

Boron-Boron Bonding in Pentaborane-9

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Calculations of the electronic structure of pentaborane-9 have been carried out using MO, VB, three-centre bond, and NPSO wavefunctions, in order to determine the approximation most suitable for this type of molecule. The best of these wavefunctions as determined by comparison with a ten-parameter CI function, was one of the NPSO functions.

Die Elektronenstruktur von Pentaboran-9 wurde unter Verwendung von MO-, VB-, NPSO- und Dreizentrenbindungs-Wellenfunktionen berechnet. Die am besten geeignete unter diesen ist nach einem Vergleich mit einer zehnp-parametrischen CI-Funktion die NPSO-Funktion.

Des calculs de la structure électronique du 9-pentaborane ont été effectués en utilisant des fonctions d'onde M.O., V.B., liaisons à trois centres et NPSO, afin de déterminer l'approximation qui convient le mieux à ce genre de molécule. La meilleure de ces fonctions d'onde, en comparaison d'une fonction d'I.C. à dix paramètres, s'avère l'une des fonctions NPSO.

Introduction

The bonding in diborane and the higher boron hydrides is usually explained in terms of three-centre, two-electron bonds. These bonds offer a degree of electron delocalization intermediate between that of the multi-centre molecular orbital and the two-centre valence bond formulations of the bonding. Although diborane itself has been extensively studied [1–6], no comparative study of these alternative bonding schemes has yet appeared for the higher hydrides; the only calculations made so far have been based on semi-empirical molecular orbital methods [7–9]. The object of the present work is to assess the relative merits of these and other approaches to the bonding in one of the higher hydrides, namely pentaborane –9, by performing wave mechanical calculations.

Basis Set

The assumption was made that the terminal hydrogens are bonded by ordinary two-electron bonds, and the bridge hydrogens by three-centre two-electron bonds. Six electrons remain to bond together the five boron atoms. The apical B–H bond was assumed to use a boron sp -hybridized orbital. The hybridization of the basal borons was assumed to be such that the resulting hybrids pointed towards the three adjacent hydrogens and the apical boron, giving an $sp^{2.366}$ hybrid pointing towards the apical boron as the basal orbital available for bonding the boron framework. Thus the present calculations for the six electrons were based on the following seven orbitals: an $sp^{2.366}$ hybrid on each basal boron ($\chi_1, \chi_2, \chi_3, \chi_4$), and p_x, p_y and $sp_z(\chi_6, \chi_7$ and $\chi_5)$ orbitals on the apical boron (see Fig. 1). The

bond lengths used in the calculations were $B_{\text{base}} - B_{\text{base}}$: 1.800 Å, and $B_{\text{base}} - B_{\text{apex}}$: 1.687 Å, as found from the microwave spectrum [10]. The orbital exponents were taken as 1.3 for the base atoms and 1.475 for that at the apex, in accordance with Slater's rules for B^+ and B^{++} cores. Molecular orbitals derived from the above atomic orbitals are given in Table 1.

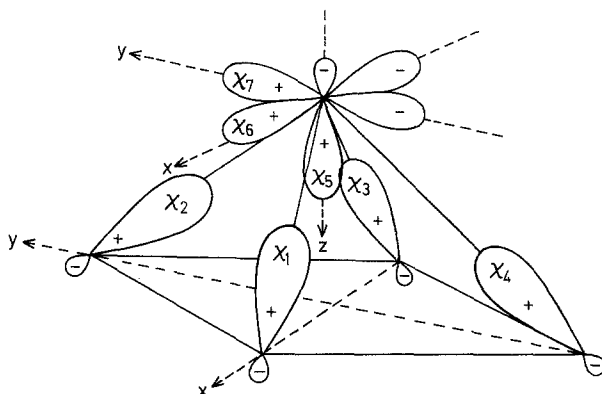


Fig. 1. The orbitals used for the pyramidal boron framework of B_5H_9 .

Table 1. *Molecular orbitals of pentaborane. For the definition of the χ see text and Fig. 1*

$$\begin{array}{l}
 \left. \begin{array}{l} \phi_7 = \chi_2 - \chi_4 - p\chi_7 \\ \phi_6 = \chi_1 - \chi_3 - p\chi_6 \end{array} \right\} (e^*) \\
 \phi_5 = \chi_1 - \chi_2 + \chi_3 - \chi_4 \quad (b) \\
 \phi_4 = \chi_1 + \chi_2 + \chi_3 + \chi_4 - q\chi_5 \quad (a^*) \\
 \left. \begin{array}{l} \phi_3 = \chi_2 - \chi_4 + r\chi_7 \\ \phi_2 = \chi_1 - \chi_3 + r\chi_6 \end{array} \right\} (e) \\
 \phi_1 = \chi_1 + \chi_2 + \chi_3 + \chi_4 + s\chi_5 \quad (a)
 \end{array}$$

A configuration interaction (CI) treatment for the six electrons using a seven orbital basis would involve 1225 Slater determinants and 74 1A_1 configurations; further simplification of the problem was considered necessary, and this was done by neglecting the high energy antibonding e^* orbitals. This left a restricted basis set of five molecular orbitals ϕ_1 to ϕ_5 , which gives only the eleven 1A_1 configurations listed in Table 2. The a^* orbital ϕ_4 is often considered to have the highest energy [11], but this is not the case here because this orbital bonds together the base atoms. This point will be discussed later.

A CI treatment was performed using the eleven configurations. This yields within the limitations set, the "best" wavefunction. This can be used for measuring the relative success of the more approximate treatments. The CI ground state energy does not depend on the values of the coefficients s and q . The value $s = 4$ was taken to give easy transformation to the equivalent bond orbital set, β_1 to β_5 , given in Table 3. In order that ϕ_4 should be orthogonal to ϕ_1 , q had to be 2.9438. The value of the coefficient r was varied to minimise the CI ground state energy, and the value thus found ($r = 1.1751$) was retained throughout the approximate treatments.

Table 2. The eleven 1A_1 configurations based on occupation of the a , e , a^* , and b molecular orbitals

$\psi_1 = (a)^2 (e)^4$	$\psi_7 = (a) (e)^2 (a^*) (b)^2$
$\psi_2 = (a) (e)^4 (a^*)$	$\psi_8 = (a)^2 (a^*)^2 (b)^2$
$\psi_3 = (a)^2 (e)^2 (a^*)^2$	$\psi_9 = (e)^4 (a^*)^2$
$\psi_4 = (a)^2 (e)^2 (a^*) (b)$	$\psi_{10} = (e)^4 (b)^2$
$\psi_5 = (a) (e)^2 (a^*)^2 (b)$	$\psi_{11} = (e)^2 (a^*)^2 (b)^2$
$\psi_6 = (a)^2 (e)^2 (b)^2$	

Table 3. The bond orbitals used for Pentaborane

$\beta_5 = 2\chi_5$
$\beta_4 = \chi_4 + \chi_5 - \frac{1}{2}\chi_7$
$\beta_3 = \chi_3 + \chi_5 - \frac{1}{2}\chi_6$
$\beta_2 = \chi_2 + \chi_5 + \frac{1}{2}\chi_7$
$\beta_1 = \chi_1 + \chi_5 + \frac{1}{2}\chi_6$

Approximate Wavefunctions

These functions have one or two adjustable parameters as against ten for the CI function; optimum values were found by applying the Variation Method.

Molecular Orbital

The simple molecular orbital (MO) function puts two electrons in each of the three lowest orbitals ϕ_1 , ϕ_2 , and ϕ_3 . Since the coefficients s and q were chosen arbitrarily a better function is

$$\Psi_{\text{MO}} = \|(\phi_1 + k\phi_4) \phi_2 \phi_3 (\phi_1 + k\phi_4) \phi_2 \phi_3\|.$$

The double lines indicate formation of a determinant, and the spins are understood to be in the order $\alpha\alpha\alpha\beta\beta\beta$. In terms of the 1A_1 configurations listed in Table 2 this function is

$$\Psi_{\text{MO}} = \psi_1 + k\psi_2 + k^2\psi_9.$$

An alternant molecular orbital (AMO) function [12] may be constructed by mixing ϕ_5 with $\phi_1 + k_1\phi_4$

$$\begin{aligned} \Psi_{\text{AMO}} &= \|(\phi_1 + k_1\phi_4 + k_2\phi_5) \phi_2 \phi_3 (\phi_1 + k\phi_4 - k_2\phi_5) \phi_2 \phi_3\| + \text{etc.} \\ &= \psi_1 + k_1\psi_2 + k_1^2\psi_9 - k_2^2\psi_{10} \end{aligned}$$

where “+ etc.” represents the addition of other determinants to form spin and symmetry eigenfunctions.

Valence Bond

Three valence bond (VB) functions are possible for B_5H_9 , apart from those involving lone pairs. The first, involving two adjacent base-apex bonds and a third bond between the remaining adjacent base atoms, cannot be written using the restricted basis set, and so was not considered. The second VB function, involving two diagonally opposite base-apex bonds and a diagonal base-base bond, can be regarded as a special case of a three-centre bond function with the coefficient of the apex orbital in the diagonal three-centre base-apex-base bond

set to zero. This function was again not considered further. The third VB function involves three base-apex bonds

$$\begin{aligned}\Psi_{\text{VBC}} &= \|(\beta_1 + k\beta_5)(\beta_2 + k\beta_5)(\beta_3 + k\beta_5)(\beta_1 + k\beta_5)(\beta_2 + k\beta_5)(\beta_3 + k\beta_5)\| + \text{etc.} \\ &= 2(1+k)^2\psi_1 - 2k(1+k)\psi_2 + (1+k)^2\psi_6 \\ &\quad + k(1+k)\psi_7 + 2k^2\psi_9 + 2\psi_{10} + k^2\psi_{11}.\end{aligned}$$

Mixing β_5 with the "pure" two-centre orbitals β_1 to β_4 is the only flexibility possible with the restricted basis set, since simultaneous mixing of the atomic orbitals χ_6 and χ_7 (giving polarization of electrons along the base-apex axes) would be equivalent to introducing the e^* molecular orbitals into the wavefunction. Nevertheless, this admixture of β_5 alone does introduce some polarization, and therefore does satisfy to a certain extent the aim of keeping electrons apart.

Three-Centre Bond

There are two ways of forming three-centre bonds in B_5H_9 which do not involve lone-pair wavefunctions for the remaining electrons: from orbitals on diagonally opposite base atoms and the apex atom (type *A*) and from orbitals on adjacent base atoms and the apex atom (type *B*). In each case the three-centre bonds can be either of σ or "closed" type or of π or "open" type. We may thus write the four three-centre bond wavefunctions

$$\Psi_{\text{C3AE}} = \|(\beta_1 + k_1\beta_5)(\beta_3 + k_1\beta_5)(\beta_2 + \beta_4 + k_2\beta_5)(\beta_1 + k_1\beta_5)(\beta_3 + k_1\beta_5)(\beta_2 + \beta_4 + k_2\beta_5)\| + \text{etc.}$$

$$\Psi_{\text{C3AH}} = \|(\beta_1 + k\beta_5)(\beta_3 + k\beta_5)(\beta_2 - \beta_4)(\beta_1 + k\beta_5)(\beta_3 + k\beta_5)(\beta_2 - \beta_4)\| + \text{etc.}$$

$$\Psi_{\text{C3BE}} = \|(\beta_1 + k_1\beta_5)(\beta_2 + k_1\beta_5)(\beta_3 + \beta_4 + k_2\beta_5)(\beta_1 + k_1\beta_5)(\beta_2 + k_1\beta_5)(\beta_3 + \beta_4 + k_2\beta_5)\| + \text{etc.}$$

$$\Psi_{\text{C3BH}} = \|(\beta_1 + k\beta_5)(\beta_2 + k\beta_5)(\beta_3 - \beta_4)(\beta_1 + k\beta_5)(\beta_2 + k\beta_5)(\beta_3 - \beta_4)\| + \text{etc.}$$

The expansions in terms of the eleven 1A_1 configurations of the three-centre bond functions and of the Non-Paired Spatial Orbital functions which follow will not be given explicitly because of their complexity.

Non-Paired Spatial Orbital

The Non-Paired Spatial Orbital (NPSO) method [13, 14] has been applied with considerable success to several systems. According to this procedure electrons with different spins may be put in different spatial orbitals; one-electron bonds and singly filled orbitals become admissible. Consequently this approach may be particularly well-suited to electron-deficient molecules such as the boron hydrides.

For pentaborane the NPSO functions will be written in terms of the orbitals

$$U_i(k) = \beta_i - k\beta_5, \quad i = 1, 2, 3, 4$$

$$V_i(k) = \beta_i + k\beta_5, \quad i = 1, 2, 3, 4$$

$$W(k) = \left(\sum_{i=1}^4 (1+k)\beta_i \right) - 4k\beta_5.$$

These orbitals are not independent, since nine orbitals are formed from five bond orbitals; but their use enables one to interpret the wavefunction readily. W is the five-centre molecular orbital which also appears in the MO function. The U orbitals are bond orbitals in which the electrons are polarized away from the C_4 axis of the molecule, and the V orbitals are bond orbitals polarized towards this axis.

Because electrons do not have to be assigned to orbitals in pairs and therefore orbitals do not have to be doubly filled, several NPSO functions for B_5H_9 are possible: three will be discussed in detail here.

The NPSO function $N1$ is an extension of the simple MO function by the addition of electron correlation. Instead of assigning two electrons to each of the two three-centre e -orbitals, ϕ_2 and ϕ_3 , one electron is assigned to each of the U orbitals. It may thus be thought of as having one electron near each of the sloping edges of the square pyramid together with two electrons in the body of the pyramid.

$$\Psi_{N1} = \|U_1(k_1) U_2(k_1) W(k_2) U_3(k_1) U_4(k_1) W(k_2)\| + etc.$$

In function $N2$ the singly filled orbitals are alternately U , V , U , V around the pyramid.

$$\Psi_{N2} = \|U_1(k_1) V_2(k_1) W(k_2) U_3(k_1) V_4(k_1) W(k_2)\| + etc.$$

Function $N3$ is a variant of the simple three-centre bond approach. The three-centre bonds of type B are localized in the sloping faces of the pyramid. Since there are four such faces a reasonable NPSO function would be one which puts one electron in each face plus two electrons in the body of the pyramid:

$$\Psi_{N3} = \|(U_1(k_1) + U_2(k_1)) (U_2(k_1) + U_3(k_1)) W(k_2) (U_3(k_1) + U_4(k_1)) \\ (U_4(k_1) + U_1(k_1)) W(k_2)\| + etc.$$

NPSO functions involving two doubly filled and two singly filled base-apex orbitals (extensions of the simple VB formulation) were also tested but gave poor results.

Results and Discussion

Table 4 gives the energies and values for the overlap with the CI function for the approximate wavefunctions; the CI results are included for comparison. The one-electron energy E_1 is the sum of the kinetic energy and the core attraction terms. All energies are given in hartrees. Table 5 gives the bond orders and gross atomic populations as defined by Mulliken [15]. Fig. 2 presents, in diagrammatic form, the coefficients of the eleven 1A_1 configurations for each normalized function; the height of each line is proportional to the value of the corresponding coefficient, negative coefficients being represented by lines below the horizontal base line.

Inspection of the coefficients of the eleven basis 1A_1 configurations for the configuration interaction (CI) function shows that the most important contribution to this function is made by the configuration ψ_3 . At first sight this is surprising, because this configuration has the orbital population $(a)^2(e)^2(a^*)^2$, with two electrons in the antibonding a^* orbital. However, it must be borne in mind that

Table 4. Mean one-electron energy (E_1), mean inter-electron repulsion energy (E_{12}) and excess energy ($E - E_{CI}$) for the various approximate wave function above that calculated using the best CI function ($E_{CI} = -10.44$ a.u.). The overlap (S) of the approximate and the CI function is also listed for each function. The number of adjustable parameters for each function is given in brackets

Function	E_1	E_{12}	$E - E_{CI}$	S
MO or AMO (1)	-13.84	3.81	0.41	0.069
C3A Σ (2)	-13.97	3.91	0.38	0.741
C3A Π (1)	-16.64	7.11	0.91	0.538
C3B Σ (2)	-13.90	3.94	0.48	0.686
C3B Π (1)	-16.04	7.39	1.79	0.134
VBC (1)	-16.57	7.12	0.99	0.444
N1 (2)	-14.86	4.44	0.02	0.987
N2 (2)	-14.76	4.34	0.02	0.991
N3 (2)	-14.66	4.32	0.10	0.928
CI (10)	-14.72	4.28	0	1.000

Table 5. Bond orders and charge distribution for the various wave-functions. The boron atoms at the base of the pyramid are labelled 1 to 4 and that at the apex 5

Function	Bond Orders			Gross Atomic Populations	
	B ₁ - B ₂	B ₁ - B ₃	B ₁ - B ₅	B ₁	B ₅
MO or AMO	0.29	0.03	-1.02	0.68	3.29
C3A Σ	0.33	0.13	-0.98	0.75	3.00
C3A Π	0.10	-0.07	+0.13	1.02	1.91
C3B Σ	0.30	0.16	-1.00	0.76	2.94
C3B Π	-0.74	0.40	+0.19	1.02	1.92
VBC	0.06	-0.04	+0.12	1.04	1.84
N1	0.21	0.09	-0.59	0.88	2.47
N ₂	0.23	0.09	-0.82	0.89	2.43
N3	0.28	0.08	-0.69	0.84	2.67
CI	0.20	0.11	-0.62	0.89	2.42

initially the coefficient s in the molecular orbital $\phi_1(a)$, and consequently q in $\phi_4(a^*)$ were chosen arbitrarily, and therefore these molecular orbitals, as used in the calculations, are not simply bonding and antibonding orbitals. Figs. 3 to 6 give the electron densities in the diagonal base-apex-base plane of the normalised molecular orbitals ϕ_1 , ϕ_2 , ϕ_4 and ϕ_5 . It can be seen that ϕ_1 has no nodes in the region of the pyramid but is diffuse, whereas ϕ_4 does have such a nodal surface, but is more localised within the pyramid. Therefore ϕ_4 may have a more favourable distribution of density than ϕ_1 , with respect both to the cores and to the other molecular orbitals.

In a simple system, such as a diatomic molecule, the bonding or antibonding nature of an orbital can be related directly to the absence or presence of nodes. This simple relationship cannot be carried over to complex molecules such as pentaborane. In a diatomic molecule the presence of nodes in a wavefunction causes a migration of charge out of the bonding region onto the nuclei and it is this migration which increases the energy. In pentaborane, orbital ϕ_4 is very similar to an atomic orbital on the apex atom alone, but in this case migration of charge

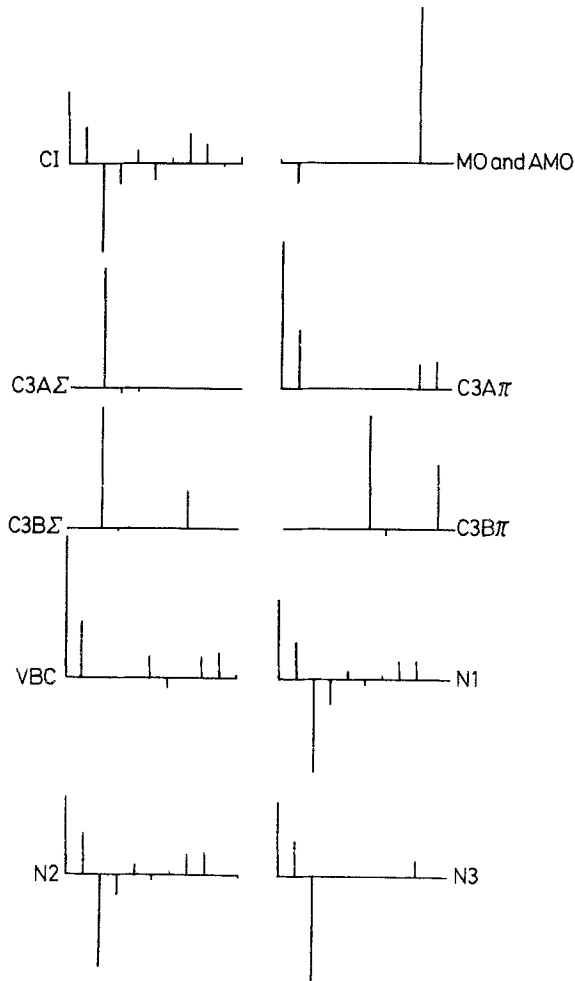


Fig. 2. Diagrammatic representation of the coefficients which measure the contribution of the eleven configurations listed in Table 2 to the configuration interaction wave function and the functions based on various approximate treatments

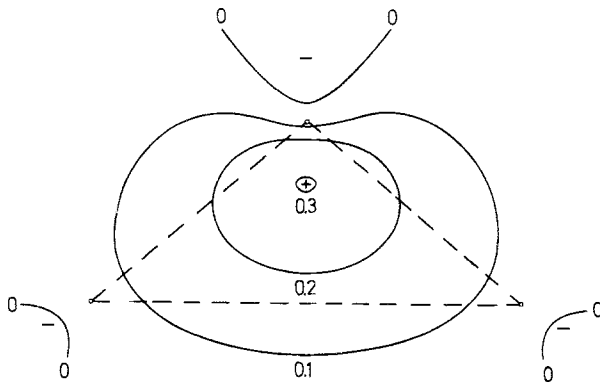


Fig. 3. The a molecular orbital: $\phi_1 = k_1(\chi_1 + \chi_2 + \chi_3 + \chi_4 + 4\chi_5)$

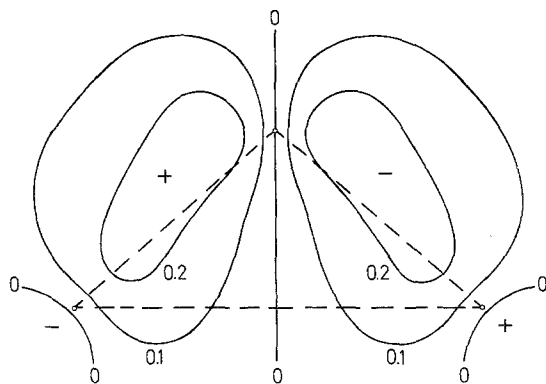


Fig. 4. An e molecular orbital: $\phi_2 = k_2(\chi_1 - \chi_3 + 1.1751\chi_6)$

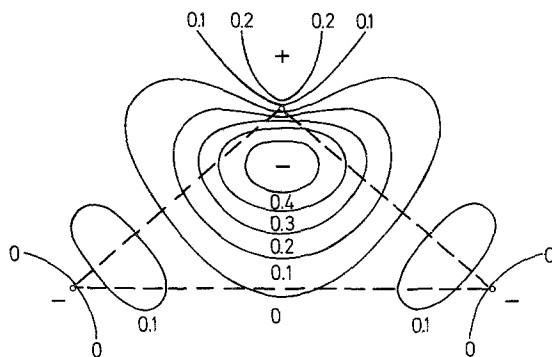


Fig. 5. The a^* molecular orbital which is orthogonal to ϕ_1 : $\phi_4^1 = k_4^1(\chi_1 + \chi_2 + \chi_3 + \chi_4 - 2.9438\chi_5)$

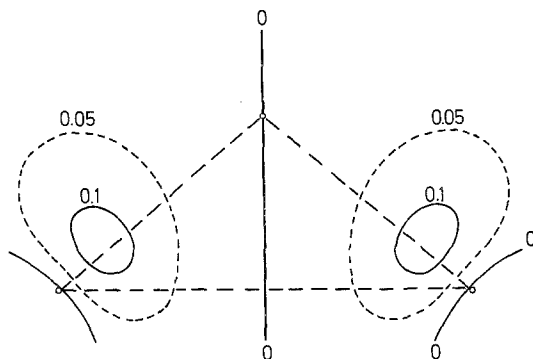


Fig. 6. The b molecular orbital: $\phi_5 = k_5(\chi_1 - \chi_2 + \chi_3 - \chi_4)$

gives a favourable location of charge, and so the energy of this orbital may well be low. Since the covalent bond order between the base and apex atoms is -0.62 (i.e. antibonding), ϕ_4 may well bind the molecule by providing strong ionic bonding between the base and apex atoms as well as some covalent bonding between the individual base atoms.

The second most important contributor to the CI function is ψ_1 . This configuration would be expected to be important, because it corresponds to the orbital population $(a)^2(e)^4$, with each of the three bonding orbitals doubly filled. The next most important contributors to the CI function are ψ_2 , ψ_8 , and ψ_9 , with the respective orbital populations $(a)(e)^4(a^*)$, $(a)^2(a^*)^2(b)^2$, and $(e)^4(a^*)^2$. The importance of ψ_2 and ψ_9 is again due to the a^* orbital not being as antibonding as its nomenclature implies. Mixing of ψ_2 and ψ_9 with ψ_1 is equivalent to allowing for a better choice for the form of the bonding a -orbital. It can also allow for some in-out correlation of the electrons with respect to the C_4 axis of the molecule.

The importance of ψ_3 and ψ_8 may be related as follows. ψ_8 may be derived from ψ_3 by exciting the two electrons in the e orbital into the b orbital. These two orbitals are respectively antisymmetric and symmetric across the diagonal of the molecule. The two-electron configurations $(e)^2$ and $(b)^2$ may be divided into terms in which the two electrons are on the same side of the molecule (always positive) and terms in which they are on opposite sides (negative for $(e)^2$ and positive for $(b)^2$). These latter terms may be given greater weight, thus keeping these two electrons apart, if ψ_3 and ψ_8 have coefficients in the CI function of opposite sign but comparable magnitude, as is observed in practice. This separation of electrons, achieved here by $(e)^2 - (b)^2$ interaction, is accomplished in the successful NPSO functions by requiring, *ab initio*, that the electrons be assigned to different orbitals.

All the remaining six configurations make small contributions to the CI function.

The bond orders and charge densities for the CI function show that there is a considerable migration of charge onto the apex atom, giving it a net charge of -0.42 , and the base atoms net charges of $+0.11$. If it is assumed that these charges are situated on the respective nuclei, then this distribution of charges corresponds to a dipole moment of 2.2 Debye, in excellent agreement numerically with the value 2.13 Debye found experimentally by Stark splitting in the microwave spectrum [10]. Although the correct sign has been obtained, the agreement of the numerical magnitude is extremely fortuitous, in view of the approximations involved. Thus, Moore's extended Hückel treatment of pentaborane [7] gives the net charge on the apex boron as -0.87 , corresponding to a dipole moment of 4.6 Debye. He finds, however, that if allowance is made for net charges of -0.1 on the apex terminal hydrogen and -0.2 on the bridge hydrogens, the calculated dipole moment becomes 1.8 Debye.

The conclusions drawn above concerning the nature of the a^* orbital are confirmed by the results for the molecular orbital functions. The simple molecular orbital function involves the three configurations ψ_1 , ψ_2 , and ψ_9 , with the respective orbital occupations $(a)^2(e)^4$, $(a)(e)^4(a^*)$ and $(e)^4(a^*)^2$. The coefficient of the last of these is by far the greatest, presumably because the a^* orbital is concentrated to a large extent along the C_4 axis of the molecule, along which axis the density of the e -orbitals is zero. For the MO function E_{12} is low. This function seems to be too successful in keeping the electrons in the different orbitals apart. The energy of the AMO function was found to be fairly insensitive to the amount of mixing between the bonding orbital $\phi_1 + k_1\phi_4$ and the antibonding orbital ϕ_5 . This is because an increase in the mixing, which separates the two electrons in the orbital $\phi_1 + k_1\phi_4$, simultaneously moves these electrons nearer

those in the e -orbitals. In fact the optimum value for the mixing coefficient is zero, and so the AMO and MO functions are identical.

The valence bond function VBC compares very poorly with the CI function: the energy is very high and E_{12} is very high. With two electrons localised in each of three adjacent two-centre orbitals, the inter-electronic repulsion must be relatively high. The net negative charge of 0.04 on the base atoms for this function, giving a dipole moment of the wrong sign, occurs because these electrons tend to keep apart by moving down the edge of the tetragonal pyramid.

The three-centre bond functions based on a diagonal type three-centre bond are more successful than the corresponding functions based on a face three-centre bond. This is probably due not to any greater inherent stability of the former type of bond but to repulsion effects between the electrons in the remaining two-centre bonds, as in the function VBC. The improvement of the Σ -type functions over the Π -type functions, however, is probably due to the greater stability of the Σ -type three-centre bond.

The NPSO functions $N1$ and $N2$ give the best approximations, by energy, overlap and charge distribution criteria, to the CI function; these two-parameter functions reproduce the coefficients of the ten-parameter CI function remarkably well. The behaviour of the function $N3$ is also good, considering that it only involves four of the eleven possible 1A_1 configurations.

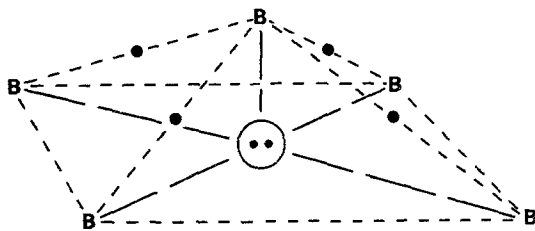


Fig. 7. A "chemical formula" for B_5H_9 based on functions $N1$ and $N2$

The best simple approximation to the electronic structure of pentaborane is thus given by functions which put two electrons in the body of the square pyramid, and one electron either in each of the sloping edges of the pyramid ($N1$ and $N2$) or in each of the sloping faces of the pyramid ($N3$) (Fig. 7).

Adamson [16] has shown that the molecular orbitals derived by Longuet-Higgins and Roberts [17] for B_5^{2-} may be transformed into an equivalent set in which the occupied orbitals are: an outward-pointing hybrid on each atom (singly filled); six three-centre bonds, each involving primarily two diagonally-opposite atoms plus a third atom (doubly filled); and a six-centre bond, composed of an inward-pointing hybrid on each atom (doubly-filled). (The criterion used in this transformation is that the overlap between the molecular orbitals be minimized, that is, that the electron pairs be separated to the maximum possible extent.) If the doubly-filled three-centre bonds are each replaced by two singly-filled two-centre bonds, so allowing for electron-correlation and changing to the NPSO form, the resulting formulation of the structure is shown in Fig. 8.

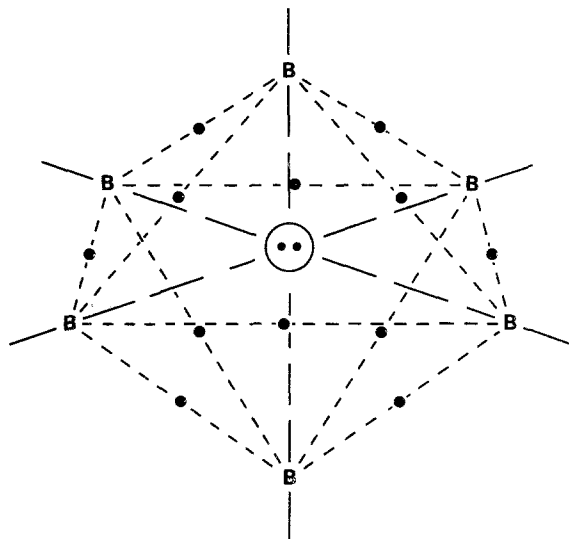


Fig. 8. A "chemical formula" for B_5^{2-} based on Adamson's calculations

This is very similar to the function $N1$ for pentaborane, in that these two electronic structures can both be described using one-electron boron-boron bonds, and a doubly-filled orbital concentrated in the centre of the molecule.

In conclusion it appears that the electronic structures of these polyhedral boron species may be represented better by functions which use two-centre one-electron boron-boron bonds, than by functions involving more delocalised electron-pair bonds.

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