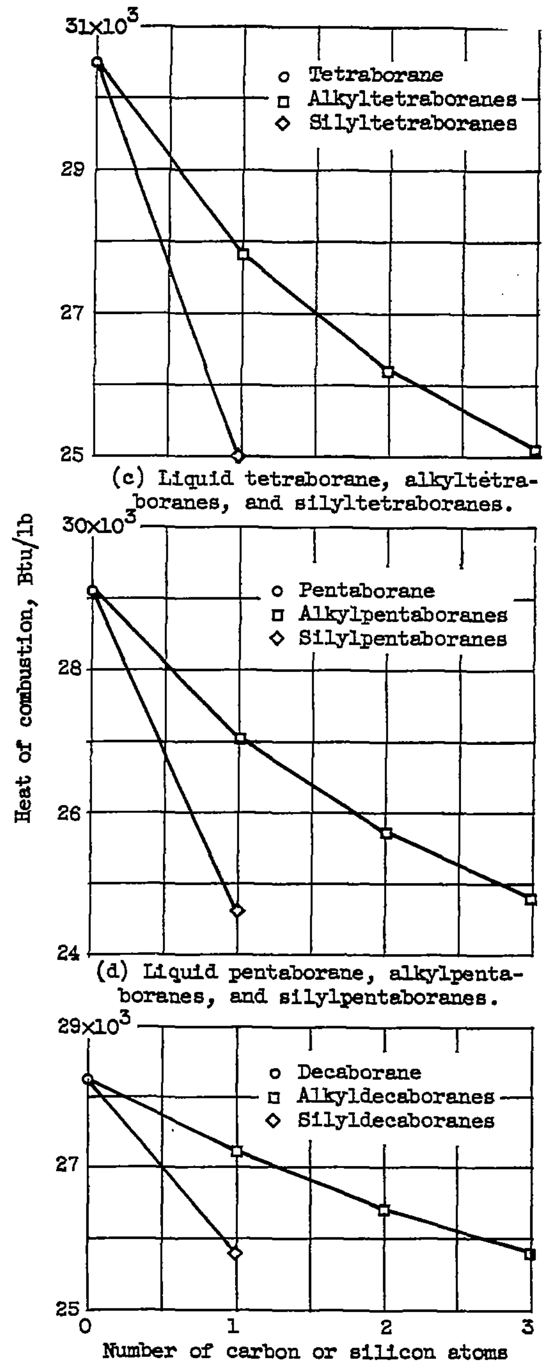
(a) Liquid borane and trialkyl- and trisilylboranes.

Figure 1. - Heats of combustion of boron-containing compounds.



(b) Liquid diborane and methyl, ethyl, and silyldiborane.

Figure 1. - Continued. Heats of combustion of boron-containing compounds.



(c) Liquid tetraborane, alkyltetraboranes, and silyltetraboranes.

(d) Liquid pentaborane, alkylpentaboranes, and silylpentaboranes.

(e) Liquid decaborane, alkyldecaboranes, and silyldecaboranes.

Figure 1. - Continued. Heats of combustion of boron-containing compounds.

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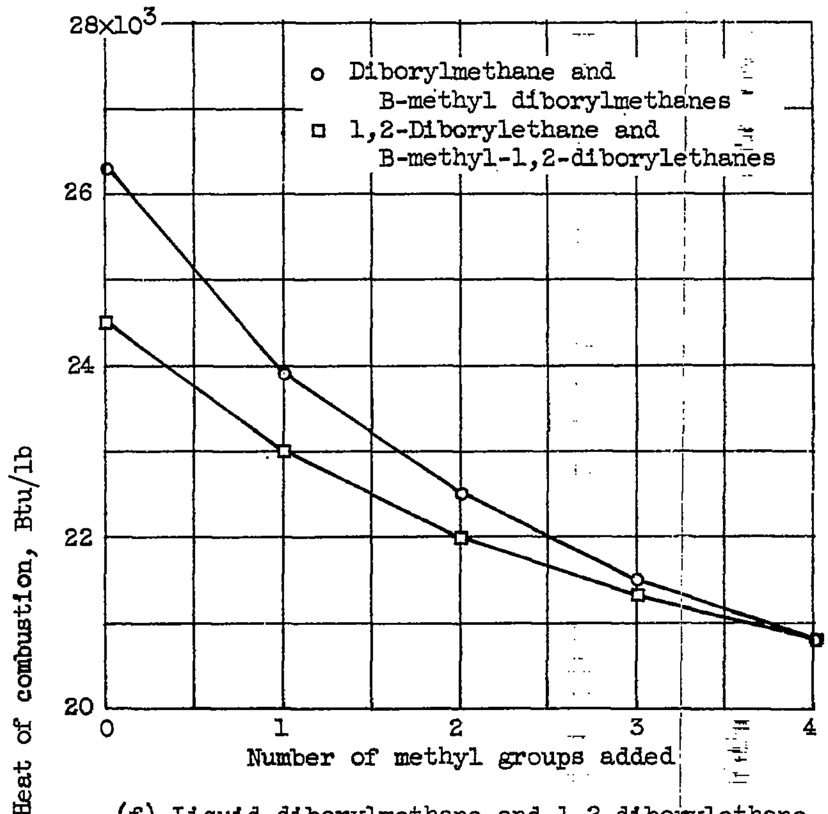
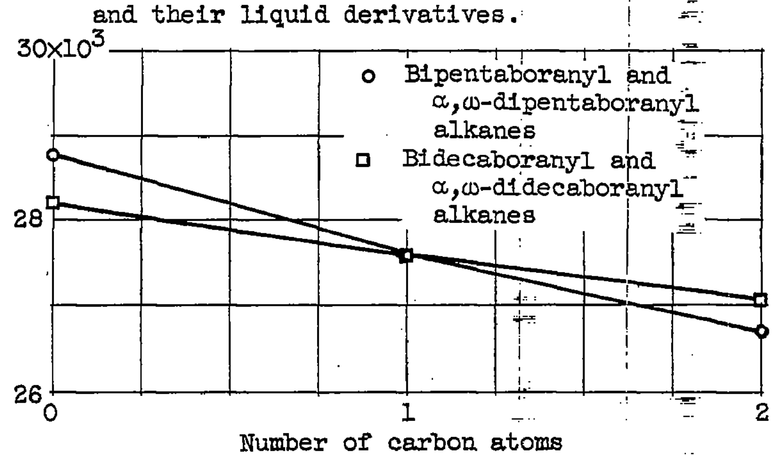


(f) Liquid diborylmethane and 1,2-diborylethane and their liquid derivatives.



(g) Bipentaboranyl-, bidecaboranyl-, dipentaboranyl-, and didecaboranyl-alkanes.

Figure 1. - Concluded. Heats of combustion of boron-containing compounds.