THE THEORY OF ATOMS IN MOLECULES FOR THE BORANES

APPLICATION OF THE THEORY OF ATOMS IN MOLECULES TO THE BORANES AND CARBORANES

By

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Abstract

The theory of Atoms in Molecules is applied to a series of borane molecules. A study of the topological features of the charge density, $\rho(\mathbf{r})$, yields a quantum mechanical definition of atoms, bonds, and the average properties of atoms within a molecule. Other topological features of the boranes studied include rings and cages, formed by bond paths in ρ which link the atoms. These bond paths which form rings are bent inward in order to maximize the binding in these electron-deficient molecules. An important result of this analysis is the unambiguous assignment of the connectivity of the boranes.

The theory of atoms and molecules allows one to quantum mechanically partition molecules into atomic basins, and calculations of average values for electron count and energies of individual atoms are performed by integration over these basins. Comparisons of atomic properties are performed to determine the transferability of atomic properties across the series.

The Laplacian of ρ, $\nabla^2\rho$, yields information about sites of electrophilic and nucleophilic attack in molecules. These sites are found to correspond to the positions of critical points in $\nabla^2\rho$, which are localized to specific atoms in the molecule. The boranes and carboranes are ranked according to their susceptibility to electrophilic and nucleophilic attack, and such reactions with boranes are predicted to be regiospecific.

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Once carbon a neighbouring hydrogen chided
"You've more charge than Mulliken provided"
The hydrogen answered with purpose
"We're split by a zero-flux surface
So we're not arbitrarily divided!"

1. Introduction

The most fundamental underlying concept in all of chemistry is the atomic hypothesis and its related theory of molecular structure. Until recently, scientists have been able to only postulate the idea that atoms exist as the distinct "building blocks" of molecules, while employing models such as that provided by Lewis to describe molecules as a network of atoms joined by bonds to give a particular structure. These models were not based on a fundamental understanding of quantum mechanics, but rather reflected experimental realities seen in the laboratory. With the theory of atoms in molecules, one can now recover the concepts of atoms, bonds, and molecular structure, so providing their unambiguous definition. With this theory, it is also possible to properly differentiate between molecular structure and molecular geometry, as well as predict the sites of relative reactivity in molecules.

The theory of atoms in molecules primarily deals with an examination of the charge density, $\rho(\mathbf{r},\mathbf{X})$ for a molecule, where $\mathbf{X}$ represents a point in configuration space, the set of nuclear coordinates representing a particular molecular geometry. The attractive forces involved in the interaction between nuclei and the surrounding electronic charge yield the first important result, that the charge density in a molecule in general attains local maxima only at the nuclear positions (Bader 1985). Therefore the nuclei make the most significant and recognizable contributions to the molecular charge distribution, a result which has made

which has made the gross structure of molecules an accessible component of chemical research for many years before the properties of the charge density were uncovered.

In deriving a quantum mechanical expression for the charge density, $\rho(\mathbf{r},\mathbf{X})$, the probability of finding each one of the N electrons in a molecular system in a particular volume element $d\tau_i = dx_i dy_i dz_i$ with spin σ_i for an arrangement of nuclei $\mathbf{X}$ is defined by

$$\psi^*(x;\mathbf{X})\psi(x;\mathbf{X})dx_1 dx_2 \cdots dx_n , \qquad d\mathbf{x}_i = d\tau_i \sigma_i \tag{1}$$

Further, one can obtain the probability of finding one electron in an elemental volume (independent of other electronic positions) by summing eqn. (1) over spin coordinates and integrating over the positions of all electrons but one, giving

$$\sum (\text{spins}) \left\{ \int d\tau_2 \int d\tau_3 \cdots \int d\tau_N \psi^*(x;\mathbf{X})\psi(x;\mathbf{X}) \right\}. \tag{2}$$

Finally, one obtains the total probability for finding electronic charge in an elemental volume $d\tau_1$ by multiplying eqn. (2) by the number of electrons N. This then defines the electronic charge density $\rho(\mathbf{r},\mathbf{X})$, where $\mathbf{r} = \mathbf{i}x + \mathbf{j}y + \mathbf{k}z$, as

$$\rho(\mathbf{r};\mathbf{X}) = N\sum(\text{spins})\left\{\int d\tau_2 \int d\tau_3 \cdots \int d\tau_N \psi^*(x;\mathbf{X})\psi(x;\mathbf{X})\right\}. \qquad (3)$$

which in a shorter form is rendered as

$$\rho(\mathbf{r};\mathbf{X}) = N\int d\tau' \psi^*(x;\mathbf{X})\psi(x;\mathbf{X}) \qquad (4)$$

where $\int d\tau'$ denotes summation over spin coordinates of all electrons, and integration over all cartesian coordinates except one.

As a physical example to illustrate the gross features of the molecular charge distribution, one can examine relief maps of B_2F_4, which show the three perpendicular molecular planes, with the charge density as a projection above each of these planes. Fig. 1a shows the plane of all six nuclei, while Fig. 1b shows the other plane still containing the boron-boron internuclear axis, obtained by rotating the plane of Fig. 1a by ninety degrees about this axis. Fig. 1c is the third plane perpendicular to the boron-boron internuclear axis, showing charge density for a plane containing the midpoint of this axis (note: the relative vertical accentuation for these three plots a, b and c is 3:3:10, so that the charge density in the midpoint of the boron-boron axis in Fig. 1c could be clearly seen).

Both Figs. 1a and 1b exhibit local maxima in $\rho(\mathbf{r})$ at the positions of each of the nuclei, showing that a nuclear maximum is visible in <u>any</u> plane containing that nucleus. Also, both these figures show a "saddle" in the midpoint of the boron-boron axis, while Fig. 1c shows a maximum there.

This points up the necessity of knowing the behaviour of $\rho(\mathbf{r})$ in all three mutually perpendicular planes. The three-dimensional form of the charge density can be summarized by expounding on the nature of the curvatures of $\rho(\mathbf{r})$ at what are known as critical points.

A critical point in the molecular charge distribution is defined as a point in space where $\nabla\rho(\mathbf{r}) = 0$. As with any scalar function, the maximal or minimal characteristics of $\rho(\mathbf{r})$ are determined by the sign of the second derivative, or curvature. Since there are three dimensions involved, there can be at most three principal non-zero curvatures for $\rho(\mathbf{r})$ (The word "principal" is used, because there are actually nine such curvatures involving cross terms in *x*, *y*, and *z*, but this 3×3 Hessian matrix can be diagonalized to give just three second derivatives with respect to the principal axes of curvature, which in the case of the central critical point in B_2F_4 coincide with the symmetry axes of the molecule).

In one dimension, a maximum is denoted by a negative curvature, while a minimum is found at a point with a positive curvature, and the combinations of the three possible signs of the curvatures can be combined into one succinct characterization for any critical point in $\rho(\mathbf{r})$. The number of non-zero curvatures is called the rank, ω, and the sum of the signs of these curvatures is called the signature, σ. Since in B_2F_4 there exists a minimum in $\rho(\mathbf{r})$ along the boron-boron internuclear axis, and a maximum along the other two perpendicular axes, the rank is three, and the signature is minus one, making this a (3,–1) or bond critical point. Note that Figs. 1a and 1b each show one positive and one negative

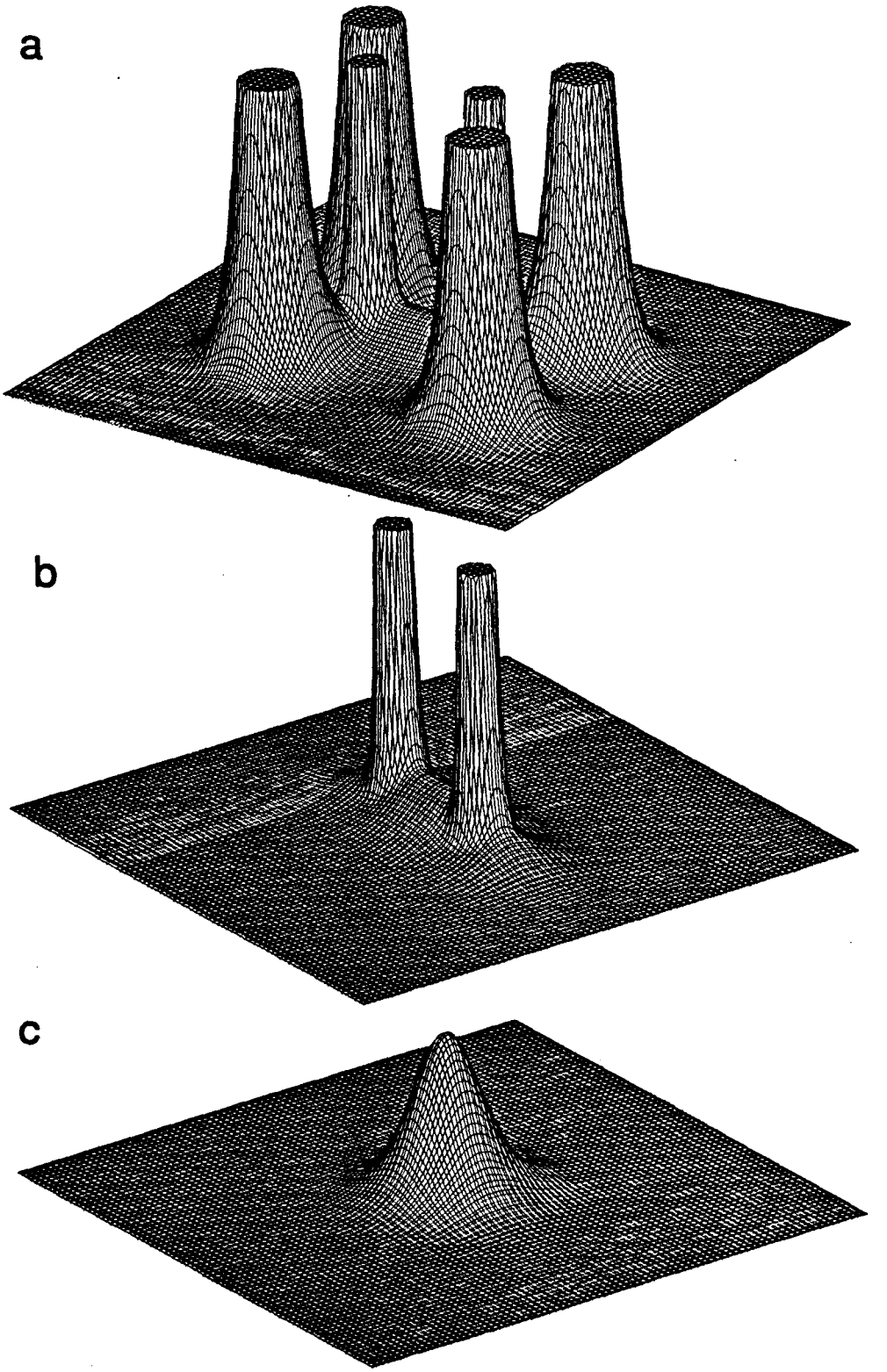

Fig. 1 Relief maps of the electronic charge density in B_2F_4 in three orthogonal planes containing the critical point midway between the boron nuclei.

curvature, while Fig. 1c shows the two negative curvatures perpendicular to the bond axis. Four more (3, –1) critical points appear between the borons and those fluorine atoms to which they are generally regarded as bonded, and these exhaust all of the available (3,–1) critical points found in this molecule.

This method of categorization also provides that the nuclear positions are known as (3, –3) critical points, although $\nabla\rho$ and $\nabla\psi$ are discontinuous because of the cusps found there. Note also that critical points of rank three are prevalent in real molecular systems, while critical points with $\omega<3$, known as degenerate critical points, are less prevalent and also unstable, since a small change in nuclear configuration will resolve these into stable critical points of rank three; the presence of these degenerate critical points marks the onset of a change in molecular structure (Bader *et al* 1981).

There are two other possible signature values for critical points of rank three, (3,+1) and (3,+3) critical points, which are characteristic of ring and cage structural elements, respectively (Bader 1985). To illustrate the nature of the (3,+1) or ring critical points, B_2H_6 will serve, as shown in Figs. 2a-2c, which also contain relief maps of $\rho(\mathbf{r})$, as in the previous figures. While the peripheral saddle points are similar to those (3,–1) or bond critical points found in B_2F_4, the critical point found in the centre of the molecule is a (3,+1) or ring critical point. This is indicated by the presence of a minimum in the plane containing the borons and the bridging hydrogens, as shown in Fig. 2b, and a saddle rather than a maximum in the

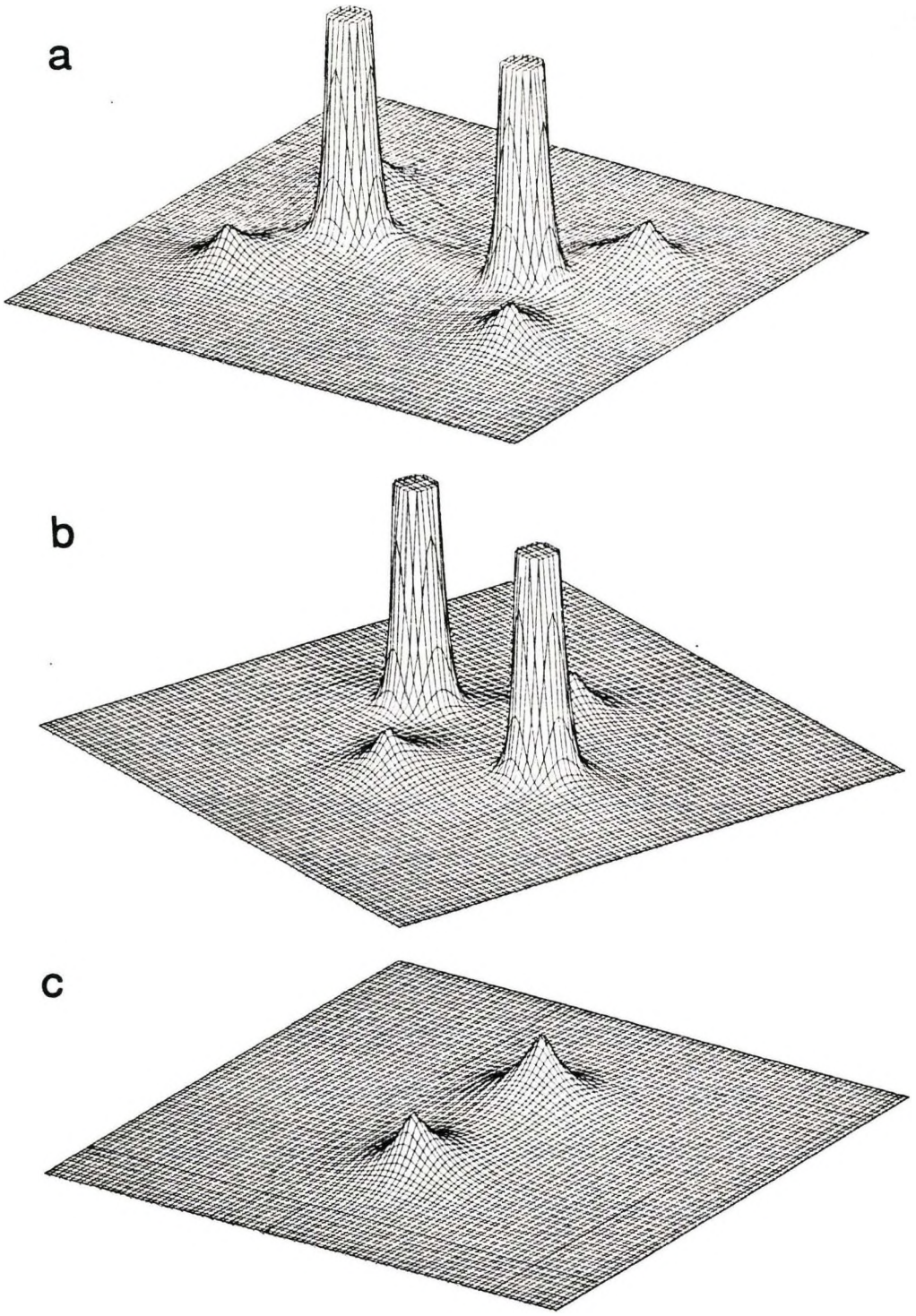

Fig. 2 Relief maps of the electronic charge density in B_2H_6 in three orthogonal planes containing the critical point midway between the boron nuclei.

plane perpendicular to the boron-boron axis and containing the bridging hydrogens, with a similar saddle appearing in the same position in Fig. 2a. This critical point is surrounded by a ring of (3, –1) bond critical points as shown in Fig. 2b, hence the name "ring" critical point. The axis of the single negative curvature is perpendicular to this ring.

Illustration of the fourth type of critical point, known as a (3, +3) or cage critical point, is served by $B_6H_6^{2-}$, shown in Figs. 3a-3b. The critical point in the centre of this molecule appears as a minimum in any plane containing the point, and the presence of the other ring and bond critical points can be deduced from examination of the (2, 0) saddles and (2,-2) maxima found in the planes represented in these figures. Thus, $B_6H_6^{2-}$ contains all the possible non-degenerate (ω=3) critical points.

After looking at the topology of $\rho(\mathbf{r})$, one can examine the properties of the gradient vector field of $\rho(\mathbf{r})$, and in so doing recover the molecular structural elements familiar to all chemists. These are directly obtainable from the charge density itself, with no reliance on arbitrary models. One can observe the gradient vector field by mapping out the trajectories of $\nabla\rho$, known as gradient paths, all of which originate and terminate at critical points, where of course $\nabla\rho(\mathbf{r})$ vanishes. These trajectories are perpendicular to the contour lines of constant density in ρ (a contour map for B_2F_4 is found in Fig. 5c), and the vector $\nabla\rho(\mathbf{r})$ is tangent to its trajectory at each point in space $\mathbf{r}$. Also, since $\nabla\rho(\mathbf{r})$ determines only one direction for each point $\mathbf{r}$, these trajectories never cross.

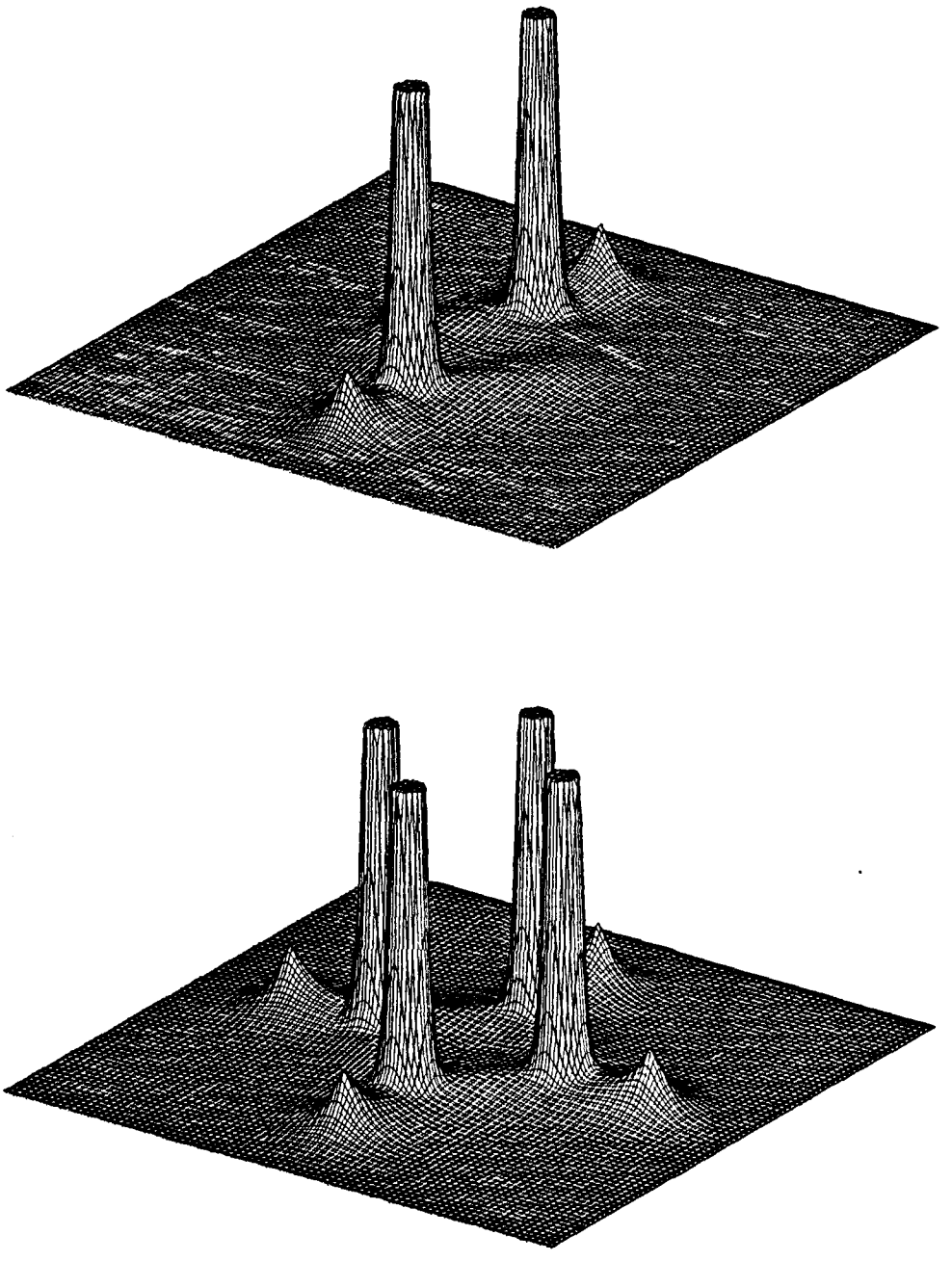

Fig. 3 Relief maps of the electronic charge density for the octahedral $B_6H_6^{2-}$ molecule in two orthogonal planes containing the central cage critical point. The third orthogonal plane is symmetrically equivalent to the lower figure.

One can examine the curvature of $\rho(\mathbf{r})$ along a line instead of along three dimensions at once, and thereby derive critical points with rank and signature (1, +1) and (1, –1). At these points, the charge density is a maximum or minimum, with the trajectories of $\nabla\rho$ originating or terminating there, respectively (see Fig. 4). For the two-dimensional case, one obtains a (2,-2) local maximum at which all gradient paths terminate, or a (2,+2) local minimum from which all gradient paths originate, or a (2,0) saddle point, at which the two gradient paths approaching the maximum terminate, and the two which approach the minimum originate, with all other off-axis paths avoiding the critical point.

In three dimensions, the two negative curvatures associated with a (3, –1) critical point define a surface, and the single positive curvature has two associated gradient paths which originate there, and which are perpendicular to the surface at the critical point; the charge density is a minimum along this line at the critical point, and a maximum at the critical point with respect to the surface. For a (3,+1) critical point, the arrows in the diagram are reversed.

Fig. 5a shows the gradient vector field of B_2F_4 in the plane containing all six atoms; these atoms, as (3, –3) critical points, are defined as point attractors, since all nearby gradient paths terminate there. The set of all gradient paths which terminate at an attractor map out the basin of that attractor. With this definition, it is possible to partition space into separate regions or basins for each attractor (nucleus). Fig. 5a shows only these paths, and illustrates that *an atom can be defined as the union of an*

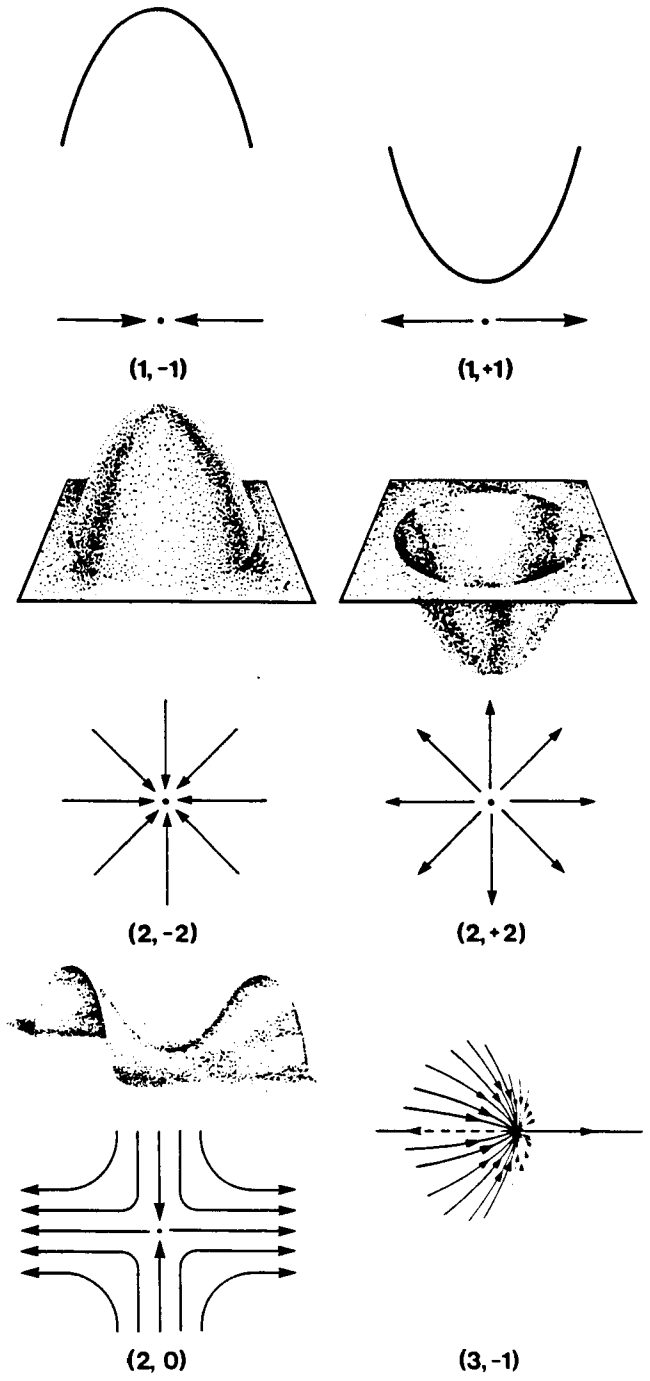

Fig. 4 Phase portraits for one-, two- and three-dimensional critical points.

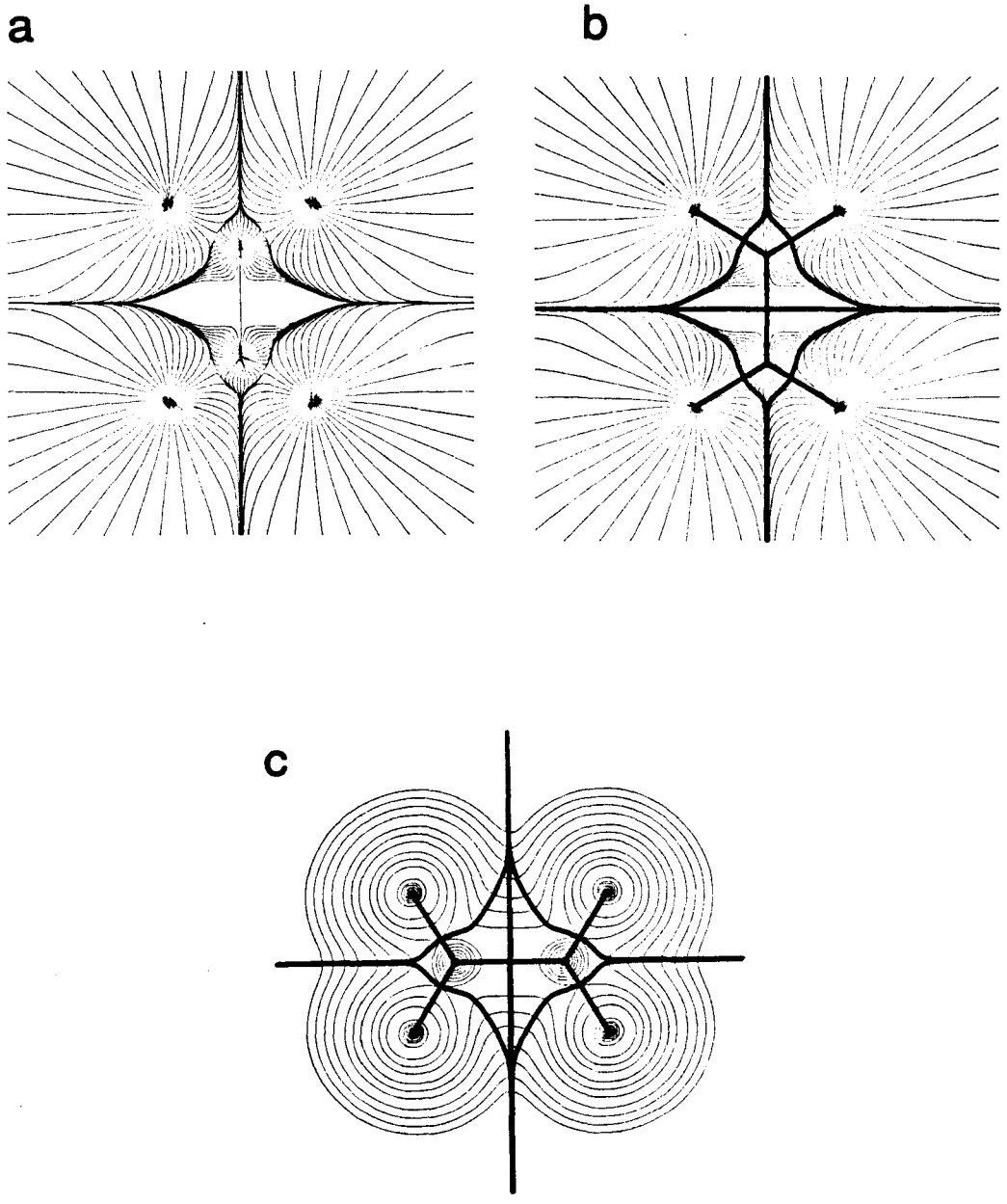

Fig. 5 a) and b) Gradient vector field of the charge density of B_2F_4 in the plane containing the nuclei. c) Contour map of $\rho(\mathbf{r})$ in same plane showing bond paths and interatomic surfaces. A bond critical point is denoted by a dot ("•")

attractor and its basin. As mentioned earlier, the paths terminating at a (3, –1) critical point and associated with a maximum in $\rho(\mathbf{r})$ define a surface, which can be called an interatomic surface, or basin boundary. These boundaries, found in any molecule, and whose intersection with the plane of the atoms has been added in Fig. 5b, provide a straightforward means of partitioning space into separate atomic regions. Note that these regions can extend infinitely far away from the nuclei, in areas where they are not enclosed by a boundary. Also added in Fig. 5b are the paths associated with the positive curvatures at the (3, –1) critical points; these originate at the critical point and terminate at the nuclei, and are called atomic interaction lines, and they always intersect the interatomic surface in a perpendicular fashion.

Through the use of the action principle, it is possible to apply quantum mechanics to a subsystem (i.e., one atom or fragment of a molecule) provided that this subsystem be bounded by a surface of zero flux in the gradient vector of the charge density. Mathematically, this can be expressed as

$$\nabla\rho(\mathbf{r}) \cdot \mathbf{n}(\mathbf{r}) = 0 \, . \qquad (5)$$

This condition is satisfied as long as the gradient vector paths do not cross this surface. In fact, the interatomic surfaces which arose out of examination of the gradient vector field at the bond critical points do satisfy the condition in eqn. (5), and as such are termed zero-flux surfaces.

Therefore, an atom, which can be defined as the region containing a point attractor and bounded by a zero-flux surface, lends itself to a quantum mechanical treatment of the same rigor as that of any total system, with no loss of generality or of the properties which are normally obtainable from the state function. Moreover, the average value of a property calculated for an atom in a system, when summed over the system, gives the same total average result as that calculated for the total system (Bader and Becker 1988), i.e.,

$$\langle M \rangle = \sum_{\Omega} M(\Omega) . \qquad (6)$$

The atomic interaction lines previously mentioned are found between every two nuclei which share an interatomic surface, and they support the contention that charge density accumulates between nuclei for a molecule in its equilibrium geometry. These atomic interaction lines are lines of maximum charge density linking the nuclei, and as such are called *bond paths* (for a molecule in an equilibrium geometry), and the (3, –1) critical points found along these paths are known as *bond critical points* (Bader 1985).

The network of bonds linking the nuclei in a molecule define what is known as a *molecular graph.* It is a property of a molecular graph that it retains its unique connectivity in spite of changes in geometry, i.e., as long as the changes in nuclear position do not induce a rupture of bonds or

formation of new bonds in the molecule. This clearly delineates the difference between molecular geometry and molecular structure. A molecular structure is defined as the set of all molecular geometries in configuration space with the same connectivity of atoms. Molecular structure abruptly and discontinuously changes with the disruption or new formation of bonds. Examples of molecular graphs of the boranes are found in Fig. 18, with bond path critical points denoted by a black dot.

The molecular graph of B_2H_6 includes an example of the ring structural element, with the presence of a (3, +1) or ring critical point located in the centre of the ring of bonded atoms. Examination of the gradient vector field in the plane of the ring in B_2H_6 (Fig. 6) shows that all gradient paths which originate at the ring critical point form a ring surface, all of which terminate at the nuclei forming the ring, except for those gradient paths which terminate at the bond critical points in the perimeter of the ring. The bond paths curve inwardly towards the centre, which is an indication of an electron-deficient structure. Again, the two paths which originate at the ring critical point and which extend in directions perpendicular to the ring surface, correspond to the unique negative curvature at the ring critical point. The axis of these two paths intersects the atomic surfaces of the borons and bridging hydrogens in the centre of the the ring surface. A ring, therefore, is that part of the molecular graph which bounds a ring surface.

An arrangement of bond paths which completely encloses a region of a molecule with ring surfaces is known as a cage structural element,

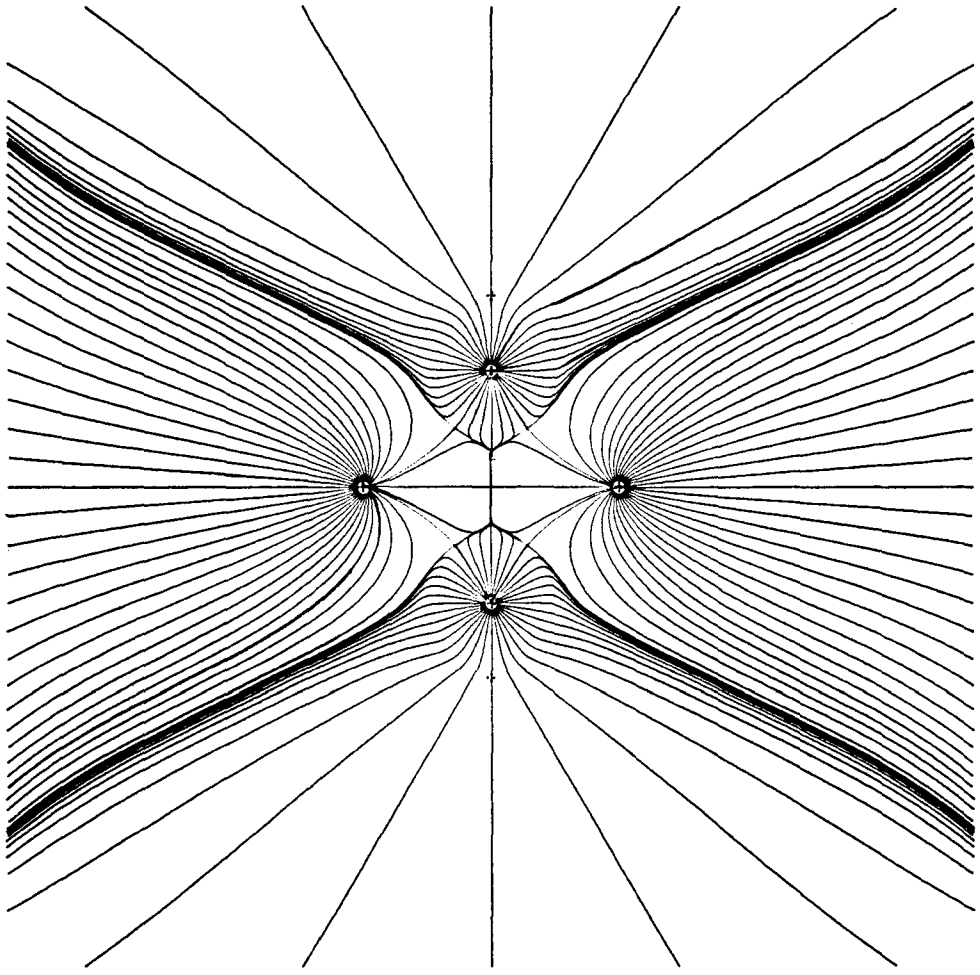

Fig. 6 Gradient vector field of $\rho(\mathbf{r})$ for B_2H_6 in same plane as that shown in Fig. 2b and containing the ring surface.

illustrated in the case of $B_6H_6^{2-}$ (see Fig. 7). Here, the gradient paths all originate from the cage critical point, and terminate at nuclei, bond and ring critical points, to give an enclosed region in three dimensions. Therefore, a cage is that part of the molecular graph which contains at least two rings which bound a region in three-dimensional space containing a (3, +3) critical point. Note that B_5H_9 does not possess this structural element, since the bottom face of the molecule is open, and there is no (3, +3) critical point in the interior of the molecule; the charge density decays monotonically as one moves in space from the apical boron atom out through the open face and beyond.

The total number of each of these four types of critical points is governed by the Poincaré-Hopf relationship (Bader *et al* 1981), eqn. (7):

$$n - b + r - c = 1 \qquad (7)$$

where n is the number of (3,–3) critical points or nuclei, b is the number of (3,–1) critical points or bond paths, r is the number of (3,+1) critical points or rings, and c is the number of (3,+3) critical points or cages. Collectively, the set of parameters (n, b, r, c) is defined as the *characteristic set* of the molecular system.

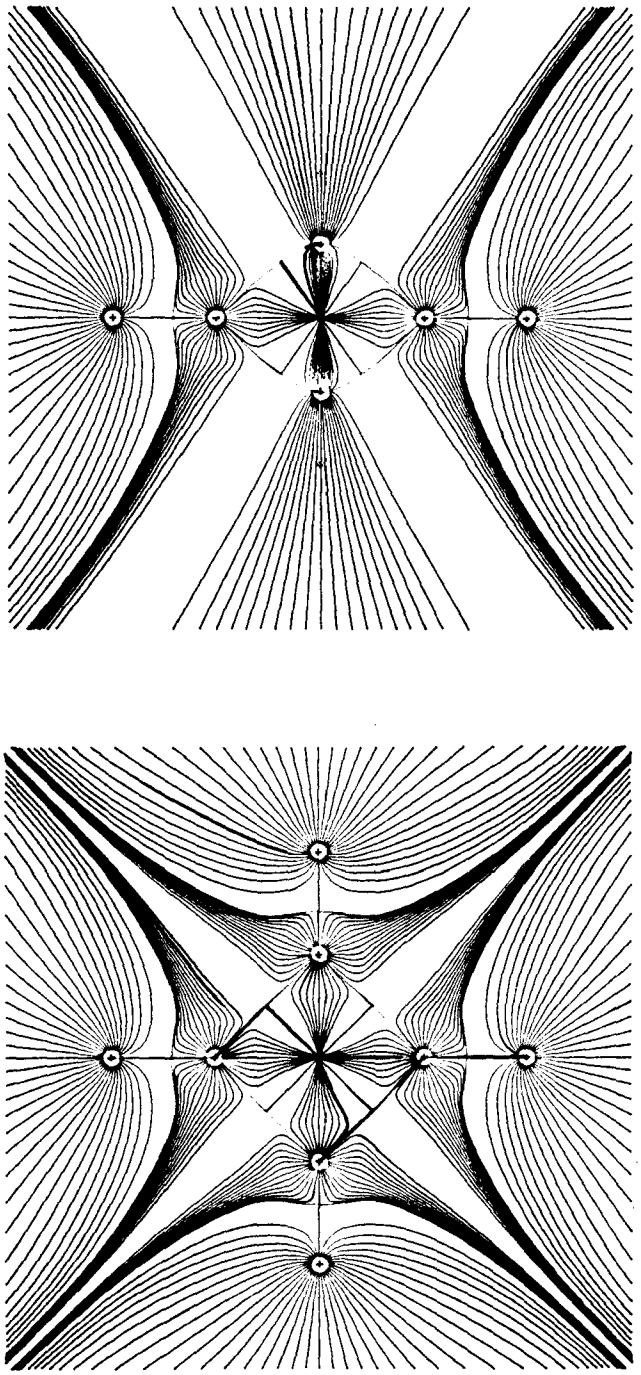

Fig. 7 Gradient vector field of $\rho(\mathbf{r})$ for $B_6H_6^{2-}$ in same planes as those shown in Fig. 3 and containing the cage critical point.

Centering on the nature of the (3,–1) critical points which appear between bonded atoms, one can now investigate the recovery from this theory of the notions of bond order, bond path angle, bond ellipticity and structural stability (Wiberg *et al* 1987).

One can describe, relatively, the bond order by looking at the value of ρ_b, the value of $\rho(\mathbf{r})$ at the bond path critical point. By selecting one bonded pair as a reference, the bond orders of other pairs of linked atoms are inferred by the ratio of these ρ_b values. One can also recover the relative electronegativities of two bonded atoms by examining the relative distances, r_A and r_B, from each atom to the bond path critical point; these are the bonded radii.

Bond paths do not always follow a straight line between the two linked atoms, but rather can bend inwardly or outwardly; this usually occurs when these bond paths form the perimeter of a ring system. In the case of small ring hydrocarbons such as cyclopropane, the bond paths curve outward, which is considered indicative of ring strain. In the case of many of the boranes under present study, the bond paths curve inwardly, signifying electron deficiency. The simplest example of this is B_2H_6. Here, the bond paths bend into the ring interior, in order to maximize the degree of binding in the system. This curvature in the bond paths is quantified by defining a bond path angle α_b, which is the angle subtended at a nucleus by the pair of bond paths linking it to the two nuclei which define the geometrical bond angle α_e. The nature of the relaxation of the charge density away from the form suggested by the geometrical

arrangement of atoms is embodied in the difference $\Delta\alpha = \alpha_b - \alpha_e$. Therefore for the boranes, $\Delta\alpha < 0$.

As mentioned before, the charge density at a bond critical point is a minimum along the bond path at that point, and is a maximum in the two perpendicular directions which define a plane tangential to the interatomic surface, giving two negative eigenvalues or curvatures, λ_1 and λ_2. One can also compare the two orthogonal planes which lie along the bond path, and which are formed on combination with one of the eigenvectors of λ_1 or λ_2. For cylindrically symmetrical bonds, of course $\lambda_1 = \lambda_2$, and both of these planes would be identical. However, if the two negative eigenvalues at the bond critical point are unequal, then by definition λ_2 is chosen to be less than λ_1, and it is in the plane formed on combination with λ_2 that charge is preferentially accumulated (Bader *et al* 1983). In this plane, $\rho(\mathbf{r})$ falls off relatively more slowly as one moves away from the critical point, making the axis of λ_2 the major axis of curvature, which determines the relative orientation of this plane in the molecule. The bond ellipticity, ε, is defined as $(\lambda_1/\lambda_2 - 1)$, which quantifies the preferential accumulation of charge in a given plane, specifically the plane defined by the bond path and the major axis of curvature λ_2. Thus $\varepsilon = 0$ for a cylindrically symmetrical bond.

A general statement can be made that in small ring systems, there is less difference between the values of ρ at the ring critical point and those at the surrounding bond critical points, relative to large ring systems. Accompanying this smaller difference is the fact that the charge density at

the bond critical point falls off much more slowly ("soft" curvature) in the direction of the ring critical point than in directions perpendicular to the ring (directions of "hard" curvature). Therefore the major axis of curvature would be tangent to the ring rather than perpendicular to it. A resulting preferential accumulation of charge over the ring surface is indicative of systems whose bond critical points possess large ellipticities.

In fact, the value of the ellipticity at the bond point approaches infinity when ring rupture is about to occur. At this point in nuclear configuration space, known as a *bifurcation point*, a (3,–1) or bond critical point and the (3,+1) or ring critical point of the charge density would coalesce, with the positive curvature of the ring point in the plane of the ring annihilating the negative curvature of the major axis of the ellipse formed at the bond point. This is of course easier to do in a three-membered ring than a larger ring system because of the closer proximity of these neighbouring points, and the fact that the values of $\rho(\mathbf{r})$ for these points of different signature are nearly the same.

Thus, large ellipticities are associated with unstable structures, since a small change in nuclear configuration can result in an abrupt and discontinuous change in molecular structure, characterized by a different set of connectivities.

Another important aspect of the role of the charge density in the theory of atoms in molecules appears in the study of the Laplacian $\rho(\mathbf{r})$ (Bader and Nguyen-Dang 1981). Mathematically, the Laplacian density $L(\mathbf{r})$ is defined as :

$$L(\mathbf{r}) = -(\hbar^2/4m)\nabla^2\rho(\mathbf{r}) \tag{8}$$

When $L(\mathbf{r})$ is integrated over the space of a subsystem, Ω, or more specifically the basin of an atom, one obtains $L(\Omega)$:

$$\begin{aligned} L(\Omega) &= \int_{\Omega} L(\mathbf{r})d\tau = -(\hbar^2/4m)\int_{\Omega} \nabla^2\rho(\mathbf{r})d\tau \\ &= -(\hbar^2/4m)\oint dS(\Omega,\mathbf{r})\nabla\rho(\mathbf{r})\bullet\mathbf{n}(\mathbf{r}) = 0 \end{aligned} \tag{9}$$

The last expression for $L(\Omega)$ in eqn. (9) shows that $L(\Omega)=0$ because of the zero-flux boundary condition, while the previous expression reaches the same conclusion, but on the basis that for the basin of an attractor, the positive and negative contributions to $\int_{\Omega}\nabla^2\rho d\tau$ cancel.

The local expression for the virial theorem relates $L(\mathbf{r})$ to the electronic potential energy density $\mathcal{V}(\mathbf{r})$ and the electronic kinetic energy density $G(\mathbf{r})$:

$$(\hbar^2/4m)\nabla^2\rho(\mathbf{r}) = 2G(\mathbf{r}) + \mathcal{V}(\mathbf{r}) , \tag{10}$$

where

$$G(\mathbf{r}) = \frac{\hbar^2}{2m}\int d\tau' \,(\nabla\psi^*)\bullet\nabla\psi \tag{11}$$

and

$$\mathscr{V}(\mathbf{r}) = -\mathbf{r}\cdot\nabla\cdot\ddot{\sigma}(\mathbf{r}) + \nabla\cdot(\mathbf{r}\cdot\ddot{\sigma}(\mathbf{r}))$$

and

$$\ddot{\sigma}(\mathbf{r}) = \int d\tau' \frac{\hbar^2}{4m}\{\psi^*\nabla\nabla\psi + \psi\nabla\nabla\psi^* - \nabla\psi^*\nabla\psi - \nabla\psi\nabla\psi^*\}$$

.

Also, the two terms on the right side of eqn. (10) can be combined in such a way as to form the electronic energy density $E_e(\mathbf{r})$

$$E_e(\mathbf{r}) = G(\mathbf{r}) + \mathscr{V}(\mathbf{r}) \tag{12}$$

Since $L(\Omega) = 0$, eqn. (10), when integrated, yields the virial theorem for an atom in a molecule:

$$2T(\Omega) = -\mathscr{V}(\Omega). \tag{13}$$

As a consequence of this theorem, the average electronic energy of an atom in a molecule is

$$E_e(\Omega) = \int_\Omega E_e(\mathbf{r})d\tau = -T(\Omega) = \frac{1}{2}\mathscr{V}(\Omega) \tag{14}$$

Another atomic property described in this thesis is the average atomic population, $N(\Omega)$. This is obtained by an integration of $\rho(\mathbf{r})$ over the basin of the atom Ω:

$$N(\Omega) = \int_{\Omega} \rho(\mathbf{r}) d\tau \qquad (15)$$

The Laplacian of the scalar function $\rho(\mathbf{r})$ is itself a scalar function, $\nabla^2\rho(\mathbf{r})$, which has its own maxima and minima. These maxima and minima correspond to regions of charge concentration and depletion, respectively. A convention in use when examining relief plots or diagrams of the scalar field of $\nabla^2\rho(\mathbf{r})$ is to deal with the negative of the function, $-\nabla^2\rho(\mathbf{r})$, which enables one to view positively-valued regions in the function as areas of charge concentration. Therefore, those regions where $-\nabla^2\rho(\mathbf{r}) > 0$ are regions of local charge concentration, and regions where $-\nabla^2\rho(\mathbf{r}) < 0$ are regions of local charge depletion (Bader 1985).

Understanding this property of the Laplacian, one can, with the aid of the local expression of the virial theorem, determine whether the electronic potential or kinetic energy makes the dominant contribution to the local energy of the charge distribution. The average virial ratio of kinetic to potential energy is 2:1, and the always negative contribution of the potential energy and always positive contribution of the kinetic energy can produce a positive or negative value for $\nabla^2\rho(\mathbf{r})$, depending on how their relative values differ from this ratio. Therefore it can be said that a region of space with a negative value of the Laplacian and the accompanying local charge concentration signifies a potential energy dominance in the electronic energy $E_e(\mathbf{r})$ and in the local virial

relationship, with a dominance by the kinetic energy producing the opposite effect.

Furthermore, since the local statement of the virial theorem requires that these two contributions exactly cancel over the system as a whole, then a region with a negative value of the Laplacian is a region of compressed charge density relative to the average, and a region with a positive value for the Laplacian has a relatively expanded charge density.

Combining information about the nature of the Laplacian with that given earlier about the nature of a (3,–1) critical point, it can be seen that a chemical bond involves the contraction of $\rho(\mathbf{r})$ towards the bond path in the plane of the interatomic surface, accompanied by an expansion of $\rho(\mathbf{r})$ away from the surface and towards the respective atomic basins. It is the net contribution of these two effects which gives rise to the sign of the Laplacian at the bond critical point. Thus, a large value of ρ_b accompanied by a large negative value of $\nabla^2\rho_b$ at the bond critical point signifies a concentration of charge in the internuclear region, which is consistent with a shared interaction, with nuclei bound by virtue of the lowering of the potential energy. Conversely, a small value of ρ_b and a positive value of $\nabla^2\rho_b$ at the bond critical point is characteristic of a closed-shell interaction, with a depletion of charge in the internuclear region, in favour of separate charge concentrations in each atomic basin. This is the case where the kinetic energy contribution to the electronic energy dominates in the internuclear region.

For an isolated atom, there are concentric and alternating shells of charge concentration and depletion, recovering the concept of the electronic shell model of atoms. The outermost region of charge concentration coincides with the valence shell of the atom, and it is called the Valence Shell Charge Concentration, or VSCC. This spherical shell is distorted upon chemical combination with other atoms, resulting in the appearance of maxima, minima and saddles on its surface (Bader *et al* 1988).

A local maximum in the VSCC corresponds to a nucleophile or Lewis base, and a local minimum in the VSCC corresponds to an electrophile or Lewis acid. Therefore a chemical reaction can be characterized as an interaction of the "lump" in the VSCC of a Lewis base with a corresponding "hole" in the VSCC of a Lewis acid. One can also speak in terms of eqn. (10) to describe this interaction as one between the base with excess potential energy and the acid with an excess of kinetic energy. At no time during this interaction does the value of $L(\Omega)$ deviate from zero, as changes in concentration and depletion in one region of an atom are counterbalanced by opposite changes in other regions.

Like the topology of $\rho(\mathbf{r})$, the scalar Laplacian function $\nabla^2\rho(\mathbf{r})$ has its own set of critical points in the VSCC's of atoms. Two types of critical points, (3,–3) and (3,+3) critical points, pinpoint the areas of local charge concentration and depletion, respectively. Regions of charge concentration, or "lumps" in the VSCC, can be found in the general area of the bond path in $\rho(\mathbf{r})$, and as such are called *bonded maxima.* They can also

be found in the areas where the "lone pairs" of the VSEPR model are located, and these are called *non-bonded maxima*. In the boranes, only bonded maxima are found, seeing as these molecules have no lone pairs. On the other hand, regions of charge depletion are marked by the presence of (3,+1) critical points in $\nabla^2\rho(\mathbf{r})$, also known as "holes" in the VSCC.

Understandably, then, a study of reactivity for the boranes would involve the identification of "lumps" and "holes" in the VSCC of these molecules, which correspond to sites of electrophilic and nucleophilic attack, respectively.

2. The Hartree-Fock Approximation and SCF Procedure

In order to perform a topological analysis and integration over the atomic basins, it is first necessary to determine equilibrium geometries for the molecules under study. This is accomplished through the application of programs utilizing the Hartree-Fock approximation and SCF procedure, both of which are described by Szabo and Ostlund (1989) and reprinted below.

One can take a set of spin orbitals $\{\chi_a\}$ to form a single determinant $|\Psi_0\rangle = \frac{1}{\sqrt{N!}} |\chi_1\chi_2\cdots\chi_a\chi_b\ldots\chi_N\rangle$ which approximates the ground state of an N-electron system. By varying these spin orbitals while maintaining their orthonormality, one can minimize the electronic energy E_0,

$$E_0 = \langle\Psi_0|\mathscr{H}|\Psi_0\rangle = \sum_a \langle a|h|a\rangle + \frac{1}{2}\sum_{ab} \langle ab||ab\rangle \ , \tag{16}$$

where

$$\langle ab||ab\rangle = \langle ab|bb\rangle - \langle ab|ba\rangle \tag{17}$$

In so doing, one obtains the Hartree-Fock integro-differential equation

$$h(1)\chi_a(1) + \sum_{b\neq a}\left[\int dx_2|\chi_b(2)|^2 r_{12}^{-1}\right]\chi_a(1) - \sum_{b\neq a}\left[\int dx_2 \chi_b^*(2)\chi_a(2) r_{12}^{-1}\right]\chi_b(1) = \varepsilon_a\chi_a(1) \tag{18}$$

In this equation,

$$h(1) = -\frac{1}{2}\nabla_1^2 - \sum_A \frac{Z_A}{r_{1A}} \tag{19}$$

is the kinetic and electron-nuclear potential energy for electron 1. The first sum over b in eqn. (18) is known as the coulomb term, and the second is called the exchange term. The two-electron coulomb potential for electron 1 is

$$v_a^{coul}(1) = \sum_{b\neq a}\int dx_2|\chi_b(2)|^2 r_{12}^{-1} \; . \tag{20}$$

Here, $v_a^{coul}(1)$ represents the average potential "felt" by electron 1 from the other N-1 electrons in their spin orbitals, and this leads to the definition of the coulomb operator $\mathscr{J}_b$:

$$\mathscr{J}_b(1) = \int dx_2|\chi_b(2)|^2 r_{12}^{-1} \; . \tag{21}$$

The second summation term in eqn. (18) is the exchange term, $\mathscr{K}_b(1)$, which when acting on $\chi_a(1)$ gives

$$\mathcal{K}_b(1)\chi_a(1) = \left[\int dx_2 \chi_b^*(2) r_{12}^{-1} \chi_a(2)\right]\chi_b(1) \qquad (22)$$

which accounts for the antisymmetric properties of the spin orbitals, and which does not have a strict physical interpretation. Now, eqn. (18) can be rewritten as

$$\left[h(1) + \sum_{b\neq a} \mathcal{J}_b(1) - \sum_{b\neq a} \mathcal{K}_b(1)\right]\chi_a(1) = \varepsilon_a\chi_a(1) \ . \qquad (23)$$

Given that

$$\left[\mathcal{J}_a(1) - \mathcal{K}_a(1)\right]\chi_a(1) = 0 \qquad (24)$$

eqn. (22) now becomes a definition of the Fock operator, f:

$$f(1) = h(1) + \sum_b \left[\mathcal{J}_b(1) - \mathcal{K}_b(1)\right] \qquad (25)$$

which transforms the Hartree-Fock equations into

$$f|\chi_a\rangle = \varepsilon_a|\chi_a\rangle. \qquad (26)$$

Furthermore, the summation term in eqn. (25) is the one-electron potential operator known as the Hartree-Fock potential $v^{HF}(1)$, so that

$$f(1) = h(1) + v^{HF}(1) . \tag{27}$$

The integro-differential eqn. (26) has spin orbitals for eigenfunctions and spin orbital energies as eigenvalues. As an aside, now one can define an approximate Hamiltonian $\mathscr{H}_0$ which has $|\Psi_0\rangle$ as its eigenfunction and eigenvalue $\sum_a \varepsilon_a$, and this is known as the Hartree-Fock Hamiltonian:

$$\mathscr{H}_0 = \sum_{i=1}^{N} f(i) . \tag{28}$$

Since all of the molecules studied in this work are closed-shell ground states, i.e., all molecular states have an even number N of electrons, filling $n = N/2$ doubly-occupied spatial orbitals, one needs discuss only one application of Hartree-Fock theory, known as Restricted Closed Shell Hartree-Fock or RHF. The spin-orbitals in this case are:

$$\chi_i(\mathbf{x}) = \begin{cases} \psi_j(\mathbf{r})\alpha(\omega) \\ \psi_j(\mathbf{r})\beta(\omega) \end{cases} \tag{29}$$

where ω is the spin variable, with $\alpha(\omega)$ and $\beta(\omega)$ corresponding to up and down spins, respectively. Another notation used for spin up and down orbitals is ψ_j and $\overline{\psi}_j$. Therefore the ground state can be expressed as

$$|\Psi_o\rangle = |\chi_1\chi_2\cdots\chi_{N-1}\chi_N\rangle = |\psi_1\overline{\psi}_1\cdots\psi_a\overline{\psi}_b\cdots\psi_{N/2}\overline{\psi}_{N/2}\rangle \tag{30}$$

By integrating the spin functions out of eqn. (26) for this case, eqn. (25) now becomes

$$f(1) = h(1) + \sum_a^{N/2} [2J_a(1) - K_a(1)] \tag{31}$$

where

$$J_a(1) = \int d\mathbf{r}_2 \psi_a^*(2) r_{12}^{-1} \psi_a(2) \tag{32}$$

and

$$K_a(1)\psi_i(1) = \left[\int d\mathbf{r}_2 \psi_a^*(2) r_{12}^{-1} \psi_i(2)\right] \psi_a(1) \ . \tag{33}$$

This now gives the spatial integro-differential equation

$$f(\mathbf{r}_1)\psi_i(\mathbf{r}_1) = \varepsilon_i \psi_i(\mathbf{r}_1) \tag{34}$$

and for the closed-shell determinant (30) the ground state energy is

$$E_0 = \langle \Psi_0 | \mathscr{H} | \Psi_0 \rangle = 2 \sum_a h_{aa} + \sum_a \sum_b [2J_{ab} - K_{ab}] \qquad (35)$$

Eqn. (34) can be solved by choosing a set of basis functions and employing standard matrix manipulations. Therefore one represents the molecular orbitals ψ_i as a linear combination of a finite number K of basis functions:

$$\psi_i = \sum_{\mu=1}^{K} C_{\mu i} \phi_\mu , \quad i=1,2,\cdots,K \ . \qquad (36)$$

Furthermore, the basis functions ϕ are made up of a fixed linear combination of Gaussian functions or primitives, which have the form $ce^{-\alpha r^2}$, where c is a normalization constant and α is a parameter. One may choose to express a basis function as a discrete sum of individual primitives (an "uncontracted" set), or one can apportion the members of the set (usually in a disjoint fashion) into any fixed linear combination (a "contracted" set). In the case where there is a combination of two or more primitives, the contraction coefficients are renormalized. For the sake of description, one might denote a contraction of a 6s set of primitives to a

combination having one group of four and two groups of one primitive each as 6s/4,1,1.

The essential aspect of solving for these molecular orbitals lies in determining the expansion coefficients $C_{\mu i}$ which can be done by substituting (36) into eqn. (34) to give

$$f(1)\sum_{\nu} C_{\nu i}\phi_{\nu}(1) = \varepsilon_i \sum_{\nu} C_{\nu i}\phi_{\nu}(1) \ . \tag{37}$$

If one multiplies by $\phi_{\mu}^{*}(1)$ and integrates, the result is

$$\sum_{\nu} C_{\nu i} \int d\mathbf{r}_1 \phi_{\mu}^{*}(1) f(1) \phi_{\nu}(1) = \varepsilon_i \sum_{\nu} C_{\nu i} \int d\mathbf{r}_1 \phi_{\mu}^{*}(1) \phi_{\nu}(1) \ . \tag{38}$$

Further, if one defines the elements of the overlap matrix **S** to be

$$S_{\mu\nu} = \int d\mathbf{r}_1 \phi_{\mu}^{*}(1) \phi_{\nu}(1) \tag{39}$$

and defines the elements of the Fock matrix **F** to be

$$F_{\mu\nu} = \int d\mathbf{r}_1 \phi_{\mu}^{*}(1) f(1) \phi_{\nu}(1) \tag{40}$$

then eqn. (37) becomes the Roothaan equations,

$$\sum_{\nu} F_{\mu\nu} C_{\nu i} = \varepsilon_i \sum_{\nu} S_{\mu\nu} C_{\nu i} \ , \ i = 1,2,\cdots, K \ , \tag{41}$$

or, in matrix form,

$$\mathbf{FC} = \mathbf{SC}\varepsilon. \tag{42}$$

One can also define the charge density matrix **P** whose elements are given by

$$P_{\mu\nu} = 2\sum_{a}^{N/2} C_{\mu a} C_{\nu a}^{*} \tag{43}$$

which determines the charge density $\rho(\mathbf{r}) = |\psi_a|^2$ through the coefficients **C**.

If eqn. (31) is expressed in terms of the basis $\{\phi_\mu\}$, one finds

$$F_{\mu\nu} = \int d\mathbf{r}_1 \phi_\mu^*(1) h(1) \phi_\nu(1) + \sum_{a}^{N/2} d\mathbf{r}_1 \phi_\mu^*(1) [2J_a(1) - K_a(1)] \phi_\nu(1) \tag{44}$$

$$= H_{\mu\nu}^{\text{core}} + \sum_{a}^{N/2} \sum_{\lambda\sigma} C_{\lambda a} C_{\sigma a}^{*} [2(\mu\nu|\sigma\lambda) - (\mu\lambda|\sigma\nu)] \tag{45}$$

$$= H_{\mu\nu}^{\text{core}} + \sum_{\lambda\sigma} P_{\lambda\sigma} \left[(\mu\nu|\sigma\lambda) - \frac{1}{2}(\mu\lambda|\sigma\nu) \right] . \tag{46}$$

The first term on the right-hand side of (44) is known as $H_{\mu\nu}^{\text{core}}$, and the second term on the right-hand side of (46) is called $G_{\mu\nu}$, the matrix element of the two-electron component **G**. Thus,

$$F_{\mu\nu} = H_{\mu\nu}^{\text{core}} + G_{\mu\nu} \tag{47}$$

In this procedure, the basis functions are normalized but not orthogonal; this problem could be dealt with by orthogonalizing the basis set, but this proves to be rather time-consuming. Rather, if one transforms **C** into **C'** (' refers to an orthogonalized basis) by the transformation

$$\mathbf{C'} = \mathbf{X^{-1}C} \tag{48}$$

where **X** is a transformation matrix possessing an inverse, and if one further transforms **F** into **F'** where

$$\mathbf{F'} = \mathbf{X^{\dagger}F} \tag{49}$$

then one obtains

$$\mathbf{F'C'} = \mathbf{C'}\varepsilon. \tag{50}$$

These are called the transformed Roothan equations, which can be solved for **C'** and ε by diagonalizing **F'**, and then **C** can be obtained from **C'**. Obtaining this solution is analagous to solving eqn. (42).

With this information in hand, one can now carry out the SCF procedure, which can be summarized in the following steps:

1. Specify the coordinates, atomic numbers, and molecular charge for the molecule under study, and provide a basis set.

2. Calculate the necessary one- and two-electron integrals.

3. Diagonalize **S** to obtain a transformation matrix for the transformation of $\mathbf{F} \rightarrow \mathbf{F'}$.

4. Guess the initial density matrix **P**, which might be just simply $H_{\mu\nu}^{\text{core}}$, i.e., no two-electron components.

5. Determine **G** from **P** and the $(\mu\nu|\lambda\sigma)$.

6. Add **G** to $\mathbf{H}^{\text{core}}$ to get **F**.

7. Obtain **F'** by determining $\mathbf{X}^{\dagger}\mathbf{F}\mathbf{X}$.

8. Diagonalize **F'**, to get **C'** and ε.

9. Obtain **C**=**XC'**.

10. Get a new **P** from **C** and eqn. (43).

11. Compare the new **P** with the previous one with a convergence criterion (a small number); if the difference is too large, repeat the procedure from step 5 with the new **P**. If the two differ by less than the convergence criterion, then use the solutions to obtain energies, wavefunctions for the molecule, etc.

In general, the SCF procedure in Hartree-Fock theory is used in conjunction with a molecular coordinate optimization algorithm which describes the molecule in terms of internal coordinates, and which adjusts these coordinates until the Hellman-Feynman forces acting in the molecule is reduced to within some small value. During each complete step of this algorithm, there is first a change in internal coordinates(except for the initial step), followed by a convergence test on these coordinates, followed by a calculation of the RHF energy via the SCF procedure. This process is repeated until an equilibrium geometry is reached, at which point a final SCF calculation provides the basis for the calculation of molecular properties. It is a distinction of the AIMPAC series of programs that they further calculate these same molecular properties, but as averages for the individual atoms in a molecule; these programs extract this information from a wavefunction data file, easily obtained from an output file from a completed SCF calculation.

The AIMPAC Series of Programs

Briefly, the AIMPAC program set consists of the following:

1. SADDLE: searches and finds critical points in ρ.
2. BUBBLE (or SADD2R): searches automatically(manually) and finds critical points in $\nabla^2\rho$.
3. PROAIM (Biegler-König *et al* 1982): determines individual average atomic energies, charges, and other expectation values of atomic properties

in molecules by defining interatomic surfaces and integrating over the individual atomic basins.

4. OMEGA (Biegler-König *et al* 1981): determines individual average atomic energies, charges, and other expectation values of atomic properties in molecules by integrating along the set of gradient vector paths which terminate at the nucleus of an atom, and which effectively map out the basin of the nuclear attractor.

AIMPAC also includes a series of programs designed to calculate and display pictorially the results of topological analyses, and these are:

1. GRID: calculates a grid of points used to plot contour maps of $\rho(\mathbf{r})$ and $\nabla^2\rho(\mathbf{r})$, and whose output can also be used to generate relief maps of these two scalar functions with the use of the program RELIEF.

2. GRDVEC: traces the gradient paths of $\rho(\mathbf{r})$ which can be plotted as a gradient vector map; can also be used to generate interatomic surface and bond path overlays for contour maps, or to generate molecular graphs.

Both GRID and GRDVEC enable the user to specify virtually any plane of interest in the molecule, either by specification of three atoms which define the plane, or by the use of Euler angles to transform the coordinate axes of the original molecular frame found in the wavefunction.

3. RELIEF: creates relief maps of scalar functions such as $\rho(\mathbf{r})$ and $\nabla^2\rho(\mathbf{r})$, which are in the form of planar mesh grids with positive and/or negative regions of the function appearing as projections out of the plane.

3. General Chemistry of the Boranes and Carboranes

The general chemistry of the boranes and carboranes involves mainly a discussion of their classification, and the two sets of rules designed for electron counting and examination of proposed structures. These topics form the basis of this discussion, and are covered by Greenwood & Earnshaw (1984).

Boranes are a class of compounds composed exclusively of boron and hydrogen atoms, whose structural features are unique and distinct from other chemical series such as the hydrocarbons. Boron has one less electron than the number of available valence orbitals, which characterizes the series as "electron-deficient". The lower members of the borane series are gaseous, but the higher molecular weight members are volatile liquids and solids; the boiling points are similar to those hydrocarbons of similar molecular weight. The icosahedral B_{12} structure is prevalent in the allotropes of boron, in metal borides and in the boranes, and the anion $B_{12}H_{12}^{2-}$ is an example of a structure studied in this work.

Boranes are named by prefixing the number of B atoms in latin, followed by the letters “borane”, followed by the number of H atoms as a number in parentheses; for anions, one changes "-ane" to "-ate", and specifies the number of H atoms in this case with a latin prefix as well. A tabulation of the names of the molecules examined in this study, along with the *styx* number assignments are given in Table I.

Table I. IUPAC Names and *styx* Number Assignments for the Borane Series

Molecule	IUPAC Name	styx Numbers
B_2H_6	*nido*-diborane(6)	2002
B_4H_{10}	*arachno*-tetraborane(10)	4012
B_5H_9	*nido*-pentaborane(9)	4120
B_6H_{10}	*nido*-hexaborane(10)	4220
$B_6H_6^{2-}$	*closo*-hexahydrohexaborate(2–)	
$B_7H_7^{2-}$	*closo*-heptahydroheptaborate(2–)	
$B_{12}H_{12}^{2-}$	*closo*-dodecahydrododecaborate(2–)	
$C_2B_3H_5$	*closo*-1,5-dicarbapentaborane(5)	
$C_2B_4H_6$	*closo*-1,6-dicarbahexaborane(6).	

Description of the information contained in Table I begins with the classification of the degree of "openness" of the boron cluster, as described with the following italicized prefixes:

closo - closed structures of *n* atoms in a *n*-atom polyhedral framework;
nido - open structures of *n* atoms in a *n+1*-atom polyhedral framework;
arachno - open structures of *n* atoms in a *n*+2-atom polyhedral framework;
hypho - open structures of *n* atoms in a *n*+3-atom polyhedral framework;
conjuncto - formed by the joining of one or more of the above together.

There are no examples of either *hypho*- or *conjucto*-boranes in this study, since their structures tend to be less symmetrical, more complex, and of higher molecular weight, making them more difficult to handle computationally.

There are two types of three-centre, two-electron bonding in the boranes, as described in molecular orbital theory, and these are B-H-B bridges and B-B-B rings. Apart from this, there are normal B-B bonds, and B-H_t bonds between borons and terminal hydrogens. As a means of classifying boranes, and predicting the stability or existence of proposed cluster structures, a set of rules was developed based on what are called the *styx* numbers. Here, *s* is the number of B-H-B bridges, *t* is the number of B-B-B rings, *y* is the number of B-B bonds, and *x* is the number of BH_2 groups. Since boron has a valency of four, there should always be four lines ("bonds") drawn to every boron in a structure, if the *styx* rules are to

be followed. Since each boron contributes 3 electron and each hydrogen adds 1 electron, the total number of valence electrons for the borane B_nH_m is $(3n + m)$, which must be equivalent to twice the total number of bonds. Therefore the *styx* rules give:

number of e^- pair bonds $= n + \sum(s + t + y + x)$

number of atoms (neutral molecule) $= 2(s + t + y + x)$.

Another scheme for electron counting has been devised in what are known as Wade's Rules, based upon molecular orbital theory:

closo-boranes have the formula $B_nH_n^{2-}$ with B's at all n corners of a n-cornered triangulated polyhedron, requiring $(n + 1)$ pairs of bonding framework e^-'s;

nido-boranes have the formula B_nH_{n+4} with B's at n corners of a $(n+1)$-cornered polyhedron, requiring $(n + 2)$ pairs of bonding framework e^-'s;

arachno-boranes have the formula B_nH_{n+6} with B's at n corners of a $(n+2)$-cornered polyhedron, requiring $(n + 3)$ pairs of bonding framework e^-'s, and

hypho-boranes have the formula B_nH_{n+6} with B's at n corners of a $(n+3)$-cornered polyhedron, requiring $(n + 4)$ pairs of bonding framework e^-'s.

In the boranes, each B-H_t group provides 2 electrons to the cluster, and each BH_2 group contributes 1 electron, where the framework includes the bridging atoms. In a neutral molecule, there are as many skeletal framework electrons as atoms.

In the case of the $B_nH_n^{2-}$ molecules, there are no B-H-B bridges, and no BH_2 groups. Each B contributes one of its three electrons to the B-H_t bonds, and the remaining 2 electrons to the framework. Therefore the framework of n+1 molecular orbitals is filled by the $2n$ e^-'s of the boron atoms, plus the two extra electrons of the anion. Thus, there are n pairs of electrons in the n(B-H_t) bonding m.o.'s, there are $(n + 1)$ pairs in the framework, and there are $(2n - 1)$ empty nonbonding and antibonding framework m.o.'s. Therefore Wade's rules point up the fact that there are just enough electrons in a stable molecule to fill the bonding m.o.'s, and no more.

In terms of reactivity, one finds generally that the *arachno*-boranes are more reactive than the *nido*-, with the *closo*-boranes being the most stable, whose cage structures produce what has been called "three-dimensional aromaticity". It is also a general observation that boranes of higher molecular weight are less reactive, although acidity appears to increase with increasing size of the borane cluster. Therefore to compare the relative acidities of B_4H_{10}, B_6H_{10}, and B_5H_9, one finds that

$$B_4H_{10} > B_6H_{10} > B_5H_9$$

which shows that the openness of the structure plays a more important role in reactivity than the relative size of the molecules. Furthermore, experimentalists have found that the regions with the greatest likelihood of electrophilic attack are found at the positions of apical boron atoms, which thus are furthest removed from the open faces of the polyhedral fragment. Conversely, nucleophilic attack is more likely to occur at those boron atoms involved in B-H-B bridging. Also, bridging H atoms are more acidic than terminal, and are the first hydrogens lost upon anion formation (this is also true for *nido-* and *arachno-* carboranes). As an example, in B_5H_9, the apical boron experiences electrophilic attack more readily than the basal borons.

One can also apply Wade's rules to the carboranes, which have the formula $[(CH)_a(BH)_mH_b]^{c-}$, and are stoichiometrically derived from boranes by the following general substitutions:

$$BH \equiv C$$
$$BH_2 \equiv CH \ ,$$

In the above formula, a = number of CH groups, m = number of BH groups, b = number of extra H_b or H_{endo}, where H_{endo} is a terminal hydrogen which points inward toward the mouth of the open face. Therefore the total number of skeletal bonding electron pairs is $\frac{1}{2}(3a + 2m + b + c)$, or $n + \frac{1}{2}(a + b + c)$, where $n = a + m$ is the number of occupied vertices of the polyhedron. Again, *closo-*, *nido-*, and *arachno*-boranes require $n + 1$, 2, or 3 pairs of framework bonding electrons, respectively,

since $a + b + c = 2$, 4, and 6, respectively. Note also that {CH} donates 3 electrons to the cluster, whereas {BH} donates only two.

There are other general observations that can be made about the carboranes, as listed below:

1. There is a tendency for carbon to have a minimal coordination number, and to be as far removed from other C's as possible, so that the most stable isomer of a particular carborane has the greatest number of B-C connections.

2. B-B interatomic distances increase with increasing coordination number.

3. B-C distances are shorter than B-B distances, since C has a smaller atomic radius.

4. According to Mulliken population analyses, the negative charge on B decreases in the following order:

B(no bond to C) > B(bonded to one C) > B(bonded to two C)

In each case, the B of lower coordination number possesses a greater negative charge than that with higher coordination number.

5. The carbons in carboranes tend to have larger geometrical bond angles as they approach normal sp^3 hybridization angles. In $C_2B_4H_6$, for example, the geometrical bond angles at carbon are usually larger than 60° or 90°, while angles at boron are less.

It is the purpose of this work to both examine and quantify these observations about boranes and carboranes through the use of the theory of atoms in molecules.

4. Computational

Examination of the boranes began with the selection of a suitable basis set. For boron, a 9s/6,1,1,1 + 5p/4,1 (Dunning Jr. 1970,1971)+1d basis set was chosen. For hydrogen, a 6s/4,1,1 + 1p set was used. Table II gives a description of the basis set in the format employed in the GAUSSIAN series of programs, with the most recent version being GAUSSIAN88 (Frisch *et al* 1988).

The description of the GAUSSIAN format is as follows: the first line gives the chemical symbol of the atom described, followed on the next line by a shell descriptor, which specifies the type of shell(s,p,d, etc.), the degree of contraction(e.g., 6 for the first set in the table), and the shell scale factor. The next *n* lines, where *n* is the degree of contraction, give the exponents and contraction coefficients for each primitive, in that order.

Table II: Borane Basis Set

```
 B 0
S    6 1.00
 0.2788410000D+04  0.2122000000D-02
 0.4190390000D+03  0.1617100000D-01
 0.9646830000D+02  0.7835600000D-01
 0.2806940000D+02  0.2632500000D+00
 0.9376000000D+01  0.5967290000D+00
 0.1305700000D+01  0.2303970000D+00
S    1 1.00
 0.3406200000D+01  0.1000000000D+01
S    1 1.00
 0.3245000000D+00  0.1000000000D+01
S    1 1.00
 0.1022000000D+00  0.1000000000D+01
P    4 1.00
 0.1134130000D+02  0.1798700000D-01
 0.2436000000D+01  0.1103390000D+00
 0.6836000000D+00  0.3831110000D+00
 0.2134000000D+00  0.6478600000D+00
P    1 1.00
 0.7010000000D-01  0.1000000000D+01
D    1 1.00
 7.5000000000D-01  0.1000000000D+01
****
H 0
S    4 1.00
82.636374        6.172045011044104D-03
12.409598        4.721337522157118D-02
2.823854         0.232534718743609
0.79767          0.790495587401532
S    1 1.00
 0.258053     1.0
S    1 1.00
 0.089891     1.0
P    1 1.00
 1.0725       1.000000
```

Both the d and p functions in the basis set were optimized variationally with B_2H_6, since this was the smallest molecule containing both bond and ring structural elements.

Geometry optimizations were performed by means of both the GAUSSIAN88(Frisch *et al* 1988) program and the GAMESS(Schmidt *et al* 1987) program. GAUSSIAN88 was used to optimize the smaller boranes, such as BH_3, B_2H_6, B_4H_{10} and B_5H_9. GAMESS was used to optimize higher-symmetry cage molecules like $B_6H_6^{2-}$, $B_7H_7^{2-}$ and the carboranes, while a Direct SCF calculation was employed in GAUSSIAN88 to optimize both B_6H_{10} and $B_{12}H_{12}^{2-}$, both of which contained too many basis functions for GAMESS to handle. GAUSSIAN88 was run on the VAX 8650 & 6240, and the Trace/Multiflow was used for the direct SCF runs, while GAMESS was run on the FPS Stellar GS1000.

Tabulation of the SCF Results for the Boranes

The borane summaries presented here contain the following information:

1. The total calculated energy.
2. Cartesian coordinates of all atoms for the calculated minimum energy geometry (standard orientation).
3. Molecular point group(D_{3h} for BH_3, for example).

Also, an identifying structure is given for each molecule, to help with assignment of the positions of the numbered atoms.

Borane Energies, Coordinates

(Energies and atomic coordinates in atomic units)

Table III. BH

BH, $C_{\infty v}$ E(RHF) = -25.124157 a.u.

Atom	x	y	z
B1	0.00000	0.00000	0.22124
H2	0.00000	0.00000	-2.11093

Table IV. BH_3

BH_3, D_{3h} E(RHF) = -26.395270 a.u.

Atom	x	y	z
B1	0.00000	0.00000	0.00000
H2	0.00000	2.25084	0.00000
H3	1.94929	-1.12542	0.00000
H4	-1.94929	-1.12542	0.00000

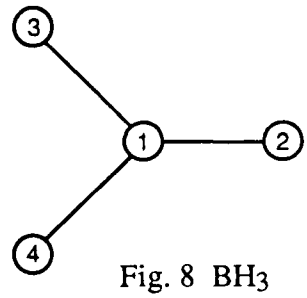

Fig. 8 BH_3

Table V. B_2H_6

B_2H_6, D_{2h} E(RHF) = -52.822442 a.u.

Atom	x	y	z
B1	-1.6982	0.0000	0.0000
H2	0.0000	0.0000	1.8514
H3	-2.7774	1.9639	0.0000
H4	-2.7774	-1.9639	0.0000
B5	1.6982	0.0000	0.0000
H6	2.7774	-1.9639	0.0000
H7	2.7774	1.9639	0.0000
H8	0.0000	0.0000	-1.8514

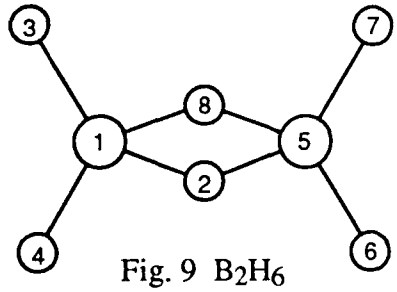

Fig. 9 B_2H_6

Table VI. B_4H_{10}

B_4H_{10}, C_{2v} E(RHF) = -104.477749 a.u.

Atom	x	y	z
B1	-1.64935	0.00000	-0.90345
B2	1.64935	0.00000	-0.90345
H3	-2.61283	0.00000	-2.91360
H4	2.61283	0.00000	-2.91360
B5	0.00000	2.71799	0.77701
B6	0.00000	-2.71799	0.77701
H7	-2.50164	-1.75440	0.44703
H8	2.50164	-1.75440	0.44703
H9	2.50164	1.75440	0.44703
H10	-2.50164	1.75440	0.44703
H11	0.00000	2.73239	3.02214
H12	0.00000	-2.73239	3.02214
H13	0.00000	4.63883	-0.37037
H14	0.00000	-4.63883	-0.37037

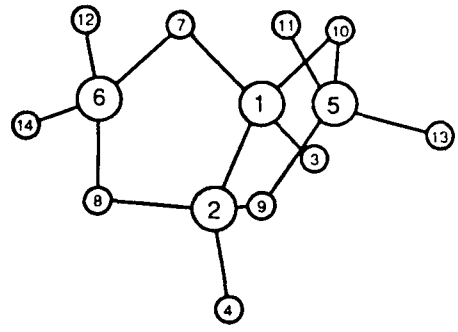

Fig. 10 B_4H_{10}

Table VII. B_5H_9

B_5H_9, C_{4v} E(RHF) = -128.597863 a.u.

Atom	x	y	z
B1	0.00000	2.43416	-0.27283
B2	2.43416	0.00000	-0.27283
B3	0.00000	-2.43416	-0.27283
B4	-2.43416	0.00000	-0.27283
B5	0.00000	0.00000	1.85481
H6	0.00000	4.64360	-0.01215
H7	4.64360	0.00000	-0.01215
H8	0.00000	-4.64360	-0.01215
H9	-4.64360	0.00000	-0.01215
H10	1.82100	1.82100	-1.96208
H11	1.82100	-1.82100	-1.96208
H12	-1.82100	-1.82100	-1.96208
H13	-1.82100	1.82100	-1.96208
H14	0.00000	0.00000	4.07958

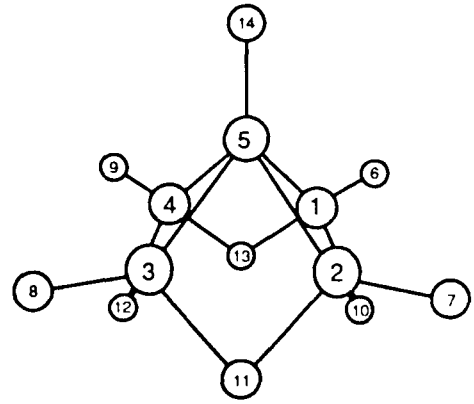

Fig. 11 B_5H_9

Table VIII. B_6H_{10}

B_6H_{10}, C_S E(RHF) = -153.860374 a.u.

Atom	x	y	z
B1	2.84236	-0.11692	0.00000
B2	0.00000	1.64075	0.00000
H3	4.91057	0.70327	0.00000
B4	0.70225	-0.21088	2.69923
B5	0.70225	-0.21088	-2.69923
H6	2.60860	-1.77117	1.79789
H7	2.60860	-1.77117	-1.79789
H8	-0.01128	3.86981	0.00000
B9	-2.43041	-0.35557	1.54956
B10	-2.43041	-0.35557	-1.54956
H11	1.36770	0.34747	4.74802
H12	1.36770	0.34747	-4.74802
H13	-0.92215	-2.10902	2.63832
H14	-0.92215	-2.10902	-2.63832
H15	-3.96890	0.26888	3.04215
H16	-3.96890	0.26888	-3.04215

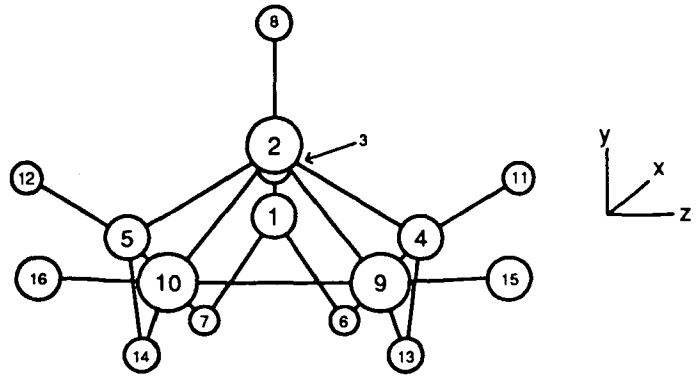

Fig. 12 B_6H_{10}

Table IX. $B_6H_6^{2-}$

$B_6H_6^{2-}$, O_h E(RHF) = -151.466097 a.u.

Atom	x	y	z
B1	0.00000	0.00000	-2.33569
B2	2.33569	0.00000	0.00000
B3	-2.33569	0.00000	0.00000
B4	0.00000	2.33569	0.00000
B5	0.00000	-2.33569	0.00000
B6	0.00000	0.00000	2.33569
H7	0.00000	0.00000	-4.63096
H8	4.63096	0.00000	0.00000
H9	-4.63096	0.00000	0.00000
H10	0.00000	4.63096	0.00000
H11	0.00000	-4.63096	0.00000
H12	0.00000	0.00000	4.63096

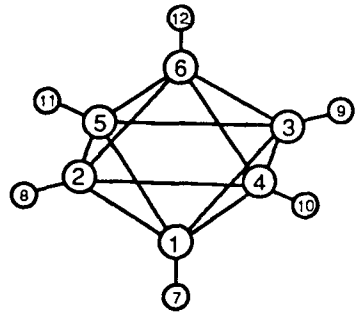

Fig. 13 $B_6H_6^{2-}$

Table X. $B_7H_7^{2-}$

$B_7H_7^{2-}$, D_{5h} E(RHF) = -176.759690 a.u.

Atom	x	y	z
B1	0.82778	2.54763	0.00000
B2	-2.16715	1.57452	0.00000
B3	-2.16715	-1.57452	0.00000
B4	0.82778	-2.54763	0.00000
B5	2.67874	0.00000	0.00000
B6	0.00000	0.00000	-2.24057
B7	0.00000	0.00000	2.24057
H8	1.53721	4.73105	0.00000
H9	-4.02447	2.92395	0.00000
H10	-4.02447	-2.92395	0.00000
H11	1.53721	-4.73105	0.00000
H12	4.97452	0.00000	0.00000
H13	0.00000	0.00000	-4.53698
H14	0.00000	0.00000	4.53698

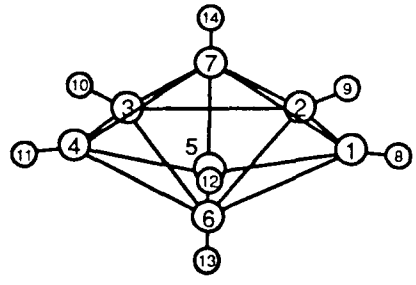

Fig. 14 $B_7H_7^{2-}$

Table XI. $B_{12}H_{12}^{2-}$

$B_{12}H_{12}^{2-}$, I_h E(RHF) = -303.326804 a.u.

Atom	x	y	z
B1	0.00000	0.00000	3.23340
B2	0.00000	2.89204	1.44602
B3	2.75050	0.89369	1.44602
B4	1.69990	-2.33971	1.44602
B5	-1.69990	-2.33971	1.44602
B6	-2.75050	0.89369	1.44602
B7	0.00000	0.00000	-3.23340
B8	0.00000	-2.89204	-1.44602
B9	2.75050	-0.89369	-1.44602
B10	1.69990	2.33971	-1.44602
B11	-1.69990	2.33971	-1.44602
B12	-2.75050	-0.89369	-1.44602
H13	0.00000	0.00000	5.50294
H14	0.00000	4.92198	2.46099
H15	4.68108	1.52097	2.46099
H16	2.89307	-3.98196	2.46099
H17	-2.89307	-3.98196	2.46099
H18	-4.68108	1.52097	2.46099
H19	0.00000	0.00000	-5.50294
H20	0.00000	-4.92198	-2.46099
H21	4.68108	-1.52097	-2.46099
H22	2.89307	3.98196	-2.46099
H23	-2.89307	3.98196	-2.46099
H24	-4.68108	-1.52097	-2.46099

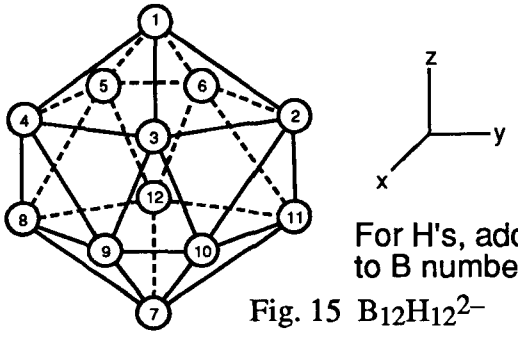

Fig. 15 $B_{12}H_{12}^{2-}$

Table XII. $C_2B_3H_5$

$C_2B_3H_5$, D_{3h} E(RHF) = -152.708566 a.u.

Atom	x	y	z
C1	0.00000	0.00000	2.10213
B2	0.00000	2.06718	0.00000
B3	-1.79023	-1.03359	0.00000
B4	1.79023	-1.03359	0.00000
C5	0.00000	0.00000	-2.10213
H6	0.00000	0.00000	4.12036
H7	0.00000	0.00000	-4.12036
H8	0.00000	4.29423	0.00000
H9	-3.71891	-2.14711	0.00000
H10	3.71891	-2.14711	0.00000

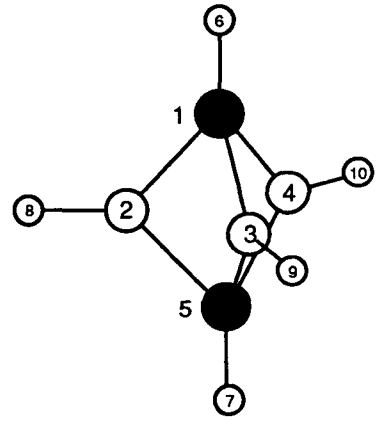

Fig. 16 $C_2B_3H_5$

Table XIII. $C_2B_4H_6$

$C_2B_4H_6$, D_{4h} E(RHF) = -177.939490 a.u.

Atom	x	y	z
B1	-2.29337	0.00000	0.00000
B2	0.00000	-2.29337	0.00000
B3	2.29337	0.00000	0.00000
B4	0.00000	2.29337	0.00000
C5	0.00000	0.00000	-2.04620
C6	0.00000	0.00000	2.04620
H7	-4.50802	0.00000	0.00000
H8	0.00000	-4.50802	0.00000
H9	4.50802	0.00000	0.00000
H10	0.00000	4.50802	0.00000
H11	0.00000	0.00000	-4.05779
H12	0.00000	0.00000	4.05779

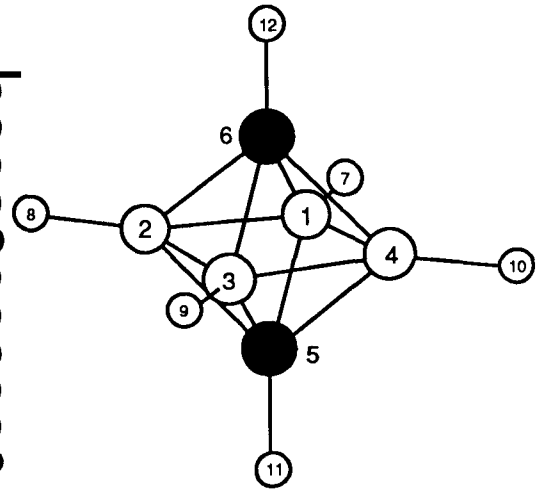

Fig. 17 $C_2B_4H_6$

Comparison of SCF Results

Before exploring the connectivity of these molecules, it will first be useful to compare the geometries obtained through these calculations with the experimental results compiled by Baudet in his contribution to the monograph on "Advances in Boron and the Boranes" (Baudet *et al* 1989). The analytical techniques used to determine his geometries were:

Microwave Spectroscopy (MW)
X-Ray Crystallography (XR), and
Electron Diffraction (ED).

Baudet took the geometry information provided by these techniques, and used them to calculate the values of internal coordinates in the borane molecules. Beaudet's article covered only the neutral boranes, so there were no comparisons for $B_6H_6^{2-}$, $B_7H_7^{2-}$, and $B_{12}H_{12}^{2-}$, but results were obtained for $B_6H_6^{2-}$ and $B_{12}H_{12}^{2-}$ (the potassium salt) in a paper by Fowler (1986), both of which came from XR results. Also, a dipole moment value was provided for comparison by Baudet for B_6H_{10}, the only C_s molecule in the series studied here.

The following is a description of the mathematics used to calculate internal coordinates from cartesian coordinates:

Taking a group of four different atoms in a molecule, and representing their coordinates in space by the vectors **A**, **B**, **C**, and **D**, one can calculate the distances between any two neighbouring atoms in the group with the following expressions:

$$R_a = |\mathbf{A} - \mathbf{B}|$$
$$R_b = |\mathbf{B} - \mathbf{C}|$$
$$R_c = |\mathbf{C} - \mathbf{D}|$$

Also, the vector differences between these same pairs can be obtained by:

$$\mathbf{r}_{AB} = \mathbf{A} - \mathbf{B}$$
$$\mathbf{r}_{BC} = \mathbf{B} - \mathbf{C}$$
$$\mathbf{r}_{CD} = \mathbf{C} - \mathbf{D}$$

and these vector differences are used in the calculation of the angle in degrees, θ_{ABC} or θ_{BCD}, formed by either set of three contiguous atoms:

$$\theta_{ABC} = \arccos\left(\frac{-\mathbf{r}_{BC}\bullet\mathbf{r}_{AB}}{R_aR_b}\right)\times\frac{360}{2\pi},$$

with a similar expression for θ_{BCD}. Finally, the torsional angle in degrees, ω_{ABCD}, created by all four atoms in the group is determined by

$$\omega_{ABCD} = \arccos\left(\frac{[\mathbf{r}_{BC}\times\mathbf{r}_{AB}]\bullet[\mathbf{r}_{CD}\times\mathbf{r}_{BC}]}{R_a R_b^2 R_c \sin(\theta_{ABC})\sin(\theta_{BCD})}\right)\times\frac{360}{2\pi}$$

It is not necessary to compare every possible combination of two, three, or four atoms in a given molecule; rather, only a fixed number of these parameters are required to unambiguously fix the geometry of a molecule (the total number of interatomic lengths and angles should be equal to $N - 1$, where N is the number of degrees of freedom). For the purpose of comparison, the same set of bond lengths and angles calculated from experiment by Baudet were chosen for calculation from geometries obtained in this work.

Furthermore, all angles are in degrees, and all lengths in angstroms. The number of significant figures for the results of this work were trimmed to match those given by Baudet, whose error values are given in parentheses.

Examination of Table XIV shows that all of the interatomic distances are in very good to excellent agreement with experiment, and most of the angles were in good agreement, except for some angles found in B_4H_{10}, B_5H_9 and B_6H_{10}.

Table XV gives a comparison of the geometrical angles and bond path angles for those bond angles which form a part of the perimeter of a ring; this restricts the atoms involved in the formation of these bond angles to borons and/or bridging hydrogens. As mentioned earlier, the difference

between the bond path angles and geometrical angles, $\Delta\alpha$, is invariably negative.

With a view towards the statements made about carboranes at the end of the General Chemistry section of the thesis, it is confirmed that B-C distances are shorter than B-B distances in the same molecule. Thus, in $C_2B_3H_5$, the B-C distance (1.56Å) is shorter than the B-B distance(1.85Å), and in $C_2B_4H_6$, the B-C distance (1.63Å) is again shorter than the B-B distance(1.72Å).

The idea that higher-coordinated boron atoms have longer B-B interatomic distances could not be approved or disproved in this research, since by the conventions of Greenwood & Earnshaw (1984), both of the carboranes studied here have pentacoordinate boron atoms, although it will be shown later that there are actually only three bonds to boron in $C_2B_3H_5$.

Finally, it has also been confirmed that there are larger angles subtended at a carbon in carboranes than at a boron in the same molecule, for in $C_2B_4H_6$ the angles subtended at carbon are greater than 60°, at 64°, and greater than 90°, at 96°, while at boron they are less than 60°, at 58°, and less than 90°, at 83°.

Table XIV. Comparison of Internal Coordinates for the Borane Series.

Molecule	Experimental	This Work
B2H6	Baudet	
Bond or Angle	MW	
B1-B5	1.743	1.797
B1-H3(Terminal)	1.184(3)	1.186
B1-H2(Bridging)	1.314(3)	1.329
H3-B1-H4	121.5(5)	122.4
H2-B1-H8	96.9(5)	94.9
B4H10	Baudet	
Bond or Angle	XR	
B1-B5	1.845(2)	1.903
B5-B6	2.786	2.877
B1-B2(B-B Bond)	1.75	1.75
B1-H10(Bridging)	1.21(4)	1.26
B5-H10(Bridging)	1.37(10)	1.43
B1-H3(Terminal)	1.14(4)	1.18
B5-H11(Terminal)	1.14(4)	1.19
B5-H13(Terminal)		1.18
H11-B5-H13	126	120
B2-B1-H3	118	116
B2-B1-H10	109	111
H10-B5-H9	135.7	135.7
B1-H10-B5	91.1	90.0
B1-B5-B2	56.6	54.6
B5-B1-B2	61.7	62.7
B5-B1-B2-B6	118.1	116.6
B2-B1-B5-H10	170	173
B5H9	Baudet	
Bond or Angle	MW	
B1-B5(Apical Bond)	1.690(5)	1.711
B1-B2(Equatorial Bond)	1.803(5)	1.822
B5-H14(Terminal Apical)	1.181(5)	1.177
B2-H7(Terminal Equatorial)	1.186(5)	1.177
B1-H10(Bridging)	1.352(5)	1.354
B1-B5-B2	64.5	64.3
B5-B1-H6	131.0(5)	132.1
B1-B2-B3-H11	116.0	116.8
B5-B2-B3-H11	193.1(29)	167.9
B5-B3-B2-B1	50.9	51.0

Table XIV(Cont'd). Comparison of Internal Coordinates for the Borane Series.

Molecule	Technique	Experimental	This Work
B6H10			
Bond or Angle		Baudet	
B1-B2	MW	1.774(13)	1.769
B2-B4	MW	1.762(4)	1.772
B2-B9	MW	1.783(11)	1.855
B1-B4	MW	1.818(5)	1.824
B4-B9	MW	1.710(6)	1.768
B9-B10	MW	1.654(3)	1.640
B2-H8	XR	1.25(6)	1.18
B1-H3	XR	1.14(6)	1.18
B4-H11	XR	1.18(4)	1.18
B9-H15	XR	1.28(5)	1.18
B1-H6	XR	1.32(6)	1.30
B4-H6	XR	1.48(5)	1.39
B4-H13	XR	1.31(4)	1.32
B9-H13	XR	1.35(4)	1.35
B5-B1-B4	MW	103.0	103.1
B1-B4-B9	MW	108.2	108.3
B4-B9-B10	MW	110.4	110.1
B1-B2-H3	XR	126.8	126.6
B2-B4-H11	XR	119.4	137.8
B2-B9-H15	XR	136.3	127.9
Dipole moment (Debyes)	MW	2.50	2.86
B6H6(2-)		Fowler(XR)	
Bond or Angle			
B1-B2		1.69(1)	1.748
B2-B3			2.472
B1-H7		1.11(7)	1.215
B7H7(2-)			
Bond or Angle		n/a	
B7-H14(Apical)			1.215
B1-H8(Equatorial)			1.215
B1-B7(Apical)			1.848
B1-B2(Equatorial)			1.666
B1-B7-H14(Apical)			129.9
B1-B2-H9(Equatorial)			126.0
H9-B2-B1-B7			134.1
B7-B1-B2-B6			91.9

Table XIV(Cont'd). Comparison of Internal Coordinates for the Borane Series.

Molecule	Technique	Experimental	This Work
B12H12(2-)		Fowler[$K_2B_{12}H_{12}$,XR]	
Bond or Angle			
B1-H13		1.07	1.201
B1-B2		1.77	1.799
C2B3H5		Baudet[ED]	
Bond or Angle			
C1-H6		1.071(7)	1.068
B2-H8		1.183(6)	1.179
C1-B2		1.556(2)	1.560
B2-B3		1.853(2)	1.895
C1-C5		2.261(3)	2.225
B2-C1-B3		73.05(1)	74.78
C1-B2-B3		53.48(1)	52.61
C1-B2-C5		93.16(1)	90.96
C2B4H6		Baudet[ED]	
Bond or Angle			
B1-C6		1.633(4)	1.626
B1-B2		1.720(4)	1.716
B1-B3		2.432(6)	2.427
C5-C6		2.179(7)	2.166
B1-H7		1.244(12)	1.172
C5-H11		1.104(22)	1.065
B1-C6-B2		63.55	63.69
C6-B2-B1		58.22	58.16
C5-B1-C6		83.73	83.48
B1-C6-B3		96.26	96.52

Table XV. Comparison of Geometric and Bond Path Angles for the Borane Series.

Molecule	Bond Angle	α_e (Geometric Angle)	α_b (Bond Path Angle)	$\Delta\alpha = \alpha_b - \alpha_e$
B_2H_6	B1-H2-B5	85.0574	1.7262	–83.3312
	H2-B1-H8	94.9426	59.1582	–35.7844
B_4H_{10}	H9-B5-H10	135.6934	92.0558	–43.6376
	B1-H10-B5	90.0361	1.8987	–88.1374
	B2-B1-H10	111.0545	101.5480	–9.5065
B_5H_9	B1-B5-B3	97.6880	93.1671	–4.5209
	B1-B5-B2	64.3349	61.8114	–2.5235
	B1-B10-B2	84.5608	1.6244	–82.9364
B_6H_{10}	B1-B2-B9	106.8640	84.5643	–22.2997
	B2-B9-H15	127.8700	140.1437	–12.2737
	B1-H6-B4	85.4123	1.2411	–84.1712
	H6-B1-B2	105.8720	91.4306	–14.4414
	B1-B2-B9	106.8640	84.5643	–22.2997
$B_6H_6^{2-}$	B2-B1-B4	60.0000	60.2804	+0.2804
	B2-B1-B3	90.0000	90.4863	+0.4863
$B_{12}H_{12}^{2-}$	B3-B1-B2	60.0000	57.0538	–2.9462
	B1-B2-B11	108.0000	101.1987	–6.8013
$C_2B_4H_6$	B2-B1-B4	90.0000	75.1615	–14.8385

With Regard to the Anionic Cage Clusters

The nature of bonding in $B_6H_6^{2-}$ and other *closo*-boranes is discussed in a paper by P.W. Fowler(1986). He points out that for a calculation with a 6-31G* basis set, the t_{2g} HOMO of $B_6H_6^{2-}$ has a positive orbital eigenvalue. He goes on to contend that "the positive t_{2g} eigenvalue appears to be stable against basis set extensions, implying that it is a 'real' feature of the SCF calculation, rather than an artefact of basis set choice."

He further states that the free $B_6H_6^{2-}$ anion in the gas phase is unbound, or unstable with respect to electron loss. It is only by modelling a crystal environment around the anion with a negative field that he obtains a stable anion, with all filled orbitals being negative in energy. Looking at $B_6H_6^{2-}$, his best SCF energy is –151.38542, compared to the value of –151.46610 obtained with the 9s/5p+1d set employed in this work, lower by 0.08 hartrees. Furthermore, although both of these calculations gave positive t_{2g} orbital eigenvalues, the HOMO energy he obtained was +0.0820, compared to only +0.0520 found in this work, making this value less positive by 0.03 hartrees. This clearly demonstrates that the positive eigenvalue of the t_{2g} HOMO is <u>not</u> stable against basis set extension, but rather it shows that the possibility of a completely stable anion cannot be ruled out, given a calculation with a sufficiently large basis set.

Tabulation of Results of Application of Theory of Atoms in Molecules

Figure 18 gives the molecular graphs of the boranes examined in this study. A molecular graph is defined as the network of bond paths linking pairs of neighbouring nuclear attractors. Again, a bond path is defined as the set of two gradient paths which originate at a (3,–1) or bond critical point and which link this point to the nuclear attractors or (3,–3) critical points on either side. This line through the charge distribution is a maximum in $\rho(\mathbf{r})$ with respect to any neighbouring line. At the bond critical point, there is a minimum in $\rho(\mathbf{r})$ with respect to neighbouring points along the bond path. Furthermore, the interatomic surface intersects the bond path at the bond critical point, which is the position of a maximum in $\rho(\mathbf{r})$ on that surface.

Table XVI gives the values of the properties associated with each of the unique bond paths in the borane series. Terminal and bridging hydrogen atoms are subscripted with the letters b and t, respectively. R_e is the geometrical distance between the two neighbouring nuclei, and R_b is the distance measured along the bond path, through the bond critical point; the presence of a value of R_b in the table is evidence of a curved bond path, curving inwardly in the case of the electron-deficient boranes. The bonded radii, r_A and r_B, are the geometrical distances from the bond critical point to the nuclei A and B, respectively, where the "bond" column gives the atoms in the form of "A-B". The value of $\rho(\mathbf{r})$ at the bond critical point is

given by ρ_b, and *n* is the ratio of ρ_b for this bond critical point to the value for the reference for this type of bond. There are three types of bonds in the borane series: B-B, B-H_t, and B-H_b. For B-B bonds, the reference has been chosen to be the B-B bond in B_4H_{10}, and for both types of B-H bond, the reference comes from B_2H_6. So, for these three references, the *n* value is 1.0000, and values of *n* greater or less than 1 in other bonds signify greater or lesser accumulations of charge in the internuclear region. Therefore it is possible to compare the bond order, and in so doing to quantify the relative strength and weaknesses of bonds. There are also references for B-C and C-H bonds in the carboranes, but these are less useful for comparison, seeing as there are only two examples of this type of molecule given.

The values of $\nabla^2\rho_b$ in Table XVI are the traces of the Hessian matrices of ρ_b, where the three eigenvalues are given as λ_1, λ_2, and λ_3, where λ_3 is the unique positive eigenvalue of the (3,–1) critical point. As mentioned earlier, information about the nature of the atomic interaction can be obtained from the value of $\nabla^2\rho_b$. The ellipticity, ε, has been defined as $(\lambda_1/\lambda_2 - 1)$. Finally, the last column gives values of $\rho(\mathbf{r})$ at ring and cage critical points when they exist, and they are denoted with subscripts r and c, respectively.

Table XVII gives a listing of the electron populations, net charges and energies of the boron atoms and the two types of hydrogen atoms in this series of molecules. These values were obtained by integration over the individual atomic basins, according to eqns. (14) and (15), and were

calculated with either PROIAIM or OMEGA. In the case where the atomic properties of one of the atoms in a molecule could not be integrated successfully, the values of the properties for that atom were calculated by difference (the difference between the total electron population or the total SCF energy for the molecule and the sum of the individual atomic properties for the other atoms), and these entries are shaded in the table. When two of the atoms in a molecule could not be integrated, the letters "n/a" for "not available" have been entered for those atoms.

Table XVIII is a listing of the total electron populations and energies for the molecules in the borane series under study, obtained by summing the individual PROAIM and/or OMEGA results according to eqn. (6). The E(SCF) results are the Restricted Hartree-Fock energy values for the molecule in atomic units from the GAUSSIAN88 SCF calculations. The differences are given as $q = \langle N \rangle - N_{molec}$, and $\Delta E = \langle E \rangle - E(SCF)$, and are tabulated in both atomic units and kcal/mol.

Table XIX repeats the information in Table XVII, but only for B_2H_6, the smallest molecule containing boron atoms as well as both types of hydrogen atoms. The atoms in B_2H_6 have been chosen as references for a comparison of the properties of the individual atoms. This comparison is given in Table XX. Values appearing in Table XX are in the form of simple differences; therefore the entries for the atoms in B_2H_6 appear in this table as zeros, and they are also shaded. The purpose of Table XX is to show how the values of these atomic properties change throughout the series.

Table XXI gives a listing of the critical points in $\nabla^2\rho(\mathbf{r})$ for the borane series. Because these points do not always lie along bond paths as the critical points in $\rho(\mathbf{r})$ do, the xyz coordinates of these points have been given, along with R, the distance from the given atom to the critical point. The value of $\nabla^2\rho(\mathbf{r})$ is given, along with eigenvalues of the Hessian of $\nabla^2\rho(\mathbf{r})$. Sites of electrophilic and nucleophilic attack are shaded.

The number of these unique critical points in the entire molecule is given by *n*, and the "designation" column describes where that unique point may be found. "Along C_n axis" means that the point lies along the axis, but inside of the cage or interior of the molecule, and therefore it is not an accessible reactive site. Two atom numbers separated by a comma signify that the critical point lies equidistant from the two nuclei, unless stated that it lies "near" one of the two. Three atom numbers separated by commas signify that the critical point can be found in the general area of the centroid of the triangle in three-dimensional space mapped out by those three nuclei. Both of these designations are used for bonded maxima which lie roughly along the bond path of a B-B bond. An atom number followed by three atom numbers in parentheses signifies that the point lies above the centroid mapped out by the three numbered nuclei in parentheses, between the plane of that triangle and the firstmentioned nucleus. Finally, "top ring" means that the point is a part of a ring of (3,+1) and/or (3,–1) critical points encircling a B-H bond and in a plane perpendicular to the B-H bond path.

Table XVI. Bond Properties for the Borane Series. (Reference values for ρ_b are shaded)

formula	bond	R_e, a_o	R_b, a_o	r_A, a_o	r_B, a_o	n	ρ_b, e/a_o^3	$\nabla^2\rho_b$, e/a_o^5	λ_1, e/a_o^5	λ_2, e/a_o^5	λ_3, e/a_o^5	ε	ρ_r and ρ_c, e/a_o^3
BH	B–H_t	2.3322		0.9626	1.3696	0.9724	0.1795	-0.4217	-0.4699	-0.4699	0.5182	0.0000	
BH_3	B–H_t	2.2508		0.9511	1.2997	0.9897	0.1827	–0.2498	–0.4758	–0.3734	0.5993	0.2741	
B_2H_6	B1–H3$_t$	2.2409	2.2415	0.9539	1.2875	1.0000	0.1846	–0.2583	–0.4342	–0.4053	0.5812	0.0714	ρ_r = 0.1083
	B1–H2$_b$	2.5123	2.6010	0.9957	1.5792	1.0000	0.1146	0.1864	–0.1671	–0.1067	0.4602	0.5657	
B_4H_{10}	B1–B2	3.2987	3.3389	1.6513	1.6513	1.0000	0.1378	–0.3058	–0.1782	–0.1480	0.0204	0.2042	ρ_r = 0.0840
	B1–H3$_t$	2.2291		0.9542	1.2750	0.9919	0.1831	–0.2095	–0.4146	–0.3723	0.5774	0.1134	
	B5-H11$_t$	2.2452	2.2462	0.9564	1.2897	1.0000	0.1846	–0.2614	–0.4240	–0.4038	0.5665	0.0498	
	B5-H13$_t$	2.2374	2.2382	0.9543	1.2838	1.0141	0.1872	–0.2782	–0.4394	–0.4117	0.5729	0.0675	
	B1–H10$_b$	2.3724	2.3915	0.9686	1.4122	1.1764	0.1348	0.1598	–0.2540	–0.1778	0.5917	0.4285	
	B5-H10$_b$	2.7010	2.8674	1.0570	1.7448	0.8264	0.0947	0.0829	–0.1010	–0.0653	0.2493	0.5467	
B_5H_9	B1-B5	3.2330	3.2336	2.1226	1.1108	0.9794	0.1350	–0.1090	–0.1646	–0.0484	0.1039	2.4039	ρ_r = 0.1110
	B1–H6$_t$	2.2248	2.2252	0.9527	1.2724	1.0125	0.1869	–0.2546	–0.4340	–0.3982	0.5776	0.0900	
	B5-H14$_t$	2.2248		0.9520	1.2727	0.9599	0.1772	–0.1363	–0.3724	–0.3724	0.6085	0.0000	
	B1-H10$_b$	2.5584	2.7080	1.0405	1.6446	0.9909	0.1136	0.0787	–0.1822	–0.0229	0.2839	6.9458	
B_6H_{10}	B1-B2	3.3419	3.3443	2.0195	1.3238	0.9154	0.1262	–0.1992	–0.1625	–0.0566	0.0198	1.8728	ρ_r = 0.1071
	B2-B4	3.3478	3.3646	1.2630	2.0869	0.9044	0.1247	–0.1870	–0.1674	–0.0479	0.0283	2.4961	ρ_r = 0.1068
	B2-B9	3.5062	3.7223	1.8332	1.7084	0.7748	0.1068	–0.0928	–0.1319	–0.0075	0.0466	16.6455	ρ_r = 0.1033
	B9-nn	1.5550		1.1675	0.3875	1.2293	0.1695	–0.4510	–0.2775	–0.2037	0.0301	0.3626	
	B1-H3$_t$	2.8434		0.9537	1.2714	1.0146	0.1873	–0.2543	–0.4273	–0.3976	0.5706	0.0748	
	B2-H8$_t$	2.2291		0.9529	1.2763	0.9821	0.1813	–0.1839	–0.3915	–0.3843	0.5918	0.0187	
	B4-H11$_t$	2.2253		0.9527	1.2730	1.0271	0.1896	–0.2838	–0.4346	–0.4239	0.5747	0.0253	
	B9-H15$_t$	2.2327		0.9537	1.2797	0.9924	0.1832	–0.2204	–0.4279	–0.3817	0.5891	0.1212	
	B1-H6$_b$	2.4543	2.5028	0.9870	1.4994	1.0946	0.1254	0.1507	–0.2232	–0.1155	0.4894	0.9335	
	B4-H6$_b$	2.6232	3.1981	1.2317	1.8511	0.9440	0.1082	–0.0864	–0.1522	–0.0161	0.0818	8.4454	
	B4-H13$_b$	2.4990	2.6314	1.0373	1.5774	1.1346	0.1300	–0.0216	–0.2252	–0.0741	0.2777	2.0396	
	B9-H13$_b$	2.5564	3.5957	1.1516	2.0857	0.9698	0.1111	–0.0550	–0.1261	–0.0111	0.0822	10.3819	

Table XVI. (Cont'd.) Bond Properties for the Borane Series.(Reference values for ρ_b are shaded)

formula	bond	R_e, a_o	R_b, a_o	r_A, a_o	r_B, a_o	n	ρ_b, e/a_o^3	$\nabla^2\rho_b$, e/a_o^5	λ_1, e/a_o^5	λ_2, e/a_o^5	λ_3, e/a_o^5	ε	ρ_r and ρ_c, e/a_o^3
$B_6H_6^{2-}$	B–B	3.3032	3.3114	1.6518	1.6518	0.9076	0.1251	–0.1692	–0.1458	–0.0445	0.0212	2.2759	$\rho_r = 0.1159$
	B–H_t	2.2953		0.9613	1.3340	0.8294	0.1531	–0.0200	–0.3114	–0.3114	0.6028	0.0000	$\rho_c = 0.0642$
$B_7H_7^{2-}$	B1-B7	3.4922		1.8076	1.6850	0.7723	0.1065	–0.0940	–0.1261	–0.0156	0.0477	7.0693	$\rho_r = 0.1042$
	B1-nn	1.5748		1.2017	0.3731	1.0749	0.1482	–0.2941	–0.1896	–0.1277	0.0231	0.4850	$\rho_c = 0.0485$
	B1-$H8_t$	2.2958		0.9627	1.3331	0.8288	0.1530	–0.0134	–0.3320	–0.2773	0.5958	0.1971	
	B7-$H14_t$	2.2964		0.9594	1.3370	0.8570	0.1582	–0.0691	–0.1199	–0.1199	–0.0713	0.0000	
$B_{12}H_{12}^{2-}$	B–B	3.3998	3.4033	1.7006	1.7006	0.8553	0.1179	–0.1614	–0.1544	–0.0407	0.0338	2.7918	$\rho_r = 0.1097$
	B–H_t	2.2695		0.9575	1.3120	0.8976	0.1657	–0.0899	–0.3467	–0.3467	0.6034	0.0000	$\rho_c = 0.0136$
$C_2B_3H_5$	B–C	2.9483	2.9557	1.9987	0.9560	1.0000	0.1685	0.0306	–0.2948	–0.2927	0.6181	0.0072	$\rho_r = 0.1003$
	C–H_t	2.0182		1.2242	0.7940	1.0000	0.2933	–1.1867	–0.7344	–0.7344	0.2820	0.0000	$\rho_c = 0.0908$
	B–H_t	2.2270		0.9501	1.2769	1.0043	0.1854	–0.2439	–0.4554	–0.3861	0.5977	0.1794	
$C_2B_4H_6$	B–C	3.0735	3.0757	1.0055	2.0682	0.8577	0.1445	0.0873	–0.2077	–0.0825	0.3775	1.5172	$\rho_r = 0.1297$
	B–B	3.2433	3.7615	1.6233	1.6233	0.9412	0.1297	–0.1279	–0.1388	–0.0024	0.0133	57.5559	$\rho_c = 0.0780$
	C–H_t	2.0116		1.2270	0.7846	1.0123	0.2969	–1.1830	–0.7400	–0.7400	0.2970	0.0000	
	B–H_t	2.2146		0.9513	1.2634	1.0060	0.1857	–0.2283	–0.4285	–0.3962	0.5965	0.0814	

Table XVII. Integrated Electron Populations, Net Charges and Energies for Atoms in the Borane Series.(Atoms by difference are shaded)

	Boron Atoms				Terminal Hydrogen Atoms				Bridging Hydrogen Atoms			
Formula	Atom	N(B), e	q(B), e	E(B), e^2/a_o	Atom	N(H_t), e	q(H_t), e	E(H_t), e^2/a_o	Atom	N(H_b), e	q(H_b), e	E(H_b), e^2/a_o
BH	B1	4.2106	+0.7894	-24.2125	H2	1.7917	-0.7917	-0.9112				
BH_3	B1	2.8385	+2.1615	-23.7544	H2	1.7199	-0.7199	-0.8804				
B_2H_6	B1	2.8764	+2.1236	-23.7300	H3	1.7042	-0.7042	-0.8751	H2	1.7133	-0.7133	-0.9305
B_4H_{10}	B1	3.6095	+1.3905	-24.0085	H3	1.6626	-0.6626	-0.8536	H7	1.7169	-0.7169	-0.9220
	B5	3.0427	+1.9574	-23.8729	H11	1.6936	-0.6936	-0.8777				
					H13	1.7003	-0.7003	-0.8804				
B_5H_9	B1	n/a	n/a	n/a	H6	1.6828	-0.6828	-0.8609	H10	1.6736	-0.6736	-0.8934
	B5	n/a	n/a	n/a	H14	1.6792	-0.6792	-0.8402				
B_6H_{10}	B1	3.5080	+1.4920	-24.0316	H3	1.6727	-0.6727	-0.8597	H6	1.7008	-0.7008	-0.9128
	B4	3.7793	+1.2207	-24.1363	H8	1.6834	-0.6834	-0.8554	H13	1.7188	-0.7188	-0.9206
	B2	n/a	n/a	n/a	H11	1.6886	-0.6886	-0.8713				
	B9	n/a	n/a	n/a	H15	1.7007	-0.7007	-0.8665				
$B_6H_6^{2-}$	B1	4.5326	+0.4674	-24.4041	H7	1.8008	-0.8008	-0.8403				
$B_7H_7^{2-}$	B1	n/a	n/a	n/a	H8	1.7684	-0.7684	-0.8349				
	B7	n/a	n/a	n/a	H14	1.7957	-0.7957	-0.8535				
$B_{12}H_{12}^{2-}$	B1	4.4274	+0.5726	-24.4198	H13	1.7393	-0.7393	-0.8574				
$C_2B_3H_5$	B2	2.8723	+2.1277	-23.7248	H8	1.7033	-0.7033	-0.8628				
$C_2B_4H_6$	B1	3.3521	+1.6479	-24.1774	H7	1.6947	-0.6947	-0.8514				

Table XVIII. Comparison of Total Integrated Electron Populations and Energies with SCF Results for Molecules in the Borane Series

Molecule	$\langle N \rangle = \sum_{\Omega} N(\Omega)$. e	$q=\langle N \rangle - N_{molec}$ e	$\langle E \rangle = \sum_{\Omega} E(\Omega)$. e^2/a_o	E(SCF), e^2/a_o	$\Delta E = \langle E \rangle - E(SCF)$, e^2/a_o	ΔE, kcal/mole
BH	6.0023	+0.0023	–25.1237	-25.1242	+0.0005	+0.3138
BH_3	7.9981	–0.0019	-26.3955	-26.3953	–0.0002	–0.1255
B_2H_6	15.9963	–0.0037	-52.8214	-52.8224	+0.001	+0.6275
B_4H_{10}	30.2851	+0.2851	-104.6740	-104.4777	–0.1963	–123.2
$C_2B_3H_5$	31.9940	–0.0060	-152.7066	-152.7085	+0.0019	+1.1923

Table XIX. Reference Values for Integrated Electron Populations and Energies for Atoms in the Borane Series

Atom	N(Ω), e	E(Ω), e^2/a_o	E(Ω), kcal/mole
B	2.8764	-23.7300	–14,890.6
H_t	1.7042	-0.8751	–549.1
H_b	1.7133	-0.9305	–628.4

Table XX. Comparison of Integrated Electron Populations and Energies for Atoms in the Borane Series.(Reference atoms are shaded)

	Boron Atom Comparison				Terminal Hydrogen Atom Comparison				Bridging Hydrogen Atom Comparison			
Formula	Atom	$\Delta N(B)$, e	$\Delta E(B)$, e^2/a_o	$\Delta E(B)$, kcal/mole	Atom	$\Delta N(H_t)$, e	$\Delta E(H_t)$, e^2/a_o	$\Delta E(H_t)$, kcal/mole	Atom	$\Delta N(H_b)$, e	$\Delta E(H_b)$, e^2/a_o	$\Delta E(H_b)$, kcal/mole
BH	B1	+1.3342	–0.4825	–302.8	H2	+0.0875	–0.0361	–22.65				
BH_3	B1	-0.0379	–0.0244	–15.31	H2	+0.0156	-0.0053	-3.313				
B_2H_6	B1	0.0000	0.0000	0.000	H3	0.0000	0.0000	0.000	H2	0.0000	0.0000	0.000
B_4H_{10}	B1	+0.7331	–0.2785	–174.8	H3	-0.0416	+0.0215	+13.47	H7	+0.0036	+0.0085	+5.328
	B5	+0.1662	–0.1429	–89.67	H11	-0.0107	-0.0026	-1.619				
					H13	-0.0040	-0.0053	-3.301				
B_5H_9	B1	n/a	n/a	n/a	H6	-0.0215	+0.0142	+8.886	H10	-0.0397	+0.0371	+23.26
	B5	n/a	n/a	n/a	H14	-0.0250	+0.0349	+21.89				
B_6H_{10}	B1	+0.6316	–0.3016	–189.3	H3	-0.0315	+0.0154	+9.657	H6	-0.0125	+0.0176	+11.07
	B4	+0.9029	–0.4063	–254.9	H8	-0.0208	+0.0197	+12.37	H13	+0.0055	+0.0099	+6.212
	B2	n/a	n/a		H11	-0.0157	+0.0038	+2.359				
	B9	n/a	n/a		H15	-0.0035	+0.0086	+5.409				
$B_6H_6^{2-}$	B1	+1.656	–0.6741	–423.0	H7	+0.0965	+0.0349	+21.87				
$B_7H_7^{2-}$	B1	n/a	n/a		H8	+0.0641	+0.0402	+25.21				
	B7	n/a	n/a		H14	+0.0915	+0.0216	+13.53				
$B_{12}H_{12}^{2-}$	B1	+1.551	–0.6898	–432.8	H13	+0.0351	+0.0177	+11.11				
$C_2B_3H_5$	B2	-0.0041	+0.0052	+3.263	H8	-0.0010	+0.0123	+7.712				
$C_2B_4H_6$	B1	+0.4757	–0.4474	–280.7	H7	-0.0095	+0.0237	+14.87				

Table XXI. Critical Points in $\nabla^2\rho$ for the Borane Series.(Sites of electrophilic and nucleophilic attack are shaded)

Molecule	x	y	z	$\nabla^2\rho$, e/a_o^5	R	λ_1, e/a_o^7	λ_3, e/a_o^7	λ_3, e/a_o^7	Desigination	n
BH_3										
(3,-1)	1.0689	0.6171	0.0000	0.00488	1.2342	-2.19943	-0.19500	1.07670	2,1,3	3
B_2H_6										
(3,-1)	-2.9783	0.0000	0.0000	0.03039	1.2801	-1.33345	-0.15506	0.84004	3,1,4	2
(3,-1)	-0.3583	0.0000	0.0000	-0.05567	1.3398	-0.89350	-0.76696	0.56002	2,1,8	2
(3,-1)	-1.3543	-0.8500	0.9502	0.03592	1.3204	-1.19882	-0.20763	0.75185	4,1,2	8
(3,+1)	-0.6886	1.0432	0.0000	0.08510	1.4517	-0.28260	0.11360	0.28787	2,3,8	4
(3,+1)	0.0000	0.0000	0.0000	-0.04507	1.6982	-0.73009	0.29090	0.38989	Centre	1
(3,+1)	-3.2205	0.0000	-0.8132	0.05541	1.7259	-0.03522	0.01025	0.14408	2,3,4	4
B_4H_{10}-B1										
(3,-1)	-0.9196	0.0000	-1.9370	-0.00631	1.2652	-1.84180	-0.28447	0.77308	2,1,3	2
(3,-1)	-0.9819	0.9483	-0.3222	-0.06434	1.2972	-1.53012	-0.67866	0.48955	2,1,7	4
(3,-1)	-2.4725	0.0000	0.1048	0.01806	1.3016	-1.59173	-0.30366	0.96243	7,1,10	2
(3,-1)	-2.6802	-0.7920	-1.0793	0.03604	1.3118	-1.11577	-0.13928	0.79065	3,1,7	4
(3,-1)	0.0000	0.0000	-0.8714	-0.30725	1.6497	-1.26474	-1.14502	0.27602	1,2 Midpt.	1
(3,+1)	-3.1271	0.0000	-0.5995	0.05369	1.5087	-0.14817	0.05994	0.08657	3,7,10	2
(3,+1)	-1.6090	-1.6253	-1.2802	0.08112	1.6689	-0.13762	0.05964	0.27904	2,3,7	4
(3,+1)	-1.3813	-0.3311	0.8727	0.10317	1.8265	-0.04566	0.06275	0.34129	2,7,10 -	2
(3,+1)	-1.3813	0.3311	0.8727	0.10317	1.8265	-0.04566	0.06275	0.34129	2,7,10 +	2
(3,-3)	-0.3565	0.0000	-0.8610	-0.31827	1.2936	-1.33950	-1.13687	-1.06169	1,2,near 1	2
(3,-3)	0.3565	0.0000	-0.8610	-0.31827	2.0063	-1.33950	-1.13687	-1.06169	1,2,near 2	2

Table XXI(Cont'd). Critical Points in $\nabla^2\rho$ for the Borane Series.(Sites of electrophilic & nucleophilic attack are shaded)

Molecule	x	y	z	$\nabla^2\rho$, e/a_o^5	R	λ_1, e/a_o^7	λ_3, e/a_o^7	λ_3, e/a_o^7	Desigination	n
B_4H_{10}-B5										
(3,-1)	0.0000	3.8246	1.4111	0.02849	1.2754	-1.44110	-0.19920	0.90690	5,11,13	2
(3,-1)	0.9773	2.1053	1.3717	0.02277	1.2977	-1.61950	-0.24372	0.77892	5,9,11	4
(3,-1)	-0.9656	2.8191	-0.1130	0.03604	1.3171	-1.28865	-0.13132	0.60671	5,10,13	4
(3,-1)	0.0000	1.5832	0.0701	-0.04524	1.3369	-1.41802	-0.47347	0.17147	5,9,10	2
(3,+1)	0.0000	2.4891	-0.6530	0.05672	1.4482	-0.32645	0.04245	0.27823	9,10,13	2
(3,+1)	0.0000	1.2965	1.2766	0.06700	1.5067	-0.20695	0.04266	0.18131	9,10,11	2
(3,+1)	1.6272	2.8764	1.4781	0.07366	1.7789	-0.05689	0.07257	0.21604	9,11,13	4
B_5H_9-B1										
(3,-1)	0.0000	2.8449	0.9620	0.01557	1.3014	-1.14874	-0.12099	0.52882	5,1,6	4
(3,-1)	1.0346	1.6209	-0.3955	-0.09403	1.3217	-1.18164	-0.83612	0.42507	2,1,6	8
(3,-1)	0.7494	3.0942	-1.1481	0.03331	1.3279	-1.03892	-0.12858	0.65463	5,1,10	8
(3,-1)	0.0000	2.1181	-1.5750	0.03232	1.3400	-1.24480	-0.20022	0.66263	13,1,10	4
(3,+1)	0.0000	1.1340	-0.8083	0.11179	1.4061	-0.56065	0.25964	0.36702	5,10,13	4
(3,+1)	0.0000	2.8879	-1.6370	0.04976	1.4376	-0.34328	0.10763	0.11191	6,10,13	4
(3,+1)	1.5726	2.7768	-0.2299	0.07640	1.6100	-0.14129	0.07623	0.23255	5,6,10	8
(3,-3)	0.0000	1.5649	0.6111	-0.30181	1.2397	-2.19429	-1.36701	-0.76389	1,5	4
(3,+3)	0.0000	0.0000	-0.0993	0.18489	2.4403	0.22223	0.22223	0.32236	lower cage	1
B_5H_9-B5										
(3,-1)	-0.7298	0.7298	1.0937	-0.13656	1.2824	-2.01867	-0.78774	0.60837	1,5,4	4
(3,-1)	0.0000	1.2782	2.4374	0.03974	1.4047	-0.42621	-0.00768	0.32774	1,5,14	4
(3,+1)	0.0000	0.0000	0.5154	0.14894	1.3394	-1.07061	0.86079	0.86079	1,3,5	1
(3,+1)	0.9127	-0.9127	2.4286	0.04126	1.4126	-0.39687	0.00706	0.29068	1,2,14	4
(3,-3)	0.0000	1.5649	0.6111	-0.30181	1.9989	-2.19429	-1.36701	-0.76389	1,5	4
(3,-3)	-1.4581	0.4539	1.1549	-0.12217	1.3253	-1.17796	-0.74501	-0.16772	2,9	2

Table XXI(Cont'd). Critical Points in $\nabla^2\rho$ for the Borane Series.(Sites of electrophilic & nucleophilic attack are shaded)

Molecule	x	y	z	$\nabla^2\rho$, e/a_o^5	R	λ_1, e/a_o^7	λ_3, e/a_o^7	λ_3, e/a_o^7	Desigination	n
B_6H_{10}-B1										
(3,-1)	2.9329	1.1790	0.0000	0.01262	1.2991	-1.24074	-0.15507	0.55156	3,1,2	1
(3,-1)	3.6982	-0.7028	0.8079	0.03673	1.3147	-1.12836	-0.14532	0.77141	3,1,6	2
(3,-1)	2.0295	-0.2087	1.0302	-0.09891	1.3154	-1.16778	-0.83229	0.34749	2,1,6	2
(3,-1)	2.7753	-1.4434	0.0000	0.03155	1.3282	-1.29883	-0.23966	0.81327	1,6,7	1
(3,+1)	3.6560	-1.4009	0.0000	0.05701	1.5201	-0.14985	0.07878	0.08677	3,6,7	1
(3,+1)	3.1624	0.1498	1.5223	0.08142	1.5783	-0.15852	0.09343	0.24635	2,3,6	2
(3,+1)	1.5084	-1.0635	0.0000	0.10187	1.6357	-0.00480	0.04887	0.08661	2,6,7	1
(3,-3)	1.8042	0.5829	0.0000	-0.26075	1.2520	-2.08961	-1.17612	-0.71443	1,2	1
B_6H_{10}-B2										
(3,-1)	-1.0820	0.9707	0.0000	-0.09773	1.2727	-2.23125	-0.68211	0.31160	9,10	1
(3,-1)	0.8276	0.9614	0.6913	-0.13443	1.2745	-2.15689	-0.85277	0.52890	1,2,4	2
(3,-1)	1.2176	2.2385	0.0000	0.03572	1.3564	-0.71545	-0.05930	0.47284	1,2,8	1
(3,-1)	-0.8213	2.2175	0.9221	0.03552	1.3629	-0.66126	-0.02360	0.41447	8,2,9	2
(3,-1)	-1.2250	0.6925	0.9085	-0.10509	1.7959	-0.73316	-0.39107	0.41623	2,9	2
(3,-1)	-1.8406	2.2305	0.0000	0.04945	1.9328	-0.04953	-0.00390	0.16440	8,2,front face	1
(3,+1)	-1.2851	2.1808	0.0000	0.03886	1.3939	-0.47950	0.01050	0.30407	top ring	1
(3,+1)	-0.0048	0.2238	0.0000	0.12277	1.4170	-0.49960	0.37952	0.43980	along c2 axis	1
(3,+1)	-1.5546	0.5446	0.0000	-0.00197	1.9022	-0.52167	0.46704	0.81388	8,9,10	1
(3,+1)	-0.7467	0.5237	1.4489	-0.05773	1.9760	-0.61529	0.51807	0.63769	4,8,9	2
(3,+1)	1.2926	0.4768	1.0096	-0.04988	2.0112	-0.59738	0.43609	0.79422	1,4,8	2
(3,-3)	1.8042	0.5829	0.0000	-0.26075	2.0914	-2.08961	-1.17612	-0.71443	1,2	1
(3,-3)	0.3225	0.5036	1.7695	-0.26471	2.1280	-2.62332	-1.21958	-0.55811	2,4	2
(3,-3)	-1.4581	0.4539	1.1549	-0.12217	2.2065	-1.17796	-0.74501	-0.16772	2,9	2

Table XXI(Cont'd). Critical Points in $\nabla^2\rho$ for the Borane Series.(Sites of electrophilic & nucleophilic attack are shaded)

Molecule	x	y	z	$\nabla^2\rho$, e/a_o^5	R	λ_1, e/a_o^7	λ_3, e/a_o^7	λ_3, e/a_o^7	Desigination	n
B_6H_{10}-B4										
(3,-1)	-0.4765	-0.4326	2.2914	-0.14804	1.2669	-1.86712	-1.00696	0.46232	2,4,13	2
(3,-1)	1.8474	-0.7334	3.0816	0.03596	1.3155	-1.24287	-0.15980	0.75387	4,6,11	2
(3,-1)	0.2343	-1.0049	3.6644	0.04272	1.3346	-0.90675	-0.11565	0.64114	4,13,11	2
(3,-1)	1.5716	-0.3041	1.6907	-0.09646	1.3347	-1.04640	-0.82100	0.25851	2,4,6	2
(3,-1)	0.5290	1.0969	2.9904	0.03445	1.3509	-0.68040	-0.06790	0.43628	2,4,11	2
(3,-1)	0.8668	-1.5429	2.4117	0.04865	1.3726	-0.93902	-0.16703	0.65241	4,6,13	2
(3,+1)	0.4717	-0.9952	1.5009	0.09790	1.4506	-0.31727	0.17221	0.25933	2,6,13	2
(3,+1)	-0.5607	-0.1965	3.5817	0.07313	1.5408	-0.14858	0.08311	0.18055	2,11,13	2
(3,+1)	1.0989	-1.6721	3.1250	0.06290	1.5728	-0.13075	0.07131	0.11201	2,6,13	2
(3,+1)	1.8264	-0.3074	1.3956	-0.08140	1.7241	-0.79549	0.19115	0.37727	2,6,11	2
(3,-3)	0.3225	0.5036	1.7695	-0.26471	1.2325	-2.62332	-1.21958	-0.55811	2,4	2
B_6H_{10}-B9										
(3,-1)	-1.7193	0.3381	0.7520	-0.10879	1.2739	-2.04157	-0.75021	0.42248	2,9,10	1
(3,-1)	-2.0499	0.6283	2.3514	0.01793	1.3250	-1.06597	-0.11143	0.46805	2,9,15	2
(3,-1)	-2.0323	-1.6409	1.3494	0.01889	1.3604	-9.85146	-0.22235	0.55410	10,9,13	2
(3,-1)	-3.6614	-0.6045	1.2760	0.01179	1.2854	-1.30486	-0.13576	0.61853	10,9,15	2
(3,-1)	-2.2434	-0.8543	2.7799	0.05264	1.3407	-1.00019	-0.04765	0.65848	13,9,15	2
(3,-1)	-1.2881	0.2750	1.5931	-0.11551	1.3055	-1.69147	-0.67389	0.11124	2,9,13	2
(3,-1)	-2.4955	-0.4799	0.0000	-0.46112	1.5559	-1.80471	-1.40751	0.12500	9,10	1
(3,-1)	-1.2250	0.6925	0.9085	-0.10509	1.7211	-0.73316	-0.39107	0.41623	2,9	2
(3,+1)	-2.0335	-0.5525	2.8035	0.05391	1.3299	-1.06431	0.06005	0.56811	10,13,15	2
(3,+1)	-1.2595	-0.8528	1.0389	0.09530	1.3708	-0.73255	0.31553	0.50310	2,10,13	2
(3,+1)	-3.0521	1.0456	0.4854	0.06253	1.8661	-0.05736	0.01939	0.23541	2,10,15	2
(3,+1)	-0.7467	0.5237	1.4489	-0.05773	1.9022	-0.61529	0.51807	0.63769	2,13,15	2
(3,-3)	-2.5044	-0.4938	0.2816	-0.46516	1.2776	-1.90928	-1.54360	-0.70579	9,10 near 9	2
(3,-3)	-1.4581	0.4539	1.1549	-0.12217	1.3253	-1.17796	-0.74501	-0.16772	2,9	2

Table XXI(Cont'd). Critical Points in $\nabla^2\rho$ for the Borane Series.(Sites of electrophilic & nucleophilic attack are shaded)

Molecule	x	y	z	$\nabla^2\rho$, e/a_o^5	R	λ_1, e/a_o^7	λ_3, e/a_o^7	λ_3, e/a_o^7	Designation	n
B_6H_6(2-)										
(3,-1)	0.8812	0.8812	-2.9969	0.03550	1.4108	-0.45637	-0.00731	0.32503	7,(1,2,4)	24
(3,-1)	0.7274	0.7274	-1.6203	-0.14372	1.2530	-2.59216	-0.73692	0.30506	2,1,4	24
(3,-1)	1.3059	0.0000	-1.3059	-0.18398	1.6631	-1.03033	-0.46054	0.14822	1,2	12
(3,+1)	0.0000	0.0000	-1.0679	0.13340	1.2678	-2.16556	0.92705	0.92705	along c4 axis	6
(3,+1)	1.2610	0.0000	-2.9977	0.03690	1.4242	-0.39262	0.00692	0.30212	7,1,2	24
(3,+1)	0.9901	0.9901	-0.9901	-0.05202	1.9420	-0.66860	0.62911	0.62911	1,2,4	8
(3,-3)	1.0941	0.0000	-1.5362	-0.18827	1.3551	-1.07772	-0.48215	-0.35005	1,2 near 1	48
(3,+3)	0.0000	0.0000	0.0000	0.25011	2.3357	0.21262	0.21262	0.21262	centre of cage	1
B_7H_7(2-) B1										
(3,-1)	-0.0311	3.5312	0.0000	0.01150	1.3058	-1.19565	-0.08248	0.55556	2,1,8	10
(3,-1)	0.3030	1.8564	0.9844	-0.10599	1.3123	-1.38354	-0.65584	0.13784	7,1,2	20
(3,-1)	0.0000	0.0000	0.0000	0.19932	2.6787	-0.02590	-0.02590	0.19608	centre of cage	1
(3,+1)	0.4301	1.3238	0.0000	0.11306	1.2868	-1.75473	0.78083	0.81957	along c2 axis	5
(3,+1)	1.1055	3.4025	-1.4535	0.05203	1.7090	-0.05868	0.01102	0.18687	6,5,12 near 5	10
(3,+1)	0.8634	2.6573	-1.9887	0.04147	1.9920	-0.03678	0.00467	0.16381	6,5,12 near 6	10
(3,-3)	0.5615	1.7281	1.0415	-0.10773	1.3517	-0.88952	-0.58472	-0.08782	1,6 near 1	10
(3,-3)	-0.7028	2.1630	0.0000	-0.32149	1.5782	-1.40227	-0.83332	-0.10889	1,2	5
(3,-3)	0.3395	1.0448	-1.5832	-0.14463	2.2369	-1.82709	-0.81895	-0.17029	1,6 near 6	10
B_7H_7(2-) B7										
(3,-1)	-0.3334	1.0261	1.6001	-0.12880	1.2547	-2.63575	-0.72449	0.16443	1,7,2	10
(3,-1)	-0.3811	1.1729	2.8902	0.03663	1.3939	-0.52080	-0.00374	0.37524	1,2,14	10
(3,-1)	0.4816	1.4822	1.2139	-0.10035	1.8662	-0.73353	-0.31296	0.33695	1,7	10
(3,-1)	0.0000	0.0000	0.0000	0.19932	2.2406	-0.02590	-0.02590	0.19608	centre of cage	1
(3,+1)	0.0000	0.0000	0.9288	0.13076	1.3118	-1.39010	0.58014	0.58014	along c5 axis	2
(3,+1)	0.3819	1.1755	2.8868	0.03708	1.3947	-0.51129	0.00376	0.36798	1,7,14	2
(3,+1)	-0.4862	1.4963	1.0853	-0.02816	1.9519	-0.53406	0.42550	0.76595	1,2,7	10
(3,-3)	0.3395	1.0448	1.5832	-0.14463	1.2802	-1.82709	-0.81895	-0.17029	1,7 near 7	10
(3,-3)	-1.4700	1.0680	1.0415	-0.10773	2.1770	-0.88952	-0.58472	-0.08782	2,7 near 2	10

Table XXI(Cont'd). Critical Points in $\nabla^2\rho$ for the Borane Series.(Sites of electrophilic & nucleophilic attack are shaded)

Molecule	x	y	z	$\nabla^2\rho$, e/a_o^5	R	λ_1, e/a_o^7	λ_3, e/a_o^7	λ_3, e/a_o^7	Desigination	n
$B_{12}H_{12}(2-)$										
(3,-1)	0.6371	0.8769	2.5934	-0.14592	1.2587	-2.47883	-0.83903	0.30988	2,1,3	60
(3,-1)	0.7299	1.0046	3.8750	0.04476	1.3977	-0.49872	-0.00678	0.38257	13,(1,2,3)	60
(3,-1)	0.0000	1.4698	2.3781	-0.16544	1.7005	-0.93278	-0.50377	0.29799	1,2	30
(3,+1)	0.0000	0.0000	1.8418	0.10881	1.3916	-0.59801	0.40055	0.40055	along c5 axis	12
(3,+1)	0.0000	1.2411	3.8706	0.04560	1.3951	-0.50943	0.00672	0.39334	13,1,2	60
(3,+1)	0.9702	1.3353	2.1606	-0.05190	1.9686	-0.60264	0.63475	0.63475	1,2,3	20
(3,-3)	0.0000	1.1464	2.5741	-0.17764	1.3225	-0.98192	-0.96057	-0.33808	1,2 near 1	60
(3,-3)	0.0000	0.0000	0.0000	0.08448	3.2334	-0.06556	-0.06556	-0.06556	centre of cage	1
$C_2B_3H_5$-C1										
(3,-1)	-0.6865	0.3963	1.5026	-0.42393	0.9938	-13.93154	-1.81647	1.48598	2,1,3	6
(3,-1)	0.0000	0.8965	2.5499	-0.07386	1.0021	-11.56675	-0.11718	2.29055	6,1,2	6
(3,-1)	-1.0393	1.1674	0.0000	0.02972	2.6195	-0.81463	-0.37499	0.36545	2,3 near 2	6
(3,+1)	-1.3196	0.7619	0.0000	0.04982	2.5963	-0.32564	0.00301	0.32036	2,3 midpoint	3
(3,+1)	-0.7913	0.4569	2.5228	-0.05256	1.0059	-10.97764	0.11659	1.94626	6,(1,2,3)	6
(3,+1)	0.0000	0.8558	0.0000	0.20515	2.2697	-3.94342	0.89317	1.70836	1,2,5 inside	3
(3,-3)	0.0000	0.8346	1.5048	-0.64414	1.0263	-8.59867	-3.12535	-1.51546	1,2 near 1	6
(3,+3)	0.0000	0.0000	0.0000	0.39371	2.1021	0.06576	0.87607	0.87607	centre of cage	1

Table XXI(Cont'd). Critical Points in $\nabla^2\rho$ for the Borane Series.(Sites of electrophilic & nucleophilic attack are shaded)

Molecule	x	y	z	$\nabla^2\rho$, e/a_o^5	R	λ_1, e/a_o^7	λ_3, e/a_o^7	λ_3, e/a_o^7	Designation	n
$C_2B_3H_5$-B2										
(3,-1)	0.0000	2.6271	1.1497	0.02076	1.2788	-1.34416	-0.10026	0.69812	1,2,8	6
(3,+1)	-0.7913	0.4569	2.5228	-0.05256	1.0059	-10.97764	0.11659	1.94626	6,(1,2,3)	6
(3,+1)	-1.1885	0.6862	0.6036	0.05163	1.9194	-0.43480	0.12958	0.75245	1,2,3 ring centre	6
(3,+1)	0.0000	0.8558	0.0000	0.20515	2.2697	-3.94342	0.89317	1.70836	1,2,5 inside	3
(3,-3)	0.0000	0.8346	-1.5048	-0.64414	1.9452	-8.59867	-3.12535	-1.51546	1,2 near 1	6
(3,+3)	0.0000	0.0000	0.0000	0.39371	2.0672	0.06576	0.87607	0.87607	centre of cage	1
$C_2B_4H_6$-B1										
(3,-1)	-1.5298	-0.7840	-0.6308	-0.12977	1.2632	-2.60579	-0.91987	0.36746	5,1,2 near 1	8
(3,-1)	-2.7942	-1.2759	0.0000	0.02509	1.3707	-0.59461	-0.05621	0.30036	7,1,2	8
(3,+1)	-1.0705	0.0000	0.0000	0.18700	1.2229	-3.85637	1.11980	1.42820	along c2 axis	4
(3,+1)	-2.6425	0.0000	-1.7476	0.06146	1.7821	-0.07323	0.01576	0.19978	5,1,7	8
(3,+1)	-2.2497	-2.2497	0.0000	0.04131	2.2501	-0.02179	0.03905	0.17363	8,2,1,7	4
(3,-3)	-1.2854	-1.2854	0.0000	-0.16907	1.6335	-1.08017	-0.39430	-0.06141	1,2 midpoint	4
(3,-3)	-0.8285	0.0000	-1.4813	-0.45293	2.0833	-10.82248	-1.98322	-0.97986	1,5 near 5	8
(3,+3)	0.0000	0.0000	0.0000	0.42823	2.2934	0.03288	0.54829	0.54829	centre of cage	1
$C_2B_4H_6$-C5										
(3,-1)	-0.5560	-0.5560	-1.4518	-0.37211	0.9857	-14.29404	-1.45504	0.99681	1,5,2	8
(3,-1)	-0.9051	0.0000	-2.4501	-0.15534	0.9912	-13.5076	-0.06271	1.39091	1,5,11	8
(3,+1)	-0.9224	-0.9224	-0.9605	-0.00951	1.6971	-0.94910	0.99536	1.40295	1,2,6	8
(3,-3)	-0.8285	0.0000	-1.4813	-0.45293	1.0028	-10.82248	-1.98322	-0.97986	1,6 near 6	8
(3,+3)	0.0000	0.0000	0.0000	0.42823	2.0462	0.03288	0.54829	0.54829	centre of cage	1

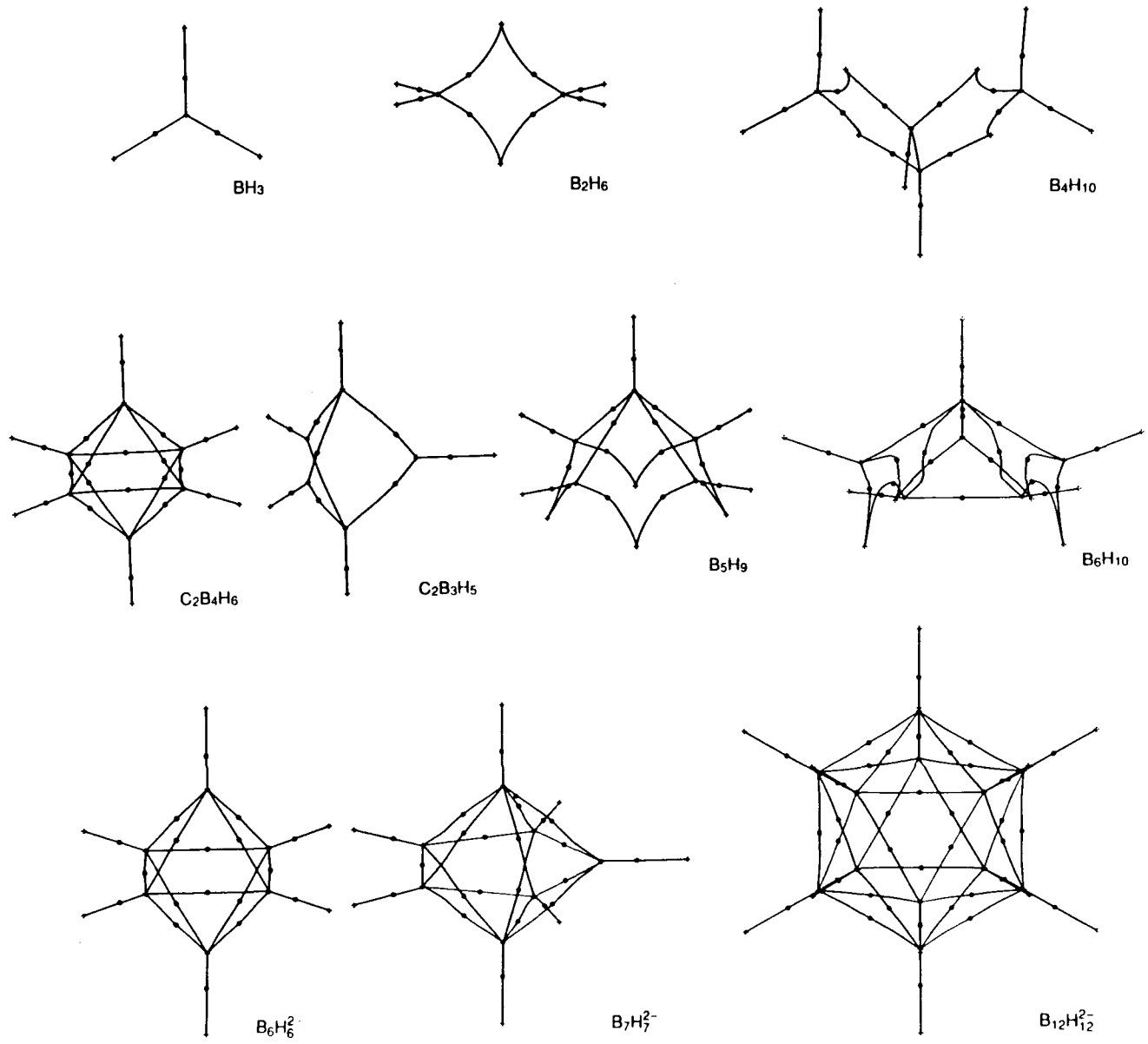

Fig. 18. Molecular Graphs of Borane Series

5. Discussion

A. Bond Properties in ρ

Examination of the molecular graphs in Figure 18 shows that the first major goal of this work has been accomplished; the non-arbitrary assignment of the connectivity of these boranes. There are several instances of connectivities which may contradict the models used by some researchers. In B_5H_9, for example, while there exists the set of four B-B bonds between the apical boron and those in the basal plane, there are no B-B bonds between adjacent basal borons, but rather there are four-membered rings formed by the apical boron, two adjacent basal borons, and a bridging hydrogen atom. Similarly, in B_6H_{10} there are no B-B bonds between those pairs of neighbouring basal boron atoms which have bridging hydrogens between them, so there are the same types of four-membered rings present here also; however, between the two basal borons labelled 9 & 10 (the two symmetrically equivalent borons which are bridged on one side only), there is a bond path, although there is a non-nuclear attractor or (3,-3) critical point in the centre of the bond path, rather than a (3,–1) critical point in ρ. Examining the bond critical points which link this attractor to the borons on either side, one finds that the values of $\rho(\mathbf{r})$ at the attractor and those at the (3,–1) points (which lie only

0.38 a.u. on either side) differ by only 0.00036 a.u. If a larger basis set were used, the non-nuclear attractor would most likely disappear, and there would be only the expected (3,–1) critical point; in any event, one treats this as a bond critical point and attaches no physical significance to the anomaly, since this is a very flat region of electron density.

For the carboranes, there are no B-B bonds in $C_2B_3H_5$, but they do exist in $C_2B_4H_6$. Comparison of the values of ρ_b between these two molecules shows that there is higher electron density at the B-C bond critical point in $C_2B_3H_5$ than in $C_2B_4H_6$, which is consistent with the fact that the carbon in $C_2B_3H_5$ is tetracoordinate, with shorter B-C bond lengths, whereas in $C_2B_4H_6$ the carbon is pentacoordinate, with longer bond lengths.

In the three anionic cage clusters, there are B-B bonds between all pairs of adjacent borons, but, as with B_6H_{10}, there are non-nuclear attractors in $\rho(\mathbf{r})$ between adjacent basal borons in $B_7H_7^{2-}$. There are no bridging hydrogens present in these cage molecules.

Having established the lines of interaction among the atoms in the borane series, these interactions can be further characterized by examining the value of the Laplacian of the charge density at the bond critical point, r_c (See Table XVI). As mentioned earlier, the nature of the pair-wise atomic interactions is determined by the predominance of either a perpendicular contraction of $\rho(\mathbf{r})$ towards the bond path (charge concentration at r_c) or a parallel expansion of $\rho(\mathbf{r})$ away from the

interatomic surface, in favour of separate charge concentrations in the individual atomic basins (charge depletion at r_c).

Examination of the values of $\nabla^2\rho(\mathbf{r})$ for the two types of B-H bond critical points shows that all values of $\nabla^2\rho_b$ are near zero, which characterizes these interactions as borderline, rather than strictly ionic or covalent. In general, values of ρ_b for the B-H_b bonds are 0.135 a.u. or less, whereas the values of ρ_b for B-H_t bonds are in the neighbourhood of 0.18 a.u. (for the non-*closo* molecules). This is the major distinction between the types of B-H bonding in the boranes, showing that B-H_b interactions are weaker, in agreement with the classification of B-H-B bridges as 3-centre, 2-electron bonds.

Another aspect of both types of B-H bonding in the boranes is that the VSCC of boron is virtually stripped away by hydrogen, as can be seen in the contour diagrams of the Laplacian of ρ for B_2H_6 (see Fig. 19a,b), for both the planes containing terminal and bridging hydrogen bonds to boron. It can also be seen from the diagrams that hydrogen is very polarizable, with a significant amount of charge density pulled back towards the boron core, seen more in the case of a terminal hydrogen bond than in the bridging case.

In order to examine the nature of the bonding between boron and a terminal hydrogen, one can compare the B-H_t bonding in the *nido*-borane reference of B_2H_6 to that in the *arachno*-B_4H_{10}. Here, one finds that the value of ρ_b differs in only the third decimal place; comparison with the two other *nido*-boranes, B_5H_9 and B_6H_{10}, reveals a maximum difference of

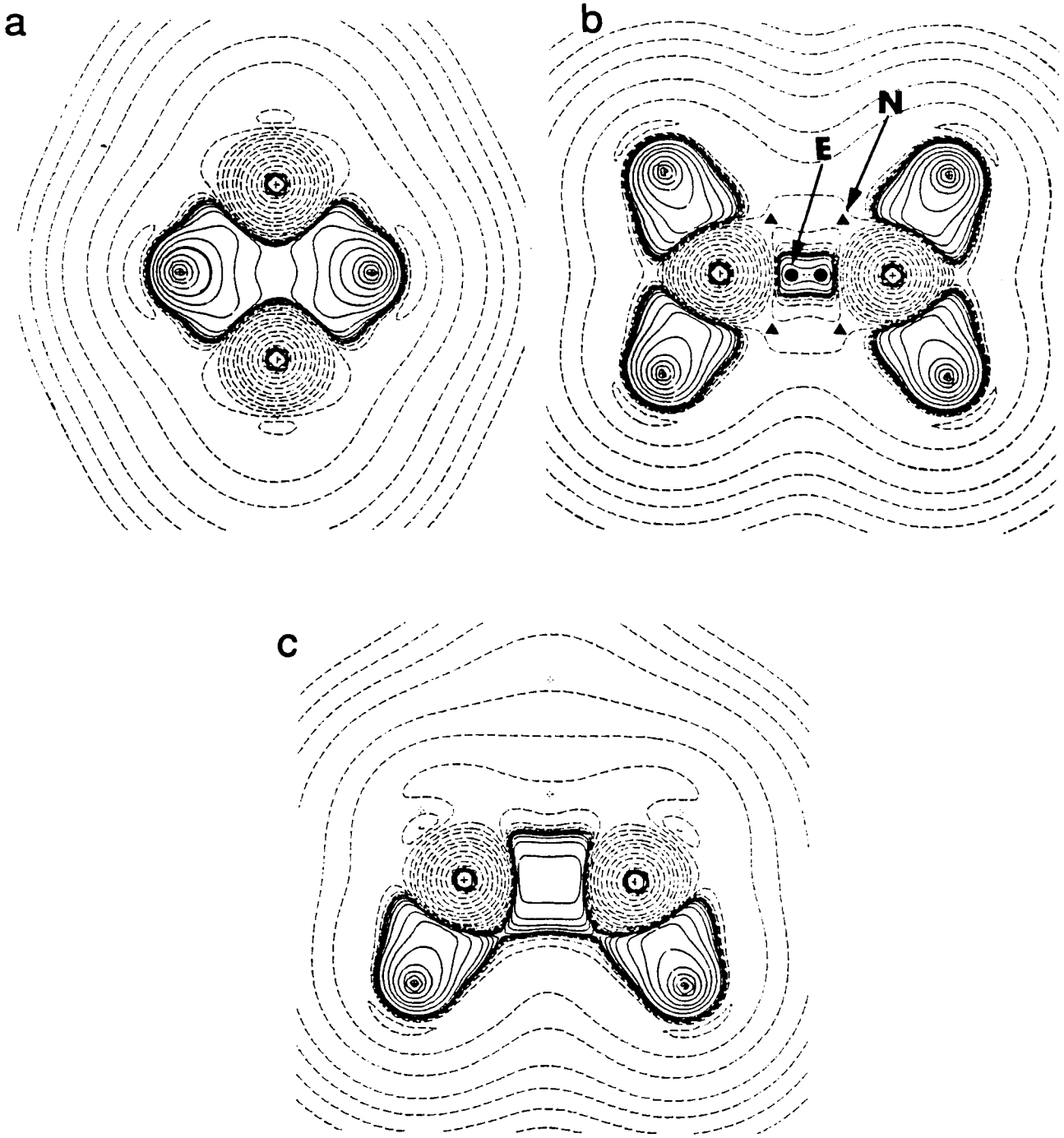

Fig. 19 Contour maps of $\nabla^2\rho(\mathbf{r})$ for a) Plane of ring in B_2H_6, b) Plane of borons and terminal hydrogens in B_2H_6, and c) Plane of bonded borons and their terminal H's in B_4H_{10}.

only .007 a.u., so there are no real differences in B-H_t bonding in these two classes of boranes.

On the other hand, comparing B-H_t bonds in the *nido*-boranes to the anionic *closo*-boranes, one finds that the value of ρ_b has been lowered from the reference value of 0.18 a.u. in the former to 0.15 a.u. in the case of $B_6H_6^{2-}$, giving this cage cluster an *n* value of 0.83. Also, the value of $\nabla^2\rho_b$ changes from the reference value of -.26 a.u. to -.02 for the same anion. These two facts suggest that the terminal hydrogen bonding in the anionic clusters is of a more ionic nature, with less accumulation of charge in the interatomic region, and more charge drawn in to the separate atomic basins. Reference to Table XVII confirms this, with the electron population on the hydrogen atom in $B_6H_6^{2-}$ increasing by 0.1 e relative to the B_2H_6 reference. Similarly, the electron population of each boron atom increases by 1.7 e relative to the reference, although it must be kept in mind that these cages have a net charge of –2, relative to the neutral *nido*- and *arachno*-boranes. Finally, comparison of B-H_t bonding in the *nido*- and *arachno*-boranes to the *closo*-carboranes shows the atomic interactions to be virtually identical.

The next type of atomic interaction in the boranes to be considered is the bonding between boron and bridging hydrogen. B-H_b bonding in the *nido*- and *arachno*-boranes is characterized by lower values of ρ_b than for B-H_t bonds, 0.11a.u. compared to 0.18 a.u., and also by mostly positive near-zero values of $\nabla^2\rho_b$. Therefore these are weaker atomic interactions, but like the B-H_t bonds, they are on the borderline with regard to the

shared nature of the interaction. In the case of *arachno*-B_4H_{10}, the bond critical points on the two sides of the bridging hydrogen differ from the reference by ±0.02 a.u., with the critical point linking to the boron involved in B-B bonding having a larger ρ_b value, and the other, linking to the boron in an environment similar to B_2H_6, having a smaller value. Both bond critical points have positive values of $\nabla^2\rho_b$, with the firstmentioned interaction being a bit more ionic.

The reference B-B bond in this study is the B-B bond in *arachno*-B_4H_{10}, with a ρ_b value of 0.14 a.u., lower than in the B-H_t interaction, but higher than in a B-H_b bond. A B-B bond exhibits a definite covalent nature, shown by a $\nabla^2\rho_b$ value of –0.31. Therefore charge density in these types of interactions is contracted towards the bond path, in the region between the two nuclei. Comparison of the diagram of $-\nabla^2\rho$ for B_2H_6 (Fig. 19a,b) with that for the plane of the B-B bond in B_4H_{10} (Fig. 19c) clearly shows that the latter is a more shared interaction.

Perusal of Table XVI shows that there is very little difference in the bond properties of the B-B bonds in the two *nido*-boranes, B_5H_9 and B_6H_{10}, except for a much weaker bond between B2 and B9 or between B2 and B10 (See Fig. 12) in B_6H_{10}, with an *n*-value of 0.77, and which is also borderline covalent. There is also a stronger bond between B9 and B10 in the same molecule, which has a *n*-value of 1.23, and a strongly covalent character ($\nabla^2\rho_b$ = -.45).

Looking at B-B bonds in the *closo*-boranes, the values of ρ_b are progressively lower as the cage is enlarged, relative to that found in B_4H_{10}

($\rho_b = 0.1378$). The charge density at the B-B bond critical point drops from a value of 0.1251 in $B_6H_6^{2-}$, down to an value of .1179 in $B_{12}H_{12}^{2-}$. In the case of $B_7H_7^{2-}$, there are five equatorial B-B bonds, each with a ρ_b value of 0.1482, and ten apical bonds with ρ_b equal to 0.1065, giving an average value for the molecule of 0.1204, which is bracketed by the values in the other two anions. Therefore the trend is apparent, that as the cage size increases, there are fewer electrons per B-B bond path. The values of $\rho(\mathbf{r})$ for both ring and cage critical points follow the same general trend, except for the value of ρ_r for $B_7H_7^{2-}$, which is smaller than that for $B_{12}H_{12}^{2-}$.

The value of ρ_b for the B-B bond in $C_2B_4H_6$, the only carborane in this study with B-B bonds, is similar to that in the reference, but it is borderline covalent.

Comparison of $\rho(\mathbf{r})$ values between a particular ring critical point and its surrounding bond critical points along with an examination of the ellipticities at these points yields information about the stability of the ring systems in the boranes. For example, the four-membered ring in B_2H_6 has a value of ρ_r of 0.1083 a.u., very close to the values of ρ_b in the bond paths that form the ring, all of which are 0.1146 a.u. As is apparent for the entire series of boranes, the charge density is delocalized over the surface of the ring, but the ellipticity of the bonds which make up the ring is only .57, making this a lesser example this effect. Similarly, in B_4H_{10}, ρ_r is only close in magnitude to ρ_b in the case of the B5-H10 bond critical point, while the other bond critical points have ρ_b larger by 0.06 a.u., and all of

the values of ε in these bond critical points are near zero. These two smaller molecules with four-membered ring systems show the least amount of charge delocalization in the borane series.

To see an example where this effect is more pronounced, one can examine the case of B_5H_9; here, the value of ρ_r is exceeded by only 0.0026 a.u. by the value for the bonds between basal borons and bridging hydrogens. The ellipticity for this bridging bond is 7.0, which suggests that charge density is more delocalized over the surface of the four-membered ring, a conclusion that is further supported by the ε value of 2.4 for the B-B bond. This is also the case in the three rings of B_6H_{10}, which have ellipticities ranging from 1.9 to 16.6 in the bonds around the perimeters of the rings.

The three-membered rings in the *closo*-boranes are also marked by B-B bonds with high ellipticities, ranging from 2.3 to 7.0, and very similar values of $\rho(\mathbf{r})$, when comparing the ring and bond critical points. The largest ellipticity found in any bond was found in the B-B bond in $C_2B_4H_6$, with $\varepsilon = 58$. Here, the value of ρ_r and ρ_b are equivalent to four decimal places! In the two cases where non-nuclear attractors between bonded atoms appear, i.e., in $B_7H_7^{2-}$ and B_6H_{10}, the ellipticities are small, and it is uncertain as to whether the presence of the attractors has affected this aspect of the topology in $\rho(\mathbf{r})$, since the other bonds in these rings have high ellipticities.

For those bonds in the boranes which have high ellipticities, it is useful to examine the orientation of the major axis of "soft" curvature,

whose eigenvalue is λ_2. All of these eigenvalues are oriented in a direction tangent to the surface of the molecule at the bond critical point, rather than pointing into or out of the interior of the molecule. This confirms the fact that charge is delocalized over the surface of the rings, rather than being concentrated in the bonds themselves.

B. Atomic Properties

The results of the integration of the properties determined over the individual atomic basins for the borane series in this study are given in Table XVII. The values in this table are divided into columns for boron atoms, terminal hydrogens, and bridging hydrogens. Before examining these results, it is useful to discuss their accuracy in general.

There are two ways of checking the validity of an integration. The first is to sum the individual values of the atomic properties, and to compare these with values for the total molecule. The total energy of the molecule can be obtained from the output of the SCF calculation, and the total electron population can be calculated from the molecular formula. The size of the difference obtained from a comparison of the energies or electron populations is the most important indicator of the success of a set of atomic integrations, since the actual results must be usable.

The second way of checking an integration is to look at the value of the Laplacian integrated over the basin of an atom, $L(\Omega)$. According to eqn. (9), the value of $L(\Omega)$ should theoretically be zero, if the region of space for integration is a true quantum mechanical subsystem bounded by a surface of zero flux. In practice, a "good" value of $L(\Omega)$ for a PROAIM integration is on the order of 10^{-5}, with 10^{-3} being marginally acceptable.

In this work, the integration results which were rejected had failed the first test, comparing the electron populations to the total for the

molecule, and most of the boron atom integrations which were acceptable had $L(\Omega)$ values on the order of 10^{-3}. When only one atomic integration in a molecule is rejected, the values of the properties for that particular atom can be obtained by subtracting the sum of the values for the other atoms in the molecule from the molecular totals (i.e., calculation by difference), but then one is no longer able to compare a complete sum of the atomic properties with the molecular values. Incomplete summations of the atomic properties are the reason that Table XVIII contains only five of the eleven molecules studied.

Four of the five molecules listed in Table XVIII have values of ΔE on the order of one kcal/mol or less, which represent an excellent agreement between the sums of the individual atomic energies and the totals for the molecules. Only B_4H_{10} had a large ΔE value, but the value of $L(\Omega)$ for both of the boron atoms in this molecule were on the order of 10^{-1}. And all of the molecules had q values on the order of 10^{-3}, except again for B_4H_{10}. These results for energy and electron population lend support to the idea that properties can be calculated for an atom (or fragment) in a molecule, and that these properties are additive to a sum which is equal to the molecular values.

The provision of electron populations and energies for the individual atoms in the boranes invites a comparison of their properties. In BH, for example, the boron atom is bonded to one terminal hydrogen, while the boron in BH_3 is bonded to three terminal hydrogens. The terminal hydrogen atom in BH withdraws 0.79 e of charge from B, while in BH_3 the

boron has a charge q(B) = +2.2, almost three times the charge transfer for one terminal hydrogen in BH. This begins to suggest that terminal hydrogen as a functional group is transferable, i.e., that one H_t in BH has the same effect as one H_t in BH_3, or indeed in other borane molecules.

In B_2H_6, q(B) = +2.12, compared to a value of q(B)=+2.16 in BH_3. The boron in B_2H_6 is surrounded by two terminal hydrogens and a pair of bridging hydrogens, while the boron in BH_3 is bonded to three terminal hydrogens. Comparison of the atomic charges on boron reveals that a terminal hydrogen withdraws slightly more charge from a boron atom than two hydrogen bridges. This may be because more charge remains in the boron atomic basin because of delocalization of charge within the ring in B_2H_6. The same comparison can be made between the boron in BH_3 and the boron in B_4H_{10} which is not involved in B-B bonding.

The boron in B_4H_{10} which is not involved in B-B bonding (B5 in Fig. 10) has an electron population of 3.04, and it has a bonding arrangement similar to the boron in B_2H_6 (N(B) = 2.88). The bond critical point linking B5 in B_4H_{10} to a neighbouring bridging hydrogen is 0.06 a.u. further away from the boron than the same critical point in B_2H_6, and thus the boron in B_4H_{10} has a slightly larger basin relative to the boron in B_2H_6, and this could account for the difference in electron count. Therefore the boron atom in B_2H_6 can be considered transferable.

The boron in B_4H_{10} which is involved in B-B bonding (B1 in Fig. 10) has a charge of +1.39, so it has 0.73 e more than the boron in B_2H_6. The major difference between B1 in B_4H_{10} and the boron in B_2H_6 is that

the boron in B_4H_{10} has a single B-B bond instead of a second terminal hydrogen bond. Since the two bonded borons in B_4H_{10} are symmetrically equivalent, there is no net transfer of charge from one boron atomic basin to the other, whereas in B_2H_6 there is another terminal hydrogen atom to withdraw charge from boron. This accounts for the difference in electron population between the B-B bonded boron in B_4H_{10} and the boron in B_2H_6.

At this point, some general statements can be made about the terminal and bridging hydrogens in the boranes. It is important to consider how the properties of atoms (or groups) in a molecule change when they appear in different members of a series of related compounds. If they change little, then it can be said that these atoms or groups are transferable, i.e., a transferable atom or group can be removed from one molecule and use to replace a similar atom or group in another molecule with little change in the charge distribution or molecular properties. Table XX gives the information which shows how the atomic properties of borons, and bridging and terminal hydrogens change throughout the borane series.

If one were to discuss relative transferability, the conclusion would be that the bridging hydrogens are the most transferable atoms in borane systems, since the values of ΔN and ΔE and their spread for this type of atom are the smallest in the table. Therefore, bridging hydrogens are the most constant in their atomic properties. Terminal hydrogens are also quite constant in their properties, even when including the anionic cages and carboranes. But there are large differences in electron population and

energy among the boron atoms as a group, with a spread in energies across the series as large as 435 kcal/mol, compared with a spread of 48 kcal/mol for terminal hydrogens, and only 18 kcal/mol for the bridging hydrogens. The large spread in boron energies suggests that there are different types of borons in the series under study, a fact already evident from examination of the topology of $\rho(\mathbf{r})$.

In the case of B_5H_9, there is a large difference between the atomic properties of the basal and apical borons. Each basal boron has one terminal hydrogen and two hydrogen bridges withdrawing charge from it, while the apical boron has only a single terminal hydrogen. The position of the bond critical point in the B-B bonds in B_5H_9 is about 2 a.u. away from the basal borons, but only about 1 a.u. away from the apical boron.

In B_6H_{10}, the two boron atoms which were successfully integrated were both basal borons, and both showed a charge increase (relative to the boron in B_2H_6—the apical boron B_6H_{10} could not be calculated)

In $C_2B_3H_5$, the boron atom is bonded to two carbons and a terminal hydrogen, with no B-B bonds found. The value of E(B) = –23.7, very close to the energy of the boron in *nido*-B_2H_6. In $C_2B_4H_6$, E(B) = –24.2, a difference of 280 kcal/mol. This is because in $C_2B_4H_6$ the carbon is withdrawing charge from four borons rather than three in $C_2B_3H_5$, and also there are equatorial B-B bonds in this molecule. The formation of these bonds is easier in $C_2B_4H_6$ than in $C_2B_3H_5$, because of the fact that the boron atoms are closer together in $C_2B_4H_6$ (R=3.24 a.u.) than in $C_2B_3H_5$ (R=3.58 a.u.).

C. Electron Counting Schemes

Having discussed the connectivity of the boranes, the nature of their bonding interactions, and their atomic electron populations, some things can be said about the electron-counting schemes that have been put forward to help predict structural stability or to classify the different boranes by means of molecular orbital theory.

First are the *styx* rules. In order for these rules to work, there have to be four bonds to each boron. The only way to represent the stable B_5H_9 structure is to draw a series of resonance structures involving B-B-B three-centre bonds. Now that the bonds in B_5H_9 have been unambiguously defined, a new set of rules for the boranes involving bonding should be developed, if possible, based on the true connectivity of the molecule, rather than on some model of bonding.

This researcher has attempted to devise a set of rules based on the true bonding in the boranes, but these attempts have been unsuccessful. The reason for this failure is obvious from the discussion on B-B bonding in part A of this section. To apportion, say, two electrons to every B-B bond in a borane molecule would not work well in the case of $B_{12}H_{12}^{2-}$, in which there are five B-B bonds around a single boron. Therefore it does not seem possible to set up an electron-counting scheme based on the number of bonds in a molecule. This leaves only the number of boron atoms in a molecule as a basis for an electron count.

In part B of this section, the atomic electron populations were discussed. The differences in the values of the populations on boron throughout the borane series makes it difficult, if not impossible to create an electron-counting scheme based on these populations.

Wade's rules are the only set of rules which can still be applied in spite of the new discoveries about the boranes outlined in this thesis, and they do correctly predict the number of electrons in the various classes of boranes. They are based on the number of borons present in the molecule, and on the number of additional vertices (borons) required to make a complete cage from these molecules.

C. Reactivity and the Laplacian of ρ

This section of the thesis deals with the scalar field derived from the second derivative of $\rho(\mathbf{r})$, $\nabla^2\rho(\mathbf{r})$. Both $\rho(\mathbf{r})$ and $\nabla^2\rho(\mathbf{r})$ are scalar fields, and as such both have the same topological features. In both are found critical points of rank three, and lines in space which link these points. In this discussion, it should be remembered that $\rho(\mathbf{r})$ and $\nabla^2\rho(\mathbf{r})$ are mapped out independently in space, and references to "bond paths", which are found only in $\rho(\mathbf{r})$, are made only in order to help the reader visualize where the critical points in $\nabla^2\rho(\mathbf{r})$ lie.

The Laplacian of ρ is a useful tool for modelling reactivity in molecules. Sites of preferential nucleophilic attack in molecules are found to correspond to the positions of "holes" in the Valence Shell Charge

Concentration (VSCC) of boron atoms, i.e., the positions of critical points with the most positive values of $\nabla^2\rho$; this correspondence is not always perfect, as steric considerations also play a role. Essentially, holes give attacking nucleophiles access to the core of the atom. For sites of electrophilic attack in the boranes, one needs to locate those critical points with the most negative values of $\nabla^2\rho$, and which are not lying strictly along bond paths in ρ. Tabulation of the critical point data for the Laplacian of ρ is found in Table XXI.

To begin this discussion, a simple example from organic chemistry will be useful. In CH_4 (see Fig. 20), there are four bonded maxima or (3,–3) critical points in the VSCC of the carbon atom which lie along the four bond paths. There are lines of maximum charge concentration, or LOMCC, which link each of these bonded maxima to the other three, and these lines originate from (3,–1) saddle points, of which there are six in the case of a tetrahedrally coordinated carbon. So the (3,–1) critical point can be approximately located in space in the centroid of the plane triangle formed by the central carbon and any two bonded atoms. The network of lines which link the bonded maxima in methane are collectively known as an *atomic graph*, and it partitions the VSCC into four areas, which gives the atomic graph the appearance of a tetrahedron with curved faces. There is a face or (3,+1) critical point in the centre of each face, topologically identical to the ring critical point found in $\rho(\mathbf{r})$. Therefore, for this molecule, the atomic graph looks like a tetrahedron in space, centered on the carbon atom, with four (3,–3) critical points, one at each of the four

corners of the tetrahedron, and six (3,–1) critical points, one along each edge, and finally with four (3,+1) critical points in the VSCC located in the centre of each face of the tetrahedron.

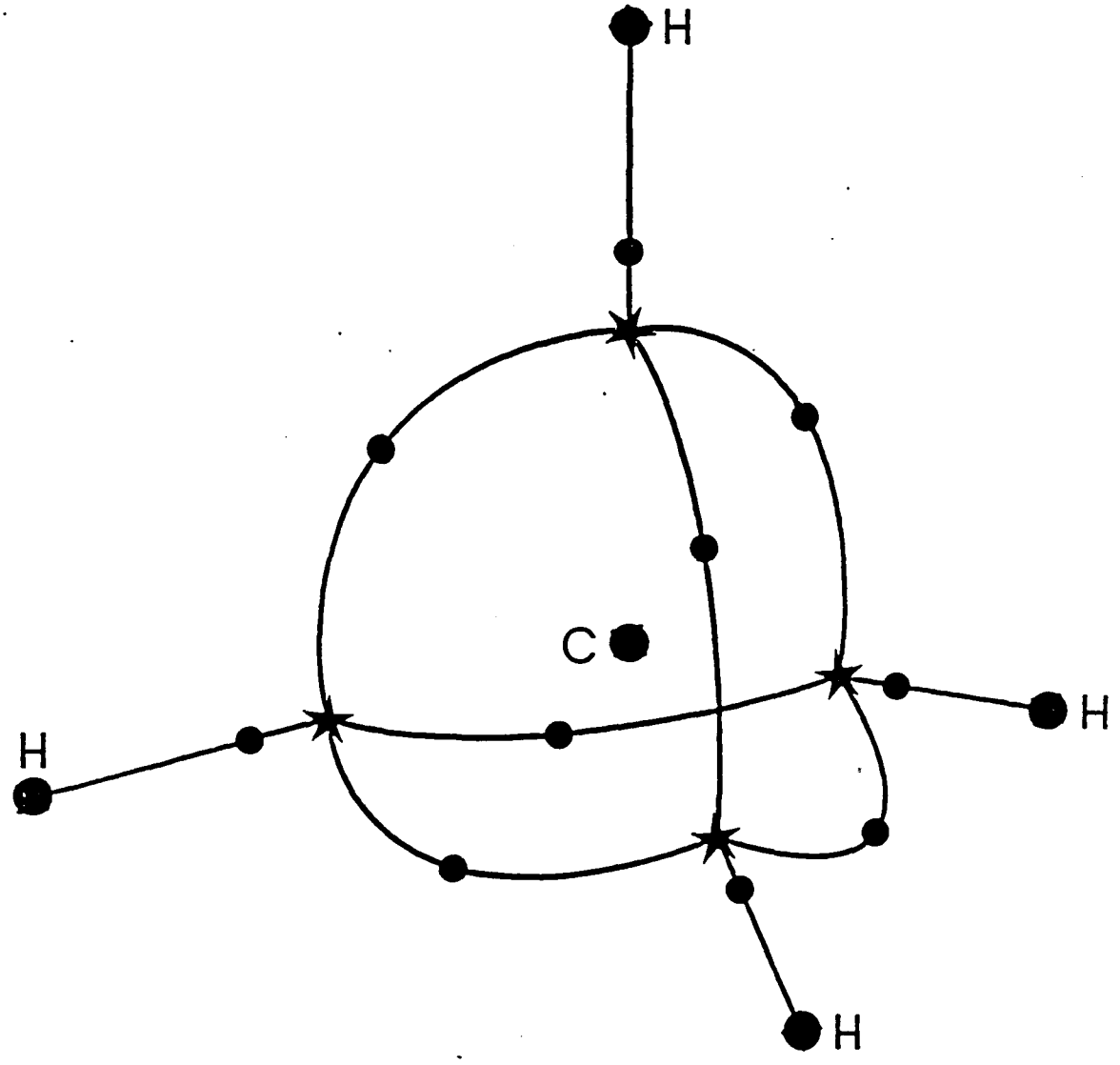

Fig. 20 Atomic Graph of CH_4. Bonded maxima appear as "★" (in this figure only)

Sites of electrophilic attack are generally found at (3,–3) or (3,–1) critical points. The (3,–3) critical points appear as either bonded or non-bonded maxima. A bonded maximum is a local concentration of electronic charge along a bond path, while a non-bonded maximum does not lie along such paths. Non-bonded maxima correspond to the lone pairs of the VSEPR model, but these are absent in the electron-deficient boranes and therefore are not found. This leaves the (3,–1) points as sites of electrophilic attack.

With the atomic graph of methane in mind, it is possible to envision the topology of $\nabla^2\rho$ for a boron atom in a borane molecule, especially the four-coordinate borons such as are found in B_2H_6 or B_4H_{10}. But there is one important difference between the atomic graphs of hydrocarbons and those of boranes; in the boranes, the hydrogen atoms have effectively stripped away the VSCC of boron, and so *there are no bonded maxima between boron and hydrogen in the boranes.* So in these molecules, the LOMCC link (3,–1) critical points to the protons, which serve as the (3,–3) critical points.

In the case of bonding between symmetrically equivalent borons, there is a (3,–1) critical point in the centre of the bond path, linking two (3,–3) bonded maxima which lie along the region of the bond path in ρ, and which are equidistant from the central saddle point.

The following is a description of the topology of $\nabla^2\rho$ for each of the boranes studied here, along with contour maps of the Laplacian which contain symbols to denote the four types of critical point: "❐" for (3,+3), "●" for (3,–1), "▲" for (3,+1), and "■" for (3,–3) critical points. Sites of electrophilic attack are marked by an arrow and the letter "**E**", and sites of nucleophilic attack are similarly marked by the letter "**N**".

i) BH_3. In BH_3, there are only three (3,–1) critical points which link the hydrogens.

ii) B_2H_6. In B_2H_6, each boron atom is tetrahedrally coordinated, so the placement of the critical points is similar to that already discussed for CH_4, but with a distortion caused by the lower symmetry of the boron environment. Here, again, the hydrogen nuclei, both terminal and bridging, serve as the (3,–3) critical points.

Electrophilic attack occurs at either of the two (3,–1) critical points in $\nabla^2\rho$, which lie inside and in the plane of the ring, at a distance of 1.34 a.u. from each boron (see Fig. 19b). At these points, $\nabla^2\rho = -0.06$. Nucleophilic attack can occur at any of the four (3,+1) points above and below the plane of the ring, 1.45 a.u. from the closest boron, and with a $\nabla^2\rho$ value of +0.09.

iii) B_4H_{10}. In B_4H_{10}, both of the boron atoms are again arranged as in methane, with six (3,–1) points about each boron. There is also a pair of bonded maxima along the B-B bond path, both lying at a distance of 0.36

a.u. from the central (3,–1) critical point. This is the smallest of the molecules to contain bonded maxima.

Figure 21 shows that electrophilic attack occurs at any of the four (3,–1) critical points which link the bonded maxima to bridging hydrogens ($\nabla^2\rho = -0.06$, $R_{B1} = 1.30$ a.u.) Note that these two borons, involved in B-B bonding, are furthest removed from the open face of the molecule. Nucleophilic attack occurs at either of the other borons, labelled B5 and B6, at any of the four (3,+1) points which are 1.80 a.u. from one of these borons, and which have a $\nabla^2\rho$ value of +0.07. There is a (3,+1) critical point in the VSCC of B1 or B2 inside the "butterfly", and although it has a larger positive value of $\nabla^2\rho$, the presence of the H_{endo}, H11 and H12, makes it sterically infeasible for nucleophilic attack to occur at B1. This finding is confirmed by Muetterties (1967), who explains that cleavage of B_4H_{10} by a nucleophile such as $:NH_3$ takes place at the boron other than the one involved in B-B bonding.

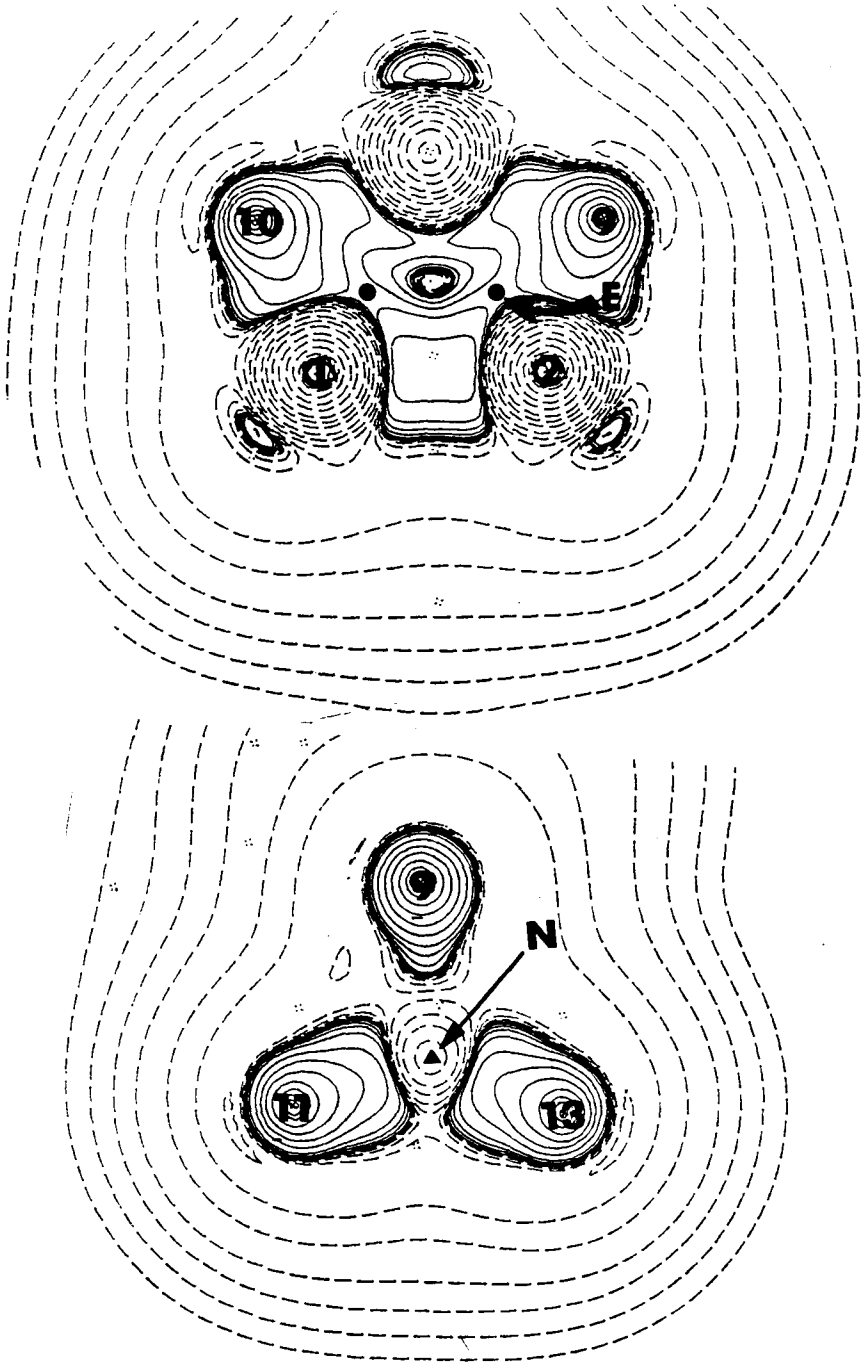

Fig. 21 Contour maps of $\nabla^2\rho(\mathbf{r})$ for B_4H_{10}, containing: a) Plane of two B-B bonded borons and two bridging hydrogens, and b) Plane of one bridging and two neighbouring terminal hydrogens.

iv) B_5H_9. In the vicinity of the basal borons in B_5H_9, there are tetrahedral arrangements of critical points in $\nabla^2\rho$ as in B_2H_6, but there is a single (3,–3) critical point or bonded maximum along each B-B bond, about 1.2 a.u. away from a basal boron, and about 2.0 a.u. from the apical boron. Rather than link to a second bonded maximum along each bond path, the (3,–3) critical points link to the proton of the apical hydrogen, through four (3,–1) critical points which lie in a plane perpendicular to the apical B-H_t bond path, just above the apical boron.

Adjacent bonded maxima are linked by (3,–1) critical points exterior to the faces of the pyramid (see Fig. 22). These saddle points are 1.28 a.u. from the apical boron, and are the sites of electrophilic attack, with a $\nabla^2\rho$ value of –0.14. The (3,+1) holes are in the face created by links between a bonded maximum, a basal terminal hydrogen, and a bridging hydrogen. ($\nabla^2\rho$ = +0.076, R_{B1} = 1.61 a.u.) This confirms the statement by Greenwood & Earnshaw (1984), that electrophilic attack occurs at borons furthest removed from an open face, and nucleophilic attack occurs at borons involved in bridging.

v) B_6H_{10} (Fig. 23). For B_6H_{10}, the site of electrophilic attack is found above the plane of the ring formed by borons 1,2, and 4, at a distance of 1.27 a.u. from the apical B2 ($\nabla^2\rho$ = –.13). Nucleophilic attack occurs, as in B_5H_9, at the basal B4 boron atom, in the face critical point formed by the links between B2, the terminal hydrogen on B4, and the bridging hydrogen between B4 and B9 ($\nabla^2\rho$ = +0.073, R_{B4} = 1.54a.u.).

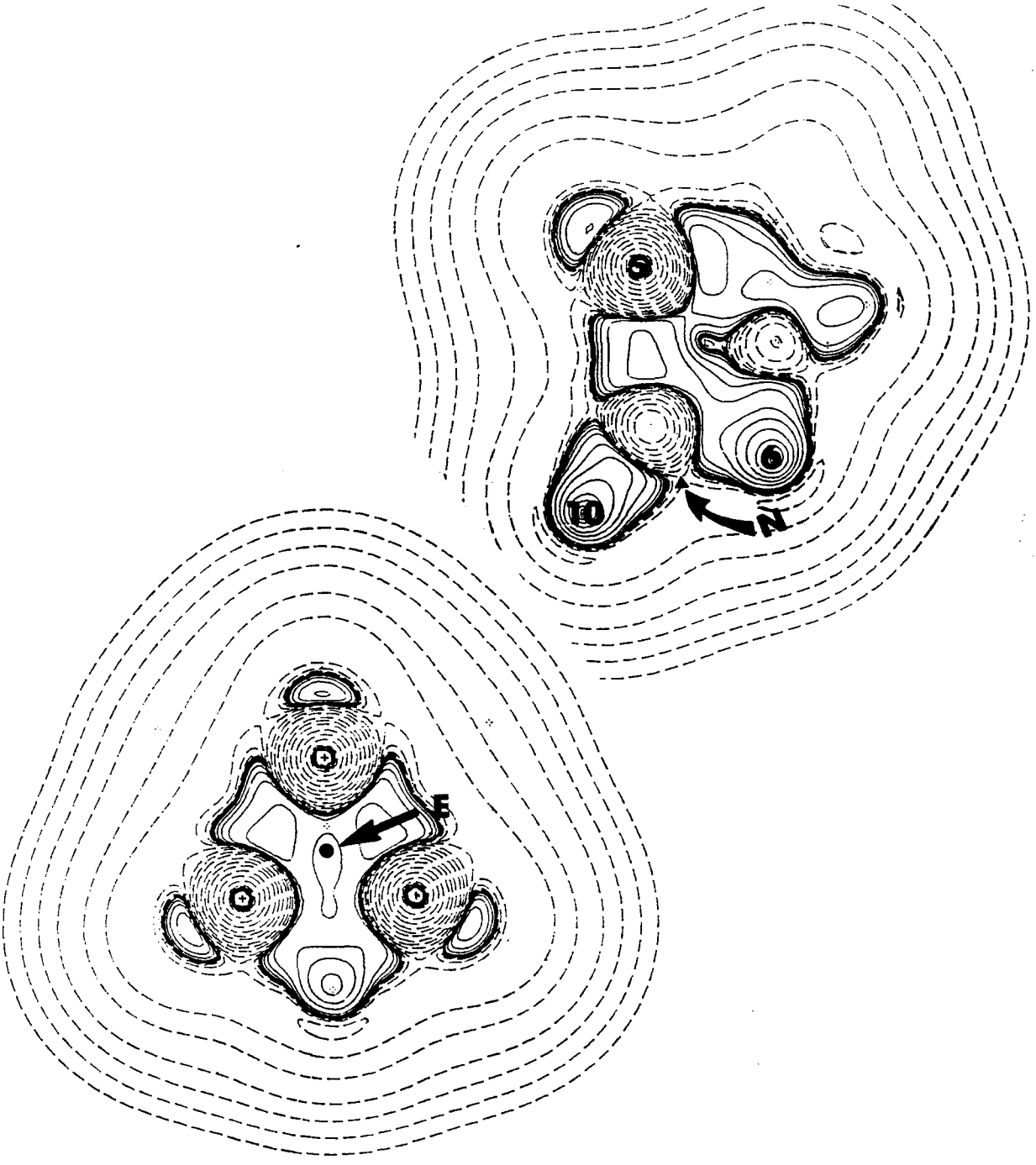

Fig. 22 Contour maps of $\nabla^2\rho(\mathbf{r})$ for B_5H_9, containing:
a) Plane of two basal borons and the apical boron, and
b) Plane of the apical boron, one bridging and one neighbouring terminal hydrogens.

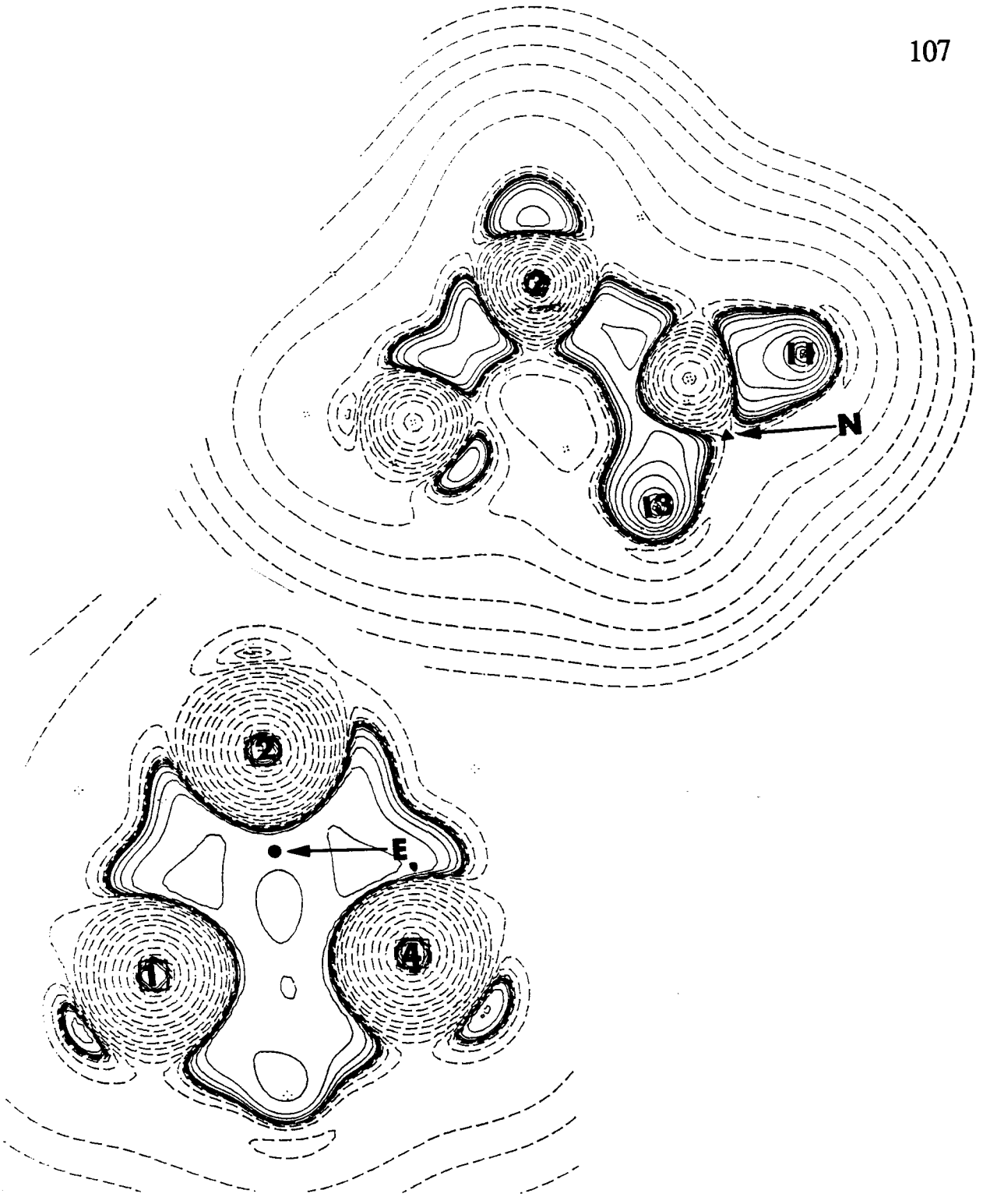

Fig. 23 Contour maps of $\nabla^2\rho(\mathbf{r})$ for B_6H_{10}, containing:
a) Plane of two basal borons and the apical boron, and
b) Plane of the apical boron, one bridging and one neighbouring terminal hydrogens.

vi & vii) $B_6H_6^{2-}$ and $B_{12}H_{12}^{2-}$. In $B_6H_6^{2-}$ and $B_{12}H_{12}^{2-}$, there are pairs of bonded maxima linked by (3,–1) critical points along each of the B-B bonds in the cage. The relief map of $\nabla^2\rho$ in Fig. 24b shows these bonded maxima as a ridge between the boron atoms. There are also three more (3,–1) critical points in the surface of the 3-membered B-B-B rings, and these link bonded maxima located on neighbouring bond paths. Again, the bonded maxima link to the terminal hydrogen nearest it, forming an alternating ring of (3,–1) and (3,+1) critical points.

In both of these anionic cages, electrophilic attack occurs at the (3,–1) critical points lying between the bond paths that make up the faces. For $B_6H_6^{2-}$, $\nabla^2\rho = -0.14$, and the points are 1.25 a.u. from the nearest boron atom (see Fig. 24a). In $B_{12}H_{12}^{2-}$, $\nabla^2\rho = -0.15$, and $R_B = 1.26$ a.u.

Nucleophilic Attack occurs at the ring of (3,+1) critical points which lie in a plane perpendicular to each B-H_t bond path (see Fig 24a). These points lie between B-B bonds and B-H_t bonds. For $B_6H_6^{2-}$, there are four such points in this ring, and in $B_{12}H_{12}^{2-}$, there are five. In $B_6H_6^{2-}$, $\nabla^2\rho = +0.037$, and $R_B = 1.42$ a.u.; in $B_{12}H_{12}^{2-}$, $\nabla^2\rho = +0.046$, $R_B = 1.40$ a.u.

viii) $B_7H_7^{2-}$. $B_7H_7^{2-}$ is similar to the other two *closo*-boranes, except that there are two bonded maxima along equatorial-apical bonds, but only one along equatorial-equatorial bonds. They also link to the terminal hydrogens as described earlier.

Electrophilic attack takes place at the same type of (3,–1) critical point as in the other two anions, but preferentially at the one closest to

axial boron. Here, $\nabla^2\rho = -.129$, and the distance to boron is 1.25 a.u. The other two (3,–1) critical points in the triangular face have $\nabla^2\rho = -.11$.

Nucleophilic attack in $B_7H_7^{2-}$ occurs at the equatorial boron, in the position shown in Fig. 25 ($\nabla^2\rho = +.052$, $R_B = 1.71$ a.u.).

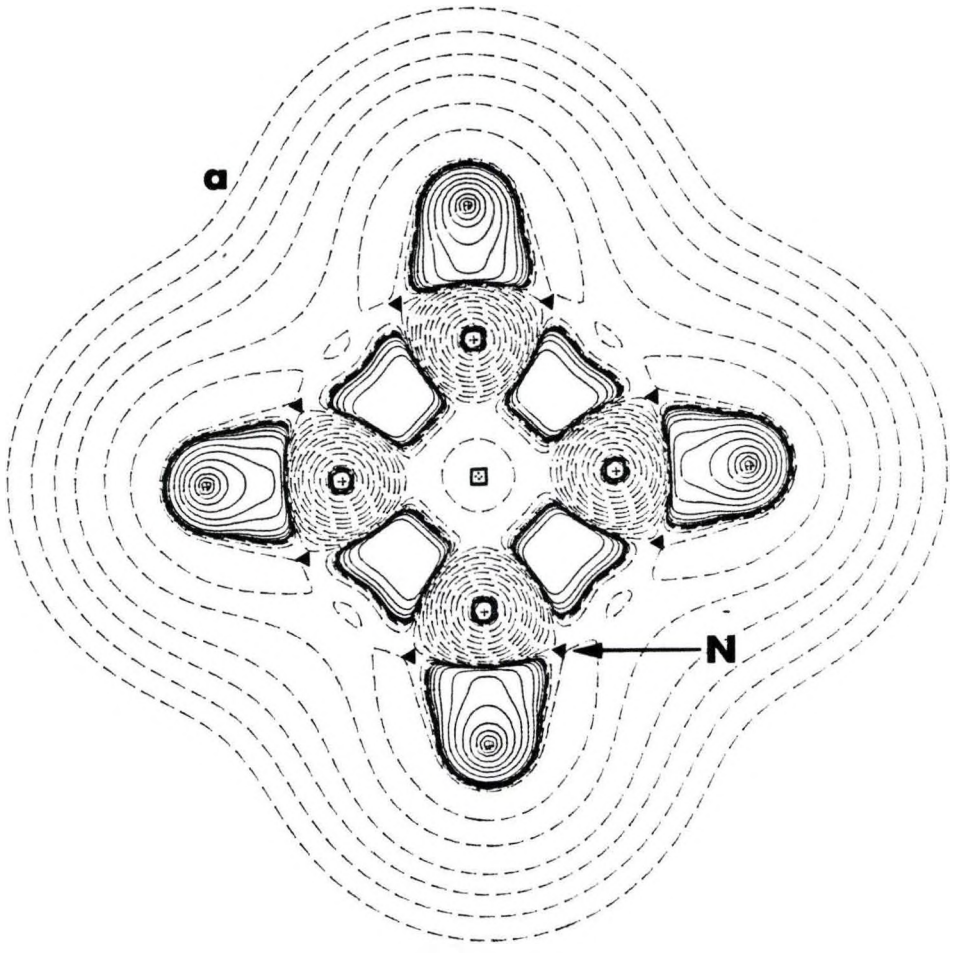

Fig. 24 a) Contour map of $\nabla^2\rho(\mathbf{r})$ for $B_6H_6^{2-}$, containing the plane of four boron atoms.

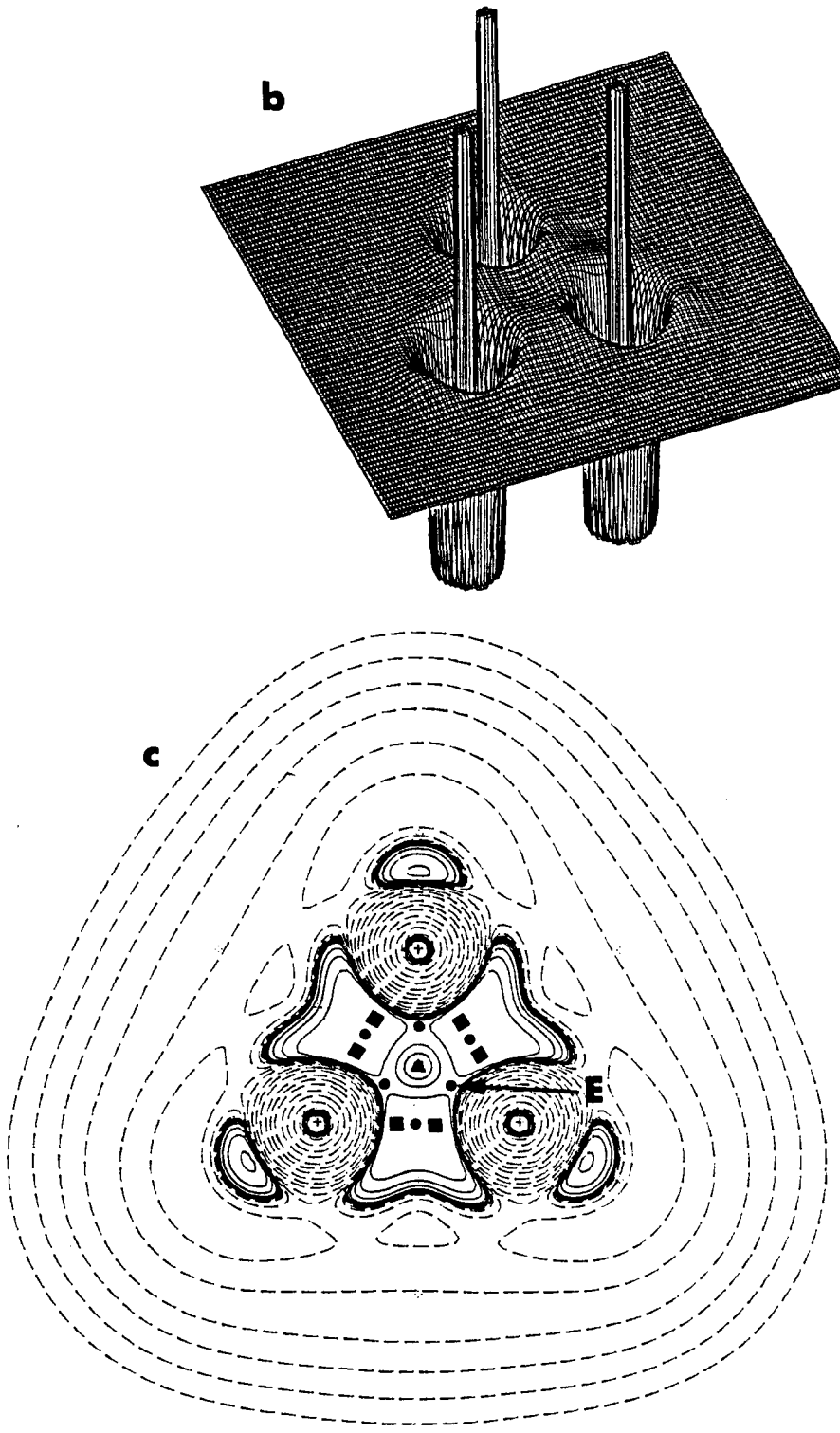

Fig. 24 b) Relief map of $\nabla^2\rho(\mathbf{r})$ for $B_6H_6^{2-}$, containing a B-B-B face.
c) Contour map of $\nabla^2\rho(\mathbf{r})$ for $B_6H_6^{2-}$, for same plane.

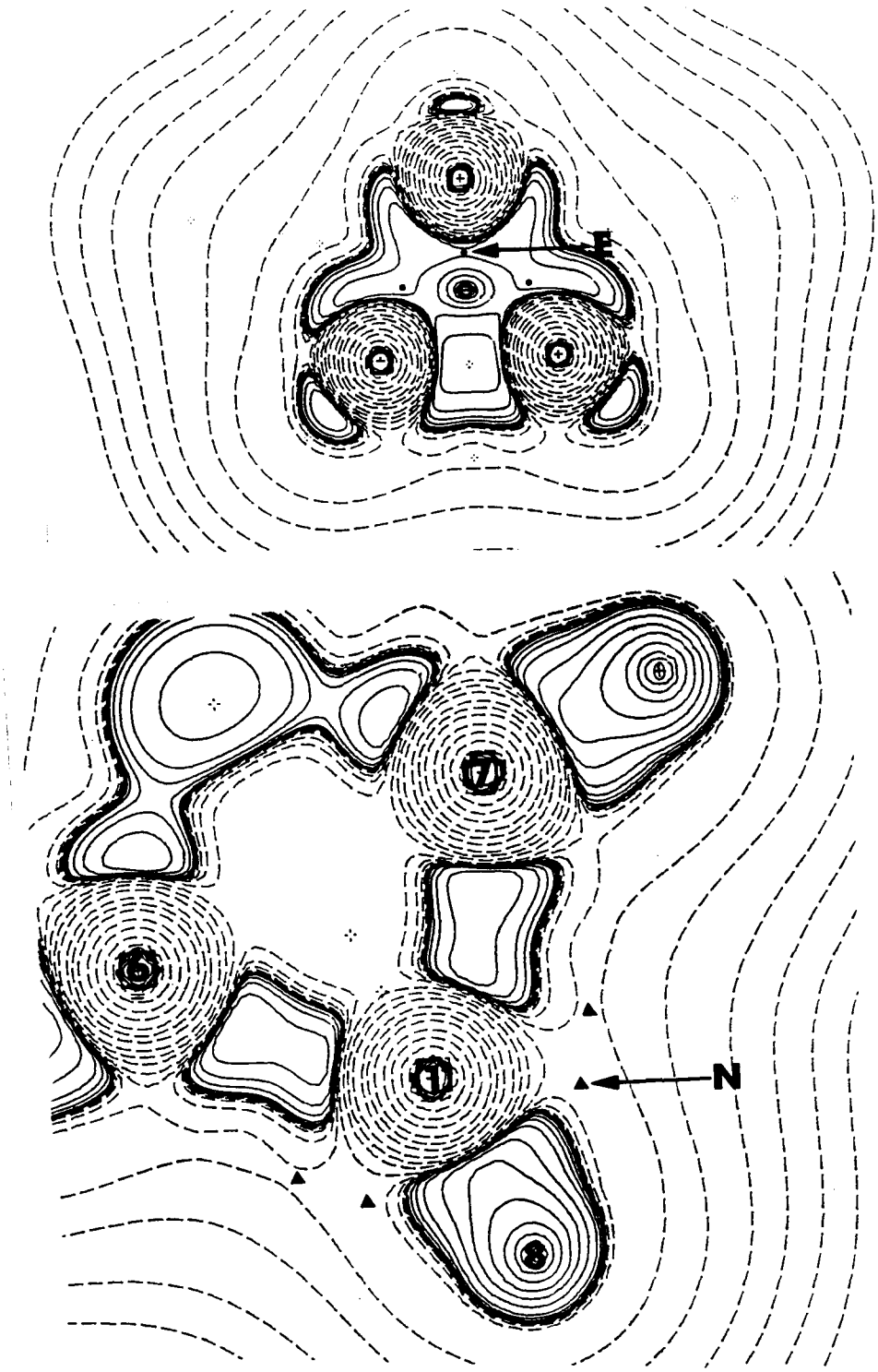

Fig. 25 a) Contour map of $\nabla^2\rho(\mathbf{r})$ for $B_7H_7^{2-}$, plane of a B-B-B face.
b) Contour map of $\nabla^2\rho(\mathbf{r})$ for $B_7H_7^{2-}$, plane containing one equatorial and the two axial borons.

ix & x) $C_2B_3H_5$ and $C_2B_4H_6$. Both of these molecules possess single bonded maxima along the B-C bonds, 1.0 a.u. from the axial carbon in each case. These link directly to the equatorial hydrogens, as there are no second bonded maxima present along the B-C bond paths.

As in the *closo*-anions, electrophilic attack occurs at the (3,–1) critical point between the B-C bonds. For $C_2B_3H_5$, $\nabla^2\rho = -0.42$, and the distance from the carbon atom is 0.994 a.u., a reasonable value for the extent of the VSCC of carbon. For $C_2B_4H_6$, $\nabla^2\rho = -0.37$, $R_c = .986$ a.u.

Nucleophilic attack occurs in $C_2B_3H_5$ in the triangular faces, at a distance from carbon of 2.03 a.u., and from boron of 1.92; therefore, the attack is at the equatorial boron ($\nabla^2\rho = +0.052$). But in $C_2B_4H_6$, the analagous face critical point has a $\nabla^2\rho$ value of –0.01, so it is not the site of nucleophilic attack. This is no doubt because of the presence of B-B bonds around the equator of the molecule. Instead, the (3,+1) critical points at which nucleophilic attack is most likely to occur are between the B-C bonds and the B-H bonds (see Fig. 26), with a value of $\nabla^2\rho$ equal to +.06, at a distance of 1.78 a.u. from the equatorial boron. This is in agreement with a statement by Onak (1988) that conversion of *closo*-$C_2B_4H_6$ to the *nido* form by addition of $(CH_3)_3N$: occurs by nucleophilic attack at boron.

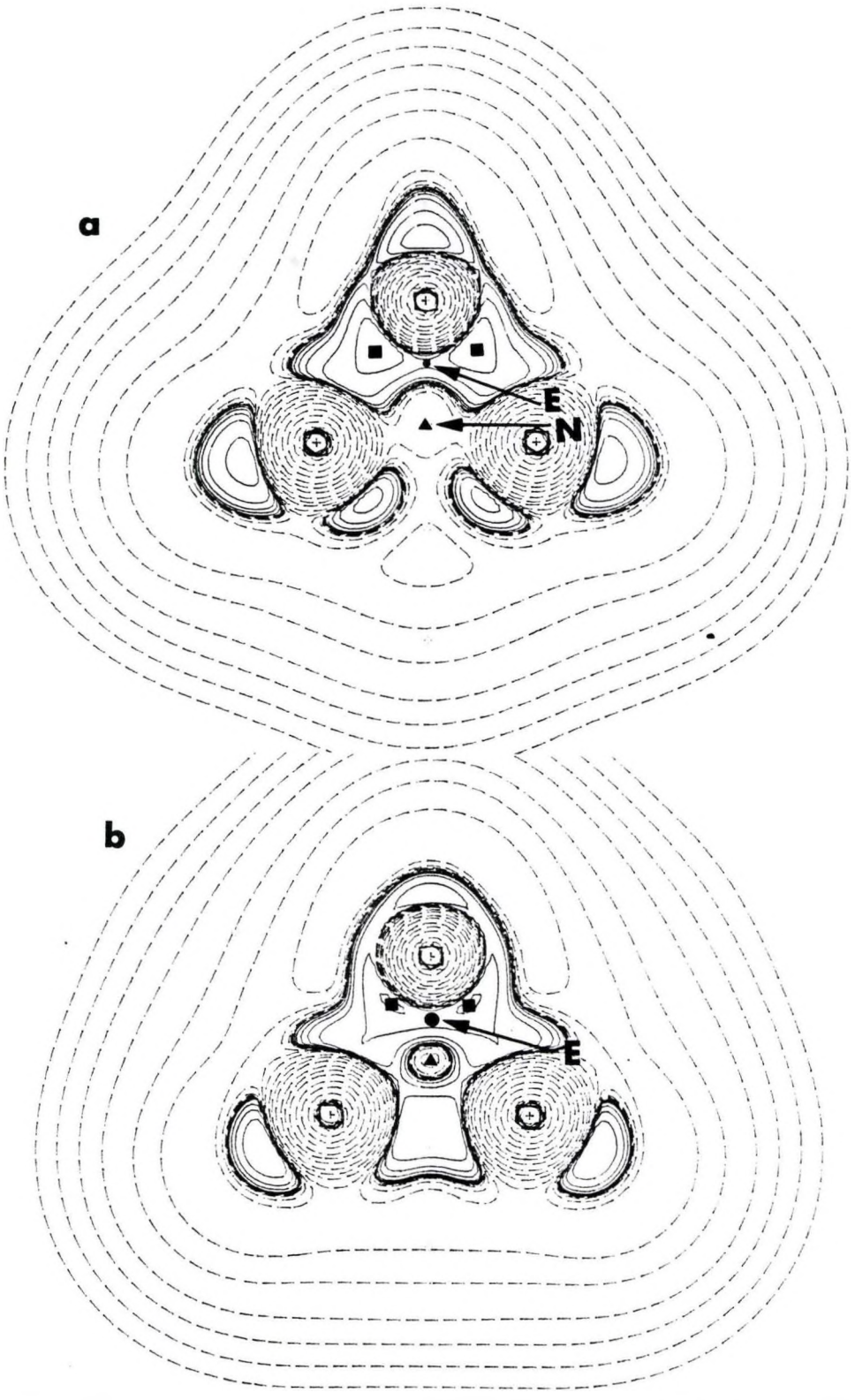

Fig. 26 a) Contour map of $\nabla^2\rho(\mathbf{r})$ for $C_2B_3H_5$, plane of a B-C-B face.
b) Contour map of $\nabla^2\rho(\mathbf{r})$ for $C_2B_4H_6$, plane of a B-C-B face.

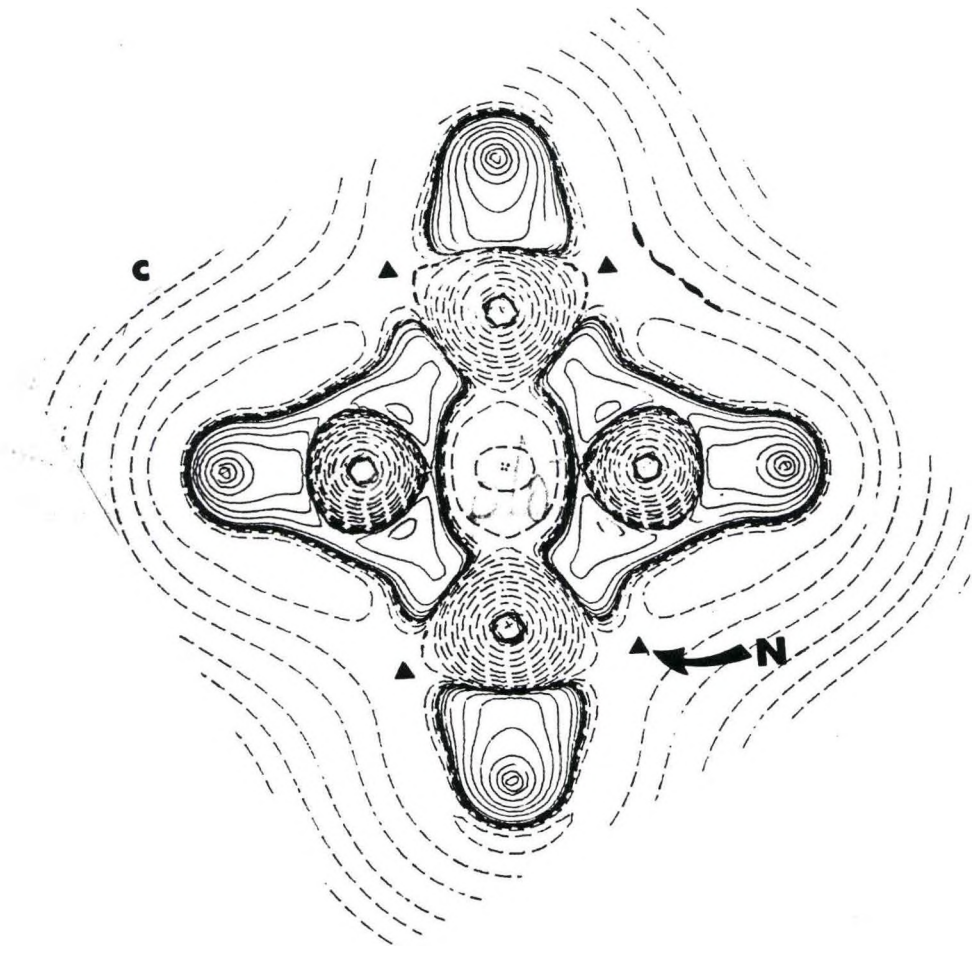

Fig. 26 c) Contour map of $\nabla^2\rho(\mathbf{r})$ for $C_2B_4H_6$, plane containing one equatorial boron and the two axial carbons.

Since the boranes are electron-deficient, nucleophilic attack should be more prevalent in these molecules than electrophilic attack. The highest value of positive $\nabla^2\rho$ for a site of nucleophilic attack in the borane series studied here is +0.09, for B_2H_6. Ranking these molecules by their $\nabla^2\rho$ value, one finds:

Susceptibility to Electrophilic Attack:

$C_2B_3H_5 > C_2B_4H_6 > B_{12}H_{12}^{2-} > B_6H_6^{2-} > B_5H_9 > B_6H_{10} > B_7H_7^{2-} > B_4H_{10} > B_2H_6$.

Susceptibility to Nucleophilic Attack:

$B_2H_6 > B_5H_9 > B_4H_{10} > B_6H_{10} > C_2B_4H_6 > B_7H_7^{2-} > C_2B_3H_5 > B_{12}H_{12}^{2-} > B_6H_6^{2-}$.

In conclusion, the information presented here on the reactivity of the boranes and carboranes leads to the following points of interest:

1. $B_7H_7^{2-}$ is more susceptible to nucleophilic attack than either of the two other *closo*-boranes, probably because of the asymmetrical axial-equatorial B-B bonds.

2. Among the *nido*-boranes, larger species are less reactive, with respect to nucleophilic attack, a confirmation of the statement by Greenwood and Earnshaw.

3. Electrophilic attack does occur preferentially at apical boron atoms, those furthest removed from the open face, and nucleophilic attack does occur most likely at basal boron atoms, which are involved in bridging, again in agreement with Greenwood & Earnshaw.

4. In compounds of carbon and boron, electrophilic attack occurs at carbon, while nucleophilic attack occurs at boron.

5. The *closo*-compounds, whether they be boranes or carboranes, are as a group less susceptible to nucleophilic attack than any of the open clusters. Therefore the cage species are the most stable.

6. B_5H_9 was found to be more susceptible to nucleophilic attack than either B_4H_{10} or B_6H_{10}, in contradiction to the statements of Greenwood and Earnshaw, but only by a difference in $\nabla^2\rho$ of 0.02-0.03.

The results contained herein have shown that the Theory of Atoms in Molecules does indeed correctly predict the connectivity, atomic properties, and relative reactivities of the boranes and carboranes. It remains to be seen how an application of this theory to heteroboranes and other normal boranes will aid in the development of our understanding of this fascinating class of inorganic compounds.

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Appendix A. PROAIM. OMEGA Output

BH-B1

```
 PROAIM STELLIX VERSION 0.95

BH OPTIMIZATION
 -V/T FOR THIS WAVEFUNCTION =        2.00070036000
 MOLECULAR SCF ENERGY (AU)  =      -25.12415719630

B1 of BH 9s/5p + 1d on B, 6s/4,1,1 + 1p on H
 INTEGRATION IS OVER ATOM   B    1
   120 PHI PLANES     96 THETA PLANES
  80 PATHS WITH  141 POINTS PER PATH
 RADIUS OF BETA SPHERE   0.9626 WITH    120 POINTS PER PATH
 VOL1 RHO CONTOUR THRESHOLD=   0.0010
 VOL2 RHO CONTOUR THRESHOLD=   0.0020

 INSERTION LIMIT USED          =    6
 INSERTION LIMIT REACHED      0 TIMES FOR SURFACE   1
 FOR SURFACE # 1 NUMBER OF INSERTED PATHS =     80
 TOTAL NUMBER OF INSERTED PATHS=    80

 RESULTS OF THE INTEGRATION
              N   4.21063532288807E+00     NET CHARGE   7.89364677111933E-01
              G   2.41977442926019E+01
              K   2.41955345365419E+01        E(ATOM)  -2.42124801211100E+01
              L  -2.20975605997717E-03
              I   2.15887839820299E+00
         R(-1)    1.09722827560107E+01
             R1   4.98807275921952E+00
             R2   1.08607455145977E+01
             R4   1.03709628246311E+02
        GR(-1)  -2.14771838637499E+01
            GR0  -1.20717859266444E+01
            GR1  -1.92502803298574E+01
            GR2  -5.33711021309990E+01
           VNEO  -5.48614137800537E+01      VNEO(COR)  -5.48806184248487E+01
           VNET  -5.63792289160715E+01      VNET(COR)  -5.63989648833123E+01
           VEET   7.94275385488764E+00      VEET(COR)   7.94553427478510E+00
            EHF  -2.42409405246419E+01
                                            VREP(COR)   7.97399467831708E+00
                                              V(ATOM)  -4.84249702049953E+01
         EL DX    4.66156944814873E-04
         EL DY   -1.72052569796800E-12
         EL DZ   -2.01404648386085E+00
  EL DIPOLE MAG   2.01404653780755E+00
           QXX    9.59439371310041E-01      QXX(DIAG)   9.60751721594765E-01
           QXY   -1.43141267233719E-11
           QXZ   -1.55926562581205E-03
           QYY    9.60751721594765E-01      QYY(DIAG)   9.59440215622743E-01
           QYZ    5.02665477618232E-12
```

```
           QZZ  -1.92019109290481E+00      QZZ(DIAG)  -1.92019193721751E+00
          FAXA  -3.76483538693656E-05
          FAYA   2.62309278302193E-13
          FAZA   1.07647265489600E+00
          FBXA  -7.29154881869253E-06
          FBYA   3.87733576564211E-14
          FBZA   5.61970322398683E-01
         RHO*L   4.04321478788050E+02
          VOL1   1.63226343922733E+02
          VOL2   1.20310879254625E+02
       N(VOL1)   4.12457949330514E+00
       N(VOL2)   4.06275891796840E+00

  THE ATOMIC OVERLAP MATRIX AOM :

 0.999011
-0.012282  0.278503
 0.003484  0.300182  0.827803

           NA   2.10531766144403E+00
           NB   2.10531766144403E+00
           N    4.21063532288807E+00
         FOOA  -1.94138979663631E+00
         FOOB  -1.94138979663631E+00
         ALOC   9.22136280044652E-01
         BLOC   9.22136280044652E-01
          FLA   1.63927864807727E-01
          FLB   1.63927864807727E-01
           FL   2.26924552625176E+00

 ERROR ESTIMATE FOR DIFFERENTIAL EQUATIONS
 FOR SURFACE # 1   EPSD   5.44984484988687E-08

 MAXIMUM DISTANCE REACHED FROM NUCLEUS =  9.9981146210E+00
```

BH-H2

```
 PROAIM STELLIX VERSION 0.95

BH OPTIMIZATION
 -V/T FOR THIS WAVEFUNCTION =        2.00070036000
 MOLECULAR SCF ENERGY (AU)  =      -25.12415719630

H2 of BH 9s/5p + 1d on B, 6s/4,1,1 + 1p on H
 INTEGRATION IS OVER ATOM   H    2
   120 PHI PLANES     96 THETA PLANES
  80 PATHS WITH  141 POINTS PER PATH
 RADIUS OF BETA SPHERE   1.3696 WITH    120 POINTS PER PATH
 VOL1 RHO CONTOUR THRESHOLD=   0.0010
```

```
VOL2 RHO CONTOUR THRESHOLD=    0.0020

INSERTION LIMIT USED           =     6
INSERTION LIMIT REACHED       0 TIMES FOR SURFACE    1
FOR SURFACE # 1 NUMBER OF INSERTED PATHS =      80
TOTAL NUMBER OF INSERTED PATHS=     80

RESULTS OF THE INTEGRATION
             N   1.79173615135739E+00     NET CHARGE  -7.91736151357386E-01
             G   9.10486029561403E-01
             K   9.10521508831770E-01        E(ATOM)  -9.11159201675696E-01
             L   3.54792703665287E-05
             I   1.48553776024578E+00
         R(-1)   1.74843201622875E+00
            R1   2.55022416992433E+00
            R2   4.54269136246203E+00
            R4   2.43830717096907E+01
        GR(-1)  -2.96393745274208E+00
           GR0  -4.30718241127402E+00
           GR1  -7.90919819322078E+00
           GR2  -1.74213996348689E+01
          VNEO  -1.74843201622875E+00      VNEO(COR)  -1.74904406782397E+00
          VNET  -5.89928692049337E+00      VNET(COR)  -5.90135200963427E+00
          VEET   1.95849414933614E+00      VEET(COR)   1.95917973473906E+00
           EHF  -3.03027126232546E+00
                                           VREP(COR)   4.07829179538882E+00
                                             V(ATOM)  -1.82306021424545E+00
         EL DX  -5.24253619047974E-07
         EL DY  -3.10731573422550E-14
         EL DZ  -5.51712669407832E-01
 EL DIPOLE MAG   5.51712669408081E-01
           QXX  -1.18397398109016E-01      QXX(DIAG)  -1.18399093403364E-01
           QXY   4.33338107371216E-13
           QXZ  -2.10857194010971E-06
           QYY  -1.18399093403364E-01      QYY(DIAG)  -1.18397398121533E-01
           QYZ  -1.25235377251072E-13
           QZZ   2.36796491512380E-01      QZZ(DIAG)   2.36796491524897E-01
          FAXA  -4.46096820296222E-08
          FAYA  -2.61341480903033E-15
          FAZA   3.53692904107110E-01
          FBXA  -1.12465044819739E-06
          FBYA  -6.66270439071904E-14
          FBZA  -1.77787147334031E+00
         RHO*L   1.02529856875571E-01
          VOL1   9.58028916597456E+01
          VOL2   7.34841174900852E+01
       N(VOL1)   1.74403707538013E+00
       N(VOL2)   1.71151634265801E+00
```

```
  THE ATOMIC OVERLAP MATRIX AOM :

 0.000989
 0.012284  0.722488
-0.003484 -0.299742  0.172392

            NA   8.95868075678693E-01
            NB   8.95868075678693E-01
            N    1.79173615135739E+00
          FOOA  -7.31725082612497E-01
          FOOB  -7.31725082612497E-01
          ALOC   8.16777718145783E-01
          BLOC   8.16777718145783E-01
           FLA   1.64142993066196E-01
           FLB   1.64142993066196E-01
            FL   1.06001106874489E+00

 ERROR ESTIMATE FOR DIFFERENTIAL EQUATIONS
 FOR SURFACE # 1   EPSD   3.56376503474895E-08

 MAXIMUM DISTANCE REACHED FROM NUCLEUS =  9.9965164172E+00
```

BH3-B1

```
 PROAIM VERSION 0.90

BH3 OPTIMIZATION USING VD SET(Renormalized) d=0.75, p=1.0725
 -V/T FOR THIS WAVEFUNCTION =        2.00175720000
 MOLECULAR SCF ENERGY (AU)  =      -26.39526969889

BH3 Integration of B
 INTEGRATION IS OVER ATOM   B    1
   120 PHI PLANES     96 THETA PLANES
  80 PATHS WITH  141 POINTS PER PATH
 RADIUS OF BETA SPHERE   0.9511 WITH    120 POINTS PER PATH
 VOL1 RHO CONTOUR THRESHOLD=   0.0010
 VOL2 RHO CONTOUR THRESHOLD=   0.0020

 INSERTION LIMIT USED          =    6
 INSERTION LIMIT REACHED      0 TIMES FOR SURFACE   1
 INSERTION LIMIT REACHED      0 TIMES FOR SURFACE   2
 INSERTION LIMIT REACHED      0 TIMES FOR SURFACE   3
 FOR SURFACE # 1 NUMBER OF INSERTED PATHS =    192
 FOR SURFACE # 2 NUMBER OF INSERTED PATHS =    192
 FOR SURFACE # 3 NUMBER OF INSERTED PATHS =    192
 TOTAL NUMBER OF INSERTED PATHS=   576

 RESULTS OF THE INTEGRATION
             N   2.83847466387523E+00     NET CHARGE   2.16152533612477E+00
             G   2.37111792776597E+01
             K   2.37126965456553E+01        E(ATOM)  -2.37543644960253E+01
```

L	1.51726799564267E-03		
I	6.74281029606683E-01		
R(-1)	1.03263310004731E+01		
R1	1.65101437836471E+00		
R2	1.76270671980631E+00		
R4	6.01038923875535E+00		
GR(-1)	-1.92104077697166E+01		
GR0	-6.70627622854193E+00		
GR1	-4.15626056248759E+00		
GR2	-5.13501158107185E+00		
VNEO	-5.16316550023656E+01	VNEO(COR)	-5.16769787530033E+01
VNET	-5.53584136503959E+01	VNET(COR)	-5.54070088568807E+01
VEET	7.97166413220649E+00	VEET(COR)	7.97866188808473E+00
EHF	-2.36740529725341E+01		
		VREP(COR)	7.89835036459347E+00
		V(ATOM)	-4.75086584922872E+01
EL DX	-4.01237772373887E-03		
EL DY	1.92822519791914E-03		
EL DZ	-1.84245975083525E-07		
EL DIPOLE MAG	4.45165446163478E-03		
QXX	3.43238042733823E-02	QXX(DIAG)	-7.67455889272106E-02
QXY	-5.96295272123438E-03		
QXZ	-5.87667162417044E-05		
QYY	4.24216825649860E-02	QYY(DIAG)	3.11650596069139E-02
QYZ	9.50114203318068E-05		
QZZ	-7.67454868383685E-02	QZZ(DIAG)	4.55805293202966E-02
FAXA	1.27237611632512E-03		
FAYA	-1.25036497140148E-03		
FAZA	-6.53406269839464E-07		
FBXA	3.35995477024341E-04		
FBYA	-3.09720785071665E-04		
FBZA	-5.89246164309999E-08		
RHO*L	3.95812632272822E+02		
VOL1	2.23884749336799E+01		
VOL2	2.01352395596544E+01		
N(VOL1)	2.83517691112919E+00		
N(VOL2)	2.83192479464181E+00		

THE ATOMIC OVERLAP MATRIX AOM :

```
 0.997366
-0.021860  0.187223
-0.000001 -0.000408  0.117551
 0.000001  0.000551  0.000286  0.117098
```

NA	1.41923733193762E+00
NB	1.41923733193762E+00
N	2.83847466387523E+00
FOOA	-1.05827756626344E+00
FOOB	-1.05827756626344E+00
ALOC	7.45666381829614E-01
BLOC	7.45666381829614E-01

```
           FLA   3.60959765674180E-01
           FLB   3.60959765674180E-01
            FL   1.78019709761180E+00

 ERROR ESTIMATE FOR DIFFERENTIAL EQUATIONS
 FOR SURFACE # 1   EPSD   4.10504636500200E-08
 FOR SURFACE # 2   EPSD   4.10504636500200E-08
 FOR SURFACE # 3   EPSD   4.10504636500200E-08

 MAXIMUM DISTANCE REACHED FROM NUCLEUS =  9.9955962036E+00
```

BH3-H2

```
 PROAIM VERSION 0.90

BH3 OPTIMIZATION USING VD SET(Renormalized) d=0.75, p=1.0725
 -V/T FOR THIS WAVEFUNCTION =        2.00175720000
 MOLECULAR SCF ENERGY (AU)  =      -26.39526969889

BH3 Integration of H
 INTEGRATION IS OVER ATOM   H    2
   120 PHI PLANES     96 THETA PLANES
  80 PATHS WITH  141 POINTS PER PATH
 RADIUS OF BETA SPHERE   1.2997 WITH    120 POINTS PER PATH
 VOL1 RHO CONTOUR THRESHOLD=   0.0010
 VOL2 RHO CONTOUR THRESHOLD=   0.0020

 INSERTION LIMIT USED          =    6
 INSERTION LIMIT REACHED      0 TIMES FOR SURFACE   1
 FOR SURFACE # 1 NUMBER OF INSERTED PATHS =    192
 TOTAL NUMBER OF INSERTED PATHS=   192

 RESULTS OF THE INTEGRATION
             N   1.71986338166556E+00     NET CHARGE  -7.19863381665558E-01
             G   8.78825867788447E-01
             K   8.78835511779175E-01        E(ATOM)  -8.80379801540474E-01
             L   9.64399072746475E-06
             I   1.11773442223603E+00
        R(-1)   1.71812834090062E+00
           R1   2.37821403055307E+00
           R2   4.10980517645047E+00
           R4   2.07639088978504E+01
       GR(-1)  -2.76490102947142E+00
          GR0  -3.90595332707110E+00
          GR1  -7.02815752816314E+00
          GR2  -1.52773846836535E+01
         VNEO  -1.71812834090062E+00      VNEO(COR)  -1.71963656333671E+00
         VNET  -6.66643943077094E+00      VNET(COR)  -6.67229142289453E+00
         VEET   2.40371781700107E+00      VEET(COR)   2.40582786958289E+00
          EHF  -3.38388610199070E+00
                                          VREP(COR)   4.90933417003311E+00
```

```
                                                    V(ATOM)   -1.76295725286142E+00
          EL DX  -6.38826634248590E-07
          EL DY   4.34018015391986E-01
          EL DZ   1.47204488725674E-06
   EL DIPOLE MAG   4.34018015394952E-01
             QXX  -4.57796539007002E-02      QXX(DIAG)   -5.58152398487724E-01
             QXY   1.95997439593407E-06
             QXZ   5.21766584896370E-05
             QYY   6.03932047027020E-01      QYY(DIAG)   -4.57796485932820E-02
             QYZ  -7.47443082100611E-06
             QZZ  -5.58152393126320E-01      QZZ(DIAG)    6.03932047081005E-01
            FAXA   2.38017711511789E-07
            FAYA  -3.49821198141421E-01
            FAZA  -4.61858687866289E-08
            FBXA   2.69537365416017E-06
            FBYA   1.96963688448871E+00
            FBZA  -3.43469261906124E-07
           RHO*L   9.91969677280422E-02
            VOL1   8.81804432036079E+01
            VOL2   6.78030104323580E+01
        N(VOL1)    1.67882094480529E+00
        N(VOL2)    1.64941845012111E+00

  THE ATOMIC OVERLAP MATRIX AOM :

  0.000878
  0.007286  0.270783
  0.009200  0.374844  0.548273
  0.000000  0.000000  0.000000  0.039998

             NA    8.59931690832779E-01
             NB    8.59931690832779E-01
             N     1.71986338166556E+00
           FOOA   -6.56818451814762E-01
           FOOB   -6.56818451814762E-01
           ALOC    7.63803054145711E-01
           BLOC    7.63803054145711E-01
            FLA    2.03113239018017E-01
            FLB    2.03113239018017E-01
             FL    1.06304492985080E+00

 ERROR ESTIMATE FOR DIFFERENTIAL EQUATIONS
 FOR SURFACE # 1   EPSD   3.45896923016946E-08

 MAXIMUM DISTANCE REACHED FROM NUCLEUS =  9.9957658742E+00
```

B2H6-B1

```
 PROAIM STELLIX VERSION 0.95

B2H6 USING D95 AND VAN DUIJNEVELDT BASES (Renormalized)
```

```
 -V/T FOR THIS WAVEFUNCTION =        2.00207143000
 MOLECULAR SCF ENERGY (AU)  =      -52.82244183403

B2H6 Integration of B1
 INTEGRATION IS OVER ATOM   B    1
   120 PHI PLANES     96 THETA PLANES
  80 PATHS WITH  141 POINTS PER PATH
 RADIUS OF BETA SPHERE   0.9539 WITH    120 POINTS PER PATH
 VOL1 RHO CONTOUR THRESHOLD=   0.0010
 VOL2 RHO CONTOUR THRESHOLD=   0.0020

 INSERTION LIMIT USED          =    6
 INSERTION LIMIT REACHED      0 TIMES FOR SURFACE   1
 INSERTION LIMIT REACHED      0 TIMES FOR SURFACE   2
 INSERTION LIMIT REACHED      1 TIMES FOR SURFACE   3
 INSERTION LIMIT REACHED      1 TIMES FOR SURFACE   4
 FOR SURFACE # 1 NUMBER OF INSERTED PATHS =     53
 FOR SURFACE # 2 NUMBER OF INSERTED PATHS =     53
 FOR SURFACE # 3 NUMBER OF INSERTED PATHS =     89
 FOR SURFACE # 4 NUMBER OF INSERTED PATHS =     89
 TOTAL NUMBER OF INSERTED PATHS=   284

 RESULTS OF THE INTEGRATION
              N   2.87639115822766E+00     NET CHARGE   2.12360884177234E+00
              G   2.36813312642053E+01
              K   2.36809650477718E+01        E(ATOM)  -2.37300185092007E+01
              L  -3.66216433510751E-04
              I   4.68296569167601E-01
         R(-1)   1.03507964448527E+01
             R1   1.69001161272838E+00
             R2   1.78543743530470E+00
             R4   5.52107513108538E+00
        GR(-1)  -1.91352832221070E+01
           GR0  -6.61851874658061E+00
           GR1  -3.96319451052202E+00
           GR2  -4.58725898509630E+00
          VNEO  -5.17539822242634E+01      VNEO(COR)  -5.18075291406183E+01
          VNET  -6.19121858819014E+01      VNET(COR)  -6.19762429166703E+01
          VEET   1.12316455464790E+01      VEET(COR)   1.12432662944632E+01
           EHF  -2.69995752876505E+01
                                           VREP(COR)   1.45128230729131E+01
                                             V(ATOM)  -4.74634198437572E+01
         EL DX   5.28777924497619E-02
         EL DY   5.11944070911604E-09
         EL DZ  -1.38375206340026E-03
  EL DIPOLE MAG   5.28958949648561E-02
           QXX   1.55352787161654E-01      QXX(DIAG)   1.26522741587297E-01
           QXY   2.98150620949584E-09
           QXZ   1.48215091328895E-03
           QYY   1.26522739922993E-01      QYY(DIAG)   1.55357811415897E-01
           QYZ   2.60736202779051E-05
           QZZ  -2.81875527084647E-01      QZZ(DIAG)  -2.81880553003195E-01
```

```
          FAXA   7.17386452088246E-02
          FAYA  -1.33890660035511E-07
          FAZA   4.55393769433029E-04
          FBXA  -1.50871219749283E+00
          FBYA  -8.09627670305894E-09
          FBZA   2.30483535479529E-04
         RHO*L   3.93805134409472E+02
          VOL1   1.88284871187015E+01
          VOL2   1.75972135628431E+01
       N(VOL1)   2.87477952517395E+00
       N(VOL2)   2.87298422998257E+00

   THE ATOMIC OVERLAP MATRIX AOM :

  0.498615
  0.498638  0.498662
 -0.011825 -0.011951  0.095202
 -0.009767 -0.009820  0.068090  0.087848
  0.000000  0.000000  0.000074  0.000079  0.063369
  0.000000  0.000000  0.000000  0.000000  0.000000  0.067461
  0.002468  0.002421 -0.000188 -0.052631 -0.000034  0.000000  0.071135
  0.000000  0.000000  0.000000  0.000000  0.000001  0.060128  0.000000
0.055906

           NA   1.43819557911383E+00
           NB   1.43819557911383E+00
           N    2.87639115822766E+00
         FOOA  -1.05110920590296E+00
         FOOB  -1.05110920590296E+00
         ALOC   7.30852758253239E-01
         BLOC   7.30852758253239E-01
          FLA   3.87086373210874E-01
          FLB   3.87086373210874E-01
           FL   1.82528195232470E+00

 ERROR ESTIMATE FOR DIFFERENTIAL EQUATIONS
 FOR SURFACE # 1   EPSD   1.20581628063488E-07
 FOR SURFACE # 2   EPSD   1.20581628066682E-07
 FOR SURFACE # 3   EPSD   3.04044187630510E-04
 FOR SURFACE # 4   EPSD   7.23323114118775E-04

 MAXIMUM DISTANCE REACHED FROM NUCLEUS =  9.9972156042E+00
```

B2H6-H2

```
 PROAIM STELLIX VERSION 0.95

B2H6 USING D95 AND VAN DUIJNEVELDT BASES (Renormalized)
 -V/T FOR THIS WAVEFUNCTION =        2.00207143000
 MOLECULAR SCF ENERGY (AU)  =      -52.82244183403
```

```
B2H6 Integration of Bridging H
 INTEGRATION IS OVER ATOM   H    2
   120 PHI PLANES     96 THETA PLANES
  80 PATHS WITH  141 POINTS PER PATH
 RADIUS OF BETA SPHERE   1.5792 WITH    120 POINTS PER PATH
 VOL1 RHO CONTOUR THRESHOLD=   0.0010
 VOL2 RHO CONTOUR THRESHOLD=   0.0020

 INSERTION LIMIT USED          =    6
 INSERTION LIMIT REACHED      1 TIMES FOR SURFACE   1
 INSERTION LIMIT REACHED      1 TIMES FOR SURFACE   2
 FOR SURFACE # 1 NUMBER OF INSERTED PATHS =     89
 FOR SURFACE # 2 NUMBER OF INSERTED PATHS =     89
 TOTAL NUMBER OF INSERTED PATHS=   178

 RESULTS OF THE INTEGRATION
              N   1.71330020378423E+00     NET CHARGE  -7.13300203784231E-01
              G   9.27507775433108E-01
              K   9.28543316287295E-01        E(ATOM)  -9.30466728768952E-01
              L   1.03554085418655E-03
              I   6.00242104975462E-01
         R(-1)   1.74013671210300E+00
            R1   2.22882905248296E+00
            R2   3.44049068716434E+00
            R4   1.20075925650597E+01
        GR(-1)  -2.24025216130865E+00
           GR0  -2.77722518826241E+00
           GR1  -4.30510035317847E+00
           GR2  -7.93754047726038E+00
          VNEO  -1.74013671210300E+00      VNEO(COR)  -1.74193713307477E+00
          VNET  -1.13228292394554E+01      VNET(COR)  -1.13345443300461E+01
          VEET   4.62634819860384E+00      VEET(COR)   4.63113481925355E+00
           EHF  -5.76793772456427E+00
                                           VREP(COR)   9.46860581504886E+00
                                             V(ATOM)  -1.86593851499723E+00
         EL DX  -2.60914601738159E-05
         EL DY  -1.16804100796610E-03
         EL DZ   4.68855427436464E-01
  EL DIPOLE MAG   4.68856883107404E-01
           QXX   4.40064505122622E-01      QXX(DIAG)   4.40064516471911E-01
           QXY  -2.73546421351362E-05
           QXZ   8.79448728962813E-05
           QYY  -1.11703854176376E-01      QYY(DIAG)  -1.11512518208618E-01
           QYZ   6.44135762147223E-03
           QZZ  -3.28360650946246E-01      QZZ(DIAG)  -3.28551998263293E-01
          FAXA   3.35597464649190E-06
          FAYA   1.13500606315245E-04
          FAZA  -3.40254750287146E-01
          FBXA   3.92498027317463E-06
          FBYA   1.73179076107756E-03
          FBZA   2.32348802113613E+00
         RHO*L   8.62093447805431E-02
```

```
          VOL1    5.91785853051270E+01
          VOL2    4.96595864321962E+01
       N(VOL1)    1.69756248385816E+00
       N(VOL2)    1.68379211007336E+00

   THE ATOMIC OVERLAP MATRIX AOM :

  0.000568
  0.000000  0.000523
  0.007069  0.000000  0.287536
  0.000000  0.001555 -0.000002  0.019753
  0.005685  0.000000  0.306703 -0.000002  0.391118
  0.000004  0.000000  0.000174  0.000000  0.000002  0.042957
  0.004127  0.000000  0.163354  0.000000  0.166190  0.000102  0.103099
  0.000000  0.000001 -0.000001  0.000004 -0.000001 -0.000003  0.000000
0.011096

            NA    8.56650101892115E-01
            NB    8.56650101892115E-01
            N     1.71330020378423E+00
          FOOA   -5.45583669733466E-01
          FOOB   -5.45583669733466E-01
          ALOC    6.36880411883936E-01
          BLOC    6.36880411883936E-01
           FLA    3.11066432158649E-01
           FLB    3.11066432158649E-01
            FL    1.16771653405076E+00

 ERROR ESTIMATE FOR DIFFERENTIAL EQUATIONS
 FOR SURFACE # 1    EPSD    2.05272494593827E-04
 FOR SURFACE # 2    EPSD    2.05272494593827E-04

 MAXIMUM DISTANCE REACHED FROM NUCLEUS =  9.9959018620E+00
```

B2H6-H3

```
 PROAIM STELLIX VERSION 0.95

B2H6 USING D95 AND VAN DUIJNEVELDT BASES (Renormalized)
 -V/T FOR THIS WAVEFUNCTION =        2.00207143000
 MOLECULAR SCF ENERGY (AU)  =      -52.82244183403

B2H6 Integration of Terminal H
 INTEGRATION IS OVER ATOM   H    3
   120 PHI PLANES      96 THETA PLANES
  80 PATHS WITH  141 POINTS PER PATH
 RADIUS OF BETA SPHERE   1.2875 WITH    120 POINTS PER PATH
 VOL1 RHO CONTOUR THRESHOLD=   0.0010
 VOL2 RHO CONTOUR THRESHOLD=   0.0020

 INSERTION LIMIT USED          =    6
```

```
INSERTION LIMIT REACHED      0 TIMES FOR SURFACE   1
FOR SURFACE # 1 NUMBER OF INSERTED PATHS =     53
TOTAL NUMBER OF INSERTED PATHS=    53

RESULTS OF THE INTEGRATION
             N   1.70423871590660E+00     NET CHARGE  -7.04238715906604E-01
             G   8.73224055120012E-01
             K   8.73292504442757E-01        E(ATOM)  -8.75101468735235E-01
             L   6.84493227445586E-05
             I   6.22408680590528E-01
        R(-1)    1.71423403800436E+00
           R1    2.32361568384050E+00
           R2    3.92575995854152E+00
           R4    1.85539460218572E+01
       GR(-1)   -2.65386705424597E+00
          GR0   -3.64482232136458E+00
          GR1   -6.35216999882664E+00
          GR2   -1.33562299880105E+01
         VNEO   -1.71423403800436E+00      VNEO(COR)  -1.71600765894522E+00
         VNET   -9.45434010491038E+00      VNET(COR)  -9.46412197554199E+00
         VEET    3.80313307712618E+00      VEET(COR)   3.80706796368013E+00
          EHF   -4.77791452334144E+00
                                           VREP(COR)   7.70988101828633E+00
                                             V(ATOM)  -1.75424095725566E+00
        EL DX   -1.77817385895831E-01
        EL DY    3.64009249168047E-01
        EL DZ   -4.48755960335572E-06
 EL DIPOLE MAG   4.05119434521291E-01
          QXX    1.21579570667562E-01      QXX(DIAG)   6.19789184955219E-01
          QXY   -3.68016708265273E-01
          QXZ   -3.86505518037816E-05
          QYY    3.47943171116139E-01      QYY(DIAG)  -1.50266438533052E-01
          QYZ   -1.11800270441938E-05
          QZZ   -4.69522741783702E-01      QZZ(DIAG)  -4.69522746422168E-01
         FAXA    1.71987471620733E-01
         FAYA   -3.05191127525399E-01
         FAZA    4.60508412338142E-08
         FBXA   -1.47123448802947E+00
         FBYA    1.94572645385979E+00
         FBZA   -5.76525967121113E-07
       RHO*L     9.79870198647061E-02
         VOL1    8.27759441879269E+01
         VOL2    6.44674718725112E+01
      N(VOL1)    1.66882671105959E+00
      N(VOL2)    1.64236861699685E+00
```

```
   THE ATOMIC OVERLAP MATRIX AOM :

  0.000408
  0.000407  0.000407
  0.002365  0.002362  0.058339
  0.004129  0.004132  0.099462  0.196213
  0.000000  0.000000  0.000000  0.000000  0.022859
  0.003782  0.003780  0.101884  0.183135  0.000001  0.194723
 -0.003307 -0.003315 -0.081814 -0.174825  0.000000 -0.156548  0.162641
  0.003948  0.003947  0.104789  0.196497  0.000000  0.203550 -0.170868
0.216530

             NA   8.52119357953302E-01
             NB   8.52119357953302E-01
             N    1.70423871590660E+00
           FOOA  -6.25526534149967E-01
           FOOB  -6.25526534149967E-01
           ALOC   7.34083234128625E-01
           BLOC   7.34083234128625E-01
            FLA   2.26592823803335E-01
            FLB   2.26592823803335E-01
             FL   1.07871218175664E+00

 ERROR ESTIMATE FOR DIFFERENTIAL EQUATIONS
 FOR SURFACE # 1   EPSD   9.66293167339648E-08

 MAXIMUM DISTANCE REACHED FROM NUCLEUS =  9.9957599157E+00
```

B4H10-B1

```
 PROAIM STELLIX VERSION 0.95

B4H10 OPTIMIZATION USING VD SET(Renormalized) d=0.75, p=1.0725
 -V/T FOR THIS WAVEFUNCTION =        2.00132087000
 MOLECULAR SCF ENERGY (AU)  =     -104.47774919276

B1 of B4H10 9s/5p + 1d on B, F
 INTEGRATION IS OVER ATOM   B    1
   120 PHI PLANES     96 THETA PLANES
  80 PATHS WITH  141 POINTS PER PATH
 RADIUS OF BETA SPHERE   0.9542 WITH    120 POINTS PER PATH
 VOL1 RHO CONTOUR THRESHOLD=   0.0010
 VOL2 RHO CONTOUR THRESHOLD=   0.0020

 INSERTION LIMIT USED          =    6
 INSERTION LIMIT REACHED      0 TIMES FOR SURFACE   1
 INSERTION LIMIT REACHED      0 TIMES FOR SURFACE   2
 INSERTION LIMIT REACHED      1 TIMES FOR SURFACE   3
 INSERTION LIMIT REACHED      0 TIMES FOR SURFACE   4
 FOR SURFACE # 1 NUMBER OF INSERTED PATHS =     12
 FOR SURFACE # 2 NUMBER OF INSERTED PATHS =     48
```

```
FOR SURFACE # 3 NUMBER OF INSERTED PATHS =     70
FOR SURFACE # 4 NUMBER OF INSERTED PATHS =     72
TOTAL NUMBER OF INSERTED PATHS=   202

RESULTS OF THE INTEGRATION
             N   3.60954230827205E+00     NET CHARGE   1.39045769172795E+00
             G   2.41714206132176E+01
             K   2.39768136246011E+01        E(ATOM)  -2.40084838784134E+01
             L  -1.94606988616520E-01
             I   4.54605475037047E-01
         R(-1)   1.07797462537176E+01
            R1   3.05727095823553E+00
            R2   4.76332467161421E+00
            R4   3.23683764801718E+01
        GR(-1)  -1.94721075343547E+01
           GR0  -7.44132382024344E+00
           GR1  -6.13328682767615E+00
           GR2  -1.17524158698944E+01
          VNEO  -5.38987312685880E+01      VNEO(COR)  -5.39343043834433E+01
          VNET  -7.97944275635592E+01      VNET(COR)  -7.98470918150122E+01
          VEET   1.97717381054962E+01      VEET(COR)   1.97847874351179E+01
           EHF  -3.60458758334619E+01
                                           VREP(COR)   3.18221793901664E+01
                                             V(ATOM)  -4.80249124248459E+01
         EL DX  -7.89535815936418E-01
         EL DY  -1.21531767199872E-01
         EL DZ  -3.62434916248905E-02
 EL DIPOLE MAG   7.99656404820390E-01
           QXX  -1.07568124184693E+00      QXX(DIAG)   2.09110781424446E-01
           QXY  -7.22955397811525E-01
           QXZ  -4.11430641010697E-01
           QYY   2.88204043081034E-01      QYY(DIAG)   1.39874499294432E+00
           QYZ  -8.18921138787287E-01
           QZZ   7.87477198765900E-01      QZZ(DIAG)  -1.60785577436877E+00
          FAXA   8.08016429205461E-01
          FAYA  -3.94139858965521E-02
          FAZA   5.58124115162565E-02
          FBXA  -3.06077050780627E+00
          FBYA   3.71001131811028E-02
          FBZA  -1.54825911000478E+00
         RHO*L   3.92349029696389E+02
          VOL1   3.11310678096135E+01
          VOL2   2.95461130686487E+01
       N(VOL1)   3.60780562973275E+00
       N(VOL2)   3.60549356850861E+00
```

```
   THE ATOMIC OVERLAP MATRIX AOM :

  0.003898
  0.003895  0.003944
 -0.000038  0.004782  0.498086
  0.000000  0.004818  0.498106  0.498136
  0.000356  0.000619 -0.006741 -0.007505  0.142001
  0.000764  0.000602 -0.000012 -0.000010  0.001737  0.037854
  0.000442  0.000463 -0.008303 -0.008419  0.070546 -0.001029  0.073853
 -0.000775 -0.000705 -0.004196 -0.004679  0.076076 -0.001652  0.043125
0.079255
  0.000799  0.000718 -0.000014 -0.000003 -0.001217  0.030735  0.001504
0.000785
  0.040153
 -0.000112 -0.000239 -0.000233 -0.000055 -0.031220 -0.000055 -0.007300
0.017153
  0.000266  0.045046
  0.000944  0.001058 -0.000006  0.000005  0.000596 -0.028348 -0.000261 -
0.001734
 -0.027175  0.000531  0.027791
  0.000731  0.000519 -0.002490 -0.002027 -0.049814  0.000687  0.006511 -
0.004271
 -0.000122  0.039923  0.001249  0.067462
  0.000352  0.000402  0.002920  0.002956 -0.010100 -0.000780 -0.017922 -
0.044664
  0.001044 -0.039527 -0.000180 -0.038929  0.062138
 -0.000241 -0.000107  0.000007  0.000009 -0.000694 -0.031117  0.000440 -
0.000384
 -0.029390  0.000800  0.025411  0.000484  0.000349  0.029437
  0.000322  0.000587  0.003207  0.002229  0.096139  0.000301 -0.011726
0.074510
  0.000094 -0.009579  0.000505 -0.073477 -0.010968  0.000164  0.195714

            NA   1.80477115413602E+00
            NB   1.80477115413602E+00
            N    3.60954230827205E+00
          FOOA  -1.17680966333664E+00
          FOOB  -1.17680966333664E+00
          ALOC   6.52054783034249E-01
          BLOC   6.52054783034249E-01
           FLA   6.27961490799388E-01
           FLB   6.27961490799388E-01
            FL   2.43273264493541E+00

 ERROR ESTIMATE FOR DIFFERENTIAL EQUATIONS
 FOR SURFACE # 1   EPSD   5.54597771882043E-07
 FOR SURFACE # 2   EPSD   5.54597771882043E-07
 FOR SURFACE # 3   EPSD   6.25185936992371E-07
 FOR SURFACE # 4   EPSD   6.25185989423958E-07

 MAXIMUM DISTANCE REACHED FROM NUCLEUS =  9.9980124934E+00
```

B4H10-H3

```
 PROAIM STELLIX VERSION 0.95

B4H10 OPTIMIZATION USING VD SET(Renormalized) d=0.75, p=1.0725
 -V/T FOR THIS WAVEFUNCTION =        2.00132087000
 MOLECULAR SCF ENERGY (AU)  =     -104.47774919276

H3 of B4H10 9s/5p + 1d on B, F
 INTEGRATION IS OVER ATOM   H    3
   120 PHI PLANES     96 THETA PLANES
  80 PATHS WITH  141 POINTS PER PATH
 RADIUS OF BETA SPHERE   1.2750 WITH    120 POINTS PER PATH
 VOL1 RHO CONTOUR THRESHOLD=   0.0010
 VOL2 RHO CONTOUR THRESHOLD=   0.0020

 INSERTION LIMIT USED          =    6
 INSERTION LIMIT REACHED      0 TIMES FOR SURFACE   1
 FOR SURFACE # 1 NUMBER OF INSERTED PATHS =     48
 TOTAL NUMBER OF INSERTED PATHS=    48

 RESULTS OF THE INTEGRATION
              N   1.66261263423254E+00     NET CHARGE  -6.62612634232541E-01
              G   8.52362581907736E-01
              K   8.52505134958878E-01        E(ATOM)  -8.53631183416491E-01
              L   1.42553051142896E-04
              I   3.57618159840303E-01
         R(-1)   1.68629936445736E+00
             R1   2.23910994248174E+00
             R2   3.72768554588357E+00
             R4   1.71426704695144E+01
        GR(-1)  -2.54029862483125E+00
            GR0  -3.42835687226674E+00
            GR1  -5.86534071274163E+00
            GR2  -1.21122416843638E+01
           VNEO  -1.68629936445736E+00      VNEO(COR)  -1.68741232054297E+00
           VNET  -1.34804963282913E+01      VNET(COR)  -1.34893934439173E+01
           VEET   5.84568594874522E+00      VEET(COR)   5.84954409628911E+00
            EHF  -6.78230524458722E+00
                                            VREP(COR)   1.17782181574598E+01
                                              V(ATOM)  -1.71117528645750E+00
         EL DX  -1.34999939778346E-01
         EL DY   1.38034939080335E-05
         EL DZ  -3.30370972577564E-01
  EL DIPOLE MAG   3.56889287388315E-01
            QXX  -1.49973315716207E-01      QXX(DIAG)  -3.18983953592454E-01
            QXY   4.23939662978942E-05
            QXZ   3.49213921781385E-01
            QYY  -3.18983861765472E-01      QYY(DIAG)  -3.07111773809944E-01
            QYZ   1.41778530083090E-05
            QZZ   4.68957177481679E-01      QZZ(DIAG)   6.26095727402397E-01
```

```
          FAXA   1.45951853781552E-01
          FAYA  -1.25442617278376E-06
          FAZA   3.10411399775002E-01
          FBXA  -1.62744410183759E+00
          FBYA  -9.97977599026031E-06
          FBZA  -2.52083038707518E+00
         RHO*L   9.42616992186894E-02
          VOL1   7.89652270350672E+01
          VOL2   6.18580883649522E+01
       N(VOL1)   1.62975021703342E+00
       N(VOL2)   1.60505976074877E+00

  THE ATOMIC OVERLAP MATRIX AOM :

  0.000000
  0.000000  0.000000
  0.000000  0.000004  0.000376
  0.000000  0.000004  0.000376  0.000375
  0.000000  0.000012  0.001469  0.001457  0.023524
  0.000000  0.000000  0.000000  0.000000  0.000000  0.004771
  0.000000  0.000019  0.002336  0.002327  0.037055  0.000000  0.064572
  0.000000  0.000027  0.003303  0.003277  0.054972  0.000000  0.088166
0.136116
  0.000001  0.000000  0.000000  0.000000  0.000000  0.006844  0.000000
0.000000
  0.010306
  0.000000  0.000016  0.002205  0.002188  0.038650  0.000000  0.062721
0.096841
  0.000000  0.069901
  0.000000  0.000000  0.000000  0.000000  0.000000 -0.004741  0.000000
0.000000
 -0.006766  0.000000  0.004804
  0.000000  0.000026  0.003154  0.003138  0.054219  0.000000  0.093722
0.137233
  0.000000  0.098772  0.000000  0.146182
  0.000000 -0.000039 -0.004913 -0.004883 -0.083308  0.000000 -0.140661 -
0.210868
  0.000000 -0.151756  0.000000 -0.220432  0.337483
 -0.000001  0.000000  0.000000  0.000000  0.000000 -0.003814  0.000000
0.000000
 -0.005694  0.000000  0.003660  0.000000  0.000000  0.003576
  0.000000  0.000000  0.000108  0.000088  0.003187  0.000000 -0.006873
0.010701
  0.000000  0.006857  0.000000 -0.001654 -0.005670  0.000000  0.029319

            NA   8.31306317116270E-01
            NB   8.31306317116270E-01
            N    1.66261263423254E+00
          FOOA  -5.85707049108468E-01
          FOOB  -5.85707049108468E-01
          ALOC   7.04562249857833E-01
          BLOC   7.04562249857833E-01
```

```
           FLA   2.45599268007802E-01
           FLB   2.45599268007802E-01
            FL   1.07690558512407E+00

 ERROR ESTIMATE FOR DIFFERENTIAL EQUATIONS
 FOR SURFACE # 1   EPSD   6.07421207955121E-08

 MAXIMUM DISTANCE REACHED FROM NUCLEUS =  9.9957538136E+00
```

B4H10-B5

```
 PROAIM VERSION 0.90

B4H10 OPTIMIZATION USING VD SET(Renormalized) d=0.75, p=1.0725
 -V/T FOR THIS WAVEFUNCTION =        2.00132087000
 MOLECULAR SCF ENERGY (AU)  =     -104.47774919276

B5 of B4H10 9s/5p + 1d on B, F
 INTEGRATION IS OVER ATOM   B    5
   120 PHI PLANES     96 THETA PLANES
  80 PATHS WITH  141 POINTS PER PATH
 RADIUS OF BETA SPHERE   0.9543 WITH    120 POINTS PER PATH
 VOL1 RHO CONTOUR THRESHOLD=   0.0010
 VOL2 RHO CONTOUR THRESHOLD=   0.0020

 INSERTION LIMIT USED          =   15
 INSERTION LIMIT REACHED      0 TIMES FOR SURFACE   1
 INSERTION LIMIT REACHED      1 TIMES FOR SURFACE   2
 INSERTION LIMIT REACHED      0 TIMES FOR SURFACE   3
 INSERTION LIMIT REACHED      0 TIMES FOR SURFACE   4
 FOR SURFACE # 1 NUMBER OF INSERTED PATHS =    130
 FOR SURFACE # 2 NUMBER OF INSERTED PATHS =    105
 FOR SURFACE # 3 NUMBER OF INSERTED PATHS =     66
 FOR SURFACE # 4 NUMBER OF INSERTED PATHS =     56
 TOTAL NUMBER OF INSERTED PATHS=   357

 RESULTS OF THE INTEGRATION
             N   3.04264717086716E+00     NET CHARGE   1.95735282913284E+00
             G   2.44391710881151E+01
             K   2.38414171977327E+01        E(ATOM)  -2.38729086104666E+01
             L  -5.97753890382418E-01
             I   3.36050966649339E-01
        R(-1)   1.04183722238174E+01
           R1   2.13853271241273E+00
           R2   3.26433899766700E+00
           R4   2.92203891495882E+01
       GR(-1)  -1.91800983878207E+01
          GR0  -6.89049474533851E+00
          GR1  -5.28040879678611E+00
          GR2  -1.10442599463640E+01
         VNEO  -5.20918611190872E+01      VNEO(COR)  -5.21262417012457E+01
```

VNET	-7.24752237072070E+01	VNET(COR)	-7.25230572906034E+01
VEET	1.61392128835397E+01	VEET(COR)	1.61498647497352E+01
EHF	-3.24945936259346E+01		
		VREP(COR)	2.47715497652031E+01
		V(ATOM)	-4.77515075254002E+01
EL DX	-1.82680216886464E-01		
EL DY	2.71494010605441E-01		
EL DZ	1.62047912821003E-01		
EL DIPOLE MAG	3.65158301954038E-01		
QXX	1.57663428499803E-01	QXX(DIAG)	1.33886746181526E+00
QXY	1.55654580458670E+00		
QXZ	8.63905470001508E-01		
QYY	-7.86623533445223E-01	QYY(DIAG)	1.28494779086713E+00
QYZ	-1.21459936323703E+00		
QZZ	6.28960104945419E-01	QZZ(DIAG)	-2.62381525268238E+00
FAXA	-1.19079744358280E-02		
FAYA	-1.82541510252048E-01		
FAZA	-1.02748412352619E-01		
FBXA	1.97746264620625E+00		
FBYA	2.86048126680490E+00		
FBZA	2.51350528403857E+00		
RHO*L	3.91762468520453E+02		
VOL1	1.94340816765278E+01		
VOL2	1.84460379954153E+01		
N(VOL1)	3.04109675822575E+00		
N(VOL2)	3.03969433571102E+00		

THE ATOMIC OVERLAP MATRIX AOM :

```
  0.498431
  0.498408  0.498386
 -0.004842 -0.004685  0.016353
  0.000000 -0.000157 -0.016313  0.016320
 -0.006567 -0.006570 -0.000705  0.000860  0.054885
 -0.009267 -0.009263  0.000343 -0.000161  0.064051  0.085925
  0.000000 -0.000004 -0.000351  0.000378 -0.001574 -0.000048  0.020726
  0.006233  0.006224 -0.001343  0.001269 -0.027717 -0.046965 -0.001011
0.046477
 -0.000001 -0.000003 -0.000199  0.000239 -0.000278 -0.000858  0.027540
0.000415
  0.043498
 -0.003492 -0.003502 -0.000342  0.000366  0.004293  0.023589 -0.000088 -
0.017086
  0.000615  0.055030
 -0.002397 -0.002402 -0.000123  0.000108 -0.000020  0.006469 -0.000055 -
0.034856
  0.000623 -0.014836  0.064179
 -0.000034 -0.000032  0.000490 -0.000539 -0.012052 -0.011916 -0.001037 -
0.017125
  0.000830 -0.016663  0.048580  0.041489
 -0.000001 -0.000010 -0.001022  0.001040  0.000326 -0.000658  0.012164
0.000710
```

```
  0.020650  0.000532  0.000513  0.000939  0.010730
 -0.002483 -0.002493 -0.000174  0.000163 -0.008517  0.008541  0.000018 -
0.016700
  0.000851  0.051825 -0.004777 -0.006594  0.000663  0.055282
 -0.001660 -0.001688 -0.003056  0.003103  0.015640  0.017292  0.002010 -
0.011109
 -0.000325 -0.009512  0.011491  0.004181 -0.000681 -0.011516  0.013613

            NA   1.52132358543358E+00
            NB   1.52132358543358E+00
            N    3.04264717086716E+00
          FOOA  -1.05914065570694E+00
          FOOB  -1.05914065570694E+00
          ALOC   6.96196828766765E-01
          BLOC   6.96196828766765E-01
           FLA   4.62182929726637E-01
           FLB   4.62182929726637E-01
            FL   1.98350651516022E+00

 ERROR ESTIMATE FOR DIFFERENTIAL EQUATIONS
 FOR SURFACE # 1   EPSD   1.12059638462374E-03
 FOR SURFACE # 2   EPSD   1.12059638462374E-03
 FOR SURFACE # 3   EPSD   1.12059638462374E-03
 FOR SURFACE # 4   EPSD   1.12059638462374E-03

 MAXIMUM DISTANCE REACHED FROM NUCLEUS =  1.0000000000E+01
```

B4H10-H7

```
 PROAIM STELLIX VERSION 0.95

B4H10 OPTIMIZATION USING VD SET(Renormalized) d=0.75, p=1.0725
 -V/T FOR THIS WAVEFUNCTION =        2.00132087000
 MOLECULAR SCF ENERGY (AU)  =     -104.47774919276

H7 of B4H10 9s/5p + 1d on B, F
 INTEGRATION IS OVER ATOM   H    7
   120 PHI PLANES     96 THETA PLANES
  80 PATHS WITH  141 POINTS PER PATH
 RADIUS OF BETA SPHERE   1.4122 WITH    120 POINTS PER PATH
 VOL1 RHO CONTOUR THRESHOLD=   0.0010
 VOL2 RHO CONTOUR THRESHOLD=   0.0020

 INSERTION LIMIT USED          =    6
 INSERTION LIMIT REACHED      1 TIMES FOR SURFACE   1
 INSERTION LIMIT REACHED      0 TIMES FOR SURFACE   2
 FOR SURFACE # 1 NUMBER OF INSERTED PATHS =     70
 FOR SURFACE # 2 NUMBER OF INSERTED PATHS =    130
 TOTAL NUMBER OF INSERTED PATHS=   200

 RESULTS OF THE INTEGRATION
```

N	1.71693446422685E+00	NET CHARGE	-7.16934464226847E-01
G	9.19625896296864E-01		
K	9.20764543058375E-01	E(ATOM)	-9.21980753320364E-01
L	1.13864676151119E-03		
I	3.55707370043976E-01		
R(-1)	1.72208232173277E+00		
R1	2.29147784159376E+00		
R2	3.75424943116469E+00		
R4	2.01707294246790E+01		
GR(-1)	-2.14294639035737E+00		
GR0	-2.65898638165277E+00		
GR1	-4.23845292099911E+00		
GR2	-8.66486430044561E+00		
VNEO	-1.72208232173277E+00	VNEO(COR)	-1.72321889453846E+00
VNET	-1.60621027065884E+01	VNET(COR)	-1.60727036801355E+01
VEET	7.00502203661239E+00	VEET(COR)	7.00964534494650E+00
EHF	-8.13631612691766E+00		
		VREP(COR)	1.42239807185438E+01
		V(ATOM)	-1.84872296159169E+00
EL DX	-5.05406121818854E-01		
EL DY	-1.89585078424802E-01		
EL DZ	2.36150850470211E-01		
EL DIPOLE MAG	5.89190185009150E-01		
QXX	-1.23366719720470E+00	QXX(DIAG)	1.13808791204040E+00
QXY	-3.26338665101227E-01		
QXZ	4.98543875549812E-01		
QYY	8.61936983082032E-01	QYY(DIAG)	2.61116856443951E-01
QYZ	-3.22537427029238E-01		
QZZ	3.71730214122668E-01	QZZ(DIAG)	-1.39920476848435E+00
FAXA	2.74399812103809E-01		
FAYA	1.46896261180138E-01		
FAZA	-1.38584595359301E-01		
FBXA	-2.35309325145992E+00		
FBYA	-1.33727313962191E+00		
FBZA	7.72539393895004E-01		
RHO*L	8.21105983005335E-02		
VOL1	5.59624606976272E+01		
VOL2	4.76086282440677E+01		
N(VOL1)	1.70321484912373E+00		
N(VOL2)	1.69110389072213E+00		

THE ATOMIC OVERLAP MATRIX AOM :

```
 0.000146
-0.000146  0.000146
-0.000008  0.000011  0.000322
-0.000008  0.000011  0.000311  0.000321
-0.001616  0.001637  0.002637  0.002518  0.116381
 0.001651 -0.001664 -0.001898 -0.001804 -0.101774  0.098280
-0.001278  0.001300  0.002983  0.003110  0.129979 -0.115377  0.166624
 0.000293 -0.000289  0.000483  0.000448 -0.005134  0.006777 -0.005826
0.011772
```

```
  0.001707 -0.001723 -0.002594 -0.002715 -0.135973  0.132111 -0.169524
0.009114
  0.190473
  0.000373 -0.000383 -0.000994 -0.000955 -0.037125  0.024152 -0.039161
0.005192
  0.032679  0.026898
 -0.000482  0.000490  0.001199  0.001130  0.041284 -0.039058  0.047017
0.007703
 -0.052764 -0.003978  0.028026
  0.000520 -0.000525 -0.000299 -0.000272 -0.010657  0.009323  0.000265 -
0.001593
  0.004535  0.002291 -0.008826  0.015770
 -0.000774  0.000782  0.000930  0.000959  0.058002 -0.050720  0.068624 -
0.012323
 -0.071680 -0.025014  0.012903 -0.003929  0.041852
 -0.000925  0.000938  0.001798  0.001707  0.076202 -0.067787  0.088098 -
0.001436
 -0.094244 -0.027176  0.027554 -0.003754  0.037751  0.056774
  0.000037 -0.000048 -0.001711 -0.001669 -0.072521  0.064207 -0.112124
0.001938
  0.106778  0.020701 -0.027980 -0.015227 -0.042123 -0.052890  0.104682

            NA   8.58467232113424E-01
            NB   8.58467232113424E-01
            N    1.71693446422685E+00
          FOOA  -5.14732898951439E-01
          FOOB  -5.14732898951439E-01
          ALOC   5.99595278301118E-01
          BLOC   5.99595278301118E-01
           FLA   3.43734333161985E-01
           FLB   3.43734333161985E-01
            FL   1.20220156527541E+00

 ERROR ESTIMATE FOR DIFFERENTIAL EQUATIONS
 FOR SURFACE # 1   EPSD   6.77871966340550E-04
 FOR SURFACE # 2   EPSD   6.77871966340550E-04

 MAXIMUM DISTANCE REACHED FROM NUCLEUS =  9.9978159098E+00
```

B4H10-H11

```
 PROAIM STELLIX VERSION 0.95

B4H10 OPTIMIZATION USING VD SET(Renormalized) d=0.75, p=1.0725
 -V/T FOR THIS WAVEFUNCTION =        2.00132087000
 MOLECULAR SCF ENERGY (AU)  =     -104.47774919276

H11 of B4H10 9s/5p + 1d on B, F
 INTEGRATION IS OVER ATOM   H   11
   120 PHI PLANES     96 THETA PLANES
  80 PATHS WITH  141 POINTS PER PATH
```

```
RADIUS OF BETA SPHERE   1.2897 WITH    120 POINTS PER PATH
VOL1 RHO CONTOUR THRESHOLD=   0.0010
VOL2 RHO CONTOUR THRESHOLD=   0.0020

INSERTION LIMIT USED          =    6
INSERTION LIMIT REACHED      0 TIMES FOR SURFACE   1
FOR SURFACE # 1 NUMBER OF INSERTED PATHS =     66
TOTAL NUMBER OF INSERTED PATHS=    66

RESULTS OF THE INTEGRATION
             N   1.69359303999623E+00     NET CHARGE  -6.93593039996230E-01
             G   8.76413391374559E-01
             K   8.76526757386021E-01        E(ATOM)  -8.77684535284049E-01
             L   1.13366011460783E-04
             I   3.63070277472310E-01
        R(-1)    1.71374565257926E+00
            R1   2.27999870751202E+00
            R2   3.77377190044459E+00
            R4   1.67668250187917E+01
       GR(-1)   -2.58114311636235E+00
           GR0   -3.45918917854526E+00
           GR1   -5.84107939574608E+00
           GR2   -1.18420246864733E+01
          VNEO   -1.71374565257926E+00      VNEO(COR)  -1.71487672319070E+00
          VNET   -1.36201400681936E+01      VNET(COR)  -1.36291293485642E+01
          VEET    5.88206025819449E+00      VEET(COR)   5.88594241275037E+00
           EHF   -6.86155305261309E+00
                                            VREP(COR)   1.18698109300794E+01
                                              V(ATOM)  -1.75931841848474E+00
        EL DX    8.46764009886081E-06
        EL DY   -8.12471355645476E-03
        EL DZ    3.85566775684772E-01
 EL DIPOLE MAG   3.85652368790893E-01
           QXX   -2.57764787929855E-01      QXX(DIAG)  -2.57765233004933E-01
           QXY   -8.23418955451435E-05
           QXZ    1.70382135620637E-05
           QYY   -2.39413258816131E-01      QYY(DIAG)  -2.42193815976970E-01
           QYZ    4.53452963484025E-02
           QZZ    4.97178046745986E-01      QZZ(DIAG)   4.99959048981903E-01
          FAXA    3.57221228874287E-07
          FAYA   -1.09969074370279E-02
          FAZA   -3.48396818174736E-01
          FBXA    3.13303280362559E-06
          FBYA    8.39281690751551E-01
          FBZA    2.78008719468831E+00
         RHO*L    9.73565487219362E-02
          VOL1    7.86239453886096E+01
          VOL2    6.23897016284862E+01
       N(VOL1)    1.66357367102601E+00
       N(VOL2)    1.64004954461410E+00
```

```
   THE ATOMIC OVERLAP MATRIX AOM :

  0.000394
  0.000394  0.000394
 -0.000004 -0.000004  0.000000
  0.000000  0.000000  0.000000  0.000000
  0.001610  0.001608 -0.000017  0.000000  0.028983
  0.002783  0.002785 -0.000027  0.000000  0.046095  0.080353
  0.000000  0.000000  0.000000  0.000003  0.000000  0.000000  0.006955
 -0.003627 -0.003627  0.000039  0.000000 -0.063812 -0.112161  0.000000
0.161005
  0.000000  0.000000  0.000000  0.000005  0.000000  0.000000  0.009741
0.000000
  0.014233
 -0.000163 -0.000158  0.000002  0.000000 -0.008025 -0.005255  0.000000
0.007088
  0.000000  0.014291
  0.004826  0.004830 -0.000049  0.000000  0.086066  0.153509  0.000000 -
0.221151
  0.000000 -0.011638  0.310176
  0.003272  0.003273 -0.000036  0.000000  0.061787  0.107928  0.000000 -
0.157453
  0.000000 -0.011312  0.219921  0.158469
  0.000000  0.000000  0.000000  0.000003  0.000000  0.000000  0.005988
0.000000
  0.008344  0.000000  0.000000  0.000000  0.005199
 -0.000083 -0.000080  0.000000  0.000000 -0.004599 -0.000282  0.000000 -
0.001489
  0.000000  0.013450 -0.000765 -0.002781  0.000000  0.014107
  0.001845  0.001844 -0.000020  0.000000  0.034671  0.060179  0.000000 -
0.088552
  0.000000 -0.007222  0.124625  0.089560  0.000000 -0.001901  0.052237

            NA   8.46796519998115E-01
            NB   8.46796519998115E-01
            N    1.69359303999623E+00
          FOOA  -6.06937409357890E-01
          FOOB  -6.06937409357890E-01
          ALOC   7.16745280624489E-01
          BLOC   7.16745280624489E-01
           FLA   2.39859110640225E-01
           FLB   2.39859110640225E-01
            FL   1.08665563063834E+00

 ERROR ESTIMATE FOR DIFFERENTIAL EQUATIONS
 FOR SURFACE # 1   EPSD   1.41906479808386E-07

 MAXIMUM DISTANCE REACHED FROM NUCLEUS =  9.9957610057E+00
```

B4H10-H13

```
 PROAIM STELLIX VERSION 0.95

B4H10 OPTIMIZATION USING VD SET(Renormalized) d=0.75, p=1.0725
 -V/T FOR THIS WAVEFUNCTION =        2.00132087000
 MOLECULAR SCF ENERGY (AU)  =     -104.47774919276

H13 of B4H10 9s/5p + 1d on B, F
 INTEGRATION IS OVER ATOM   H   13
   120 PHI PLANES     96 THETA PLANES
  80 PATHS WITH  141 POINTS PER PATH
 RADIUS OF BETA SPHERE   1.2838 WITH    120 POINTS PER PATH
 VOL1 RHO CONTOUR THRESHOLD=   0.0010
 VOL2 RHO CONTOUR THRESHOLD=   0.0020

 INSERTION LIMIT USED          =    6
 INSERTION LIMIT REACHED      0 TIMES FOR SURFACE   1
 FOR SURFACE # 1 NUMBER OF INSERTED PATHS =     56
 TOTAL NUMBER OF INSERTED PATHS=    56

 RESULTS OF THE INTEGRATION
              N   1.70028248487267E+00     NET CHARGE  -7.00282484872674E-01
              G   8.79093365692239E-01
              K   8.79194944377953E-01        E(ATOM)  -8.80356246604133E-01
              L   1.01578685713290E-04
              I   3.65110354360603E-01
         R(-1)   1.71848533904382E+00
            R1   2.29757323368980E+00
            R2   3.82978386646082E+00
            R4   1.74594447946970E+01
        GR(-1)  -2.62097817451986E+00
           GR0  -3.54661657980782E+00
           GR1  -6.06385787778445E+00
           GR2  -1.24783220177573E+01
          VNEO  -1.71848533904382E+00      VNEO(COR)  -1.71961953784413E+00
          VNET  -1.32960338277834E+01      VNET(COR)  -1.33048091983226E+01
          VEET   5.71910238183454E+00      VEET(COR)   5.72287698433648E+00
           EHF  -6.69773650157087E+00
                                           VREP(COR)   1.15402572393032E+01
                                             V(ATOM)  -1.76455195901936E+00
         EL DX   1.03791868339624E-06
         EL DY   3.35816155775271E-01
         EL DZ  -2.11126377442170E-01
  EL DIPOLE MAG   3.96669683404986E-01
           QXX  -2.99629674565116E-01      QXX(DIAG)  -2.99629676456025E-01
           QXY  -1.53849943507491E-06
           QXZ  -1.00236383318665E-05
           QYY   3.76633413129353E-01      QYY(DIAG)  -2.50690361345938E-01
           QYZ  -3.30087487317559E-01
           QZZ  -7.70037385642364E-02      QZZ(DIAG)   5.50320037801962E-01
```

```
          FAXA   5.40105534795250E-07
          FAYA  -3.05988824879958E-01
          FAZA   1.75995356928586E-01
          FBXA   7.09756256720090E-06
          FBYA   2.79510929980510E+00
          FBZA  -9.66756585142204E-01
         RHO*L   9.87333477941389E-02
          VOL1   7.98975854431337E+01
          VOL2   6.27343203947054E+01
       N(VOL1)   1.66741337879011E+00
       N(VOL2)   1.64262113863834E+00

   THE ATOMIC OVERLAP MATRIX AOM :

  0.000403
  0.000403  0.000403
 -0.000003 -0.000003  0.000000
  0.000000  0.000000  0.000000  0.000000
  0.001432  0.001431 -0.000010  0.000000  0.021457
  0.003054  0.003053 -0.000024  0.000000  0.044981  0.098176
  0.000000  0.000000  0.000000  0.000004  0.000000  0.000000  0.005851
 -0.002143 -0.002145  0.000020  0.000000 -0.029316 -0.069101  0.000000
0.056180
  0.000000  0.000000  0.000000  0.000007  0.000000  0.000000  0.009607
0.000000
  0.015824
  0.004540  0.004541 -0.000038  0.000000  0.069911  0.157304  0.000000 -
0.114581
  0.000000  0.262910
 -0.001344 -0.001343  0.000006  0.000000 -0.024186 -0.048401  0.000000
0.025287
  0.000000 -0.079271  0.039610
 -0.002001 -0.002001  0.000013  0.000000 -0.032130 -0.068879  0.000000
0.044250
  0.000000 -0.114531  0.044697  0.057078
  0.000000  0.000000  0.000000  0.000003  0.000000  0.000000  0.003154
0.000000
  0.005274  0.000000  0.000000  0.000000  0.002379
  0.004553  0.004555 -0.000041  0.000000  0.069635  0.160507  0.000000 -
0.121651
  0.000000  0.272724 -0.077080 -0.116129  0.000000  0.286469
 -0.000351 -0.000352  0.000002  0.000000 -0.005971 -0.013204  0.000000
0.009092
  0.000000 -0.022033  0.008301  0.010672  0.000000 -0.022583  0.003402

            NA   8.50141242436337E-01
            NB   8.50141242436337E-01
            N    1.70028248487267E+00
          FOOA  -6.17696988537365E-01
          FOOB  -6.17696988537365E-01
          ALOC   7.26581605154418E-01
          BLOC   7.26581605154418E-01
```

```
           FLA   2.32444253898972E-01
           FLB   2.32444253898972E-01
            FL   1.08258549633531E+00

 ERROR ESTIMATE FOR DIFFERENTIAL EQUATIONS
 FOR SURFACE # 1   EPSD   1.17753203968139E-07

 MAXIMUM DISTANCE REACHED FROM NUCLEUS =  9.9957581231E+00
```

B5H9-H6 (B1 & B5 n/a)

```
 PROAIM STELLIX VERSION 0.95

B5H9 SINGLE POINT USING VD SET(Renormalized) d=0.75, p=1.0725
 -V/T FOR THIS WAVEFUNCTION =        2.00144494000
 MOLECULAR SCF ENERGY (AU)  =     -128.59786257587

B5H9 Integration of H6 (Terminal at plane)
 INTEGRATION IS OVER ATOM   H    6
   120 PHI PLANES     96 THETA PLANES
  80 PATHS WITH  141 POINTS PER PATH
 RADIUS OF BETA SPHERE   1.2724 WITH    120 POINTS PER PATH
 VOL1 RHO CONTOUR THRESHOLD=   0.0010
 VOL2 RHO CONTOUR THRESHOLD=   0.0020

 INSERTION LIMIT USED          =    6
 INSERTION LIMIT REACHED      0 TIMES FOR SURFACE   1
 FOR SURFACE # 1 NUMBER OF INSERTED PATHS =     46
 TOTAL NUMBER OF INSERTED PATHS=    46

 RESULTS OF THE INTEGRATION
             N   1.68278486606256E+00     NET CHARGE  -6.82784866062559E-01
             G   8.59606986565143E-01
             K   8.59699527890584E-01        E(ATOM)  -8.60941742126414E-01
             L   9.25413254402518E-05
             I   3.26401255933370E-01
         R(-1)   1.69591584011694E+00
            R1   2.28846337893534E+00
            R2   3.85700247042721E+00
            R4   1.82321311091933E+01
        GR(-1)  -2.60273862370003E+00
           GR0  -3.56036289137520E+00
           GR1  -6.17900917062421E+00
           GR2  -1.29420501621178E+01
          VNEO  -1.69591584011694E+00      VNEO(COR)  -1.69714020386787E+00
          VNET  -1.43372554497144E+01      VNET(COR)  -1.43476062085464E+01
          VEET   6.25074233636126E+00      VEET(COR)   6.25525504987687E+00
           EHF  -7.22681358546253E+00
                                           VREP(COR)   1.26211268932130E+01
```

```
                                                V(ATOM)   -1.72647931533340E+00
        EL DX    4.34331379984838E-06
        EL DY    3.97375624469444E-01
        EL DZ    5.29842218450188E-02
  EL DIPOLE MAG  4.00892397914786E-01
           QXX  -2.84581883997205E-01      QXX(DIAG)   -2.84581884522349E-01
           QXY  -2.20428412673105E-05
           QXZ  -4.17829420527383E-06
           QYY   6.39860654384235E-01      QYY(DIAG)   -3.88388966736418E-01
           QYZ   1.84514354051375E-01
           QZZ  -3.55278770387031E-01      QZZ(DIAG)    6.72970851258767E-01
          FAXA  -6.93881809459939E-07
          FAYA  -3.50900240008978E-01
          FAZA  -4.72306892112481E-02
          FBXA  -7.10637469233854E-06
          FBYA   3.17599232131289E+00
          FBZA   2.22336664470782E-01
         RHO*L   9.63831337471319E-02
          VOL1   8.15278131400665E+01
          VOL2   6.32655911066545E+01
       N(VOL1)   1.64765564814653E+00
       N(VOL2)   1.62125164528025E+00

   THE ATOMIC OVERLAP MATRIX AOM :

  0.000200
  0.000000  0.000000
  0.000282  0.000000  0.000399
  0.000200  0.000000  0.000282  0.000200
 -0.000002  0.000000 -0.000002 -0.000002  0.000000
  0.000687  0.000000  0.000972  0.000688 -0.000005  0.009911
  0.000000  0.000003  0.000000  0.000000  0.000000  0.000000  0.004652
  0.002054  0.000000  0.002906  0.002058 -0.000015  0.029414  0.000000
0.090333
 -0.000689  0.000000 -0.000976 -0.000692  0.000009 -0.010000  0.000000 -
0.032302
  0.016685
  0.002812  0.000000  0.003981  0.002821 -0.000020  0.041125  0.000000
0.129678
 -0.045483  0.191679
  0.002384  0.000000  0.003375  0.002392 -0.000016  0.035250  0.000000
0.110838
 -0.037417  0.164240  0.141413
  0.000000  0.000006  0.000000  0.000000  0.000000  0.000000  0.007948
0.000000
  0.000000  0.000000  0.000000  0.013682
  0.000000 -0.000002  0.000000  0.000000  0.000000  0.000000 -0.003426
0.000000
  0.000000  0.000000  0.000000 -0.005921  0.002709
  0.003368  0.000000  0.004767  0.003380 -0.000022  0.050334  0.000000
0.160213
 -0.053485  0.240651  0.207303  0.000000  0.000000  0.305892
```

```
 -0.000967  0.000000 -0.001368 -0.000970  0.000004 -0.014388  0.000000 -
0.045421
  0.012927 -0.069119 -0.060228  0.000000  0.000000 -0.089461  0.027458
  0.000000  0.000001  0.000000  0.000000  0.000000  0.000000  0.001298
0.000000
  0.000000  0.000000  0.000000  0.002129 -0.000731  0.000000  0.000000
0.001219
 -0.000537  0.000000 -0.000761 -0.000541  0.000013 -0.008626  0.000000 -
0.030823
  0.022025 -0.043750 -0.034202  0.000000  0.000000 -0.049024  0.009149
0.000000
  0.034961

            NA   8.41392433031279E-01
            NB   8.41392433031279E-01
            N    1.68278486606256E+00
          FOOA  -6.06250235064147E-01
          FOOB  -6.06250235064147E-01
          ALOC   7.20532074290249E-01
          BLOC   7.20532074290249E-01
           FLA   2.35142197967132E-01
           FLB   2.35142197967132E-01
            FL   1.07653463099841E+00

 ERROR ESTIMATE FOR DIFFERENTIAL EQUATIONS
 FOR SURFACE # 1   EPSD   3.81707798297546E-08

 MAXIMUM DISTANCE REACHED FROM NUCLEUS =  9.9957525913E+00
```

B5H9-H10

```
 OMEGA DEVELOPMENT VERSION

B5H9 SINGLE POINT USING VD SET(Renormalized) d=0.75, p=1.0725
 -V/T FOR THIS WAVEFUNCTION =        2.00144494000
 MOLECULAR SCF ENERGY (AU)  =     -128.59786257587

B5H9_H10
 INTEGRATION IS OVER ATOM   H   10
 QUADRATURE ORDER OVER THETA  64 PHI  64 AND S  64 WITH 200 POINTS/PATH
 RADIUS OF BETA SPHERE   1.6446
 VOL1 RHO CONTOUR THRESHOLD=   0.0020
 VOL2 RHO CONTOUR THRESHOLD=   0.0010

 RESULTS OF THE INTEGRATION
             N   1.67363376047203E+00     NET CHARGE  -6.73633760472032E-01
             G   8.92105943672869E-01
             K   8.92122127338700E-01        E(ATOM)  -8.93411190285377E-01
             L   1.61836658310642E-05
          VNEO  -1.70027251918397E+00      VNEO(COR)  -1.70150002823244E+00
          VNET  -1.69657018952196E+01      VNET(COR)  -1.69779502567940E+01
```

VEET	7.48355926908721E+00	VEET(COR)	7.48896201283207E+00
		VREP(COR)	1.51855713213403E+01
		V(ATOM)	-1.79237893545366E+00
EL DX	1.22779940828305E-01		
EL DY	1.22779940828320E-01		
EL DZ	-3.66623648147176E-01		
EL DIPOLE MAG	4.05663317444839E-01		
QXX	1.98416908565869E-01		
QXY	-2.41312830355038E-01		
QXZ	3.18747111346181E-02		
QYY	1.98416908565869E-01		
QYZ	3.18747111345817E-02		
QZZ	-3.96833817131739E-01		
FAXA	-1.09342083836614E-01		
FAYA	-1.09342083836624E-01		
FAZA	2.78564387655329E-01		
FBXA	1.43463214618769E+00		
FBYA	1.43463214618769E+00		
FBZA	-2.42293358214650E+00		
VOL1	4.82615272401620E+01		
VOL2	5.74118045553173E+01		
N(VOL1)	1.64523025574756E+00		
N(VOL2)	1.65839938152720E+00		

B5H9-H14

```
 PROAIM STELLIX VERSION 0.95

B5H9 SINGLE POINT USING VD SET(Renormalized) d=0.75, p=1.0725
 -V/T FOR THIS WAVEFUNCTION =        2.00144494000
 MOLECULAR SCF ENERGY (AU)  =     -128.59786257587

B5H9 Integration of H14(Apex)
 INTEGRATION IS OVER ATOM   H   14
   120 PHI PLANES      96 THETA PLANES
  80 PATHS WITH  141 POINTS PER PATH
 RADIUS OF BETA SPHERE   1.2727 WITH    120 POINTS PER PATH
 VOL1 RHO CONTOUR THRESHOLD=   0.0010
 VOL2 RHO CONTOUR THRESHOLD=   0.0020

 INSERTION LIMIT USED          =    6
 INSERTION LIMIT REACHED      0 TIMES FOR SURFACE   1
 FOR SURFACE # 1 NUMBER OF INSERTED PATHS =     36
 TOTAL NUMBER OF INSERTED PATHS=    36

 RESULTS OF THE INTEGRATION
              N   1.67919810622205E+00     NET CHARGE  -6.79198106222046E-01
              G   8.38914385132822E-01
              K   8.38998018456750E-01        E(ATOM)  -8.40210320253539E-01
              L   8.36333239280315E-05
              I   3.27487261887332E-01
```

R(-1)	1.68356013614969E+00		
R1	2.30415490942622E+00		
R2	3.93594489712059E+00		
R4	1.93584206340820E+01		
GR(-1)	-2.57182920044222E+00		
GR0	-3.53975200856947E+00		
GR1	-6.21982011921170E+00		
GR2	-1.32615563800560E+01		
VNEO	-1.68356013614969E+00	VNEO(COR)	-1.68477557971974E+00
VNET	-1.46978273731966E+01	VNET(COR)	-1.47084384463569E+01
VEET	6.48539863157493E+00	VEET(COR)	6.49008075483070E+00
EHF	-7.37343072316488E+00		
		VREP(COR)	1.30233011577420E+01
		V(ATOM)	-1.68513728861481E+00
EL DX	-1.35978197597441E-06		
EL DY	-1.22407099423630E-05		
EL DZ	3.55311741666443E-01		
EL DIPOLE MAG	3.55311741879895E-01		
QXX	-3.88453494114149E-01	QXX(DIAG)	-3.88434526044639E-01
QXY	4.22610583005137E-05		
QXZ	1.43662032310680E-06		
QYY	-3.88528681307952E-01	QYY(DIAG)	-3.88547651891906E-01
QYZ	5.41160072060502E-05		
QZZ	7.76982175422101E-01	QZZ(DIAG)	7.76982177936545E-01
FAXA	3.94498486094982E-08		
FAYA	1.36838763849384E-06		
FAZA	-3.35741549129296E-01		
FBXA	1.22559454369627E-07		
FBYA	1.00956840536270E-05		
FBZA	3.22602946941167E+00		
RHO*L	9.23189979757792E-02		
VOL1	8.36591205940314E+01		
VOL2	6.50696081010147E+01		
N(VOL1)	1.64233229303064E+00		
N(VOL2)	1.61557468804323E+00		

THE ATOMIC OVERLAP MATRIX AOM :

```
  0.000000
  0.000000  0.000000
  0.000000  0.000000  0.000000
  0.000000  0.000000  0.000000  0.000000
  0.000006  0.000000  0.000000  0.000000  0.000768
  0.000013  0.000000  0.000000  0.000000  0.001007  0.005930
  0.000000  0.000004  0.000000  0.000000  0.000000  0.000000  0.001931
  0.000000  0.000000  0.000004  0.000000  0.000000  0.000000  0.000000
0.001931
  0.000049  0.000000  0.000000  0.000000  0.004657  0.026706  0.000000
0.000000
  0.127674
  0.000000  0.000000  0.000000  0.000001  0.000000  0.000000  0.000000
0.000000
```

```
  0.000000  0.000240
  0.000041  0.000000  0.000000  0.000000  0.004062  0.023898  0.000000
0.000000
  0.116383  0.000000  0.106970
  0.000000  0.000000  0.000000  0.000000  0.000000  0.000000  0.000000
0.000000
  0.000000  0.000000  0.000000  0.000098
  0.000000  0.000001  0.000000  0.000000  0.000000  0.000000  0.000539
0.000000
  0.000000  0.000000  0.000000  0.000000  0.000332
  0.000000  0.000000  0.000001  0.000000  0.000000  0.000000  0.000000
0.000539
  0.000000  0.000000  0.000000  0.000000  0.000000  0.000332
  0.000080  0.000000  0.000000  0.000000  0.008700  0.051581  0.000000
0.000000
  0.257240  0.000000  0.237736  0.000000  0.000000  0.000000  0.533624
  0.000000  0.000016  0.000000  0.000000  0.000000  0.000000  0.007534
0.000000
  0.000000  0.000000  0.000000  0.000000  0.002191  0.000000  0.000000
0.029884
  0.000000  0.000000  0.000016  0.000000  0.000000  0.000000  0.000000
0.007534
  0.000001  0.000000  0.000001  0.000000  0.000000  0.002191  0.000001 -
0.000001
  0.029885

            NA   8.39599053111022E-01
            NB   8.39599053111022E-01
            N    1.67919810622204E+00
          FOOA  -5.95166557128449E-01
          FOOB  -5.95166557128449E-01
          ALOC   7.08869971831362E-01
          BLOC   7.08869971831362E-01
           FLA   2.44432495982573E-01
           FLB   2.44432495982573E-01
            FL   1.08403154909360E+00

 ERROR ESTIMATE FOR DIFFERENTIAL EQUATIONS
 FOR SURFACE # 1   EPSD   1.81362428494212E-08

 MAXIMUM DISTANCE REACHED FROM NUCLEUS =  9.9957527366E+00
```

B6H10-B1

```
 OMEGA DEVELOPMENT VERSION

B6H10 OPTIMIZATION USING VD SET(Renormalized) d=0.75, p=1.0725
 -V/T FOR THIS WAVEFUNCTION =        2.00128156000
 MOLECULAR SCF ENERGY (AU)  =     -153.86037391838
```

```
B6H10_B1
 INTEGRATION IS OVER ATOM   B     1
 QUADRATURE ORDER OVER THETA  64 PHI  64 AND S  64 WITH 200 POINTS/PATH
 RADIUS OF BETA SPHERE   0.9870
 VOL1 RHO CONTOUR THRESHOLD=   0.0020
 VOL2 RHO CONTOUR THRESHOLD=   0.0010

 RESULTS OF THE INTEGRATION
              N   3.50797611235428E+00     NET CHARGE   1.49202388764572E+00
              G   2.40006412878527E+01
              K   2.40008582133470E+01        E(ATOM)  -2.40316167531989E+01
              L   2.16925494310568E-04
           VNEO  -5.37899015794385E+01      VNEO(COR)  -5.38243470006355E+01
           VNET  -8.49482581260142E+01      VNET(COR)  -8.50026564135215E+01
           VEET   2.23554890638078E+01      VEET(COR)   2.23698048408265E+01
                                            VREP(COR)   3.69300989364870E+01
                                              V(ATOM)  -4.80725574770344E+01
         EL DX   4.58703443101503E-01
         EL DY  -3.79222060077531E-01
         EL DZ   6.50608981966894E-07
  EL DIPOLE MAG   5.95162347232286E-01
           QXX  -2.07261483239994E-01
           QXY   6.14110573651539E-01
           QXZ  -1.68788197969783E-06
           QYY  -2.16951000921685E-01
           QYZ   1.09799681800860E-06
           QZZ   4.24212484161678E-01
          FAXA  -7.84459949543004E-01
          FAYA   5.05923552381802E-01
          FAZA  -4.64525982124542E-07
          FBXA   4.38230954404520E+00
          FBYA  -1.47023848469395E-01
          FBZA   1.37726539832517E-07
          VOL1   2.80903824183712E+01
          VOL2   2.97243726849131E+01
       N(VOL1)   3.50367150053717E+00
       N(VOL2)   3.50603797565461E+00
```

B6H10-B2 (not available)

B6H10-H3

```
 PROAIM STELLIX VERSION 0.95

B6H10 OPTIMIZATION USING VD SET(Renormalized) d=0.75, p=1.0725
 -V/T FOR THIS WAVEFUNCTION =        2.00128156000
 MOLECULAR SCF ENERGY (AU)  =     -153.86037391838

B6H10_H3
```

```
INTEGRATION IS OVER ATOM    H     3
  120 PHI PLANES      96 THETA PLANES
 80 PATHS WITH  141 POINTS PER PATH
RADIUS OF BETA SPHERE    1.2714 WITH     120 POINTS PER PATH
VOL1 RHO CONTOUR THRESHOLD=    0.0010
VOL2 RHO CONTOUR THRESHOLD=    0.0020

INSERTION LIMIT USED           =     6
INSERTION LIMIT REACHED       0 TIMES FOR SURFACE    1
FOR SURFACE # 1 NUMBER OF INSERTED PATHS =      30
TOTAL NUMBER OF INSERTED PATHS=     30

RESULTS OF THE INTEGRATION
              N    1.67270485891950E+00     NET CHARGE  -6.72704858919497E-01
              G    8.58485353420571E-01
              K    8.58604724340066E-01        E(ATOM)  -8.59705077810591E-01
              L    1.19370919493893E-04
              I    2.81995730167497E-01
         R(-1)    1.69235728001815E+00
            R1    2.26148638332394E+00
            R2    3.78329232965790E+00
            R4    1.75753566652362E+01
        GR(-1)   -2.57269873657130E+00
           GR0   -3.48965390109662E+00
           GR1   -5.99394961964082E+00
           GR2   -1.24073543519514E+01
          VNEO   -1.69235728001815E+00      VNEO(COR)  -1.69344101428080E+00
          VNET   -1.56697344477633E+01      VNET(COR)  -1.56797688703455E+01
          VEET    6.91492456525035E+00      VEET(COR)   6.91935267317028E+00
           EHF   -7.89620515817291E+00
                                            VREP(COR)   1.39558527535326E+01
                                              V(ATOM)  -1.72391611681287E+00
         EL DX    3.58009046494397E-01
         EL DY    1.47089110735672E-01
         EL DZ   -2.87303298567512E-06
 EL DIPOLE MAG    3.87047392288196E-01
           QXX    4.74237499272135E-01      QXX(DIAG)   6.59442310068864E-01
           QXY    4.06114452530727E-01
           QXZ   -1.16739629122048E-05
           QYY   -2.31079636154901E-01      QYY(DIAG)  -4.16284450018137E-01
           QYZ    2.00246686718436E-05
           QZZ   -2.43157863117235E-01      QZZ(DIAG)  -2.43157860050727E-01
          FAXA   -3.26718473638726E-01
          FAYA   -1.33544016100482E-01
          FAZA    5.85569852418911E-08
          FBXA    3.17850743252954E+00
          FBYA    9.09264926419164E-01
          FBZA   -2.38707329206926E-07
         RHO*L    9.60252759514233E-02
          VOL1    8.00422024328400E+01
          VOL2    6.24601475242027E+01
       N(VOL1)    1.63895790775575E+00
```

N(VOL2) 1.61361084755188E+00

THE ATOMIC OVERLAP MATRIX AOM :

```
  0.000000
  0.000000  0.000001
  0.000000  0.000030  0.000773
  0.000000  0.000000  0.000000  0.000000
  0.000000  0.000000  0.000000  0.000000  0.000000
  0.000000  0.000000 -0.000004  0.000000  0.000000  0.000000
  0.000000  0.000064  0.001641  0.000001  0.000000 -0.000006  0.014238
  0.000002  0.000000  0.000000  0.000000  0.000000  0.000000  0.000000
0.003175
  0.000000  0.000147  0.003786  0.000002  0.000000 -0.000016  0.032769
0.000000
  0.078033
  0.000000  0.000025  0.000626  0.000000  0.000000  0.000001  0.005800
0.000000
  0.011546  0.007337
  0.000004  0.000000  0.000000  0.000000  0.000000  0.000000  0.000000
0.005951
  0.000000  0.000000  0.011208
  0.000000 -0.000117 -0.003037 -0.000002  0.000000  0.000015 -0.026331
0.000000
 -0.065290 -0.007564  0.000000  0.057415
  0.000000  0.000240  0.006250  0.000004  0.000000 -0.000026  0.056514
0.000000
  0.136821  0.023270  0.000000 -0.116530  0.248893
 -0.000002  0.000000  0.000000  0.000000  0.000000  0.000000  0.000000 -
0.002662
  0.000000  0.000000 -0.005048  0.000000  0.000000  0.002852
  0.000000  0.000276  0.007194  0.000004  0.000000 -0.000027  0.065967
0.000000
  0.159599  0.031096  0.000000 -0.136074  0.295334  0.000000  0.354640
 -0.000003  0.000000  0.000000  0.000000  0.000000  0.000000  0.000000 -
0.004102
  0.000000  0.000000 -0.007735  0.000000  0.000000  0.003591  0.000000
0.005383
  0.000000 -0.000064 -0.001677 -0.000001  0.000000  0.000006 -0.015584
0.000000
 -0.037383 -0.008180  0.000000  0.031367 -0.069948  0.000000 -0.084681
0.000000
  0.020951
  0.000000 -0.000003 -0.000111 -0.000001  0.000000  0.000006 -0.001202
0.000000
 -0.006283  0.006381  0.000000  0.008488 -0.008127  0.000000 -0.004590
0.000000
 -0.000362  0.010501
  0.000000  0.000000  0.000000  0.000000  0.000000  0.000000  0.000000 -
0.000132
```

```
  0.000000  0.000000 -0.000362  0.000000  0.000000  0.000393  0.000000
0.000235
  0.000000  0.000000  0.000581
  0.000000 -0.000032 -0.000856 -0.000001  0.000000  0.000011 -0.007718
0.000000
 -0.023256  0.004421  0.000000  0.024411 -0.039776  0.000000 -0.042466
0.000000
  0.008565  0.012754  0.000000  0.020370

            NA   8.36352429459748E-01
            NB   8.36352429459748E-01
            N    1.67270485891950E+00
          FOOA  -5.96355937210708E-01
          FOOB  -5.96355937210708E-01
          ALOC   7.13043827224764E-01
          BLOC   7.13043827224764E-01
           FLA   2.39996492249040E-01
           FLB   2.39996492249040E-01
            FL   1.07634892170879E+00

 ERROR ESTIMATE FOR DIFFERENTIAL EQUATIONS
 FOR SURFACE # 1   EPSD   4.40457291031235E-08

 MAXIMUM DISTANCE REACHED FROM NUCLEUS =  9.9957520941E+00
```

B6H10-B4

```
 OMEGA DEVELOPMENT VERSION

B6H10 OPTIMIZATION USING VD SET(Renormalized) d=0.75, p=1.0725
 -V/T FOR THIS WAVEFUNCTION =        2.00128156000
 MOLECULAR SCF ENERGY (AU)  =     -153.86037391838

B6H10_B4
 INTEGRATION IS OVER ATOM   B    4
 QUADRATURE ORDER OVER THETA  64 PHI  64 AND S  64 WITH 200 POINTS/PATH
 RADIUS OF BETA SPHERE   0.9527
 VOL1 RHO CONTOUR THRESHOLD=   0.0020
 VOL2 RHO CONTOUR THRESHOLD=   0.0010

 RESULTS OF THE INTEGRATION
             N   3.77928097794298E+00     NET CHARGE   1.22071902205702E+00
             G   2.41052970916774E+01
             K   2.41054272624513E+01        E(ATOM)  -2.41363198138138E+01
             L   1.30170773931560E-04
          VNEO  -5.44151590269754E+01      VNEO(COR)  -5.44500048440740E+01
          VNET  -8.86131316269145E+01      VNET(COR)  -8.86698767882339E+01
          VEET   2.40486505647015E+01      VEET(COR)   2.40640505909815E+01
                                           VREP(COR)   4.03867845769294E+01
                                             V(ATOM)  -4.82830922113045E+01
        EL DX   3.92037431820375E-01
```

```
         EL DY  -7.96707875179496E-01
         EL DZ   7.55732569546060E-01
  EL DIPOLE MAG   1.16600536147740E+00
           QXX   1.16135709184301E+00
           QXY   1.13038634468558E+00
           QXZ  -6.95422210254328E-01
           QYY  -8.19946480656695E-01
           QYZ   1.40252114991514E+00
           QZZ  -3.41410611186319E-01
          FAXA  -3.17117723701131E-01
          FAYA   6.43425400838034E-01
          FAZA  -9.37732468413390E-01
          FBXA   1.26038851615795E+00
          FBYA  -2.94844684924364E-01
          FBZA   4.72325595272576E+00
          VOL1   3.36351444917007E+01
          VOL2   3.55037074443572E+01
       N(VOL1)   3.77442210415179E+00
       N(VOL2)   3.77712867442037E+00
```

B6H10-H6

```
 OMEGA DEVELOPMENT VERSION

B6H10 OPTIMIZATION USING VD SET(Renormalized) d=0.75, p=1.0725
 -V/T FOR THIS WAVEFUNCTION =        2.00128156000
 MOLECULAR SCF ENERGY (AU)  =     -153.86037391838

B6H10_H6
 INTEGRATION IS OVER ATOM   H    6
 QUADRATURE ORDER OVER THETA  64 PHI  64 AND S  64 WITH 200 POINTS/PATH
 RADIUS OF BETA SPHERE   1.4994
 VOL1 RHO CONTOUR THRESHOLD=   0.0020
 VOL2 RHO CONTOUR THRESHOLD=   0.0010

 RESULTS OF THE INTEGRATION
             N   1.70077874666383E+00     NET CHARGE  -7.00778746663831E-01
             G   9.11652099678939E-01
             K   9.11666270603710E-01        E(ATOM)  -9.12834625629465E-01
             L   1.41709247711506E-05
          VNEO  -1.71592552715173E+00      VNEO(COR)  -1.71702435380488E+00
          VNET  -1.87791436293304E+01      VNET(COR)  -1.87911692232252E+01
          VEET   8.35466646015256E+00      VEET(COR)   8.36001653510587E+00
                                           VREP(COR)   1.69599928080506E+01
                                             V(ATOM)  -1.83117641517461E+00
         EL DX   1.76593314502407E-01
         EL DY  -4.34247530008916E-01
         EL DZ   1.53476155517653E-01
  EL DIPOLE MAG   4.93265695501186E-01
           QXX   1.60218672228304E-01
           QXY   2.30897871830219E-01
```

```
          QXZ  -2.90768860054938E-01
          QYY  -6.32090139669447E-01
          QYZ  -1.88570614359579E-02
          QZZ   4.71871467441141E-01
         FAXA  -1.30390803905582E-01
         FAYA   2.84774286748083E-01
         FAZA  -1.21535047415928E-01
         FBXA   1.82769479947222E+00
         FBYA  -2.31681490060750E+00
         FBZA   1.39298009019296E+00
         VOL1   4.81573840087751E+01
         VOL2   5.69277050113039E+01
      N(VOL1)   1.67368655229294E+00
      N(VOL2)   1.68630760056994E+00
```

B6H10-H8

```
 PROAIM STELLIX VERSION 0.95

B6H10 OPTIMIZATION USING VD SET(Renormalized) d=0.75, p=1.0725
 -V/T FOR THIS WAVEFUNCTION =        2.00128156000
 MOLECULAR SCF ENERGY (AU)  =     -153.86037391838

B6H10_H8
 INTEGRATION IS OVER ATOM   H    8
   120 PHI PLANES     96 THETA PLANES
  80 PATHS WITH  141 POINTS PER PATH
 RADIUS OF BETA SPHERE   1.2763 WITH    120 POINTS PER PATH
 VOL1 RHO CONTOUR THRESHOLD=   0.0010
 VOL2 RHO CONTOUR THRESHOLD=   0.0020

 INSERTION LIMIT USED          =    6
 INSERTION LIMIT REACHED      0 TIMES FOR SURFACE   1
 FOR SURFACE # 1 NUMBER OF INSERTED PATHS =     28
 TOTAL NUMBER OF INSERTED PATHS=    28

 RESULTS OF THE INTEGRATION
             N   1.68340504606343E+00     NET CHARGE  -6.83405046063434E-01
             G   8.54173545021851E-01
             K   8.54292986131487E-01        E(ATOM)  -8.55387813850794E-01
             L   1.19441109636866E-04
             I   2.84351771015803E-01
         R(-1)   1.69683660674887E+00
            R1   2.28664423993142E+00
            R2   3.84391522250878E+00
            R4   1.79729609776004E+01
        GR(-1)  -2.56788522235097E+00
           GR0  -3.48467747791210E+00
           GR1  -5.99601092589080E+00
           GR2  -1.24424646651501E+01
          VNEO  -1.69683660674887E+00      VNEO(COR)  -1.69792320943648E+00
```

VNET	-1.67885858826331E+01	VNET(COR)	-1.67993367837326E+01
VEET	7.50830744245602E+00	VEET(COR)	7.51311553476960E+00
EHF	-8.42598545404561E+00		
		VREP(COR)	1.50837131749644E+01
		V(ATOM)	-1.71562360876815E+00
EL DX	3.57856686473226E-03		
EL DY	3.61012437996471E-01		
EL DZ	3.20811099810046E-06		
EL DIPOLE MAG	3.61030174001084E-01		
QXX	-3.68938128493064E-01	QXX(DIAG)	-3.70863317788765E-01
QXY	-4.46406610631977E-02		
QXZ	-4.65188201996484E-07		
QYY	6.64249764634106E-01	QYY(DIAG)	6.66174953944969E-01
QYZ	-4.50801926802728E-06		
QZZ	-2.95311636141042E-01	QZZ(DIAG)	-2.95311636156204E-01
FAXA	1.68810840964978E-03		
FAYA	-3.41548179862225E-01		
FAZA	-2.98013378785537E-07		
FBXA	-3.88411051274603E-02		
FBYA	3.47278724793792E+00		
FBZA	-2.50533436989359E-06		
RHO*L	9.45590549930682E-02		
VOL1	8.13960610534643E+01		
VOL2	6.35193310178447E+01		
N(VOL1)	1.64986542331414E+00		
N(VOL2)	1.62414216609349E+00		

THE ATOMIC OVERLAP MATRIX AOM :

```
  0.000000
  0.000000  0.000000
  0.000000  0.000000  0.000000
  0.000000  0.000000  0.000000  0.000000
  0.000000  0.000000  0.000000  0.000000  0.000000
  0.000000  0.000005  0.000004  0.000019  0.000000  0.000764
  0.000000  0.000013  0.000010  0.000035  0.000000  0.001392  0.010757
  0.000004  0.000000  0.000000  0.000000  0.000001  0.000000  0.000000
0.002259
  0.000000 -0.000005 -0.000001 -0.000018  0.000000 -0.000637 -0.004569
0.000000
  0.004970
  0.000000  0.000042  0.000035  0.000130  0.000000  0.005275  0.040704
0.000000
 -0.018281  0.162851
  0.000000  0.000000  0.000000  0.000000  0.000000  0.000000  0.000000 -
0.000031
  0.000000  0.000000  0.000213
  0.000000  0.000023  0.000020  0.000072  0.000000  0.002972  0.023573
0.000000
 -0.009719  0.095337  0.000000  0.056755
  0.000000  0.000018  0.000015  0.000060  0.000000  0.002428  0.019751
0.000000
```

```
 -0.010037  0.080494  0.000000  0.047004  0.040849
  0.000002  0.000000  0.000000  0.000000  0.000000  0.000000  0.000000
0.001132
  0.000000  0.000000  0.000000  0.000000  0.000000  0.000850
  0.000000  0.000002  0.000003  0.000003  0.000000  0.000175  0.001614
0.000000
  0.001145  0.006383  0.000000  0.004299  0.002563  0.000000  0.001723
 -0.000003  0.000000  0.000000  0.000000 -0.000001  0.000000  0.000000 -
0.001672
  0.000000  0.000000  0.000148  0.000000  0.000000 -0.000861  0.000000
0.001427
  0.000000  0.000054  0.000047  0.000185  0.000000  0.007543  0.060322
0.000000
 -0.028400  0.251156  0.000000  0.148402  0.126023  0.000000  0.009572
0.000000
  0.398462
  0.000000 -0.000024 -0.000015 -0.000093  0.000000 -0.003586 -0.028283
0.000000
  0.019153 -0.119395  0.000000 -0.068789 -0.062171  0.000000 -0.001061
0.000000
 -0.191378  0.103424
  0.000013  0.000000  0.000000  0.000000  0.000003  0.000000  0.000000
0.007478
  0.000000  0.000000 -0.000084  0.000000  0.000000  0.003709  0.000000 -
0.005482
  0.000000  0.000000  0.024953
  0.000000  0.000010  0.000016  0.000024  0.000000  0.001253  0.011229
0.000000
  0.001626  0.047327  0.000000  0.030291  0.021473  0.000000  0.006426
0.000000
  0.075160 -0.022727  0.000000  0.031445

            NA   8.41702523031717E-01
            NB   8.41702523031717E-01
            N    1.68340504606343E+00
          FOOA  -5.97326515973104E-01
          FOOB  -5.97326515973104E-01
          ALOC   7.09664637598569E-01
          BLOC   7.09664637598569E-01
           FLA   2.44376007058613E-01
           FLB   2.44376007058613E-01
            FL   1.08607853009033E+00

 ERROR ESTIMATE FOR DIFFERENTIAL EQUATIONS
 FOR SURFACE # 1   EPSD   2.55806253206157E-08

 MAXIMUM DISTANCE REACHED FROM NUCLEUS =  9.9957544428E+00
```

B6H10-B9 (not available)

B6H10-H11

```
 PROAIM STELLIX VERSION 0.95

B6H10 OPTIMIZATION USING VD SET(Renormalized) d=0.75, p=1.0725
 -V/T FOR THIS WAVEFUNCTION =        2.00128156000
 MOLECULAR SCF ENERGY (AU)  =     -153.86037391838

B6H10_H11
 INTEGRATION IS OVER ATOM   H   11
   120 PHI PLANES     96 THETA PLANES
  80 PATHS WITH  141 POINTS PER PATH
 RADIUS OF BETA SPHERE   1.2730 WITH    120 POINTS PER PATH
 VOL1 RHO CONTOUR THRESHOLD=   0.0010
 VOL2 RHO CONTOUR THRESHOLD=   0.0020

 INSERTION LIMIT USED          =    6
 INSERTION LIMIT REACHED      0 TIMES FOR SURFACE   1
 FOR SURFACE # 1 NUMBER OF INSERTED PATHS =     25
 TOTAL NUMBER OF INSERTED PATHS=    25

 RESULTS OF THE INTEGRATION
              N   1.68855443272503E+00     NET CHARGE  -6.88554432725032E-01
              G   8.70105188688871E-01
              K   8.70222778960726E-01        E(ATOM)  -8.71338021665331E-01
              L   1.17590271854761E-04
              I   2.84443068654535E-01
         R(-1)   1.70613676656944E+00
            R1   2.28573095031045E+00
            R2   3.82290699479039E+00
            R4   1.75791668322028E+01
        GR(-1)  -2.61281192350508E+00
           GR0  -3.54711483061426E+00
           GR1  -6.08053535431602E+00
           GR2  -1.25207468418131E+01
          VNEO  -1.70613676656944E+00      VNEO(COR)  -1.70722932479726E+00
          VNET  -1.58604631757013E+01      VNET(COR)  -1.58706197351748E+01
          VEET   6.99764798377156E+00      VEET(COR)   7.00212906525920E+00
           EHF  -7.99259241296902E+00
                                           VREP(COR)   1.41233834565629E+01
                                             V(ATOM)  -1.74723627861195E+00
         EL DX   1.20862341676508E-01
         EL DY   1.06108609470715E-01
         EL DZ   3.76606977461368E-01
  EL DIPOLE MAG   4.09511365058316E-01
           QXX  -1.35395927826233E-01      QXX(DIAG)  -4.26375346025709E-01
           QXY   6.47532283236647E-02
           QXZ   1.91474783738281E-01
           QYY  -3.32707931412415E-01      QYY(DIAG)  -1.89724231110571E-01
           QYZ   2.89405350515376E-01
           QZZ   4.68103859238648E-01      QZZ(DIAG)   6.16099577136279E-01
```

```
          FAXA  -1.03365848018030E-01
          FAYA  -9.43651304862180E-02
          FAZA  -3.30254187906054E-01
          FBXA   9.53749043548952E-01
          FBYA   5.95936514707352E-01
          FBZA   3.15675852387577E+00
         RHO*L   9.83077546137186E-02
          VOL1   8.05059771110096E+01
          VOL2   6.29365088755945E+01
       N(VOL1)   1.65516079340407E+00
       N(VOL2)   1.62978610662280E+00

   THE ATOMIC OVERLAP MATRIX AOM :

  0.000404
  0.000404  0.000404
 -0.000015 -0.000015  0.000001
 -0.000002 -0.000002  0.000000  0.000000
 -0.000002 -0.000002  0.000000  0.000000  0.000000
 -0.000002 -0.000002  0.000000  0.000000  0.000000  0.000000
  0.001099  0.001098 -0.000041 -0.000005 -0.000006 -0.000006  0.012303
  0.002316  0.002315 -0.000088 -0.000010 -0.000012 -0.000013  0.025665
0.055371
  0.000444  0.000444 -0.000014 -0.000003 -0.000004 -0.000003  0.005407
0.010093
  0.006403
 -0.001468 -0.001467  0.000057  0.000006  0.000008  0.000011 -0.016101 -
0.036981
 -0.006172  0.029747
  0.001930  0.001931 -0.000070 -0.000010 -0.000013 -0.000011  0.022395
0.046548
  0.015280 -0.029928  0.050469
  0.004325  0.004326 -0.000166 -0.000019 -0.000023 -0.000023  0.049110
0.107819
  0.019233 -0.071103  0.093391  0.219961
  0.001742  0.001742 -0.000067 -0.000009 -0.000010 -0.000009  0.020636
0.044988
  0.008817 -0.029190  0.040162  0.092099  0.039240
  0.004648  0.004649 -0.000180 -0.000021 -0.000026 -0.000024  0.053973
0.119306
  0.020969 -0.078022  0.104304  0.247856  0.104241  0.281525
 -0.000743 -0.000743  0.000027  0.000004  0.000005  0.000004 -0.008732 -
0.018271
 -0.006319  0.011685 -0.020669 -0.037662 -0.016205 -0.042564  0.009133
  0.001120  0.001121 -0.000045 -0.000004 -0.000005 -0.000008  0.012281
0.029397
  0.002222 -0.023171  0.020786  0.059625  0.023904  0.066671 -0.007888
0.020949
 -0.002197 -0.002197  0.000084  0.000011  0.000013  0.000011 -0.025819 -
0.056183
 -0.011943  0.035263 -0.052797 -0.118236 -0.050212 -0.135016  0.021715 -
0.029629
```

```
  0.066493
 -0.001024 -0.001024  0.000038  0.000005  0.000006  0.000007 -0.012214 -
0.027372
 -0.006973  0.020714 -0.026912 -0.055613 -0.023312 -0.062225  0.011001 -
0.015832
  0.029910  0.017194
 -0.000704 -0.000704  0.000027  0.000004  0.000005  0.000010 -0.008595 -
0.021368
 -0.005818  0.022905 -0.020123 -0.039311 -0.016063 -0.041889  0.007898 -
0.015561
  0.018238  0.016014  0.025228
  0.000545  0.000545 -0.000019 -0.000003 -0.000004 -0.000004  0.007130
0.014845
  0.006716 -0.009989  0.019463  0.031545  0.013717  0.035656 -0.007810
0.006776
 -0.018903 -0.010306 -0.008491  0.009451

            NA   8.44277216362516E-01
            NB   8.44277216362516E-01
            N    1.68855443272503E+00
          FOOA  -6.11456825392761E-01
          FOOB  -6.11456825392761E-01
          ALOC   7.24237032034527E-01
          BLOC   7.24237032034527E-01
           FLA   2.32820390969755E-01
           FLB   2.32820390969755E-01
            FL   1.07709760733227E+00

 ERROR ESTIMATE FOR DIFFERENTIAL EQUATIONS
 FOR SURFACE # 1   EPSD   3.60151196437524E-08

 MAXIMUM DISTANCE REACHED FROM NUCLEUS =  9.9957528597E+00
```

B6H10-H13

```
 OMEGA DEVELOPMENT VERSION

B6H10 OPTIMIZATION USING VD SET(Renormalized) d=0.75, p=1.0725
 -V/T FOR THIS WAVEFUNCTION =        2.00128156000
 MOLECULAR SCF ENERGY (AU)  =     -153.86037391838

B6H10_H13
 INTEGRATION IS OVER ATOM   H   13
 QUADRATURE ORDER OVER THETA  64 PHI  64 AND S  64 WITH 200 POINTS/PATH
 RADIUS OF BETA SPHERE   1.5774
 VOL1 RHO CONTOUR THRESHOLD=   0.0020
 VOL2 RHO CONTOUR THRESHOLD=   0.0010

 RESULTS OF THE INTEGRATION
             N   1.71883620817223E+00     NET CHARGE  -7.18836208172234E-01
             G   9.19379222342972E-01
```

K	9.19394543789713E-01	E(ATOM)	-9.20572803061252E-01
L	1.53214467411983E-05		
VNEO	-1.72582806860141E+00	VNEO(COR)	-1.72693323654170E+00
VNET	-1.90307459545517E+01	VNET(COR)	-1.90429326669429E+01
VEET	8.48502995205652E+00	VEET(COR)	8.49046350783533E+00
		VREP(COR)	1.71962121634796E+01
		V(ATOM)	-1.84672050346335E+00
EL DX	-3.69353694003519E-02		
EL DY	-4.48634924103093E-01		
EL DZ	9.94430510618108E-02		
EL DIPOLE MAG	4.61005896971189E-01		
QXX	5.00395613859065E-01		
QXY	7.67018146136258E-03		
QXZ	8.21657381909888E-02		
QYY	-5.48557931249652E-01		
QYZ	-4.71028413201757E-02		
QZZ	4.81623173905866E-02		
FAXA	NaN0xffffffffffff		
FAYA	NaN0xffffffffffff		
FAZA	NaN0xffffffffffff		
FBXA	-5.84806969247165E-01		
FBYA	-2.80280086708306E+00		
FBZA	1.71926191269175E+00		
VOL1	5.00994108073769E+01		
VOL2	5.98228226592961E+01		
N(VOL1)	1.68845480786696E+00		
N(VOL2)	1.70243666977697E+00		

B6H10-H15

```
 PROAIM STELLIX VERSION 0.95

B6H10 OPTIMIZATION USING VD SET(Renormalized) d=0.75, p=1.0725
 -V/T FOR THIS WAVEFUNCTION =        2.00128156000
 MOLECULAR SCF ENERGY (AU)  =     -153.86037391838

B6H10_H15
 INTEGRATION IS OVER ATOM   H   15
   120 PHI PLANES     96 THETA PLANES
  80 PATHS WITH  141 POINTS PER PATH
 RADIUS OF BETA SPHERE   1.2797 WITH    120 POINTS PER PATH
 VOL1 RHO CONTOUR THRESHOLD=   0.0010
 VOL2 RHO CONTOUR THRESHOLD=   0.0020

 INSERTION LIMIT USED          =    6
 INSERTION LIMIT REACHED      0 TIMES FOR SURFACE   1
 FOR SURFACE # 1 NUMBER OF INSERTED PATHS =     50
 TOTAL NUMBER OF INSERTED PATHS=    50

 RESULTS OF THE INTEGRATION
             N   1.70069703105939E+00     NET CHARGE  -7.00697031059390E-01
```

G	8.65263277378957E-01		
K	8.65371966045888E-01	E(ATOM)	-8.66480992142694E-01
L	1.08688666930458E-04		
I	2.87658460060504E-01		
R(-1)	1.70750000161219E+00		
R1	2.32459303971316E+00		
R2	3.94231784940900E+00		
R4	1.89312580924849E+01		
GR(-1)	-2.61738931583945E+00		
GR0	-3.58434572073517E+00		
GR1	-6.23204432256008E+00		
GR2	-1.30906148375076E+01		
VNEO	-1.70750000161219E+00	VNEO(COR)	-1.70859343281438E+00
VNET	-1.58104692442768E+01	VNET(COR)	-1.58205937891532E+01
VEET	7.00224957347874E+00	VEET(COR)	7.00673360168484E+00
EHF	-7.94284770475213E+00		
		VREP(COR)	1.40831003142943E+01
		V(ATOM)	-1.73749347485897E+00
EL DX	-2.62145945257587E-01		
EL DY	1.22065425289498E-01		
EL DZ	2.63233586272284E-01		
EL DIPOLE MAG	3.91040132988761E-01		
QXX	3.08187926551054E-01	QXX(DIAG)	-5.33835614867044E-01
QXY	-2.80367588167379E-01		
QXZ	-3.69251700850293E-01		
QYY	-4.40327906864368E-01	QYY(DIAG)	-1.47501200294571E-01
QYZ	1.31760918522026E-01		
QZZ	1.32139980313313E-01	QZZ(DIAG)	6.81336815161614E-01
FAXA	2.43701674110835E-01		
FAYA	-9.87722967568209E-02		
FAZA	-2.27109803659572E-01		
FBXA	-2.51768613990229E+00		
FBYA	5.73635741978374E-01		
FBZA	2.07300476877528E+00		
RHO*L	9.62254140440785E-02		
VOL1	8.29544854696553E+01		
VOL2	6.45533924959749E+01		
N(VOL1)	1.66544275229673E+00		
N(VOL2)	1.63889936334930E+00		

THE ATOMIC OVERLAP MATRIX AOM :

```
  0.000000
  0.000000  0.000000
  0.000000  0.000000  0.000000
  0.000002  0.000002  0.000000  0.000402
  0.000002  0.000002  0.000000  0.000402  0.000402
  0.000000  0.000000  0.000000 -0.000009 -0.000009  0.000000
  0.000007  0.000008 -0.000001  0.000758  0.000756 -0.000017  0.006199
  0.000013  0.000014 -0.000001  0.001334  0.001335 -0.000032  0.010936
0.020621
```

```
 -0.000014 -0.000015  0.000001 -0.001749 -0.001744  0.000041 -0.013822 -
0.024399
  0.032425
 -0.000007 -0.000007  0.000000 -0.000772 -0.000772  0.000020 -0.005996 -
0.012633
  0.014135  0.010470
 -0.000022 -0.000024  0.000001 -0.002730 -0.002729  0.000066 -0.021821 -
0.040692
  0.051311  0.025362  0.085133
 -0.000005 -0.000006  0.000000 -0.001117 -0.001109  0.000027 -0.007799 -
0.012840
  0.020737  0.008057  0.031451  0.017763
  0.000024  0.000026 -0.000001  0.003326  0.003318 -0.000080  0.026765
0.047985
 -0.065164 -0.028656 -0.105003 -0.044259  0.136495
  0.000009  0.000010  0.000000  0.001158  0.001158 -0.000027  0.010045
0.018205
 -0.024007 -0.010139 -0.039171 -0.015135  0.050743  0.019827
 -0.000015 -0.000017  0.000000 -0.002433 -0.002425  0.000058 -0.019491 -
0.033921
  0.048800  0.019236  0.077283  0.035590 -0.104236 -0.038720  0.081865
 -0.000030 -0.000034  0.000000 -0.004354 -0.004348  0.000104 -0.035400 -
0.064139
  0.086874  0.037925  0.141866  0.059298 -0.184453 -0.069186  0.141648
0.252099
  0.000008  0.000009  0.000000  0.000826  0.000829 -0.000021  0.007122
0.014761
 -0.016398 -0.010702 -0.029772 -0.008695  0.033886  0.012588 -0.023337 -
0.046290
  0.012708
  0.000021  0.000024 -0.000001  0.002679  0.002682 -0.000066  0.022488
0.043856
 -0.053774 -0.028872 -0.092706 -0.032690  0.113469  0.042967 -0.083289 -
0.155407
  0.034235  0.104909
 -0.000009 -0.000010  0.000000 -0.001488 -0.001485  0.000039 -0.011708 -
0.022857
  0.030182  0.017761  0.051453  0.022146 -0.065236 -0.023050  0.048672
0.088101
 -0.018973 -0.058031  0.037906
 -0.000010 -0.000011  0.000001 -0.000483 -0.000496  0.000006 -0.006287 -
0.011933
  0.010665  0.001582  0.019532 -0.001107 -0.020187 -0.011348  0.013892
0.030848
 -0.007093 -0.022467  0.000906  0.031126

            NA    8.50348515529695E-01
            NB    8.50348515529695E-01
            N     1.70069703105939E+00
          FOOA   -6.13666229825418E-01
          FOOB   -6.13666229825418E-01
          ALOC    7.21664374804202E-01
```

```
          BLOC   7.21664374804202E-01
           FLA   2.36682285704277E-01
           FLB   2.36682285704277E-01
            FL   1.08703080123397E+00

 ERROR ESTIMATE FOR DIFFERENTIAL EQUATIONS
 FOR SURFACE # 1   EPSD   6.10427306056258E-08

 MAXIMUM DISTANCE REACHED FROM NUCLEUS =  9.9957561066E+00
```

B6H6(2-)-B1(difference)

B6H6(2-)-H7

```
 PROAIM VERSION 0.90

B6H6(2-) OPTIMIZATION USING VD SET(Renormalized); d=0.75, p=1.0725
 -V/T FOR THIS WAVEFUNCTION =        2.00103013000
 MOLECULAR SCF ENERGY (AU)  =     -151.46609702870

H7 of B6H6 9s/5p + 1d on B, F
 INTEGRATION IS OVER ATOM   H    7
   120 PHI PLANES     96 THETA PLANES
  80 PATHS WITH  141 POINTS PER PATH
 RADIUS OF BETA SPHERE   1.3340 WITH    120 POINTS PER PATH
 VOL1 RHO CONTOUR THRESHOLD=   0.0010
 VOL2 RHO CONTOUR THRESHOLD=   0.0020

 INSERTION LIMIT USED          =   15
 INSERTION LIMIT REACHED      0 TIMES FOR SURFACE   1
 FOR SURFACE # 1 NUMBER OF INSERTED PATHS =     24
 TOTAL NUMBER OF INSERTED PATHS=    24

 RESULTS OF THE INTEGRATION
             N   1.80074679715924E+00     NET CHARGE  -8.00746797159236E-01
             G   8.39306651714599E-01
             K   8.39388440877932E-01        E(ATOM)  -8.40253120092534E-01
             L   8.17891633335982E-05
             I   3.27082109441133E-01
         R(-1)   1.73030378041836E+00
            R1   2.63535558866732E+00
            R2   4.91837399154160E+00
            R4   3.10078177019374E+01
        GR(-1)  -2.70105107396883E+00
           GR0  -3.89693556340408E+00
           GR1  -7.35325420128882E+00
           GR2  -1.72793921506833E+01
          VNEO  -1.73030378041836E+00      VNEO(COR)  -1.73119454053567E+00
          VNET  -1.53854136448303E+01      VNET(COR)  -1.53933340533840E+01
          VEET   7.12401786835160E+00      VEET(COR)   7.12768531164328E+00
```

```
          EHF  -7.42200733560075E+00

                                          VREP(COR)   1.37094395271515E+01
                                            V(ATOM)  -1.68389452623252E+00

        EL DX  -6.14172604600043E-06
        EL DY   1.18796372204766E-06
        EL DZ  -2.44187416347490E-01
 EL DIPOLE MAG   2.44187416427617E-01
          QXX  -4.34946467703815E-01      QXX(DIAG)  -4.35160044362610E-01
          QXY  -4.86455143049101E-06
          QXZ  -5.59684818249574E-06
          QYY  -4.35159933560785E-01      QYY(DIAG)  -4.34946356930297E-01
          QYZ   2.37002430564518E-06
          QZZ   8.70106401264601E-01      QZZ(DIAG)   8.70106401292907E-01
         FAXA   3.16563965031239E-07
         FAYA  -4.73087754393007E-08
         FAZA   2.84704533173427E-01
         FBXA   2.28323922633363E-06
         FBYA  -3.70169050196273E-07
         FBZA  -3.22900591364439E+00
        RHO*L   8.85536435172818E-02
         VOL1   1.04312143005762E+02
         VOL2   7.83426380356486E+01
      N(VOL1)   1.75020577547282E+00
      N(VOL2)   1.71389482855467E+00

 THE ATOMIC OVERLAP MATRIX AOM :

  0.000122
  0.000212  0.000368
  0.000000  0.000000  0.000000
  0.000000  0.000000  0.000000  0.000000
  0.000163  0.000283  0.000000  0.000000  0.000217
 -0.000058 -0.000101  0.000000  0.000000 -0.000078  0.000028
  0.000418  0.000722  0.000000  0.000000  0.000554 -0.000198  0.006776
 -0.002101 -0.003635  0.000000  0.000000 -0.002794  0.000999 -0.034651
0.189224
 -0.000001 -0.000002  0.000004  0.000000 -0.000001  0.000000 -0.000016
0.000087
  0.003724
  0.000003  0.000005  0.000000  0.000004  0.000004 -0.000001  0.000049 -
0.000262
  0.000000  0.003724
 -0.001551 -0.002685  0.000000  0.000000 -0.002065  0.000738 -0.026524
0.148112
  0.000070 -0.000209  0.116907
  0.002319  0.004016  0.000000  0.000000  0.003089 -0.001104  0.039397 -
0.221256
 -0.000104  0.000312 -0.174782  0.261824
  0.000419  0.000726  0.000000  0.000000  0.000558 -0.000200  0.007118 -
0.039975
 -0.000019  0.000056 -0.031578  0.047267  0.008750
```

```
  0.001926  0.003340  0.000000  0.000000  0.002571 -0.000919  0.035056 -
0.204241
 -0.000095  0.000295 -0.163387  0.245317  0.044322  0.234354
 -0.000003 -0.000006  0.000000  0.000004 -0.000005  0.000002 -0.000062
0.000367
 -0.000071  0.003899  0.000289 -0.000434 -0.000078 -0.000407  0.004281
  0.000001  0.000001 -0.000004  0.000000  0.000001  0.000000  0.000010 -
0.000055
 -0.003899 -0.000071 -0.000046  0.000068  0.000012  0.000064  0.000000
0.004280
  0.000000  0.000000 -0.000013  0.000000  0.000000  0.000000  0.000000
0.000005
 -0.010829 -0.000031  0.000000  0.000000  0.000000 -0.000003  0.000173
0.011227
  0.032512
  0.000000  0.000000  0.000000  0.000013  0.000000  0.000000  0.000000
0.000015
 -0.000031  0.010829  0.000000  0.000000  0.000000  0.000020  0.011227 -
0.000173
  0.000001  0.032514
  0.000000  0.000000  0.000000  0.000000  0.000000  0.000000  0.000000
0.000000
  0.000078  0.000054  0.000000  0.000000  0.000000  0.000000  0.000055 -
0.000082
 -0.000230  0.000158  0.000768

            NA   9.00373398579618E-01
            NB   9.00373398579618E-01
            N    1.80074679715924E+00
          FOOA  -6.59600320425087E-01
          FOOB  -6.59600320425087E-01
          ALOC   7.32585304569901E-01
          BLOC   7.32585304569901E-01
           FLA   2.40773078154532E-01
           FLB   2.40773078154532E-01
            FL   1.14114647673415E+00

 ERROR ESTIMATE FOR DIFFERENTIAL EQUATIONS
 FOR SURFACE # 1   EPSD   3.28904670960360E-08

 MAXIMUM DISTANCE REACHED FROM NUCLEUS =  9.9957825546E+00
```

B7H7(2-)-B1(not available)

```
 PROAIM STELLIX VERSION 0.95

B7H7 2- OPTIMIZATION USING VD SET ON H & 9S/5P+1D ON B
 -V/T FOR THIS WAVEFUNCTION =        2.00104940000
 MOLECULAR SCF ENERGY (AU)  =     -176.75968995430

B7 of B7H7(2-) 9s/5p + 1d on B, F
```

```
INTEGRATION IS OVER ATOM   B     7
  120 PHI PLANES      96 THETA PLANES
 80 PATHS WITH  141 POINTS PER PATH
RADIUS OF BETA SPHERE   0.9594 WITH     120 POINTS PER PATH
VOL1 RHO CONTOUR THRESHOLD=   0.0010
VOL2 RHO CONTOUR THRESHOLD=   0.0020

INSERTION LIMIT USED           =     6
INSERTION LIMIT REACHED       0 TIMES FOR SURFACE   1
INSERTION LIMIT REACHED       3 TIMES FOR SURFACE   2
INSERTION LIMIT REACHED       2 TIMES FOR SURFACE   3
INSERTION LIMIT REACHED       2 TIMES FOR SURFACE   4
INSERTION LIMIT REACHED       2 TIMES FOR SURFACE   5
INSERTION LIMIT REACHED       2 TIMES FOR SURFACE   6
FOR SURFACE # 1 NUMBER OF INSERTED PATHS =      15
FOR SURFACE # 2 NUMBER OF INSERTED PATHS =      21
FOR SURFACE # 3 NUMBER OF INSERTED PATHS =      20
FOR SURFACE # 4 NUMBER OF INSERTED PATHS =      21
FOR SURFACE # 5 NUMBER OF INSERTED PATHS =      21
FOR SURFACE # 6 NUMBER OF INSERTED PATHS =      21
TOTAL NUMBER OF INSERTED PATHS=   119

RESULTS OF THE INTEGRATION
             N   1.42552628463911E+01     NET CHARGE  -9.25526284639111E+00
             G   5.20939579501510E+01
             K   4.81707637386635E+01        E(ATOM)  -4.82213141381309E+01
             L  -3.92319421148749E+00
             I   1.79713636800870E+00
        R(-1)   1.21564664204503E+01
           R1   4.64892868775494E+01
           R2   1.92708223375180E+02
           R4   4.56713080297892E+03
       GR(-1)  -2.15444631825038E+01
          GR0  -3.56127370727284E+01
          GR1  -1.63773015865307E+02
          GR2  -8.88976036717321E+02
         VNEO  -6.07823321022513E+01      VNEO(COR)  -6.08142078666917E+01
         VNET  -2.60295554492543E+02      VNET(COR)  -2.60432059945574E+02
         VEET   9.04385391049488E+01      VEET(COR)   9.04859673208322E+01
          EHF  -1.21686251648931E+02
                                          VREP(COR)   1.63950904831632E+02
                                            V(ATOM)  -9.64811551139419E+01
        EL DX  -2.20721100688676E+00
        EL DY  -3.45692652078140E+00
        EL DZ   2.81058381125221E+01
 EL DIPOLE MAG   2.84035254397461E+01
           QXX   5.26041602646179E+01      QXX(DIAG)   6.83341701383365E+01
           QXY   1.91421177858890E+01
           QXZ   1.20548169543276E+01
           QYY   2.51063512223305E+01      QYY(DIAG)   2.18497631830605E+01
           QYZ   3.75511922200811E+01
           QZZ  -7.77105114869484E+01      QZZ(DIAG)  -9.01839333213970E+01
```

```
          FAXA   4.89304165142979E-01
          FAYA  -2.13674338726150E+00
          FAZA   3.28304808515742E+00
          FBXA  -1.18669739431977E+01
          FBYA  -2.13182572003148E+02
          FBZA  -8.18858173271039E+01
         RHO*L   6.93095079558815E+02
          VOL1   3.87753523037049E+02
          VOL2   3.18981312884027E+02
       N(VOL1)   1.41320154320612E+01
       N(VOL2)   1.40331438964283E+01

  THE ATOMIC OVERLAP MATRIX AOM :

  0.415588
  0.407221  0.415564
 -0.005071 -0.002074  0.242178
 -0.000029  0.001690  0.136691  0.212501
  0.000026 -0.002155 -0.176148 -0.052305  0.271604
 -0.000002  0.000154  0.012939  0.186964  0.087608  0.382973
  0.000014 -0.001035 -0.083949  0.011534  0.119183  0.070589  0.100781
 -0.003981  0.004914  0.027302 -0.000490  0.011426 -0.003552  0.001842
0.479510
 -0.001498  0.000245 -0.009758  0.019575  0.002210 -0.014567  0.004493
0.047791
  0.392493
 -0.000293 -0.001053 -0.018934 -0.002074 -0.016761  0.009476  0.000600 -
0.026141
  0.056175  0.426787
  0.004282 -0.005594 -0.013449 -0.008048  0.008251 -0.000478  0.004769
0.048247
 -0.035869 -0.035918  0.324852
 -0.000754  0.001671  0.015454  0.011719 -0.014657  0.001623 -0.007478
0.045917
  0.010095  0.040576  0.034488  0.220548
  0.004017  0.000392  0.005083 -0.001398  0.004494 -0.001076  0.001270
0.025162
 -0.002260 -0.014985 -0.036153  0.007365  0.158202
  0.000199 -0.000104  0.004989  0.011138 -0.003589 -0.001308  0.006966 -
0.026640
  0.001661 -0.039722  0.008702  0.003404 -0.002466  0.168696
 -0.000012  0.000019 -0.003240  0.018340  0.011760  0.015901  0.001284
0.009841
  0.026334 -0.030482  0.001330 -0.016666  0.003058 -0.016914  0.245119
 -0.000329  0.000927  0.000082  0.007350  0.024302  0.007968  0.011600
0.020736
  0.024837 -0.129805  0.014798 -0.002117  0.004921 -0.002745 -0.019656
0.266191
 -0.001494  0.000092  0.009828  0.026562 -0.016975  0.005947 -0.001676
0.038466
  0.156177  0.088385 -0.025551  0.009241  0.000276 -0.019296 -0.004525 -
0.016945
```

```
  0.282225
 -0.006012 -0.000249  0.019380  0.011425 -0.011737  0.000677 -0.006791 -
0.029984
  0.034818  0.039428 -0.173910 -0.043546  0.014886 -0.008198 -0.002180 -
0.018166
  0.023756  0.275427
 -0.000378  0.000445  0.011769 -0.013527 -0.003636  0.020477  0.004069
0.063555
 -0.064347  0.117888 -0.009759 -0.030905  0.013041 -0.036002 -0.089934 -
0.000521
  0.004375  0.008191  0.417220
  0.000239 -0.000329  0.001246 -0.001182  0.002880  0.010633  0.011180 -
0.052561
 -0.004449  0.070219 -0.009159  0.039223 -0.012475  0.056788 -0.188807
0.019886
 -0.019212  0.015290  0.030610  0.492844
  0.000795 -0.002362 -0.016616 -0.021547  0.010758 -0.014409 -0.001528 -
0.060908
 -0.011751 -0.023992  0.055511  0.009019  0.012236  0.004670  0.021037
0.025609
  0.039066 -0.035806 -0.008709  0.021431  0.465447
  0.001384 -0.000243  0.011330  0.000049 -0.024249 -0.010537 -0.011589
0.042175
  0.017075 -0.002259 -0.003027 -0.004703 -0.003629 -0.012692  0.033988
0.057088
 -0.010156 -0.008196 -0.028564 -0.041427 -0.055934  0.470882

            NA   7.12763142319556E+00
            NB   7.12763142319556E+00
            N    1.42552628463911E+01
          FOOA  -3.63355413713479E+00
          FOOB  -3.63355413713479E+00
          ALOC   5.09784235659278E-01
          BLOC   5.09784235659278E-01
           FLA   3.49407728606076E+00
           FLB   3.49407728606076E+00
            FL   1.06217087092563E+01

 ERROR ESTIMATE FOR DIFFERENTIAL EQUATIONS
 FOR SURFACE # 1   EPSD   3.82716945995915E-08
 FOR SURFACE # 2   EPSD   2.38878791124776E-02
 FOR SURFACE # 3   EPSD   2.38878791124776E-02
 FOR SURFACE # 4   EPSD   2.38889550021266E-02
 FOR SURFACE # 5   EPSD   2.38889550021266E-02
 FOR SURFACE # 6   EPSD   2.39547605277163E-02

 MAXIMUM DISTANCE REACHED FROM NUCLEUS =  1.0000000000E+01
```

B7H7(2-)-B7(not available)

B7H7(2-)-H14

```
 PROAIM STELLIX VERSION 0.95

B7H7 2- OPTIMIZATION USING VD SET ON H & 9S/5P+1D ON B
 -V/T FOR THIS WAVEFUNCTION =        2.00104940000
 MOLECULAR SCF ENERGY (AU)  =     -176.75968995430

H14 of B7H7(2-) 9s/5p + 1d on B, F
 INTEGRATION IS OVER ATOM   H   14
   120 PHI PLANES     96 THETA PLANES
  80 PATHS WITH  141 POINTS PER PATH
 RADIUS OF BETA SPHERE   1.3370 WITH    120 POINTS PER PATH
 VOL1 RHO CONTOUR THRESHOLD=   0.0010
 VOL2 RHO CONTOUR THRESHOLD=   0.0020

 INSERTION LIMIT USED          =    6
 INSERTION LIMIT REACHED      0 TIMES FOR SURFACE   1
 FOR SURFACE # 1 NUMBER OF INSERTED PATHS =     15
 TOTAL NUMBER OF INSERTED PATHS=    15

 RESULTS OF THE INTEGRATION
              N   1.79569026860446E+00     NET CHARGE  -7.95690268604455E-01
              G   8.52552551019213E-01
              K   8.52645069916092E-01        E(ATOM)  -8.53539835652462E-01
              L   9.25188968789713E-05
              I   2.86102900767294E-01
         R(-1)   1.73870578492261E+00
            R1   2.59376200289450E+00
            R2   4.74772090487417E+00
            R4   2.83634138984197E+01
        GR(-1)  -2.70971090804039E+00
           GR0  -3.86426209805032E+00
           GR1  -7.15671494080445E+00
           GR2  -1.64102808636530E+01
          VNEO  -1.73870578492261E+00      VNEO(COR)  -1.73961760541574E+00
          VNET  -1.73235455241544E+01      VNET(COR)  -1.73326304216453E+01
          VEET   8.06603077741448E+00      VEET(COR)   8.07026080426830E+00
           EHF  -8.40486967682387E+00
                                           VREP(COR)   1.56215906454397E+01
                                             V(ATOM)  -1.71103977620555E+00
         EL DX   1.01963039455530E-05
         EL DY   1.04204756298558E-05
         EL DZ   2.67934453439259E-01
  EL DIPOLE MAG  2.67934453835906E-01
           QXX  -3.52865375701862E-01      QXX(DIAG)  -3.52814791924183E-01
           QXY  -7.20362553420585E-05
```

```
          QXZ  -3.41766215832166E-05
          QYY  -3.52917377964891E-01      QYY(DIAG)  -3.52967963326018E-01
          QYZ  -2.25477956500224E-05
          QZZ   7.05782753666753E-01      QZZ(DIAG)   7.05782755250201E-01
         FAXA  -5.73207535397311E-07
         FAYA  -4.00736470521334E-07
         FAZA  -2.94129793313684E-01
         FBXA  -4.34293589546628E-06
         FBYA  -3.00942125998268E-06
         FBZA   3.48897716033879E+00
        RHO*L   9.11397811390659E-02
         VOL1   1.02048367701089E+02
         VOL2   7.71590880905324E+01
      N(VOL1)   1.74965479737104E+00
      N(VOL2)   1.71589026654640E+00

   THE ATOMIC OVERLAP MATRIX AOM :

  0.000374
  0.000374  0.000374
 -0.000005 -0.000005  0.000000
  0.000000  0.000000  0.000000  0.000000
  0.000000  0.000000  0.000000  0.000000  0.000000
  0.000000  0.000000  0.000000  0.000000  0.000000  0.000000
  0.000000  0.000000  0.000000  0.000000  0.000000  0.000000  0.000000
  0.000821  0.000821 -0.000008  0.000000  0.000000  0.000000  0.000000
0.008210
  0.000000  0.000000  0.000000  0.000004 -0.000001  0.000000  0.000000
0.000000
  0.003687
  0.000000  0.000000  0.000000 -0.000001 -0.000004  0.000000  0.000000
0.000000
  0.000000  0.003687
  0.003922  0.003922 -0.000045  0.000000  0.000000  0.000000  0.000000
0.040407
  0.000000  0.000000  0.212188
 -0.000524 -0.000524  0.000006  0.000000  0.000000  0.000000  0.000000 -
0.005984
  0.000000  0.000000 -0.032061  0.005020
 -0.004952 -0.004952  0.000060  0.000000  0.000000  0.000000  0.000000 -
0.052464
  0.000000  0.000000 -0.282812  0.043049  0.380882
  0.000000  0.000000  0.000000  0.000000  0.000000  0.000000  0.000000
0.000000
  0.000000  0.000000  0.000000  0.000000  0.000000  0.000224
  0.000000  0.000000  0.000000  0.000000  0.000000  0.000000  0.000000
0.000000
  0.000000  0.000000  0.000000  0.000000  0.000000  0.000000  0.000224
  0.000000  0.000000  0.000000  0.000002  0.000003  0.000000  0.000000
0.000000
  0.001175 -0.002903  0.000000  0.000000  0.000000  0.000000  0.000000
0.002841
```

```
  0.000000  0.000000  0.000000  0.000003 -0.000002  0.000000  0.000000
0.000000
  0.002903  0.001175  0.000000  0.000000  0.000000  0.000000  0.000000
0.000000
  0.002841
  0.003172  0.003173 -0.000043  0.000000  0.000000  0.000000  0.000000
0.036336
  0.000000  0.000000  0.205625 -0.031771 -0.282127  0.000000  0.000000
0.000000
  0.000000  0.215945
  0.000000  0.000000  0.000000  0.000000  0.000000  0.000000  0.000000
0.000000
  0.000000  0.000000  0.000000  0.000000  0.000000 -0.000190 -0.000114
0.000000
  0.000000  0.000000  0.000373
  0.000000  0.000000  0.000000  0.000000  0.000000  0.000000  0.000000
0.000000
  0.000000  0.000000  0.000000  0.000000  0.000000  0.000114 -0.000190
0.000000
  0.000000  0.000000  0.000000  0.000373
  0.000000  0.000000  0.000000  0.000014 -0.000003  0.000000  0.000000
0.000000
  0.010332  0.001225 -0.000001  0.000000  0.000001  0.000000  0.000000
0.002276
  0.008331  0.000000  0.000000  0.000000  0.030302
  0.000000  0.000000  0.000000  0.000003  0.000014  0.000000  0.000000
0.000000
  0.001225 -0.010331  0.000000  0.000000  0.000000  0.000000  0.000000
0.008331
 -0.002276  0.000000  0.000000  0.000000  0.000000  0.030301

            NA   8.97845134302228E-01
            NB   8.97845134302228E-01
            N    1.79569026860446E+00
          FOOA  -6.62657729074756E-01
          FOOB  -6.62657729074756E-01
          ALOC   7.38053483566238E-01
          BLOC   7.38053483566238E-01
           FLA   2.35187405227472E-01
           FLB   2.35187405227472E-01
            FL   1.13303253952970E+00

 ERROR ESTIMATE FOR DIFFERENTIAL EQUATIONS
 FOR SURFACE # 1   EPSD   2.94889278462971E-08

 MAXIMUM DISTANCE REACHED FROM NUCLEUS =  9.9957840200E+00
```

B12H12(2-)-B1(difference)

B12H12(2-)-H13

```
 PROAIM VERSION 0.90

B12H12 OPTIMIZATION USING VD SET(Renormalized) d=0.75, p=1.0725
 -V/T FOR THIS WAVEFUNCTION =        2.00077777000
 MOLECULAR SCF ENERGY (AU)  =     -303.32680385098

B12H12(2-) Integration of H13
 INTEGRATION IS OVER ATOM   H   13
   120 PHI PLANES     96 THETA PLANES
  80 PATHS WITH  141 POINTS PER PATH
 RADIUS OF BETA SPHERE   1.3120 WITH    120 POINTS PER PATH
 VOL1 RHO CONTOUR THRESHOLD=   0.0010
 VOL2 RHO CONTOUR THRESHOLD=   0.0020

 INSERTION LIMIT USED          =   15
 INSERTION LIMIT REACHED      0 TIMES FOR SURFACE   1
 FOR SURFACE # 1 NUMBER OF INSERTED PATHS =     30
 TOTAL NUMBER OF INSERTED PATHS=    30

 RESULTS OF THE INTEGRATION
              N   1.73930321163559E+00     NET CHARGE  -7.39303211635592E-01
              G   8.56592185636492E-01
              K   8.56726349009029E-01        E(ATOM)  -8.57392685061498E-01
              L   1.34163372535944E-04
              I   1.74819248524263E-01
         R(-1)   1.72593404948332E+00
            R1   2.41988375263777E+00
            R2   4.20577669621930E+00
            R4   2.17214188239885E+01
        GR(-1)  -2.63270039078098E+00
           GR0  -3.62460435958095E+00
           GR1  -6.38839842082387E+00
           GR2  -1.37445243634467E+01
          VNEO  -1.72593404948332E+00      VNEO(COR)  -1.72660497843195E+00
          VNET  -2.41010155604970E+01      VNET(COR)  -2.41103844405163E+01
          VEET   1.14149708824525E+01      VEET(COR)   1.14194082677715E+01
           EHF  -1.18293183290355E+01
                                           VREP(COR)   2.23913339117455E+01
                                             V(ATOM)  -1.71905052877084E+00
         EL DX  -6.12392827532609E-06
         EL DY  -5.94151331159713E-06
         EL DZ   2.71748299310967E-01
  EL DIPOLE MAG   2.71748299444922E-01
            QXX  -2.71918910820894E-01      QXX(DIAG)  -2.71846156363324E-01
```

```
          QXY  -3.17248602973391E-05
          QXZ   1.65486481635199E-05
          QYY  -2.71859990107817E-01      QYY(DIAG)  -2.71932744942060E-01
          QYZ   5.77916051216250E-06
          QZZ   5.43778900928711E-01      QZZ(DIAG)   5.43778901305384E-01
         FAXA   5.46101809414013E-07
         FAYA   1.93374812368979E-07
         FAZA  -3.05155534694159E-01
         FBXA   3.94414788716782E-06
         FBYA   1.85005323027382E-06
         FBZA   4.26358577491424E+00
        RHO*L   9.30195406499754E-02
         VOL1   8.78980973569109E+01
         VOL2   6.83937819963783E+01
      N(VOL1)   1.69959887287177E+00
      N(VOL2)   1.67060530937222E+00

   THE ATOMIC OVERLAP MATRIX AOM :

  0.000062
  0.000108  0.000186
 -0.000001 -0.000002  0.000000
  0.000000  0.000000  0.000000  0.000000
  0.000139  0.000240 -0.000003  0.000000  0.000309
  0.000000 -0.000001  0.000000  0.000000 -0.000001  0.000000
  0.000000  0.000000  0.000000  0.000000  0.000000  0.000000  0.000000
  0.000000  0.000000  0.000000  0.000000  0.000000  0.000000  0.000000
0.000000
  0.000000  0.000000  0.000000  0.000000  0.000000  0.000000  0.000000
0.000000
  0.000000
  0.000107  0.000186 -0.000002  0.000000  0.000240 -0.000001  0.000000
0.000000
  0.000000  0.000186
  0.000000  0.000000  0.000000  0.000000  0.000000  0.000000  0.000000
0.000000
  0.000000  0.000000  0.000000
  0.000000  0.000000  0.000000  0.000000  0.000000  0.000000  0.000000
0.000000
  0.000000  0.000000  0.000000  0.000000
  0.000246  0.000424 -0.000005  0.000000  0.000544 -0.000001  0.000000
0.000000
  0.000000  0.000421  0.000000  0.000000  0.004247
  0.000000  0.000000  0.000001  0.000000  0.000000  0.000000  0.000000
0.000002
  0.000000  0.000000  0.000000  0.000000 -0.000001  0.001270
  0.000000  0.000000  0.000000 -0.000001  0.000000  0.000000  0.000000
0.000000
  0.000002  0.000000  0.000000  0.000000  0.000000  0.000000  0.001270
  0.000705  0.001215 -0.000014  0.000000  0.001562 -0.000004  0.000000 -
0.000001
```

```
  0.000000  0.001209  0.000001  0.000000  0.012138 -0.000004  0.000000
0.035467
 -0.000001 -0.000001  0.000000  0.000000 -0.000002  0.000000  0.000000
0.000000
  0.000000 -0.000001  0.000000  0.000000 -0.000012  0.000000  0.000000 -
0.000037
  0.000249
  0.000000  0.000000  0.000000  0.000000  0.000000  0.000000  0.000000
0.000000
  0.000000  0.000000  0.000000  0.000000  0.000000  0.000000 -0.000001
0.000000
  0.000000  0.000249
  0.001433  0.002472 -0.000028  0.000000  0.003181 -0.000007  0.000000 -
0.000002
  0.000000  0.002464  0.000001  0.000000  0.025016 -0.000008  0.000000
0.074862
 -0.000079  0.000000  0.162358
  0.000000  0.000000  0.000003  0.000000  0.000000  0.000000  0.000000
0.000005
  0.000000  0.000000  0.000000  0.000000 -0.000002  0.002737  0.000001 -
0.000007
  0.000001  0.000000 -0.000015  0.005947
  0.000000  0.000000  0.000000  0.000003  0.000000  0.000000  0.000000
0.000000
 -0.000005  0.000000  0.000000  0.000000  0.000000  0.000001 -0.002737
0.000000
  0.000000  0.000001  0.000000  0.000000  0.005947
  0.000775  0.001336 -0.000015  0.000000  0.001720 -0.000004  0.000000 -
0.000001
  0.000000  0.001332  0.000001  0.000000  0.014181 -0.000005  0.000000
0.042577
 -0.000045  0.000000  0.092692 -0.000009  0.000000  0.053310
 -0.000020 -0.000034  0.000000  0.000000 -0.000044  0.000000  0.000000
0.000000
  0.000000 -0.000034  0.000000  0.000000 -0.000349  0.000000  0.000000 -
0.001061
  0.000309 -0.000001 -0.002340  0.000000  0.000000 -0.001339  0.000450
  0.000000  0.000000  0.000000  0.000000  0.000000  0.000000  0.000000
0.000000
  0.000000  0.000000  0.000000  0.000000  0.000000  0.000000  0.000000
0.000000
  0.000001  0.000308  0.000000  0.000000  0.000000  0.000000  0.000000
0.000416
  0.001513  0.002611 -0.000029  0.000000  0.003364 -0.000008  0.000000 -
0.000002
  0.000000  0.002606  0.000001  0.000000  0.026907 -0.000009  0.000000
0.081789
 -0.000084  0.000000  0.180352 -0.000017  0.000000  0.103153 -0.002621
0.000000
  0.202397
  0.000000  0.000000  0.000000  0.000000  0.000000  0.000000  0.000000
0.000000
```

```
  0.000000  0.000000  0.000000  0.000000  0.000000  0.000000  0.000204
0.000000
  0.000000  0.000000  0.000000  0.000000 -0.000548  0.000000  0.000000
0.000000
  0.000000  0.000369
  0.000001  0.000002  0.000000  0.000000  0.000003  0.000000  0.000000
0.000000
  0.000000  0.000002  0.000000  0.000000  0.000025  0.000204  0.000000
0.000076
  0.000000  0.000000  0.000168  0.000547  0.000000  0.000097 -0.000002
0.000000
  0.000189  0.000000  0.000369
  0.001263  0.002178 -0.000024  0.000000  0.002806 -0.000007  0.000000 -
0.000002
  0.000000  0.002174  0.000001  0.000000  0.023515 -0.000008  0.000000
0.071617
 -0.000078  0.000000  0.158313 -0.000015  0.000000  0.091165 -0.002308
0.000000
  0.177834  0.000000  0.000167  0.157244
  0.000000  0.000000  0.000000  0.000000  0.000000  0.000000  0.000000
0.000000
  0.000000  0.000000  0.000000  0.000000 -0.000003 -0.000001  0.000000 -
0.000010
  0.000139  0.000000 -0.000022 -0.000003  0.000000 -0.000013  0.000227
0.000001
 -0.000022  0.000000  0.000000 -0.000022  0.000173
  0.000000  0.000000  0.000000  0.000000  0.000000  0.000000  0.000000
0.000000
  0.000000  0.000000  0.000000  0.000000  0.000000  0.000000  0.000002
0.000000
  0.000000 -0.000139  0.000000  0.000000 -0.000003  0.000000  0.000001 -
0.000227
  0.000000  0.000000  0.000000  0.000000  0.000000  0.000173
  0.001297  0.002239 -0.000025  0.000000  0.002887 -0.000007  0.000000 -
0.000002
  0.000000  0.002238  0.000001  0.000000  0.024351 -0.000011  0.000000
0.075485
 -0.000083  0.000000  0.169839 -0.000021  0.000000  0.097700 -0.002503
0.000000
  0.192856  0.000000  0.000181  0.170222 -0.000024  0.000000  0.186613
 -0.000001 -0.000002 -0.000003  0.000000 -0.000003  0.000000  0.000000 -
0.000004
  0.000000 -0.000002  0.000000  0.000000 -0.000023 -0.002464  0.000002 -
0.000072
 -0.000001  0.000000 -0.000162 -0.005237 -0.000005 -0.000093  0.000002
0.000000
 -0.000183  0.000000 -0.000078 -0.000161  0.000003  0.000000 -0.000172
0.005156
  0.000000  0.000000  0.000000  0.000003  0.000000  0.000000  0.000000
0.000000
 -0.000004  0.000000  0.000000  0.000000  0.000000 -0.000002 -0.002464
0.000000
```

```
  0.000000  0.000001  0.000000 -0.000005  0.005237  0.000000  0.000000
0.000000
  0.000000 -0.000078  0.000000  0.000000  0.000000 -0.000003  0.000000
0.000000
  0.005156
  0.000000  0.000000  0.000000  0.000000  0.000000  0.000000  0.000000
0.000000
  0.000000  0.000000  0.000000  0.000000  0.000000  0.000000  0.000000
0.000000
  0.000001  0.000301  0.000000  0.000000 -0.000001  0.000000  0.000000
0.000356
  0.000000  0.000000  0.000000  0.000000  0.000000 -0.000113  0.000000
0.000000
 -0.000001  0.000489
  0.000000  0.000000  0.000000  0.000000  0.000000  0.000000  0.000000
0.000000
  0.000000  0.000000  0.000000  0.000000  0.000000 -0.000002  0.000000
0.000000
 -0.000300  0.000001  0.000000 -0.000003  0.000000  0.000000 -0.000356
0.000000
 -0.000005  0.000000  0.000000  0.000000 -0.000113  0.000000  0.000000
0.000003
  0.000000  0.000000  0.000489
  0.000000  0.000000  0.000006  0.000000  0.000000  0.000001  0.000000
0.000009
  0.000001  0.000000  0.000000  0.000000  0.000000  0.004941  0.000001
0.000001
  0.000002  0.000000  0.000001  0.010745  0.000001  0.000000  0.000000
0.000000
  0.000000  0.000000  0.000925 -0.000001 -0.000005  0.000000 -0.000009 -
0.009603
 -0.000009  0.000000 -0.000006  0.019552
  0.000000  0.000000  0.000000  0.000006  0.000000  0.000000  0.000000
0.000001
 -0.000009  0.000000  0.000000  0.000000  0.000000  0.000001 -0.004941
0.000000
  0.000000  0.000002  0.000000  0.000000  0.010745  0.000000  0.000000
0.000000
  0.000000 -0.000925  0.000000  0.000000  0.000000 -0.000006  0.000000 -
0.000009
  0.009603 -0.000002  0.000000  0.000000  0.019552

            NA   8.69651605817797E-01
            NB   8.69651605817797E-01
            N    1.73930321163559E+00
          FOOA  -6.31439588182893E-01
          FOOB  -6.31439588182893E-01
          ALOC   7.26083392428286E-01
          BLOC   7.26083392428286E-01
           FLA   2.38212017634904E-01
           FLB   2.38212017634904E-01
            FL   1.10786362345270E+00
```

```
 ERROR ESTIMATE FOR DIFFERENTIAL EQUATIONS
 FOR SURFACE # 1   EPSD   3.45525240107631E-08

 MAXIMUM DISTANCE REACHED FROM NUCLEUS =  9.9957718517E+00
```

C2B3H5-C1

```
 PROAIM STELLIX VERSION 0.95

C2B3H5 USING D95 AND VAN DUIJNEVELDT BASES (Renormalized)
 -V/T FOR THIS WAVEFUNCTION =        2.00085433000
 MOLECULAR SCF ENERGY (AU)  =     -152.70856566945

C1 of C2B3H5 9s/5p +1d on B, C 6s/4,1,1 + 1d on H
 INTEGRATION IS OVER ATOM   C    1
   120 PHI PLANES     96 THETA PLANES
  80 PATHS WITH  141 POINTS PER PATH
 RADIUS OF BETA SPHERE   1.2242 WITH    120 POINTS PER PATH
 VOL1 RHO CONTOUR THRESHOLD=   0.0010
 VOL2 RHO CONTOUR THRESHOLD=   0.0020

 INSERTION LIMIT USED          =    6
 INSERTION LIMIT REACHED      0 TIMES FOR SURFACE   1
 INSERTION LIMIT REACHED      0 TIMES FOR SURFACE   2
 INSERTION LIMIT REACHED      0 TIMES FOR SURFACE   3
 INSERTION LIMIT REACHED      0 TIMES FOR SURFACE   4
 FOR SURFACE # 1 NUMBER OF INSERTED PATHS =     24
 FOR SURFACE # 2 NUMBER OF INSERTED PATHS =     16
 FOR SURFACE # 3 NUMBER OF INSERTED PATHS =     16
 FOR SURFACE # 4 NUMBER OF INSERTED PATHS =     16
 TOTAL NUMBER OF INSERTED PATHS=    72

 RESULTS OF THE INTEGRATION
             N   8.10313645838131E+00     NET CHARGE  -2.10313645838131E+00
             G   3.88016623991965E+01
             K   3.88017737732856E+01        E(ATOM)  -3.88349232926733E+01
             L   1.11374089025115E-04
             I   1.19671580759378E+00
        R(-1)   1.59347752722598E+01
           R1   1.08985084272131E+01
           R2   2.08356178133575E+01
           R4   1.18633471719430E+02
       GR(-1)  -2.88764652944701E+01
          GR0  -1.74105946270234E+01
          GR1  -2.67358475929877E+01
          GR2  -6.06317055744567E+01
         VNEO  -9.56086516335590E+01      VNEO(COR)  -9.56494748649784E+01
         VNET  -1.60398658930278E+02      VNET(COR)  -1.60467146367984E+02
         VEET   4.75908267880783E+01      VEET(COR)   4.76111472434160E+01
          EHF  -7.40060583689142E+01
```

		VREP(COR)	8.27822823196569E+01
		V(ATOM)	-7.76848640483269E+01
EL DX	-2.11078958301664E-07		
EL DY	9.72056122781488E-05		
EL DZ	2.00914567560409E+00		
EL DIPOLE MAG	2.00914567795558E+00		
QXX	-2.25922849148033E+00	QXX(DIAG)	-2.25920443475293E+00
QXY	-1.10221705402586E-04		
QXZ	-1.59378753719784E-04		
QYY	-2.25970912624328E+00	QYY(DIAG)	-2.25973326600144E+00
QYZ	7.33095474120840E-04		
QZZ	4.51893761772361E+00	QZZ(DIAG)	4.51893770075436E+00
FAXA	-8.85823425994525E-06		
FAYA	-2.33317900894759E-05		
FAZA	-2.00818304927861E+00		
FBXA	4.42054564550771E-06		
FBYA	-2.87228275479324E-05		
FBZA	1.23391706559768E+01		
RHO*L	1.03100464608994E+03		
VOL1	1.34177105214986E+02		
VOL2	1.17432689673593E+02		
N(VOL1)	8.07660452663413E+00		
N(VOL2)	8.05256573090993E+00		

THE ATOMIC OVERLAP MATRIX AOM :

```
  0.499995
  0.499995  0.499995
 -0.000119 -0.000116  0.001065
  0.000000  0.000000  0.000000  0.001016
  0.000000  0.000000  0.000000  0.000000  0.001016
 -0.000311 -0.000234  0.011536  0.000000  0.000000  0.427239
 -0.000458 -0.000469  0.006713  0.000000  0.000000  0.341317  0.388942
 -0.000515 -0.000574 -0.004073  0.000000  0.000000 -0.025365  0.143502
0.273805
  0.000000  0.000000  0.000000  0.005982  0.000000  0.000000 -0.000002 -
0.000003
  0.189309
  0.000000  0.000000  0.000000  0.000000  0.005982  0.000000  0.000000
0.000000
  0.000000  0.189309
  0.000104  0.000083 -0.000934  0.000000  0.000000 -0.052051 -0.041635 -
0.005170
  0.000000  0.000000  0.034332
 -0.000452 -0.000461 -0.007283  0.000000  0.000000 -0.214354 -0.089654
0.198781
 -0.000002  0.000000  0.004502  0.288901
  0.000000  0.000000  0.000000 -0.005738  0.000001  0.000000  0.000002
0.000004
 -0.188957 -0.000002  0.000000  0.000003  0.225922
  0.000000  0.000000  0.000000  0.000000  0.005738  0.000001  0.000000 -
0.000001
```

```
 -0.000002  0.188956  0.000000  0.000000  0.000000  0.225922
  0.000000  0.000000  0.000000  0.000000 -0.007246  0.000000  0.000000
0.000000
  0.000000 -0.257736  0.000000  0.000000  0.000001 -0.253579  0.402399
  0.000000  0.000000  0.000000  0.007246  0.000000 -0.000002 -0.000004 -
0.000006
  0.257738 -0.000001  0.000001 -0.000005 -0.253582 -0.000002  0.000001
0.402402

             NA   4.05156822919066E+00
             NB   4.05156822919066E+00
             N    8.10313645838131E+00
           FOOA  -3.12919100611633E+00
           FOOB  -3.12919100611633E+00
           ALOC   7.72340691086281E-01
           BLOC   7.72340691086281E-01
            FLA   9.22377223074326E-01
            FLB   9.22377223074326E-01
             FL   4.97394545226498E+00

 ERROR ESTIMATE FOR DIFFERENTIAL EQUATIONS
 FOR SURFACE # 1   EPSD   7.40854805071791E-06
 FOR SURFACE # 2   EPSD   3.50120080092734E-02
 FOR SURFACE # 3   EPSD   3.50158873266090E-02
 FOR SURFACE # 4   EPSD   3.50158889376883E-02

 MAXIMUM DISTANCE REACHED FROM NUCLEUS =  9.9981467064E+00
```

C2B3H5-B2

```
 PROAIM STELLIX VERSION 0.95

C2B3H5 USING D95 AND VAN DUIJNEVELDT BASES (Renormalized)
 -V/T FOR THIS WAVEFUNCTION =        2.00085433000
 MOLECULAR SCF ENERGY (AU)  =     -152.70856566945

B2 of C2B3H5 9s/5p +1d on B, C 6s/4,1,1 + 1d on H
 INTEGRATION IS OVER ATOM   B    2
   120 PHI PLANES     96 THETA PLANES
  80 PATHS WITH  141 POINTS PER PATH
 RADIUS OF BETA SPHERE   0.9501 WITH    120 POINTS PER PATH
 VOL1 RHO CONTOUR THRESHOLD=   0.0010
 VOL2 RHO CONTOUR THRESHOLD=   0.0020

 INSERTION LIMIT USED          =    6
 INSERTION LIMIT REACHED      0 TIMES FOR SURFACE   1
 INSERTION LIMIT REACHED      0 TIMES FOR SURFACE   2
 INSERTION LIMIT REACHED      0 TIMES FOR SURFACE   3
 FOR SURFACE # 1 NUMBER OF INSERTED PATHS =     96
 FOR SURFACE # 2 NUMBER OF INSERTED PATHS =     16
 FOR SURFACE # 3 NUMBER OF INSERTED PATHS =     16
```

```
TOTAL NUMBER OF INSERTED PATHS=   128

RESULTS OF THE INTEGRATION
             N   2.87231604364235E+00     NET CHARGE   2.12768395635765E+00
             G   2.37041732419884E+01
             K   2.37045970384459E+01        E(ATOM)  -2.37248485868338E+01
             L   4.23796457484551E-04
             I   2.96614502376363E-01
         R(-1)   1.03517273022969E+01
            R1   1.69256697280122E+00
            R2   1.83009501998325E+00
            R4   6.41300259812505E+00
        GR(-1)  -1.91422033685233E+01
           GR0  -6.66307776929486E+00
           GR1  -4.12881317535596E+00
           GR2  -5.16134270585846E+00
          VNEO  -5.17586365114844E+01      VNEO(COR)  -5.17807365490873E+01
          VNET  -7.46301385181887E+01      VNET(COR)  -7.46620042893667E+01
          VEET   1.75988858925349E+01      VEET(COR)   1.76064003107307E+01
           EHF  -3.33266555872079E+01
                                           VREP(COR)   2.72082073111048E+01
                                             V(ATOM)  -4.74537969782619E+01
         EL DX  -9.38130097164408E-04
         EL DY  -1.75772490704479E-01
         EL DZ   3.05979875615121E-05
 EL DIPOLE MAG   1.75774996836217E-01
           QXX  -3.51459086902961E-01      QXX(DIAG)  -3.51470410226994E-01
           QXY  -3.39600911113033E-03
           QXZ  -2.77480459602437E-05
           QYY   6.69164168906318E-01      QYY(DIAG)   6.69175490320804E-01
           QYZ  -1.46436766723505E-04
           QZZ  -3.17705082003356E-01      QZZ(DIAG)  -3.17705080093810E-01
          FAXA   1.51605420273468E-04
          FAYA   6.22788868550726E-02
          FAZA  -2.85596089915433E-05
          FBXA   1.69477789893336E-04
          FBYA   4.28858039430607E+00
          FBZA   4.33486067489704E-05
         RHO*L   3.93973998752544E+02
          VOL1   2.18127253695636E+01
          VOL2   1.96439587936249E+01
       N(VOL1)   2.86947328941295E+00
       N(VOL2)   2.86632258544392E+00

 THE ATOMIC OVERLAP MATRIX AOM :

0.000000
0.000000  0.000000
0.000000  0.000078  0.332344
0.000000  0.000110  0.470027  0.664751
0.000000  0.000000  0.000000  0.000000  0.000000
0.000000  0.000067 -0.008146 -0.011603  0.000000  0.038954
```

```
  0.000039  0.000000  0.000000  0.000000  0.000000 -0.000007  0.015257
  0.000000 -0.000024  0.002390  0.003414  0.000000 -0.013571  0.000004
0.007343
  0.000000  0.000078 -0.009711 -0.013810  0.000000  0.049516 -0.000001 -
0.005981
  0.117482
  0.000000  0.000000  0.000000 -0.000001  0.000016 -0.000014  0.000000
0.000004
 -0.000019  0.013718
  0.000000  0.000015 -0.003161 -0.004473  0.000000  0.012985  0.000002
0.005875
  0.067910 -0.000011  0.053237
 -0.000044  0.000000  0.000000  0.000000  0.000000  0.000010 -0.017220 -
0.000005
  0.000002  0.000000 -0.000003  0.019800
  0.000000 -0.000041  0.001807  0.002615  0.000000 -0.020046  0.000002
0.015551
  0.018252  0.000000  0.035441 -0.000002  0.048223
  0.000000  0.000000 -0.000001 -0.000001  0.000027 -0.000021  0.000000
0.000005
 -0.000029  0.022820 -0.000017  0.000000 -0.000001  0.038057
  0.000000  0.000000  0.000000  0.000000  0.000000  0.000000  0.000004
0.000000
  0.000000  0.000000  0.000000 -0.000002  0.000000  0.000000  0.001533
  0.000087  0.000000  0.000000  0.000000  0.000000 -0.000003  0.035834
0.000002
 -0.000001  0.000000  0.000001 -0.040085  0.000001  0.000000  0.000014
0.085459

            NA   1.43615802182117E+00
            NB   1.43615802182117E+00
            N    2.87231604364235E+00
          FOOA  -1.05224055375370E+00
          FOOB  -1.05224055375370E+00
          ALOC   7.32677419730853E-01
          BLOC   7.32677419730853E-01
           FLA   3.83917468067470E-01
           FLB   3.83917468067470E-01
            FL   1.82007548988864E+00

 ERROR ESTIMATE FOR DIFFERENTIAL EQUATIONS
 FOR SURFACE # 1   EPSD   1.15987619707011E-05
 FOR SURFACE # 2   EPSD   3.38289672895031E-02
 FOR SURFACE # 3   EPSD   3.38289672895031E-02

 MAXIMUM DISTANCE REACHED FROM NUCLEUS =  9.9980060079E+00
```

C2B3H5-H6

```
 PROAIM STELLIX VERSION 0.95

C2B3H5 USING D95 AND VAN DUIJNEVELDT BASES (Renormalized)
 -V/T FOR THIS WAVEFUNCTION =        2.00085433000
 MOLECULAR SCF ENERGY (AU)  =     -152.70856566945

H6 of C2B3H5 9s/5p +1d on B, C 6s/4,1,1 + 1d on H
 INTEGRATION IS OVER ATOM   H    6
   120 PHI PLANES     96 THETA PLANES
  80 PATHS WITH  141 POINTS PER PATH
 RADIUS OF BETA SPHERE   0.7940 WITH    120 POINTS PER PATH
 VOL1 RHO CONTOUR THRESHOLD=   0.0010
 VOL2 RHO CONTOUR THRESHOLD=   0.0020

 INSERTION LIMIT USED          =    6
 INSERTION LIMIT REACHED      0 TIMES FOR SURFACE   1
 FOR SURFACE # 1 NUMBER OF INSERTED PATHS =     24
 TOTAL NUMBER OF INSERTED PATHS=    24

 RESULTS OF THE INTEGRATION
              N   1.03048190669061E+00     NET CHARGE  -3.04819066906079E-02
              G   6.36345188075564E-01
              K   6.36422148974628E-01        E(ATOM)  -6.36965863509161E-01
              L   7.69608990632914E-05
              I   2.05324327728400E-01
         R(-1)   1.31070142267701E+00
            R1   1.14096807564720E+00
            R2   1.66541403074919E+00
            R4   7.23059837922681E+00
        GR(-1)  -1.85746228541086E+00
           GR0  -2.17352618872189E+00
           GR1  -3.32380865958111E+00
           GR2  -6.38434221456790E+00
          VNEO  -1.31070142267701E+00      VNEO(COR)  -1.31126106938874E+00
          VNET  -9.03271314293090E+00      VNET(COR)  -9.03656995434575E+00
          VEET   3.85972833410359E+00      VEET(COR)   3.86137637097376E+00
           EHF  -4.53656265985268E+00
                                           VREP(COR)   7.76097316731728E+00
                                             V(ATOM)  -1.27559678702848E+00
         EL DX  -9.38021532008058E-06
         EL DY  -1.65469985021097E-05
         EL DZ  -8.42764932702719E-02
  EL DIPOLE MAG   8.42764954167281E-02
           QXX  -2.53459609192919E-01      QXX(DIAG)  -2.53531502758376E-01
           QXY   5.30071821821104E-05
           QXZ   1.29324712546127E-05
           QYY  -2.53492420513762E-01      QYY(DIAG)  -2.53420527235055E-01
```

```
          QYZ   7.12654898990188E-06
          QZZ   5.06952029706682E-01      QZZ(DIAG)   5.06952029993431E-01
         FAXA   2.89926834343092E-06
         FAYA   2.47269326410777E-06
         FAZA  -2.44206986404587E-01
         FBXA   7.75265988755541E-06
         FBYA   8.09723666100120E-06
         FBZA   2.11583089616130E+00
       RHO*L   9.13157357731435E-02
         VOL1   4.79055355369642E+01
         VOL2   3.65482809586754E+01
      N(VOL1)   1.00519327613759E+00
      N(VOL2)   9.89018661007735E-01

 THE ATOMIC OVERLAP MATRIX AOM :

  0.000004
  0.000004  0.000004
  0.000000  0.000000  0.000000
  0.000000  0.000000  0.000000  0.000000
  0.000000  0.000000  0.000000  0.000000  0.000000
  0.000131  0.000132 -0.000001  0.000000  0.000000  0.008771
  0.000395  0.000398 -0.000007  0.000000  0.000000  0.026902  0.083518
  0.000604  0.000610 -0.000013  0.000000  0.000000  0.042431  0.132721
0.212053
  0.000000  0.000000  0.000000  0.000002  0.000000  0.000000  0.000000
0.000000
  0.001843
  0.000000  0.000000  0.000000  0.000000  0.000002  0.000000  0.000000
0.000000
  0.000000  0.001843
 -0.000104 -0.000105  0.000002  0.000000  0.000000 -0.007261 -0.022698 -
0.036236
  0.000000  0.000000  0.006272
  0.000524  0.000528 -0.000012  0.000000  0.000000  0.038117  0.120112
0.192950
  0.000000  0.000000 -0.032972  0.176585
  0.000000  0.000000  0.000000 -0.000002  0.000000  0.000000  0.000000
0.000000
 -0.002123  0.000000  0.000000  0.000000  0.002541
  0.000000  0.000000  0.000000  0.000000  0.000002  0.000000  0.000000
0.000000
  0.000000  0.002123  0.000000  0.000000  0.000000  0.002541
  0.000000  0.000000  0.000000  0.000000 -0.000004  0.000000  0.000001
0.000001
  0.000000 -0.004204  0.000000  0.000001  0.000000 -0.004884  0.009632
  0.000000  0.000000  0.000000  0.000004  0.000000  0.000000  0.000001
0.000001
  0.004204  0.000000  0.000000  0.000001 -0.004884  0.000000  0.000000
0.009633

            NA   5.15240953345304E-01
```

```
            NB   5.15240953345304E-01
             N   1.03048190669061E+00
          FOOA  -2.36066431042767E-01
          FOOB  -2.36066431042767E-01
          ALOC   4.58167056617023E-01
          BLOC   4.58167056617023E-01
           FLA   2.79174522302537E-01
           FLB   2.79174522302537E-01
            FL   7.94415475647841E-01

 ERROR ESTIMATE FOR DIFFERENTIAL EQUATIONS
 FOR SURFACE # 1   EPSD   2.63323810653399E-09

 MAXIMUM DISTANCE REACHED FROM NUCLEUS =  9.9955197656E+00
```

C2B3H5-H8

```
 PROAIM STELLIX VERSION 0.95

C2B3H5 USING D95 AND VAN DUIJNEVELDT BASES (Renormalized)
 -V/T FOR THIS WAVEFUNCTION =        2.00085433000
 MOLECULAR SCF ENERGY (AU)  =     -152.70856566945

H8 of C2B3H5 9s/5p +1d on B, C 6s/4,1,1 + 1d on H
 INTEGRATION IS OVER ATOM   H    8
   120 PHI PLANES     96 THETA PLANES
  80 PATHS WITH  141 POINTS PER PATH
 RADIUS OF BETA SPHERE   1.2769 WITH    120 POINTS PER PATH
 VOL1 RHO CONTOUR THRESHOLD=   0.0010
 VOL2 RHO CONTOUR THRESHOLD=   0.0020

 INSERTION LIMIT USED          =    6
 INSERTION LIMIT REACHED      0 TIMES FOR SURFACE   1
 FOR SURFACE # 1 NUMBER OF INSERTED PATHS =     96
 TOTAL NUMBER OF INSERTED PATHS=    96

 RESULTS OF THE INTEGRATION
             N   1.70325897554193E+00     NET CHARGE  -7.03258975541928E-01
             G   8.62035172573210E-01
             K   8.62075494266486E-01        E(ATOM)  -8.62811991223503E-01
             L   4.03216932761300E-05
             I   3.50278355140750E-01
        R(-1)   1.70345754883351E+00
           R1   2.35185417472863E+00
           R2   4.05688540498637E+00
           R4   2.04022608900061E+01
       GR(-1)  -2.69720004868839E+00
          GR0  -3.77665230544589E+00
          GR1  -6.73577267189266E+00
          GR2  -1.45267204606562E+01
         VNEO  -1.70345754883351E+00      VNEO(COR)  -1.70418489558028E+00
```

VNET	-1.43455264798146E+01	VNET(COR)	-1.43516517701237E+01
VEET	6.25436653560978E+00	VEET(COR)	6.25703704134438E+00
EHF	-7.22908444993830E+00		
		VREP(COR)	1.26233095000592E+01
		V(ATOM)	-1.72834227006450E+00
EL DX	-1.41493054485529E-06		
EL DY	4.20537469650127E-01		
EL DZ	-5.13602155140060E-07		
EL DIPOLE MAG	4.20537469652821E-01		
QXX	-5.30518740031098E-01	QXX(DIAG)	7.00219494342795E-01
QXY	7.61680971653428E-06		
QXZ	2.84429071324539E-05		
QYY	7.00219494290726E-01	QYY(DIAG)	-5.30518742320360E-01
QYZ	2.07053232572192E-06		
QZZ	-1.69700754259629E-01	QZZ(DIAG)	-1.69700752022435E-01
FAXA	1.59114339767807E-07		
FAYA	-3.52643417080758E-01		
FAZA	1.01082334304649E-07		
FBXA	1.62569493612693E-06		
FBYA	3.28351641514366E+00		
FBZA	1.14977449439453E-06		
RHO*L	9.75765313140557E-02		
VOL1	8.69371061869513E+01		
VOL2	6.67955391266952E+01		
N(VOL1)	1.66352265215446E+00		
N(VOL2)	1.63441693681671E+00		

THE ATOMIC OVERLAP MATRIX AOM :

```
  0.000000
  0.000000  0.000000
  0.000000  0.000000  0.000280
  0.000000  0.000000  0.000396  0.000561
  0.000000  0.000000  0.000000  0.000000  0.000000
  0.000000  0.000001  0.000448  0.000633  0.000000  0.003455
  0.000004  0.000000  0.000000  0.000000  0.000000  0.000000  0.003105
  0.000000  0.000000  0.000339  0.000479  0.000000  0.002312  0.000000
0.002026
  0.000000  0.000001  0.004099  0.005809  0.000000  0.028767  0.000000
0.022832
  0.277242
  0.000000  0.000000  0.000000  0.000000  0.000001  0.000000  0.000000
0.000000
  0.000000  0.003103
  0.000000  0.000000  0.003784  0.005366  0.000000  0.026569  0.000000
0.021720
  0.263956  0.000000  0.253002
 -0.000004  0.000000  0.000000  0.000000  0.000000  0.000000 -0.003088
0.000000
  0.000000  0.000000  0.000000  0.003207
  0.000000 -0.000002  0.003575  0.005076  0.000000  0.025350  0.000000
0.021928
```

```
  0.265234  0.000000  0.256859  0.000000  0.265266
  0.000000  0.000000  0.000000  0.000000  0.000002  0.000000  0.000000
0.000000
  0.000000  0.005565  0.000000  0.000000  0.000000  0.010075
  0.000000  0.000000  0.000000  0.000000  0.000000  0.000000  0.000000
0.000000
  0.000000  0.000000  0.000000  0.000000  0.000000  0.000000  0.000456
  0.000011  0.000000  0.000000  0.000000  0.000000  0.000000  0.009499
0.000000
  0.000000  0.000000  0.000000 -0.009438  0.000000  0.000000  0.000000
0.029853

            NA   8.51629487770963E-01
            NB   8.51629487770963E-01
            N    1.70325897554193E+00
          FOOA  -6.32291333970070E-01
          FOOB  -6.32291333970070E-01
          ALOC   7.42448850174289E-01
          BLOC   7.42448850174289E-01
           FLA   2.19338153800893E-01
           FLB   2.19338153800893E-01
            FL   1.07096764157186E+00

 ERROR ESTIMATE FOR DIFFERENTIAL EQUATIONS
 FOR SURFACE # 1   EPSD   2.29236980888057E-08

 MAXIMUM DISTANCE REACHED FROM NUCLEUS =  9.9957547805E+00
```

C2B4H6-B1 (not used)

```
 PROAIM VERSION 0.90

C2B4H6 OPTIMIZATION USING VD SET(Renormalized); d=0.75, p=1.0725
 -V/T FOR THIS WAVEFUNCTION =        1.99999917000
 MOLECULAR SCF ENERGY (AU)  =     -177.93948958540

B1 of C2B4H6  9s/5p + 1d on B, 6s/4,1,1 + 1p on H, D95* on C
 INTEGRATION IS OVER ATOM   B    1
   120 PHI PLANES     96 THETA PLANES
  80 PATHS WITH  141 POINTS PER PATH
 RADIUS OF BETA SPHERE   0.9513 WITH    120 POINTS PER PATH
 VOL1 RHO CONTOUR THRESHOLD=   0.0010
 VOL2 RHO CONTOUR THRESHOLD=   0.0020

 INSERTION LIMIT USED          =   15
 INSERTION LIMIT REACHED      0 TIMES FOR SURFACE   1
 INSERTION LIMIT REACHED      1 TIMES FOR SURFACE   2
 INSERTION LIMIT REACHED      2 TIMES FOR SURFACE   3
 INSERTION LIMIT REACHED      3 TIMES FOR SURFACE   4
 INSERTION LIMIT REACHED      4 TIMES FOR SURFACE   5
 FOR SURFACE # 1 NUMBER OF INSERTED PATHS =     34
```

```
FOR SURFACE # 2 NUMBER OF INSERTED PATHS =    201
FOR SURFACE # 3 NUMBER OF INSERTED PATHS =    181
FOR SURFACE # 4 NUMBER OF INSERTED PATHS =    171
FOR SURFACE # 5 NUMBER OF INSERTED PATHS =    156
TOTAL NUMBER OF INSERTED PATHS=   743

RESULTS OF THE INTEGRATION
             N   3.88894943048254E+00     NET CHARGE   1.11105056951746E+00
             G   2.45060966842442E+01
             K   2.40822016402892E+01        E(ATOM)  -2.40821816520619E+01
             L  -4.23895043954916E-01
             I   4.40847431178414E-01
         R(-1)   1.08042761637345E+01
            R1   4.74197746575767E+00
            R2   1.34490868832680E+01
            R4   2.63766931381640E+02
        GR(-1)  -1.97929389357993E+01
           GR0  -9.08099758196928E+00
           GR1  -1.49499498783720E+01
           GR2  -6.02729509829059E+01
          VNEO  -5.40213808186723E+01     VNEO(COR)  -5.40213583997899E+01
          VNET  -9.05369736541524E+01     VNET(COR)  -9.05369360812927E+01
          VEET   2.49936095364642E+01     VEET(COR)   2.49935991641119E+01
           EHF  -4.14611624773989E+01
                                          VREP(COR)   4.23725799894490E+01
                                            V(ATOM)  -4.81643560918437E+01
         EL DX  -9.21492740151795E-01
         EL DY  -1.21972524359266E+00
         EL DZ   3.35995663521777E-01
 EL DIPOLE MAG   1.56517463112429E+00
           QXX   3.75647794301294E+00     QXX(DIAG)   6.79891865585010E+00
           QXY  -7.88105546911312E+00
           QXZ   2.15087666924656E+00
           QYY  -1.29473420541713E+01     QYY(DIAG)   1.00471859624293E+01
           QYZ   3.95418095448295E+00
           QZZ   9.19086411115834E+00     QZZ(DIAG)  -1.68461046182794E+01
          FAXA   3.79920530857507E-01
          FAYA   1.78031846309422E-01
          FAZA  -3.07305905263249E-02
          FBXA  -6.14777665806513E+00
          FBYA   4.46689543769777E-01
          FBZA  -7.87442283012301E-01
         RHO*L   3.93007416909655E+02
          VOL1   6.36845386639410E+01
          VOL2   5.35911057155735E+01
       N(VOL1)   3.87147994532255E+00
       N(VOL2)   3.85701677713484E+00

 THE ATOMIC OVERLAP MATRIX AOM :

0.000000
0.000000  0.000000
```

```
  0.000004  0.000055  0.252221
 -0.000006 -0.000031 -0.125561  0.064404
  0.000002 -0.000064 -0.329774  0.160083  0.440058
  0.000004 -0.000045 -0.246790  0.118369  0.332451  0.252242
  0.000007  0.000100 -0.002215 -0.000716  0.007452  0.007268  0.062124
 -0.000038 -0.000004 -0.001841  0.002449 -0.000901 -0.001823 -0.003073
0.016998
 -0.000001 -0.000104  0.006008 -0.002922 -0.008616 -0.006911 -0.071824
0.000551
  0.132383
 -0.000013 -0.000024 -0.003928  0.005478 -0.001831 -0.003625 -0.014904
0.006821
  0.004747  0.080965
 -0.000002 -0.000036  0.000414  0.000279 -0.001789 -0.001801 -0.021259
0.000652
  0.017306  0.002875  0.010045
  0.000006  0.000016 -0.001053 -0.000420  0.003807  0.003795  0.020016 -
0.004201
 -0.060638 -0.020228  0.006599  0.091890
  0.000006 -0.000017  0.004913 -0.003676 -0.003551 -0.001608 -0.011353 -
0.004227
  0.051378 -0.020063  0.000402 -0.009794  0.083136
  0.000044  0.000005  0.002241 -0.002981  0.001098  0.002221  0.003792 -
0.019262
 -0.000605 -0.008283 -0.000803  0.005033  0.005119  0.022227
  0.000000 -0.000044 -0.000832  0.000443  0.000747  0.000357 -0.024280
0.000346
 -0.001233  0.003194  0.017193  0.042810 -0.040169 -0.000380  0.070183
  0.000002 -0.000011 -0.000496  0.000564 -0.000079 -0.000308 -0.003469 -
0.002796
  0.002137 -0.003444  0.004562  0.026451  0.026940  0.003314  0.001624
0.072769
  0.000066  0.000000  0.000051 -0.000084  0.000018  0.000048  0.000304 -
0.031409
 -0.002149 -0.000884 -0.000003  0.000467  0.000514  0.035171 -0.001032
0.000263
  0.072964
  0.000017  0.000009  0.004225 -0.005539  0.002035  0.004189  0.006684 -
0.006795
 -0.001492 -0.016243 -0.000847  0.013080  0.013424  0.007960 -0.000985
0.009854
  0.000673  0.020971
 -0.000002 -0.000009 -0.000455  0.001044 -0.000080 -0.000128 -0.005756
0.001300
  0.017369  0.094344  0.002146 -0.001638 -0.001691 -0.001472  0.008896
0.035228
 -0.004283 -0.002715  0.198894

            NA    1.94447471524127E+00
            NB    1.94447471524127E+00
            N     3.88894943048254E+00
          FOOA   -1.16520062222670E+00
```

```
          FOOB  -1.16520062222670E+00
          ALOC   5.99236705467842E-01
          BLOC   5.99236705467842E-01
           FLA   7.79274093014572E-01
           FLB   7.79274093014572E-01
            FL   2.72374880825584E+00

 ERROR ESTIMATE FOR DIFFERENTIAL EQUATIONS
 FOR SURFACE # 1   EPSD   2.31255146824405E-02
 FOR SURFACE # 2   EPSD   2.32235720699789E-02
 FOR SURFACE # 3   EPSD   2.32235720699789E-02
 FOR SURFACE # 4   EPSD   2.36358436747061E-02
 FOR SURFACE # 5   EPSD   2.36358436747061E-02

 MAXIMUM DISTANCE REACHED FROM NUCLEUS =  9.9977365554E+00
```

C2B4H6-C5

```
 PROAIM VERSION 0.90

C2B4H6 OPTIMIZATION USING VD SET(Renormalized); d=0.75, p=1.0725
 -V/T FOR THIS WAVEFUNCTION =        1.99999917000
 MOLECULAR SCF ENERGY (AU)  =     -177.93948958540

C5 of C2B4H6  9s/5p + 1d on B, 6s/4,1,1 + 1p on H, D95* on C
 INTEGRATION IS OVER ATOM   C    5
   120 PHI PLANES     96 THETA PLANES
  80 PATHS WITH  141 POINTS PER PATH
 RADIUS OF BETA SPHERE   1.2270 WITH    120 POINTS PER PATH
 VOL1 RHO CONTOUR THRESHOLD=   0.0010
 VOL2 RHO CONTOUR THRESHOLD=   0.0020

 INSERTION LIMIT USED          =   15
 INSERTION LIMIT REACHED      1 TIMES FOR SURFACE   1
 INSERTION LIMIT REACHED      1 TIMES FOR SURFACE   2
 INSERTION LIMIT REACHED      2 TIMES FOR SURFACE   3
 INSERTION LIMIT REACHED      4 TIMES FOR SURFACE   4
 INSERTION LIMIT REACHED      0 TIMES FOR SURFACE   5
 FOR SURFACE # 1 NUMBER OF INSERTED PATHS =    201
 FOR SURFACE # 2 NUMBER OF INSERTED PATHS =    196
 FOR SURFACE # 3 NUMBER OF INSERTED PATHS =    181
 FOR SURFACE # 4 NUMBER OF INSERTED PATHS =    252
 FOR SURFACE # 5 NUMBER OF INSERTED PATHS =      8
 TOTAL NUMBER OF INSERTED PATHS=   838

 RESULTS OF THE INTEGRATION
             N   8.00318113656391E+00     NET CHARGE  -2.00318113656391E+00
             G   3.87554388145008E+01
             K   3.87578333200647E+01        E(ATOM)  -3.87578011510631E+01
```

L	2.39450556391561E-03		
I	1.01916716191064E+00		
R(-1)	1.58878320870242E+01		
R1	1.06005673561004E+01		
R2	1.97843914960734E+01		
R4	1.03984848280511E+02		
GR(-1)	-2.81021351970077E+01		
GR0	-1.54824937493989E+01		
GR1	-2.16506353887147E+01		
GR2	-4.61076186561693E+01		
VNEO	-9.53269925221451E+01	VNEO(COR)	-9.53269529614268E+01
VNET	-1.72430338217858E+02	VNET(COR)	-1.72430266659238E+02
VEET	5.34742011346809E+01	VEET(COR)	5.34741789428782E+01
EHF	-8.01983037631123E+01		
		VREP(COR)	9.49146815549275E+01
		V(ATOM)	-7.75155851043104E+01
EL DX	-3.75707738061035E-02		
EL DY	4.92818359636564E-02		
EL DZ	-1.59336787408274E+00		
EL DIPOLE MAG	1.59457249586191E+00		
QXX	-2.74362552943825E+00	QXX(DIAG)	-2.91855078175617E+00
QXY	-1.80770478114299E-01		
QXZ	-1.61359037897593E-01		
QYY	-2.73159720537010E+00	QYY(DIAG)	-2.56493378718347E+00
QYZ	2.01033918099512E-01		
QZZ	5.47522273480835E+00	QZZ(DIAG)	5.48348456893963E+00
FAXA	1.25146504009484E-02		
FAYA	-1.43690236658928E-02		
FAZA	1.55151091968528E+00		
FBXA	2.70335578559280E-02		
FBYA	-2.90904403448946E-02		
FBZA	-1.39745917787429E+01		
RHO*L	1.03267915630149E+03		
VOL1	1.13877503717660E+02		
VOL2	1.02125050724206E+02		
N(VOL1)	7.98610430504920E+00		
N(VOL2)	7.96919516555806E+00		

THE ATOMIC OVERLAP MATRIX AOM :

```
  0.499996
  0.499996  0.499996
 -0.000102 -0.000100  0.000629
  0.000000  0.000000  0.000002  0.000586
  0.000000  0.000000  0.000001  0.000000  0.000588
  0.000000  0.000000  0.000000  0.000000  0.000000  0.000545
 -0.000304 -0.000265  0.008895  0.000064  0.000021 -0.000010  0.392178
  0.000448  0.000471 -0.005456 -0.000017 -0.000006  0.000002 -0.326465
0.388385
  0.000002  0.000003  0.000060  0.002080  0.005764  0.000008  0.001902 -
0.000594
  0.238452
```

```
  0.000002  0.000003  0.000063  0.005720 -0.002155  0.000008  0.002091 -
0.000683
 -0.001978  0.238330
 -0.000502 -0.000546 -0.002611 -0.000027 -0.000009  0.000004 -0.005591 -
0.163647
 -0.000728 -0.000764  0.275449
  0.000082  0.000064 -0.000705  0.000001 -0.000001  0.000000 -0.055424
0.043998
  0.000229  0.000443 -0.004222  0.030268
  0.000000  0.000000 -0.000001  0.000001  0.000000  0.000886 -0.000017
0.000006
  0.000021  0.000025  0.000006 -0.000006  0.012122
  0.000445  0.000443  0.005771  0.000021  0.000007 -0.000003  0.209247 -
0.082402
  0.000702  0.000799 -0.193227 -0.012257 -0.000007  0.287849
  0.000001  0.000002  0.000041  0.001351  0.003744  0.000005  0.001238 -
0.000332
  0.148655 -0.001126 -0.000513 -0.000006  0.000013  0.000404  0.107019
  0.000001  0.000002  0.000040  0.003715 -0.001400  0.000005  0.001275 -
0.000346
 -0.001136  0.148591 -0.000525  0.000003  0.000011  0.000421 -0.000724
0.106973
 -0.000001 -0.000001 -0.000020 -0.002033 -0.005562 -0.000002 -0.000661
0.000248
 -0.289563  0.000790  0.000231 -0.000153 -0.000007 -0.000288 -0.178458
0.000418
  0.396376
 -0.000001 -0.000001 -0.000022 -0.005547  0.002059 -0.000003 -0.000763
0.000292
  0.000782 -0.289501  0.000253 -0.000254 -0.000011 -0.000336  0.000410 -
0.178428
 -0.000344  0.396345
  0.000002  0.000004  0.000076 -0.000077 -0.000026 -0.000006  0.002407 -
0.000854
 -0.003247 -0.002739 -0.000850  0.000528 -0.000018  0.000994 -0.001486 -
0.001417
  0.001346  0.001147  0.129506

            NA   4.00159056828196E+00
            NB   4.00159056828196E+00
            N    8.00318113656392E+00
          FOOA  -2.93672288555361E+00
          FOOB  -2.93672288555361E+00
          ALOC   7.33888896288172E-01
          BLOC   7.33888896288172E-01
           FLA   1.06486768272835E+00
           FLB   1.06486768272835E+00
            FL   5.06645825101030E+00

 ERROR ESTIMATE FOR DIFFERENTIAL EQUATIONS
 FOR SURFACE # 1   EPSD   2.67904499798986E-02
 FOR SURFACE # 2   EPSD   2.67904556159878E-02
```

```
 FOR SURFACE # 3    EPSD    2.67904556159878E-02
 FOR SURFACE # 4    EPSD    2.71792536656819E-02
 FOR SURFACE # 5    EPSD    2.71792536656819E-02

 MAXIMUM DISTANCE REACHED FROM NUCLEUS =  9.9981460757E+00
```

C2B4H6-H7

```
 PROAIM VERSION 0.90

C2B4H6 OPTIMIZATION USING VD SET(Renormalized); d=0.75, p=1.0725
 -V/T FOR THIS WAVEFUNCTION =         1.99999917000
 MOLECULAR SCF ENERGY (AU)  =      -177.93948958540

H7 of C2B4H6  9s/5p + 1d on B, 6s/4,1,1 + 1p on H, D95* ON C
 INTEGRATION IS OVER ATOM    H     7
   120 PHI PLANES      96 THETA PLANES
  80 PATHS WITH  141 POINTS PER PATH
 RADIUS OF BETA SPHERE   1.2634 WITH     120 POINTS PER PATH
 VOL1 RHO CONTOUR THRESHOLD=    0.0010
 VOL2 RHO CONTOUR THRESHOLD=    0.0020

 INSERTION LIMIT USED           =    15
 INSERTION LIMIT REACHED       0 TIMES FOR SURFACE    1
 FOR SURFACE # 1 NUMBER OF INSERTED PATHS =      34
 TOTAL NUMBER OF INSERTED PATHS=     34

 RESULTS OF THE INTEGRATION
              N   1.69472037265554E+00      NET CHARGE  -6.94720372655540E-01
              G   8.51335716242103E-01
              K   8.51410682561489E-01         E(ATOM)  -8.51409975890623E-01
              L   7.49663193855213E-05
              I   3.00779415289706E-01
         R(-1)    1.69580989071493E+00
            R1    2.33668762276984E+00
            R2    4.02132289351011E+00
            R4    2.01312588459062E+01
        GR(-1)   -2.63873526204675E+00
           GR0   -3.66399283043740E+00
           GR1   -6.48402544052692E+00
           GR2   -1.38901806486695E+01
          VNEO   -1.69580989071493E+00       VNEO(COR)  -1.69580918695354E+00
          VNET   -1.60075402686225E+01       VNET(COR)  -1.60075336254905E+01
          VEET    7.09621347032448E+00       VEET(COR)   7.09621052539467E+00
           EHF   -8.05991611573648E+00
                                             VREP(COR)   1.43047166652405E+01
                                               V(ATOM)  -1.70281696024995E+00
         EL DX   -4.08217697351173E-01
         EL DY   -5.94775837641725E-13
         EL DZ   -1.53945332744948E-13
  EL DIPOLE MAG   4.08217697351173E-01
```

```
          QXX   8.24180818511461E-01      QXX(DIAG)   8.24180818511461E-01
          QXY  -1.38095032906831E-12
          QXZ  -9.70436983236620E-13
          QYY  -4.09569170852913E-01      QYY(DIAG)  -4.09569125614901E-01
          QYZ  -1.51034324554802E-05
          QZZ  -4.14611647658549E-01      QZZ(DIAG)  -4.14611692896561E-01
         FAXA   3.53797928667319E-01
         FAYA   2.67176815814027E-14
         FAZA   3.43695086588274E-14
         FBXA  -3.53043956305592E+00
         FBYA   2.59168163131693E-13
         FBZA   3.99389744071252E-13
        RHO*L   9.60510946336808E-02
         VOL1   8.53812197999240E+01
         VOL2   6.59135433746884E+01
      N(VOL1)   1.65624275880377E+00
      N(VOL2)   1.62811623194034E+00

   THE ATOMIC OVERLAP MATRIX AOM :

  0.000000
  0.000000  0.000000
  0.000000  0.000000  0.000201
  0.000000  0.000000 -0.000098  0.000048
  0.000000  0.000000 -0.000267  0.000130  0.000354
  0.000000  0.000000 -0.000201  0.000098  0.000267  0.000201
  0.000000  0.000000  0.000268 -0.000130 -0.000353 -0.000266  0.001794
 -0.000003  0.000000  0.000000  0.000000  0.000000  0.000000  0.000000
0.002093
  0.000000  0.000000 -0.002094  0.001021  0.002771  0.002086 -0.012268
0.000000
  0.094820
  0.000000  0.000000  0.000000  0.000004 -0.000001  0.000000  0.000000
0.000000
  0.000000  0.003985
  0.000000  0.000000  0.000212 -0.000103 -0.000280 -0.000211  0.001239
0.000000
 -0.009672  0.000000  0.001107
  0.000000 -0.000002  0.002743 -0.001338 -0.003632 -0.002735  0.016027
0.000000
 -0.129373  0.000000  0.013146  0.179436
  0.000000  0.000003 -0.002859  0.001394  0.003786  0.002851 -0.016612
0.000000
  0.135603  0.000000 -0.013861 -0.188620  0.198862
  0.000003  0.000000  0.000000  0.000000  0.000000  0.000000  0.000000 -
0.002099
  0.000000  0.000000  0.000000  0.000000  0.000000  0.002265
  0.000000 -0.000005  0.003423 -0.001670 -0.004535 -0.003416  0.020048
0.000000
 -0.167441  0.000000  0.017052  0.234940 -0.247946  0.000000  0.310590
  0.000000  0.000000  0.000000  0.000002 -0.000001  0.000000  0.000000
0.000000
```

```
  0.000000  0.001874  0.000000  0.000000  0.000000  0.000000  0.000000
0.001028
  0.000008  0.000000  0.000000  0.000000  0.000000  0.000000  0.000000 -
0.006302
  0.000000  0.000000  0.000000  0.000000  0.000000  0.006266  0.000000
0.000000
  0.020054
  0.000000  0.000000  0.000000  0.000000  0.000000  0.000000  0.000000
0.000000
  0.000000  0.000000  0.000000  0.000000  0.000000  0.000000  0.000000
0.000000
  0.000000  0.000396
  0.000000  0.000000  0.000000  0.000012 -0.000004  0.000000  0.000000
0.000000
  0.000000  0.010738  0.000000  0.000000  0.000000  0.000000  0.000000
0.004850
  0.000000  0.000000  0.030127

            NA   8.47360186327770E-01
            NB   8.47360186327770E-01
            N    1.69472037265554E+00
          FOOA  -6.13747213890230E-01
          FOOB  -6.13747213890230E-01
          ALOC   7.24304993075076E-01
          BLOC   7.24304993075076E-01
           FLA   2.33612972437540E-01
           FLB   2.33612972437540E-01
            FL   1.08097315876531E+00

 ERROR ESTIMATE FOR DIFFERENTIAL EQUATIONS
 FOR SURFACE # 1   EPSD   1.62162870787286E-08

 MAXIMUM DISTANCE REACHED FROM NUCLEUS =  9.9957481695E+00
```

C2B4H6-H11

```
 PROAIM VERSION 0.90

C2B4H6 OPTIMIZATION USING VD SET(Renormalized); d=0.75, p=1.0725
 -V/T FOR THIS WAVEFUNCTION =        1.99999917000
 MOLECULAR SCF ENERGY (AU)  =     -177.93948958540

H1 1of C2B4H6  9s/5p + 1d on B, 6s/4,1,1 + 1p on H, D95* ON C
 INTEGRATION IS OVER ATOM   H   11
   120 PHI PLANES     96 THETA PLANES
  80 PATHS WITH  141 POINTS PER PATH
 RADIUS OF BETA SPHERE   0.7846 WITH    120 POINTS PER PATH
 VOL1 RHO CONTOUR THRESHOLD=   0.0010
 VOL2 RHO CONTOUR THRESHOLD=   0.0020

 INSERTION LIMIT USED          =   15
```

```
INSERTION LIMIT REACHED      0 TIMES FOR SURFACE   1
FOR SURFACE # 1 NUMBER OF INSERTED PATHS =      8
TOTAL NUMBER OF INSERTED PATHS=     8

RESULTS OF THE INTEGRATION
             N   9.88952122393712E-01     NET CHARGE   1.10478776062878E-02
             G   6.27659405023357E-01
             K   6.27753095078199E-01        E(ATOM)  -6.27752574043130E-01
             L   9.36900548423319E-05
             I   1.69614501015834E-01
         R(-1)   1.28284759283460E+00
            R1   1.07022233562541E+00
            R2   1.52320349000818E+00
            R4   6.27255375601138E+00
       GR(-1)  -1.80024034261296E+00
           GR0  -2.06933534166171E+00
           GR1  -3.10321413841353E+00
           GR2  -5.82669818943966E+00
          VNEO  -1.28284759283460E+00      VNEO(COR)  -1.28284706045263E+00
          VNET  -9.88613346004028E+00      VNET(COR)  -9.88612935729319E+00
          VEET   4.28954247950746E+00      VEET(COR)   4.28954069934659E+00
           EHF  -4.96883788545462E+00
                                           VREP(COR)   8.63062601075809E+00
                                             V(ATOM)  -1.25550334653511E+00
        EL DX  -1.19433272346517E-05
        EL DY   4.38636659492029E-07
        EL DZ   8.36465355724948E-02
 EL DIPOLE MAG   8.36465364262987E-02
           QXX  -2.23863825939210E-01      QXX(DIAG)  -2.23944840148932E-01
           QXY  -1.97748178261688E-06
           QXZ  -8.54849407974452E-06
           QYY  -2.23944791880393E-01      QYY(DIAG)  -2.23863777779471E-01
           QYZ   4.20103599545057E-08
           QZZ   4.47808617819603E-01      QZZ(DIAG)   4.47808617928404E-01
          FAXA   2.99838738516793E-06
          FAYA  -7.84881254390866E-08
          FAZA   2.44751859471421E-01
          FBXA   8.35227766491836E-06
          FBYA  -2.39889447974117E-07
          FBZA  -2.23054936637918E+00
         RHO*L   9.11827002216045E-02
          VOL1   4.48541162356032E+01
          VOL2   3.45172460729587E+01
      N(VOL1)   9.65436961494520E-01
      N(VOL2)   9.50789844182718E-01

 THE ATOMIC OVERLAP MATRIX AOM :

0.000004
0.000004  0.000004
0.000000  0.000000  0.000000
0.000000  0.000000  0.000000  0.000000
```

```
  0.000000  0.000000  0.000000  0.000000  0.000000
  0.000000  0.000000  0.000000  0.000000  0.000000  0.000000
  0.000114  0.000115 -0.000001  0.000000  0.000000  0.000000  0.006671
 -0.000386 -0.000388  0.000007  0.000000  0.000000  0.000000 -0.023063
0.080567
  0.000000  0.000000  0.000000  0.000000  0.000001  0.000000  0.000000
0.000000
  0.001937
  0.000000  0.000000  0.000000  0.000001  0.000000  0.000000  0.000000
0.000000
  0.000000  0.001937
  0.000596  0.000599 -0.000014  0.000000  0.000000  0.000000  0.036611 -
0.128720
  0.000000  0.000000  0.206632
 -0.000087 -0.000088  0.000002  0.000000  0.000000  0.000000 -0.005311
0.018695
  0.000000  0.000000 -0.029997  0.004445
  0.000000  0.000000  0.000000  0.000000  0.000000  0.000000  0.000000
0.000000
  0.000000  0.000000  0.000000  0.000000  0.000063
 -0.000516 -0.000519  0.000013  0.000000  0.000000  0.000000 -0.032988
0.116768
  0.000000  0.000000 -0.188434  0.027396  0.000000  0.172982
  0.000000  0.000000  0.000000  0.000000  0.000001  0.000000  0.000000
0.000000
  0.001332  0.000000  0.000000  0.000000  0.000000  0.000000  0.000970
  0.000000  0.000000  0.000000  0.000001  0.000000  0.000000  0.000000
0.000000
  0.000000  0.001332  0.000000  0.000000  0.000000  0.000000  0.000000
0.000970
  0.000000  0.000000  0.000000 -0.000001 -0.000002  0.000000  0.000000
0.000001
 -0.004059  0.000000 -0.000001  0.000000  0.000000  0.000001 -0.002773
0.000000
  0.008583
  0.000000  0.000000  0.000000 -0.000002  0.000001  0.000000  0.000000
0.000000
  0.000000 -0.004059  0.000000  0.000000  0.000000  0.000000  0.000000 -
0.002773
  0.000000  0.008584
  0.000000  0.000000  0.000000  0.000000  0.000000  0.000000  0.000000
0.000000
  0.000000  0.000000  0.000000  0.000000  0.000000  0.000000  0.000000
0.000000
  0.000000  0.000000  0.000126

           NA    4.94476061196856E-01
           NB    4.94476061196856E-01
           N     9.88952122393712E-01
         FOOA   -2.20837687396565E-01
         FOOB   -2.20837687396565E-01
         ALOC    4.46609461461163E-01
```

```
          BLOC    4.46609461461163E-01
           FLA    2.73638373800291E-01
           FLB    2.73638373800291E-01
            FL    7.68114434997147E-01

ERROR ESTIMATE FOR DIFFERENTIAL EQUATIONS
FOR SURFACE # 1    EPSD    1.38635976382147E-09

MAXIMUM DISTANCE REACHED FROM NUCLEUS =   9.9955151541E+00
```

Appendix B: SADDLE Output

BH

```
 SADDLE
BH OPTIMIZATION

       B    1          0.00000000      0.00000000      0.22123918
       H    2          0.00000000      0.00000000     -2.11093683

 SEARCHING BETWEEN ATOMS    1   2
 NUMBER OF PERFORMED NEWTON ITERATION STEPS :    6

 COORDINATES OF CRITICAL POINT
          X =   0.00000000E+00
          Y =   0.00000000E+00
          Z =  -7.41358640E-01
          R =   7.41358640E-01

 VECTORS FROM NUCLEI TO CRITICAL POINT
 LENGTHS AND ANGLES MADE WITH PROJECTIONS ONTO YZ/XZ/XY PLANES OF MCS

 NUCLEUS         LENGTH         YZ ANGLE         XZ ANGLE         XY ANGLE
   B    1   9.62597820E-01  0.00000000E+00  0.00000000E+00  9.00000000E+01
   H    2   1.36957819E+00  0.00000000E+00  0.00000000E+00  9.00000000E+01

 EIGENVALUES OF THE HESSIAN
    -4.69926200E-01   -4.69926200E-01    5.18153214E-01

 THE ELLIPTICITY IS      0.00000

 EIGENVECTORS OF THE HESSIAN
     1.00000000E+00    0.00000000E+00    0.00000000E+00
     0.00000000E+00    1.00000000E+00    0.00000000E+00
     0.00000000E+00    0.00000000E+00    1.00000000E+00

 EIGENVALUES OF THE STRESSIAN
    -1.17481550E-01   -1.17481550E-01   -8.31113135E-02

 THE TRACE OF THE STRESSIAN IS  -0.31807441

 EIGENVECTORS OF THE STRESSIAN
     1.00000000E+00    0.00000000E+00    0.00000000E+00
     0.00000000E+00    1.00000000E+00    0.00000000E+00
     0.00000000E+00    0.00000000E+00    1.00000000E+00

 VALUES
 RHO         1.7952824469E-01
 GRAD        4.5102810375E-17
 DEL2       -4.2169918564E-01
```

```
G(X)        1.0632480844E-01
K(X)        2.1174960485E-01
L(X)        1.0542479641E-01

COMPONENTS OF THE DIVERGENCE OF THE STRESSIAN
    0.00000000E+00    0.00000000E+00   -5.98402649E-01

MAGNITUDE OF THE DIVERGENCE OF THE STRESSIAN        0.598403

CRITICAL POINTS
 0.00000000E+00  0.00000000E+00 -7.41358640E-01  B    1  H    2
```

BH3

```
SADDLE
BH3
       B    1          0.00000000     0.00000000     0.00000000
       H    2          0.00000000     2.25084129     0.00000000
       H    3          1.94928573    -1.12542064     0.00000000
       H    4         -1.94928573    -1.12542064     0.00000000

SEARCHING BETWEEN ATOMS    1   2
NUMBER OF PERFORMED NEWTON ITERATION STEPS :    6

COORDINATES OF CRITICAL POINT
         X =   3.17375445E-18
         Y =   9.51101516E-01
         Z =   0.00000000E+00
         R =   9.51101516E-01

VECTORS FROM NUCLEI TO CRITICAL POINT
LENGTHS 'AND ANGLES MADE WITH PROJECTIONS ONTO YZ/XZ/XY PLANES OF MCS

NUCLEUS         LENGTH         YZ ANGLE         XZ ANGLE         XY ANGLE
  B    1   9.51101516E-01  0.00000000E+00  9.00000000E+01  0.00000000E+00
  H    2   1.29973977E+00  0.00000000E+00  9.00000000E+01  0.00000000E+00
  H    3   2.84809746E+00  4.31897585E+01  4.68102415E+01  0.00000000E+00
  H    4   2.84809746E+00  4.31897585E+01  4.68102415E+01  0.00000000E+00

EIGENVALUES OF THE HESSIAN
   -4.75745806E-01   -3.73411847E-01    5.99325496E-01

THE ELLIPTICITY IS      0.27405

EIGENVECTORS OF THE HESSIAN
    0.00000000E+00    1.00000000E+00    0.00000000E+00
    0.00000000E+00    0.00000000E+00    1.00000000E+00
    1.00000000E+00    0.00000000E+00    0.00000000E+00

EIGENVALUES OF THE STRESSIAN
   -1.50207847E-01   -1.18936452E-01   -8.68420865E-02
```

```
 THE TRACE OF THE STRESSIAN IS  -0.35598638

 EIGENVECTORS OF THE STRESSIAN
     1.00000000E+00    0.00000000E+00    0.00000000E+00
     0.00000000E+00    0.00000000E+00    1.00000000E+00
     0.00000000E+00    1.00000000E+00    0.00000000E+00

 VALUES
 RHO         1.8269295555E-01
 GRAD        3.1918939349E-16
 DEL2       -2.4983215695E-01
 G(X)        1.4676417281E-01
 K(X)        2.0922221204E-01
 L(X)        6.2458039238E-02

 COMPONENTS OF THE DIVERGENCE OF THE STRESSIAN
     1.39347508E-19    6.28300077E-01    0.00000000E+00

 MAGNITUDE OF THE DIVERGENCE OF THE STRESSIAN        0.628300

 CRITICAL POINTS
  3.17375445E-18  9.51101516E-01  0.00000000E+00  B    1  H    2
  8.23678077E-01 -4.75550758E-01  0.00000000E+00  B    1  H    3
 -8.23678077E-01 -4.75550758E-01  0.00000000E+00  B    1  H    4
```

B2H6

```
 SADDLE
B2H6 USING D95 AND VAN DUIJNEVELDT BASES (Renormalized)

        B    1        -1.69819114     0.00000000     0.00000000
        H    2         0.00000000     0.00000000     1.85138799
        H    3        -2.77735215     1.96393642     0.00000000
        H    4        -2.77735215    -1.96393642     0.00000000
        B    5         1.69819114     0.00000000     0.00000000
        H    6         2.77735215    -1.96393642     0.00000000
        H    7         2.77735215     1.96393642     0.00000000
        H    8         0.00000000     0.00000000    -1.85138799

 SEARCHING BETWEEN ATOMS    1   2
 NUMBER OF PERFORMED NEWTON ITERATION STEPS :    8

 COORDINATES OF CRITICAL POINT
          X =  -8.49030624E-01
          Y =  -6.15050639E-18
          Z =   5.19879641E-01
          R =   9.95554037E-01

 VECTORS FROM NUCLEI TO CRITICAL POINT
```

LENGTHS AND ANGLES MADE WITH PROJECTIONS ONTO YZ/XZ/XY PLANES OF MCS

NUCLEUS		LENGTH	YZ ANGLE	XZ ANGLE	XY ANGLE
B	1	9.95664814E-01	5.85238749E+01	0.00000000E+00	3.14761251E+01
H	2	1.57916671E+00	3.25234475E+01	0.00000000E+00	5.74765525E+01
H	3	2.80102571E+00	4.35062794E+01	4.45192626E+01	1.06963087E+01
H	4	2.80102571E+00	4.35062794E+01	4.45192626E+01	1.06963087E+01
B	5	2.59973336E+00	7.84645487E+01	0.00000000E+00	1.15354513E+01
H	6	4.15667814E+00	6.07414732E+01	2.81952296E+01	7.18485248E+00
H	7	4.15667814E+00	6.07414732E+01	2.81952296E+01	7.18485248E+00
H	8	2.51868283E+00	1.96998692E+01	0.00000000E+00	7.03001308E+01

EIGENVALUES OF THE HESSIAN

-1.67080384E-01 -1.06713421E-01 4.60169150E-01

THE ELLIPTICITY IS 0.56569

EIGENVECTORS OF THE HESSIAN

0.00000000E+00	-6.17682489E-01	7.86427583E-01
1.00000000E+00	0.00000000E+00	0.00000000E+00
0.00000000E+00	7.86427583E-01	6.17682489E-01

EIGENVALUES OF THE STRESSIAN

-1.01856408E-01 -8.66526211E-02 -4.65946678E-02

THE TRACE OF THE STRESSIAN IS -0.23510370

EIGENVECTORS OF THE STRESSIAN

0.00000000E+00	-5.75334588E-01	8.17918157E-01
1.00000000E+00	0.00000000E+00	0.00000000E+00
0.00000000E+00	8.17918157E-01	5.75334588E-01

VALUES

RHO	1.1459637618E-01
GRAD	1.9711279093E-17
DEL2	1.8637534514E-01
G(X)	1.4084876667E-01
K(X)	9.4254930388E-02
L(X)	-4.6593836285E-02

COMPONENTS OF THE DIVERGENCE OF THE STRESSIAN

2.95354764E-01 -6.58147148E-19 1.78679698E-01

MAGNITUDE OF THE DIVERGENCE OF THE STRESSIAN 0.345197

SEARCHING BETWEEN ATOMS 1 3
NUMBER OF PERFORMED NEWTON ITERATION STEPS : 6

COORDINATES OF CRITICAL POINT

X = -2.13735907E+00
Y = 8.46772431E-01

```
          Z =  -3.80860217E-19
          R =   2.29898398E+00

VECTORS FROM NUCLEI TO CRITICAL POINT
LENGTHS AND ANGLES MADE WITH PROJECTIONS ONTO YZ/XZ/XY PLANES OF MCS

NUCLEUS          LENGTH          YZ ANGLE          XZ ANGLE          XY ANGLE
  B     1   9.53882602E-01   2.74129473E+01   6.25870527E+01   0.00000000E+00
  H     2   2.95177317E+00   4.63934703E+01   1.66706045E+01   3.88447381E+01
  H     3   1.28749622E+00   2.98072304E+01   6.01927696E+01   0.00000000E+00
  H     4   2.88265076E+00   1.28274393E+01   7.71725607E+01   0.00000000E+00
  B     5   3.92790898E+00   7.75505356E+01   1.24494644E+01   0.00000000E+00
  H     6   5.66166677E+00   6.02348881E+01   2.97651119E+01   0.00000000E+00
  H     7   5.04008350E+00   7.71936924E+01   1.28063076E+01   0.00000000E+00
  H     8   2.95177317E+00   4.63934703E+01   1.66706045E+01   3.88447381E+01

EIGENVALUES OF THE HESSIAN
   -4.34188854E-01   -4.05270084E-01    5.81163742E-01

THE ELLIPTICITY IS      0.07136

EIGENVECTORS OF THE HESSIAN
    0.00000000E+00    8.71695670E-01    4.90047608E-01
    0.00000000E+00    4.90047608E-01   -8.71695670E-01
    1.00000000E+00    0.00000000E+00    0.00000000E+00

EIGENVALUES OF THE STRESSIAN
   -1.42728340E-01   -1.30824183E-01   -8.48900654E-02

THE TRACE OF THE STRESSIAN IS  -0.35844259

EIGENVECTORS OF THE STRESSIAN
    8.82320932E-01    0.00000000E+00    4.70648248E-01
    4.70648248E-01    0.00000000E+00   -8.82320932E-01
    0.00000000E+00    1.00000000E+00    0.00000000E+00

VALUES
RHO         1.8457846428E-01
GRAD        5.0040504828E-17
DEL2       -2.5829519615E-01
G(X)        1.4693439468E-01
K(X)        2.1150819372E-01
L(X)        6.4573799038E-02

COMPONENTS OF THE DIVERGENCE OF THE STRESSIAN
   -2.97342648E-01    5.57266148E-01    6.68366615E-13

MAGNITUDE OF THE DIVERGENCE OF THE STRESSIAN        0.631631


STARTING COORDINATES
0.000000 0.000000 0.000000
```

NUMBER OF PERFORMED NEWTON ITERATION STEPS : 1

COORDINATES OF CRITICAL POINT
X = 7.17196068E-15
Y = 8.54063072E-19
Z = 1.01423736E-17
R = 7.17196790E-15

VECTORS FROM NUCLEI TO CRITICAL POINT
LENGTHS AND ANGLES MADE WITH PROJECTIONS ONTO YZ/XZ/XY PLANES OF MCS

NUCLEUS		LENGTH	YZ ANGLE	XZ ANGLE	XY ANGLE
B	1	1.69819114E+00	9.00000000E+01	0.00000000E+00	0.00000000E+00
H	2	1.85138799E+00	0.00000000E+00	0.00000000E+00	9.00000000E+01
H	3	3.40157776E+00	5.47348968E+01	3.52651032E+01	0.00000000E+00
H	4	3.40157776E+00	5.47348968E+01	3.52651032E+01	0.00000000E+00
B	5	1.69819114E+00	9.00000000E+01	0.00000000E+00	0.00000000E+00
H	6	3.40157776E+00	5.47348968E+01	3.52651032E+01	0.00000000E+00
H	7	3.40157776E+00	5.47348968E+01	3.52651032E+01	0.00000000E+00
H	8	1.85138799E+00	0.00000000E+00	0.00000000E+00	9.00000000E+01

EIGENVALUES OF THE HESSIAN
-1.58120842E-01 2.10472539E-03 1.10948387E-01

EIGENVECTORS OF THE HESSIAN
-1.23599048E-16 -1.00000000E+00 0.00000000E+00
-1.00000000E+00 -2.09467860E-16 0.00000000E+00
0.00000000E+00 0.00000000E+00 1.00000000E+00

EIGENVALUES OF THE STRESSIAN
-5.61895421E-02 -4.65533502E-02 -2.62873798E-03

THE TRACE OF THE STRESSIAN IS -0.10537163

EIGENVECTORS OF THE STRESSIAN
-3.70580303E-16 0.00000000E+00 -1.00000000E+00
-1.00000000E+00 0.00000000E+00 1.48535698E-16
0.00000000E+00 1.00000000E+00 0.00000000E+00

VALUES
RHO 1.0831268377E-01
GRAD 2.6195550005E-17
DEL2 -4.5067729130E-02
G(X) 4.7052349019E-02
K(X) 5.8319281302E-02
L(X) 1.1266932283E-02

COMPONENTS OF THE DIVERGENCE OF THE STRESSIAN
6.15823559E-13 -1.29160260E-19 -2.69230055E-13

MAGNITUDE OF THE DIVERGENCE OF THE STRESSIAN 0.000000

```
CRITICAL POINTS
-8.49030624E-01 -6.15050639E-18  5.19879641E-01  B    1  H    2
-8.49030624E-01  9.62010927E-19 -5.19879641E-01  B    1  H    8
-2.13735907E+00  8.46772431E-01 -3.80860217E-19  B    1  H    3
-2.13735907E+00 -8.46772431E-01 -1.25739511E-18  B    1  H    4
 7.17196068E-15  8.54063072E-19  1.01423736E-17
```

B4H10

```
SADDLE
B4H10 USING VD SET(Renormalized) d=0.75, p=1.0725
       B    1        -1.64935284     0.00000000    -0.90345247
       B    2         1.64935284     0.00000000    -0.90345247
       H    3        -2.61283291     0.00000000    -2.91359814
       H    4         2.61283291     0.00000000    -2.91359814
       B    5         0.00000000     2.71798625     0.77700618
       B    6         0.00000000    -2.71798625     0.77700618
       H    7        -2.50163768    -1.75439713     0.44702994
       H    8         2.50163768    -1.75439713     0.44702994
       H    9         2.50163768     1.75439713     0.44702994
       H   10        -2.50163768     1.75439713     0.44702994
       H   11         0.00000000     2.73238695     3.02214344
       H   12         0.00000000    -2.73238695     3.02214344
       H   13         0.00000000     4.63882914    -0.37037368
       H   14         0.00000000    -4.63882914    -0.37037368

SEARCHING BETWEEN ATOMS    1   2   B-B Bond
NUMBER OF PERFORMED NEWTON ITERATION STEPS :    3

COORDINATES OF CRITICAL POINT
         X =   1.22279194E-17
         Y =   2.30062967E-18
         Z =  -8.23212564E-01
         R =   8.23212564E-01

VECTORS FROM NUCLEI TO CRITICAL POINT
LENGTHS AND ANGLES MADE WITH PROJECTIONS ONTO YZ/XZ/XY PLANES OF MCS

NUCLEUS        LENGTH         YZ ANGLE         XZ ANGLE         XY ANGLE
  B    1   1.65130350E+00  8.72147948E+01  0.00000000E+00  2.78520520E+00
  B    2   1.65130350E+00  8.72147948E+01  0.00000000E+00  2.78520520E+00
  H    3   3.34613324E+00  5.13385973E+01  0.00000000E+00  3.86614027E+01
  H    4   3.34613324E+00  5.13385973E+01  0.00000000E+00  3.86614027E+01
  B    5   3.15406869E+00  0.00000000E+00  5.95124827E+01  3.04875173E+01
  B    6   3.15406869E+00  0.00000000E+00  5.95124827E+01  3.04875173E+01
  H    7   3.30902046E+00  4.91133062E+01  3.20180395E+01  2.25737718E+01
  H    8   3.30902046E+00  4.91133062E+01  3.20180395E+01  2.25737718E+01
  H    9   3.30902046E+00  4.91133062E+01  3.20180395E+01  2.25737718E+01
  H   10   3.30902046E+00  4.91133062E+01  3.20180395E+01  2.25737718E+01
  H   11   4.71727689E+00  0.00000000E+00  3.53963832E+01  5.46036168E+01
```

```
  H    12    4.71727689E+00  0.00000000E+00  3.53963832E+01  5.46036168E+01
  H    13    4.66087962E+00  0.00000000E+00  8.44244965E+01  5.57550350E+00
  H    14    4.66087962E+00  0.00000000E+00  8.44244965E+01  5.57550350E+00

EIGENVALUES OF THE HESSIAN
   -1.78178604E-01   -1.47958835E-01    2.03548016E-02

THE ELLIPTICITY IS      0.20424

EIGENVECTORS OF THE HESSIAN
    0.00000000E+00    3.46944695E-17    1.00000000E+00
    0.00000000E+00   -1.00000000E+00    2.08166817E-17
    1.00000000E+00    0.00000000E+00    0.00000000E+00

EIGENVALUES OF THE STRESSIAN
   -6.45684557E-02   -6.25270712E-02    1.14145826E-03

THE TRACE OF THE STRESSIAN IS  -0.12595407

EIGENVECTORS OF THE STRESSIAN
    0.00000000E+00    6.93889390E-18   -1.00000000E+00
    0.00000000E+00   -1.00000000E+00    1.38777878E-17
    1.00000000E+00    0.00000000E+00    0.00000000E+00

VALUES
RHO         1.3783595298E-01
GRAD        9.9792341496E-18
DEL2       -3.0578263729E-01
G(X)        2.4754204698E-02
K(X)        1.0119986402E-01
L(X)        7.6445659322E-02

COMPONENTS OF THE DIVERGENCE OF THE STRESSIAN
   -2.43043830E-13   -7.94168894E-14    1.88926782E-03

MAGNITUDE OF THE DIVERGENCE OF THE STRESSIAN        0.001889

SEARCHING BETWEEN ATOMS    1   3
NUMBER OF PERFORMED NEWTON ITERATION STEPS :    5

COORDINATES OF CRITICAL POINT
         X =  -2.06761096E+00
         Y =  -4.04663287E-19
         Z =  -1.76110078E+00
         R =   2.71596963E+00

VECTORS FROM NUCLEI TO CRITICAL POINT
LENGTHS AND ANGLES MADE WITH PROJECTIONS ONTO YZ/XZ/XY PLANES OF MCS

NUCLEUS        LENGTH         YZ ANGLE         XZ ANGLE         XY ANGLE
  B    1   9.54201489E-01  2.59975760E+01  0.00000000E+00  6.40024240E+01
  B    2   3.81462718E+00  7.70070306E+01  0.00000000E+00  1.29929694E+01
```

```
  H     3   1.27495770E+00  2.53178340E+01  0.00000000E+00  6.46821660E+01
  H     4   4.82024947E+00  7.61668696E+01  0.00000000E+00  1.38331304E+01
  B     5   4.25493258E+00  2.90735997E+01  3.97012645E+01  3.66203034E+01
  B     6   4.25493258E+00  2.90735997E+01  3.97012645E+01  3.66203034E+01
  H     7   2.85344174E+00  8.74901473E+00  3.79399646E+01  5.07007218E+01
  H     8   5.36952360E+00  5.83162146E+01  1.90705627E+01  2.42823770E+01
  H     9   5.36952360E+00  5.83162146E+01  1.90705627E+01  2.42823770E+01
  H    10   2.85344174E+00  8.74901473E+00  3.79399646E+01  5.07007218E+01
  H    11   5.88390846E+00  2.05730267E+01  2.76702969E+01  5.43838402E+01
  H    12   5.88390846E+00  2.05730267E+01  2.76702969E+01  5.43838402E+01
  H    13   5.26572623E+00  2.31197696E+01  6.17568898E+01  1.53140321E+01
  H    14   5.26572623E+00  2.31197696E+01  6.17568898E+01  1.53140321E+01

EIGENVALUES OF THE HESSIAN
   -4.14545303E-01   -3.72324233E-01    5.77421700E-01

THE ELLIPTICITY IS      0.11340

EIGENVECTORS OF THE HESSIAN
    0.00000000E+00    9.04107154E-01    4.27305808E-01
    1.00000000E+00    0.00000000E+00    0.00000000E+00
    0.00000000E+00   -4.27305808E-01    9.04107154E-01

EIGENVALUES OF THE STRESSIAN
   -1.41202139E-01   -1.34208278E-01   -8.47333443E-02

THE TRACE OF THE STRESSIAN IS  -0.36014376

EIGENVECTORS OF THE STRESSIAN
    8.90992457E-01    0.00000000E+00    4.54018108E-01
    0.00000000E+00    1.00000000E+00    0.00000000E+00
   -4.54018108E-01    0.00000000E+00    8.90992457E-01

VALUES
RHO         1.8314334158E-01
GRAD        5.2858686965E-16
DEL2       -2.0944783581E-01
G(X)        1.5389090085E-01
K(X)        2.0625285980E-01
L(X)        5.2361958952E-02

COMPONENTS OF THE DIVERGENCE OF THE STRESSIAN
   -2.73140175E-01   -9.81499753E-14   -5.63784669E-01

MAGNITUDE OF THE DIVERGENCE OF THE STRESSIAN        0.626465

SEARCHING BETWEEN ATOMS    5  10
NUMBER OF PERFORMED NEWTON ITERATION STEPS :    9

COORDINATES OF CRITICAL POINT
         X =  -7.88541936E-01
         Y =   2.08481150E+00
```

Z = 4.69579194E-01
R = 2.27788103E+00

VECTORS FROM NUCLEI TO CRITICAL POINT
LENGTHS AND ANGLES MADE WITH PROJECTIONS ONTO YZ/XZ/XY PLANES OF MCS

NUCLEUS		LENGTH	YZ ANGLE	XZ ANGLE	XY ANGLE
B	1	2.64057765E+00	1.90257711E+01	5.21414774E+01	3.13305059E+01
B	2	3.48926724E+00	4.43215067E+01	3.66905316E+01	2.31725451E+01
H	3	4.37268401E+00	2.46580415E+01	2.84753570E+01	5.06879743E+01
H	4	5.23083920E+00	4.05607657E+01	2.34882862E+01	4.02989085E+01
B	5	1.05698628E+00	4.82475192E+01	3.68010171E+01	1.69089942E+01
B	6	4.87679977E+00	9.30514852E+00	8.00059238E+01	3.61424637E+00
H	7	4.20413230E+00	2.40465694E+01	6.59512159E+01	3.07312710E-01
H	8	5.05621531E+00	4.05958967E+01	4.94029501E+01	2.55523410E-01
H	9	3.30680571E+00	8.42520817E+01	5.73453487E+00	3.90705478E-01
H	10	1.74481493E+00	7.90583174E+01	1.09159791E+01	7.40487164E-01
H	11	2.74895191E+00	1.66695743E+01	1.36253287E+01	6.82113041E+01
H	12	5.50842841E+00	8.23027383E+00	6.09875246E+01	2.76062350E+01
H	13	2.80184320E+00	1.63459794E+01	6.57203108E+01	1.74447397E+01
H	14	6.82163196E+00	6.63790593E+00	8.02768148E+01	7.07282355E+00

EIGENVALUES OF THE HESSIAN
-1.01022988E-01 -6.53150933E-02 2.49271294E-01

THE ELLIPTICITY IS 0.54670

EIGENVECTORS OF THE HESSIAN
-2.37235293E-01 -5.19049518E-01 -8.21161990E-01
7.12465604E-01 4.81662933E-01 -5.10287745E-01
-6.60387900E-01 7.06107936E-01 -2.55537481E-01

EIGENVALUES OF THE STRESSIAN
-7.77906838E-02 -6.25851348E-02 -2.85052844E-02

THE TRACE OF THE STRESSIAN IS -0.16888110

EIGENVECTORS OF THE STRESSIAN
-4.06572178E-02 5.90271642E-01 -8.06180116E-01
4.87589455E-01 -6.92533728E-01 -5.31651727E-01
-8.72125859E-01 -4.14700404E-01 -2.59653734E-01

VALUES
RHO 9.4712721178E-02
GRAD 6.9932747303E-18
DEL2 8.2933212036E-02
G(X) 9.4807203006E-02
K(X) 7.4073899997E-02
L(X) -2.0733303009E-02

COMPONENTS OF THE DIVERGENCE OF THE STRESSIAN
-1.80893778E-01 -1.40713924E-01 -6.90891070E-02

MAGNITUDE OF THE DIVERGENCE OF THE STRESSIAN 0.239366

SEARCHING BETWEEN ATOMS 1 10
NUMBER OF PERFORMED NEWTON ITERATION STEPS : 6

COORDINATES OF CRITICAL POINT
X = -1.90456356E+00
Y = 7.34684647E-01
Z = -3.26222341E-01
R = 2.06725540E+00

VECTORS FROM NUCLEI TO CRITICAL POINT
LENGTHS AND ANGLES MADE WITH PROJECTIONS ONTO YZ/XZ/XY PLANES OF MCS

NUCLEUS		LENGTH	YZ ANGLE	XZ ANGLE	XY ANGLE
B	1	9.68549774E-01	1.52777100E+01	4.93357379E+01	3.65820715E+01
B	2	3.67468066E+00	7.52703085E+01	1.15329571E+01	9.03762769E+00
H	3	2.78135228E+00	1.47528042E+01	1.53162476E+01	6.84751011E+01
H	4	5.25748475E+00	5.92304041E+01	8.03284249E+00	2.94807997E+01
B	5	2.96276235E+00	4.00034492E+01	4.20215148E+01	2.18615370E+01
B	6	4.09455881E+00	2.77196066E+01	5.74832064E+01	1.56308097E+01
H	7	2.67393805E+00	1.29025750E+01	6.85704340E+01	1.68089346E+01
H	8	5.11938048E+00	5.93941808E+01	2.90916224E+01	8.68743923E+00
H	9	4.58828312E+00	7.38045629E+01	1.28407925E+01	9.70222085E+00
H	10	1.41217214E+00	2.50118364E+01	4.62271356E+01	3.31999396E+01
H	11	4.33932371E+00	2.60342231E+01	2.74111022E+01	5.05007667E+01
H	12	5.18261529E+00	2.15609529E+01	4.19884731E+01	4.02464334E+01
H	13	4.34415192E+00	2.60031213E+01	6.39893697E+01	5.82329764E-01
H	14	5.70122462E+00	1.95155201E+01	7.04790241E+01	4.43713565E-01

EIGENVALUES OF THE HESSIAN
-2.54033332E-01 -1.77833163E-01 5.91668814E-01

THE ELLIPTICITY IS 0.42849

EIGENVECTORS OF THE HESSIAN
-8.58779169E-02 9.57921780E-01 2.73881083E-01
5.74025697E-01 2.72256988E-01 -7.72250369E-01
-8.14321486E-01 9.08955263E-02 -5.73252580E-01

EIGENVALUES OF THE STRESSIAN
-1.20855458E-01 -1.13908380E-01 -5.53680903E-02

THE TRACE OF THE STRESSIAN IS -0.29013193

EIGENVECTORS OF THE STRESSIAN
9.17297355E-01 3.02778015E-01 2.58633016E-01
-1.54432558E-03 6.52200653E-01 -7.58044803E-01
3.98199922E-01 -6.94953079E-01 -5.98729522E-01

VALUES

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RHO          1.3482172022E-01
GRAD         4.6100908736E-18
DEL2         1.5980231867E-01
G(X)         1.6504125409E-01
K(X)         1.2509067442E-01
L(X)        -3.9950579668E-02

COMPONENTS OF THE DIVERGENCE OF THE STRESSIAN
   -1.17185719E-01    3.32820055E-01    2.53714710E-01

MAGNITUDE OF THE DIVERGENCE OF THE STRESSIAN        0.434595

SEARCHING BETWEEN ATOMS    5  11
NUMBER OF PERFORMED NEWTON ITERATION STEPS :    6

COORDINATES OF CRITICAL POINT
         X =  -1.64072020E-19
         Y =   2.69259426E+00
         Z =   1.73302154E+00
         R =   3.20209736E+00

VECTORS FROM NUCLEI TO CRITICAL POINT
LENGTHS AND ANGLES MADE WITH PROJECTIONS ONTO YZ/XZ/XY PLANES OF MCS

NUCLEUS         LENGTH         YZ ANGLE         XZ ANGLE         XY ANGLE
  B     1   4.11356583E+00  2.36378641E+01  4.08866381E+01  3.98605901E+01
  B     2   4.11356583E+00  2.36378641E+01  4.08866381E+01  3.98605901E+01
  H     3   5.97227211E+00  2.59440942E+01  2.67981825E+01  5.10807520E+01
  H     4   5.97227211E+00  2.59440942E+01  2.67981825E+01  5.10807520E+01
  B     5   9.56352511E-01  0.00000000E+00  1.52143169E+00  8.84785683E+01
  B     6   5.49439230E+00  0.00000000E+00  7.99796247E+01  1.00203753E+01
  H     7   5.26191010E+00  2.83869520E+01  5.76857306E+01  1.41461625E+01
  H     8   5.26191010E+00  2.83869520E+01  5.76857306E+01  1.41461625E+01
  H     9   2.96516093E+00  5.75304490E+01  1.84457629E+01  2.57026297E+01
  H    10   2.96516093E+00  5.75304490E+01  1.84457629E+01  2.57026297E+01
  H    11   1.28973591E+00  0.00000000E+00  1.76804819E+00  8.82319518E+01
  H    12   5.57604307E+00  0.00000000E+00  7.66328948E+01  1.33671052E+01
  H    13   2.86567648E+00  0.00000000E+00  4.27775482E+01  4.72224518E+01
  H    14   7.62719086E+00  0.00000000E+00  7.39917435E+01  1.60082565E+01

EIGENVALUES OF THE HESSIAN
   -4.23952191E-01   -4.03844210E-01    5.66449326E-01

THE ELLIPTICITY IS      0.04979

EIGENVECTORS OF THE HESSIAN
    1.00000000E+00    2.30025132E-18   -3.62990061E-20
    2.30053771E-18   -9.99875512E-01    1.57784878E-02
    0.00000000E+00    1.57784878E-02    9.99875512E-01

EIGENVALUES OF THE STRESSIAN
   -1.41957327E-01   -1.33543213E-01   -8.34664680E-02
```

THE TRACE OF THE STRESSIAN IS -0.35896701

EIGENVECTORS OF THE STRESSIAN

1.17464994E-16	1.00000000E+00	1.63652772E-19
-9.99999029E-01	1.17465108E-16	-1.39320326E-03
-1.39320326E-03	0.00000000E+00	9.99999029E-01

VALUES

RHO	1.8463048969E-01
GRAD	1.8733420948E-16
DEL2	-2.6134707571E-01
G(X)	1.4681511920E-01
K(X)	2.1215188813E-01
L(X)	6.5336768928E-02

COMPONENTS OF THE DIVERGENCE OF THE STRESSIAN

-2.74086484E-13	-8.49495085E-03	6.27977766E-01

MAGNITUDE OF THE DIVERGENCE OF THE STRESSIAN 0.628035

SEARCHING BETWEEN ATOMS 5 13
NUMBER OF PERFORMED NEWTON ITERATION STEPS : 6

COORDINATES OF CRITICAL POINT

X =	1.13544397E-19
Y =	3.52300347E+00
Z =	2.64534545E-01
R =	3.53292117E+00

VECTORS FROM NUCLEI TO CRITICAL POINT
LENGTHS AND ANGLES MADE WITH PROJECTIONS ONTO YZ/XZ/XY PLANES OF MCS

NUCLEUS		LENGTH	YZ ANGLE	XZ ANGLE	XY ANGLE
B	1	4.06154058E+00	2.39594784E+01	6.01585510E+01	1.67126754E+01
B	2	4.06154058E+00	2.39594784E+01	6.01585510E+01	1.67126754E+01
H	3	5.41654656E+00	2.88409494E+01	4.05729032E+01	3.59263762E+01
H	4	5.41654656E+00	2.88409494E+01	4.05729032E+01	3.59263762E+01
B	5	9.54295502E-01	0.00000000E+00	5.75192875E+01	3.24807125E+01
B	6	6.26199488E+00	0.00000000E+00	8.53057552E+01	4.69424481E+00
H	7	5.84315435E+00	2.53490305E+01	6.45788179E+01	1.78977244E+00
H	8	5.84315435E+00	2.53490305E+01	6.45788179E+01	1.78977244E+00
H	9	3.06911454E+00	5.45973289E+01	3.51878820E+01	3.40892702E+00
H	10	3.06911454E+00	5.45973289E+01	3.51878820E+01	3.40892702E+00
H	11	2.86870725E+00	0.00000000E+00	1.59977901E+01	7.40022099E+01
H	12	6.83625015E+00	0.00000000E+00	6.62103295E+01	2.37896705E+01
H	13	1.28381283E+00	0.00000000E+00	6.03599912E+01	2.96400088E+01
H	14	8.18649009E+00	0.00000000E+00	8.55519242E+01	4.44807580E+00

EIGENVALUES OF THE HESSIAN

-4.39432003E-01	-4.11650179E-01	5.72862655E-01

THE ELLIPTICITY IS 0.06749

EIGENVECTORS OF THE HESSIAN

1.00000000E+00	9.28095801E-20	-1.59220126E-19
-1.84295053E-19	5.03592357E-01	-8.63941398E-01
0.00000000E+00	8.63941398E-01	5.03592357E-01

EIGENVALUES OF THE STRESSIAN

-1.43569060E-01	-1.34195566E-01	-8.57366048E-02

THE TRACE OF THE STRESSIAN IS -0.36350123

EIGENVECTORS OF THE STRESSIAN

3.47219200E-19	1.00000000E+00	-5.75411389E-19
5.16652085E-01	-6.72056128E-19	-8.56195435E-01
8.56195435E-01	0.00000000E+00	5.16652085E-01

VALUES

RHO	1.8715238892E-01
GRAD	1.1553530283E-17
DEL2	-2.7821952679E-01
G(X)	1.4697317445E-01
K(X)	2.1652805615E-01
L(X)	6.9554881698E-02

COMPONENTS OF THE DIVERGENCE OF THE STRESSIAN

-2.00407223E-13	5.44332363E-01	-3.37968498E-01

MAGNITUDE OF THE DIVERGENCE OF THE STRESSIAN 0.640719

1-2-5 Ring

NUMBER OF PERFORMED NEWTON ITERATION STEPS : 7

COORDINATES OF CRITICAL POINT

X =	-1.15851246E-17
Y =	1.39930475E+00
Z =	-3.17042787E-02
R =	1.39966387E+00

VECTORS FROM NUCLEI TO CRITICAL POINT
LENGTHS AND ANGLES MADE WITH PROJECTIONS ONTO YZ/XZ/XY PLANES OF MCS

NUCLEUS		LENGTH	YZ ANGLE	XZ ANGLE	XY ANGLE
B	1	2.33202991E+00	4.50124640E+01	3.68725636E+01	2.19511030E+01
B	2	2.33202991E+00	4.50124640E+01	3.68725636E+01	2.19511030E+01
H	3	4.13403699E+00	3.92000071E+01	1.97845288E+01	4.41958928E+01
H	4	4.13403699E+00	3.92000071E+01	1.97845288E+01	4.41958928E+01
B	5	1.54691095E+00	0.00000000E+00	5.84803758E+01	3.15196242E+01
B	6	4.19596208E+00	0.00000000E+00	7.88875374E+01	1.11124626E+01
H	7	4.05378997E+00	3.81054574E+01	5.10745198E+01	6.78219928E+00
H	8	4.05378997E+00	3.81054574E+01	5.10745198E+01	6.78219928E+00

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  H     9   2.57166641E+00  7.65983300E+01  7.93668466E+00  1.07286072E+01
  H    10   2.57166641E+00  7.65983300E+01  7.93668466E+00  1.07286072E+01
  H    11   3.33213056E+00  0.00000000E+00  2.35824932E+01  6.64175068E+01
  H    12   5.13778768E+00  0.00000000E+00  5.35308675E+01  3.64691325E+01
  H    13   3.25717903E+00  0.00000000E+00  8.40318104E+01  5.96818964E+00
  H    14   6.04762415E+00  0.00000000E+00  8.67897337E+01  3.21026627E+00

EIGENVALUES OF THE HESSIAN
   -1.00371144E-01    2.99419602E-02    4.26577631E-02

EIGENVECTORS OF THE HESSIAN
    1.94980329E-21    1.00000000E+00    3.15360537E-21
   -5.25880987E-01    3.70768927E-21   -8.50558163E-01
    8.50558163E-01    0.00000000E+00   -5.25880987E-01

EIGENVALUES OF THE STRESSIAN
   -3.99254597E-02   -2.98658903E-02   -3.02863609E-03

THE TRACE OF THE STRESSIAN IS  -0.07281999

EIGENVECTORS OF THE STRESSIAN
   -5.81181632E-18    1.00000000E+00   -9.19265130E-18
   -5.34382792E-01   -1.08757550E-17   -8.45242588E-01
    8.45242588E-01    0.00000000E+00   -5.34382792E-01

VALUES
RHO         8.3987372112E-02
GRAD        2.6324718745E-18
DEL2       -2.7771420607E-02
G(X)        3.2938565466E-02
K(X)        3.9881420618E-02
L(X)        6.9428551519E-03

COMPONENTS OF THE DIVERGENCE OF THE STRESSIAN
    9.07432116E-15   -4.93556417E-02   -3.07082269E-02

MAGNITUDE OF THE DIVERGENCE OF THE STRESSIAN        0.058129


CRITICAL POINTS
 1.22279194E-17  2.30062967E-18 -8.23212564E-01   1   2 B-B Bond
-2.06761096E+00 -4.04663287E-19 -1.76110078E+00   1   3
 2.06761096E+00 -3.47107465E-19 -1.76110078E+00   2   4
-1.90456356E+00 -7.34684647E-01 -3.26222341E-01   1   7
-7.88541936E-01 -2.08481150E+00  4.69579194E-01   6   7
 7.88541936E-01 -2.08481150E+00  4.69579194E-01   6   8
 1.90456356E+00 -7.34684647E-01 -3.26222341E-01   2   8
 1.90456356E+00  7.34684647E-01 -3.26222341E-01   2   9
 7.88541936E-01  2.08481150E+00  4.69579194E-01   5   9
-7.88541936E-01  2.08481150E+00  4.69579194E-01   5  10
-1.90456356E+00  7.34684647E-01 -3.26222341E-01   1  10
-1.64072020E-19  2.69259426E+00  1.73302154E+00   5  11
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 1.13544397E-19  3.52300347E+00  2.64534545E-01   5  13
 4.89434994E-20 -2.69259426E+00  1.73302154E+00   6  12
 1.04727149E-19 -3.52300347E+00  2.64534545E-01   6  14
-1.15851246E-17  1.39930475E+00 -3.17042787E-02   1-2-5 Ring
-2.94267484E-17 -1.39930475E+00 -3.17042787E-02   1-2-6 Ring
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B5H9

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SADDLE
B5H9 Using 9s/5p+1d on B, 6s/4,1,1+1p on H
       B    1          0.00000000     2.43415605    -0.27283475
       B    2          2.43415605     0.00000000    -0.27283475
       B    3          0.00000000    -2.43415605    -0.27283475
       B    4         -2.43415605     0.00000000    -0.27283475
       B    5          0.00000000     0.00000000     1.85480774
       H    6          0.00000000     4.64360457    -0.01214649
       H    7          4.64360457     0.00000000    -0.01214649
       H    8          0.00000000    -4.64360457    -0.01214649
       H    9         -4.64360457     0.00000000    -0.01214649
       H   10          1.82099785     1.82099785    -1.96208496
       H   11          1.82099785    -1.82099785    -1.96208496
       H   12         -1.82099785    -1.82099785    -1.96208496
       H   13         -1.82099785     1.82099785    -1.96208496
       H   14          0.00000000     0.00000000     4.07958214

SEARCHING BETWEEN ATOMS    1   5
NUMBER OF PERFORMED NEWTON ITERATION STEPS :    8

COORDINATES OF CRITICAL POINT
         X =  -3.55919379E-16
         Y =   8.18940526E-01
         Z =   1.10430863E+00
         R =   1.37483131E+00

VECTORS FROM NUCLEI TO CRITICAL POINT
LENGTHS 'AND ANGLES MADE WITH PROJECTIONS ONTO YZ/XZ/XY PLANES OF MCS

NUCLEUS         LENGTH         YZ ANGLE         XZ ANGLE         XY ANGLE
  B    1   2.12260337E+00  0.00000000E+00  4.95488719E+01  4.04511281E+01
  B    2   2.91415565E+00  5.66457244E+01  1.63211832E+01  2.82012694E+01
  B    3   3.53258563E+00  0.00000000E+00  6.70554524E+01  2.29445476E+01
  B    4   2.91415565E+00  5.66457244E+01  1.63211832E+01  2.82012694E+01
  B    5   1.11081614E+00  0.00000000E+00  4.74970194E+01  4.25029806E+01
  H    6   3.98428502E+00  0.00000000E+00  7.37269826E+01  1.62730174E+01
  H    7   4.84563711E+00  7.33967363E+01  9.73001620E+00  1.33208696E+01
  H    8   5.57547047E+00  0.00000000E+00  7.84487657E+01  1.15512343E+01
  H    9   4.84563711E+00  7.33967363E+01  9.73001620E+00  1.33208696E+01
  H   10   3.70444621E+00  2.94438828E+01  1.56940962E+01  5.58693518E+01
  H   11   4.43712491E+00  2.42299900E+01  3.65102070E+01  4.37153987E+01
  H   12   4.43712491E+00  2.42299900E+01  3.65102070E+01  4.37153987E+01
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```
  H    13   3.70444621E+00  2.94438828E+01  1.56940962E+01  5.58693518E+01
  H    14   3.08592224E+00  0.00000000E+00  1.53895045E+01  7.46104955E+01

EIGENVALUES OF THE HESSIAN
   -1.64580032E-01   -4.83504622E-02    1.03899732E-01

THE ELLIPTICITY IS      2.40390

EIGENVECTORS OF THE HESSIAN
   -2.62461961E-16    1.00000000E+00    3.07619700E-16
    6.49061769E-01    4.04371315E-16   -7.60735710E-01
    7.60735710E-01    0.00000000E+00    6.49061769E-01

EIGENVALUES OF THE STRESSIAN
   -9.70830955E-02   -9.18329343E-02   -2.96326719E-02

THE TRACE OF THE STRESSIAN IS  -0.21854870

EIGENVECTORS OF THE STRESSIAN
    1.00000000E+00    2.07235443E-16    1.91248120E-16
    2.81997114E-16   -7.34884980E-01   -6.78191763E-01
    0.00000000E+00   -6.78191763E-01    7.34884980E-01

VALUES
RHO         1.3499858609E-01
GRAD        1.0409563458E-16
DEL2       -1.0903076243E-01
G(X)        9.5645505563E-02
K(X)        1.2290319617E-01
L(X)        2.7257690609E-02

COMPONENTS OF THE DIVERGENCE OF THE STRESSIAN
   -2.78565276E-14    1.89003785E-01   -1.60126463E-01

MAGNITUDE OF THE DIVERGENCE OF THE STRESSIAN        0.247715


SEARCHING BETWEEN ATOMS    1   6
NUMBER OF PERFORMED NEWTON ITERATION STEPS :    6

COORDINATES OF CRITICAL POINT
         X =  -1.52837156E-18
         Y =   3.38237572E+00
         Z =  -1.80731906E-01
         R =   3.38720084E+00

VECTORS FROM NUCLEI TO CRITICAL POINT
LENGTHS 'AND ANGLES MADE WITH PROJECTIONS ONTO YZ/XZ/XY PLANES OF MCS

NUCLEUS        LENGTH         YZ ANGLE         XZ ANGLE         XY ANGLE
  B    1   9.52682256E-01  0.00000000E+00  8.44521278E+01  5.54787222E+00
  B    2   4.16822074E+00  3.57309390E+01  5.42395603E+01  1.26613586E+00
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  B     3   5.81726094E+00  0.00000000E+00  8.90928162E+01  9.07183773E-01
  B     4   4.16822074E+00  3.57309390E+01  5.42395603E+01  1.26613586E+00
  B     5   3.94764324E+00  0.00000000E+00  5.89601485E+01  3.10398515E+01
  H     6   1.27244617E+00  0.00000000E+00  8.23865407E+01  7.61345933E+00
  H     7   5.74734286E+00  5.38967799E+01  3.60514304E+01  1.68088432E+00
  H     8   8.02775066E+00  0.00000000E+00  8.87966812E+01  1.20331876E+00
  H     9   5.74734286E+00  5.38967799E+01  3.60514304E+01  1.68088432E+00
  H    10   2.98783412E+00  3.75512530E+01  3.15053716E+01  3.65983764E+01
  H    11   5.79347464E+00  1.83196937E+01  6.39151461E+01  1.79071741E+01
  H    12   5.79347464E+00  1.83196937E+01  6.39151461E+01  1.79071741E+01
  H    13   2.98783412E+00  3.75512530E+01  3.15053716E+01  3.65983764E+01
  H    14   5.43973725E+00  0.00000000E+00  3.84469881E+01  5.15530119E+01

EIGENVALUES OF THE HESSIAN
   -4.34028730E-01   -3.98182816E-01    5.77573963E-01

THE ELLIPTICITY IS      0.09002

EIGENVECTORS OF THE HESSIAN
    1.00000000E+00   -5.72725482E-19   -4.55843567E-18
   -4.59427364E-18   -1.24660725E-01   -9.92199427E-01
    0.00000000E+00    9.92199427E-01   -1.24660725E-01

EIGENVALUES OF THE STRESSIAN
   -1.40105306E-01   -1.33388826E-01   -8.91865162E-02

THE TRACE OF THE STRESSIAN IS  -0.36268065

EIGENVECTORS OF THE STRESSIAN
    2.07168258E-19    1.00000000E+00    2.31206137E-18
   -8.92457198E-02    2.32132429E-18   -9.96009639E-01
    9.96009639E-01    0.00000000E+00   -8.92457198E-02

VALUES
RHO         1.8690945034E-01
GRAD        6.7655281192E-17
DEL2       -2.5463758215E-01
G(X)        1.4951062610E-01
K(X)        2.1317002164E-01
L(X)        6.3659395537E-02

COMPONENTS OF THE DIVERGENCE OF THE STRESSIAN
    5.04661125E-19    6.37728855E-01    6.86708727E-02

MAGNITUDE OF THE DIVERGENCE OF THE STRESSIAN        0.641415


SEARCHING BETWEEN ATOMS     5  14
NUMBER OF PERFORMED NEWTON ITERATION STEPS :     6

COORDINATES OF CRITICAL POINT
         X =  -1.27430319E-18
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          Y =  -8.94102280E-19
          Z =   2.80683740E+00
          R =   2.80683740E+00

VECTORS FROM NUCLEI TO CRITICAL POINT
LENGTHS 'AND ANGLES MADE WITH PROJECTIONS ONTO YZ/XZ/XY PLANES OF MCS

NUCLEUS          LENGTH          YZ ANGLE          XZ ANGLE          XY ANGLE
  B     1   3.92549312E+00  0.00000000E+00  3.83226516E+01  5.16773484E+01
  B     2   3.92549312E+00  3.83226516E+01  0.00000000E+00  5.16773484E+01
  B     3   3.92549312E+00  0.00000000E+00  3.83226516E+01  5.16773484E+01
  B     4   3.92549312E+00  3.83226516E+01  0.00000000E+00  5.16773484E+01
  B     5   9.52029664E-01  0.00000000E+00  0.00000000E+00  9.00000000E+01
  H     6   5.43228622E+00  0.00000000E+00  5.87394008E+01  3.12605992E+01
  H     7   5.43228622E+00  5.87394008E+01  0.00000000E+00  3.12605992E+01
  H     8   5.43228622E+00  0.00000000E+00  5.87394008E+01  3.12605992E+01
  H     9   5.43228622E+00  5.87394008E+01  0.00000000E+00  3.12605992E+01
  H    10   5.41984196E+00  1.96325839E+01  1.96325839E+01  6.16303790E+01
  H    11   5.41984196E+00  1.96325839E+01  1.96325839E+01  6.16303790E+01
  H    12   5.41984196E+00  1.96325839E+01  1.96325839E+01  6.16303790E+01
  H    13   5.41984196E+00  1.96325839E+01  1.96325839E+01  6.16303790E+01
  H    14   1.27274474E+00  0.00000000E+00  0.00000000E+00  9.00000000E+01

EIGENVALUES OF THE HESSIAN
   -3.72363680E-01   -3.72363680E-01    6.08473153E-01

THE ELLIPTICITY IS      0.00000

EIGENVECTORS OF THE HESSIAN
    5.34256688E-01   -8.45322300E-01    0.00000000E+00
   -8.45322300E-01   -5.34256688E-01    0.00000000E+00
    0.00000000E+00    0.00000000E+00    1.00000000E+00

EIGENVALUES OF THE STRESSIAN
   -1.32686028E-01   -1.32686028E-01   -8.42078979E-02

THE TRACE OF THE STRESSIAN IS  -0.34957995

EIGENVECTORS OF THE STRESSIAN
    6.94077898E-01   -7.19899904E-01    0.00000000E+00
   -7.19899904E-01   -6.94077898E-01    0.00000000E+00
    0.00000000E+00    0.00000000E+00    1.00000000E+00

VALUES
RHO        1.7721521619E-01
GRAD       1.4573939566E-16
DEL2      -1.3625420748E-01
G(X)       1.5775820120E-01
K(X)       1.9182175307E-01
L(X)       3.4063551869E-02

COMPONENTS OF THE DIVERGENCE OF THE STRESSIAN
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   -1.01844386E-18   -9.35544752E-19    6.06705634E-01

MAGNITUDE OF THE DIVERGENCE OF THE STRESSIAN        0.606706

SEARCHING BETWEEN ATOMS    1  10
NUMBER OF PERFORMED NEWTON ITERATION STEPS :    9

COORDINATES OF CRITICAL POINT
         X =   7.97172045E-01
         Y =   1.90177103E+00
         Z =  -6.77580053E-01
         R =   2.17056008E+00

VECTORS FROM NUCLEI TO CRITICAL POINT
LENGTHS 'AND ANGLES MADE WITH PROJECTIONS ONTO YZ/XZ/XY PLANES OF MCS

NUCLEUS        LENGTH         YZ ANGLE         XZ ANGLE         XY ANGLE
  B    1   1.04054593E+00  5.00057926E+01  3.07731374E+01  2.28906731E+01
  B    2   2.54170582E+00  4.00944371E+01  4.84369637E+01  9.16287878E+00
  B    3   4.42713967E+00  1.03735346E+01  7.83493033E+01  5.24551438E+00
  B    4   3.77121109E+00  5.89637141E+01  3.02840035E+01  6.16113749E+00
  B    5   3.26576243E+00  1.41286426E+01  3.56150127E+01  5.08445240E+01
  H    6   2.93188271E+00  1.57772199E+01  6.92569943E+01  1.31184302E+01
  H    7   4.34218586E+00  6.23536651E+01  2.59747814E+01  8.81523035E+00
  H    8   6.62723373E+00  6.90868371E+00  8.09853177E+01  5.76271997E+00
  H    9   5.80186048E+00  6.96793978E+01  1.91344747E+01  6.58592582E+00
  H   10   1.64459613E+00  3.85018092E+01  2.81517451E+00  5.13564281E+01
  H   11   4.06905152E+00  1.45729751E+01  6.61913081E+01  1.84016726E+01
  H   12   4.72903527E+00  3.36169004E+01  5.19260324E+01  1.57607438E+01
  H   13   2.91741165E+00  6.38221552E+01  1.58652754E+00  2.61223361E+01
  H   14   5.18486340E+00  8.84429970E+00  2.15179620E+01  6.65646827E+01

EIGENVALUES OF THE HESSIAN
   -1.82212873E-01   -2.29319107E-02    2.83854408E-01

THE ELLIPTICITY IS      6.94582

EIGENVECTORS OF THE HESSIAN
   -6.08163375E-01   -2.17592444E-01   -7.63407386E-01
   -6.60896420E-01    6.71508709E-01    3.35099949E-01
   -4.39719492E-01   -7.08328725E-01    5.52193070E-01

EIGENVALUES OF THE STRESSIAN
   -8.88780989E-02   -8.34605285E-02   -3.89868087E-02

THE TRACE OF THE STRESSIAN IS  -0.21132544

EIGENVECTORS OF THE STRESSIAN
    1.19370515E-02    6.59111640E-01    7.51950366E-01
    7.17003933E-01    5.18517126E-01   -4.65881262E-01
   -6.96966905E-01    5.44712619E-01   -4.66396072E-01
```

VALUES

RHO	1.1355555229E-01
GRAD	5.6638123765E-17
DEL2	7.8709624208E-02
G(X)	1.1550142105E-01
K(X)	9.5824014998E-02
L(X)	-1.9677406052E-02

COMPONENTS OF THE DIVERGENCE OF THE STRESSIAN

2.31030164E-01 -1.49766152E-01 -1.08738288E-01

MAGNITUDE OF THE DIVERGENCE OF THE STRESSIAN 0.296022

1-5-2-10 RING

NUMBER OF PERFORMED NEWTON ITERATION STEPS : 3

COORDINATES OF CRITICAL POINT

X =	1.23152620E+00
Y =	1.23152620E+00
Z =	-2.77838961E-01
R =	1.76366325E+00

VECTORS FROM NUCLEI TO CRITICAL POINT
LENGTHS 'AND ANGLES MADE WITH PROJECTIONS ONTO YZ/XZ/XY PLANES OF MCS

NUCLEUS		LENGTH	YZ ANGLE	XZ ANGLE	XY ANGLE
B	1	1.72133680E+00	4.56798897E+01	4.43196259E+01	1.66568550E-01
B	2	1.72133680E+00	4.43196259E+01	4.56798897E+01	1.66568550E-01
B	3	3.86702834E+00	1.85703235E+01	7.14295176E+01	7.41448540E-02
B	4	3.86702834E+00	7.14295176E+01	1.85703235E+01	7.41448540E-02
B	5	2.75345156E+00	2.65684299E+01	2.65684299E+01	5.07629620E+01
H	6	3.63724182E+00	1.97908668E+01	6.97340588E+01	4.18906108E+00
H	7	3.63724182E+00	6.97340588E+01	1.97908668E+01	4.18906108E+00
H	8	6.00869460E+00	1.18270031E+01	7.78968121E+01	2.53433123E+00
H	9	6.00869460E+00	7.78968121E+01	1.18270031E+01	2.53433123E+00
H	10	1.87926535E+00	1.82806215E+01	1.82806215E+01	6.36663105E+01
H	11	3.53582586E+00	9.59681835E+00	5.96906145E+01	2.84464620E+01
H	12	4.63384190E+00	4.12042930E+01	4.12042930E+01	2.13132350E+01
H	13	3.53582586E+00	5.96906145E+01	9.59681835E+00	2.84464620E+01
H	14	4.69259334E+00	1.52149179E+01	1.52149179E+01	6.82136385E+01

EIGENVALUES OF THE HESSIAN

-1.56521078E-01 2.87858638E-02 4.90381870E-02

EIGENVECTORS OF THE HESSIAN

-6.29462766E-01	7.07106781E-01	-3.22143796E-01
-6.29462766E-01	-7.07106781E-01	-3.22143796E-01
-4.55580126E-01	0.00000000E+00	8.90194781E-01

EIGENVALUES OF THE STRESSIAN

-5.29483553E-02 -4.91299146E-02 -9.17235813E-05

THE TRACE OF THE STRESSIAN IS -0.10216999

EIGENVECTORS OF THE STRESSIAN

5.12711243E-01	-4.86957063E-01	7.07106781E-01
5.12711243E-01	-4.86957063E-01	-7.07106781E-01
6.88661283E-01	7.25083193E-01	-5.12471356E-15

VALUES

RHO	1.1095363237E-01
GRAD	3.0456626572E-17
DEL2	-7.8697026912E-02
G(X)	4.1247868364E-02
K(X)	6.0922125092E-02
L(X)	1.9674256728E-02

COMPONENTS OF THE DIVERGENCE OF THE STRESSIAN

2.36047981E-03 2.36047981E-03 2.37127971E-03

MAGNITUDE OF THE DIVERGENCE OF THE STRESSIAN 0.004095

CRITICAL POINTS

-3.55919379E-16	8.18940526E-01	1.10430863E+00	B	1	B	5
8.18940526E-01	5.95729360E-17	1.10430863E+00	B	2	B	5
2.56322460E-16	-8.18940526E-01	1.10430863E+00	B	3	B	5
-8.18940526E-01	-1.82814063E-16	1.10430863E+00	B	4	B	5
-1.52837156E-18	3.38237572E+00	-1.80731906E-01	B	1	H	6
3.38237572E+00	-4.54931409E-19	-1.80731906E-01	B	2	H	7
3.47604404E-20	-3.38237572E+00	-1.80731906E-01	B	3	H	8
-3.38237572E+00	7.05647129E-20	-1.80731906E-01	B	4	H	9
-1.27430319E-18	-8.94102280E-19	2.80683740E+00	B	5	H	14
7.97172045E-01	1.90177103E+00	-6.77580053E-01	B	1	H	10
1.90177103E+00	7.97172045E-01	-6.77580053E-01	B	2	H	10
1.90177103E+00	-7.97172045E-01	-6.77580053E-01	B	2	H	11
7.97172045E-01	-1.90177103E+00	-6.77580053E-01	B	3	H	11
-7.97172045E-01	-1.90177103E+00	-6.77580053E-01	B	3	H	12
-1.90177103E+00	-7.97172045E-01	-6.77580053E-01	B	4	H	12
-1.90177103E+00	7.97172045E-01	-6.77580053E-01	B	4	H	13
-7.97172045E-01	1.90177103E+00	-6.77580053E-01	B	1	H	13
1.23152620E+00	1.23152620E+00	-2.77838961E-01	B	1	B	2
1.23152620E+00	-1.23152620E+00	-2.77838961E-01	B	2	B	3
-1.23152620E+00	-1.23152620E+00	-2.77838961E-01	B	3	B	4
-1.23152620E+00	1.23152620E+00	-2.77838961E-01	B	1	B	4

B6H10

SADDLE

B6H10 OPTIMIZATION USING VD SET(Renormalized) d=0.75, p=1.0725

B	1	2.84236207	-0.11692499	0.00000000
B	2	0.00000000	1.64074943	0.00000000
H	3	4.91057066	0.70327194	0.00000000
B	4	0.70224922	-0.21088470	2.69922671
B	5	0.70224922	-0.21088470	-2.69922671
H	6	2.60859821	-1.77116675	1.79789076
H	7	2.60859821	-1.77116675	-1.79789076
H	8	-0.01128123	3.86981331	0.00000000
B	9	-2.43040813	-0.35556816	1.54955953
B	10	-2.43040813	-0.35556816	-1.54955953
H	11	1.36769926	0.34747057	4.74802345
H	12	1.36769926	0.34747057	-4.74802345
H	13	-0.92214902	-2.10902166	2.63831555
H	14	-0.92214902	-2.10902166	-2.63831555
H	15	-3.96890378	0.26887843	3.04215026
H	16	-3.96890378	0.26887843	-3.04215026

SEARCHING BETWEEN ATOMS 1 2
NUMBER OF PERFORMED NEWTON ITERATION STEPS : 6

COORDINATES OF CRITICAL POINT
X = 1.10054963E+00
Y = 9.05150686E-01
Z = 1.35635635E-16
R = 1.42495869E+00

VECTORS FROM NUCLEI TO CRITICAL POINT
LENGTHS AND ANGLES MADE WITH PROJECTIONS ONTO YZ/XZ/XY PLANES OF MCS

NUCLEUS		LENGTH	YZ ANGLE	XZ ANGLE	XY ANGLE
B	1	2.01954184E+00	5.95960752E+01	3.04039248E+01	0.00000000E+00
B	2	1.32375036E+00	5.62415432E+01	3.37584568E+01	0.00000000E+00
H	3	3.81536568E+00	8.69669476E+01	3.03305244E+00	0.00000000E+00
B	4	2.94788111E+00	7.76521998E+00	2.22463099E+01	6.62981746E+01
B	5	2.94788111E+00	7.76521998E+00	2.22463099E+01	6.62981746E+01
H	6	3.55939555E+00	2.50672090E+01	4.87554242E+01	3.03387381E+01
H	7	3.55939555E+00	2.50672090E+01	4.87554242E+01	3.03387381E+01
H	8	3.16629000E+00	2.05574410E+01	6.94425590E+01	0.00000000E+00
B	9	4.05687188E+00	6.05010386E+01	1.81051169E+01	2.24550928E+01
B	10	4.05687188E+00	6.05010386E+01	1.81051169E+01	2.24550928E+01
H	11	4.78812100E+00	3.19843603E+00	6.68851199E+00	8.25797671E+01
H	12	4.78812100E+00	3.19843603E+00	6.68851199E+00	8.25797671E+01
H	13	4.48745515E+00	2.67915022E+01	4.21975238E+01	3.60103473E+01
H	14	4.48745515E+00	2.67915022E+01	4.21975238E+01	3.60103473E+01
H	15	5.94633320E+00	5.84884006E+01	6.14254892E+00	3.07705333E+01
H	16	5.94633320E+00	5.84884006E+01	6.14254892E+00	3.07705333E+01

EIGENVALUES OF THE HESSIAN
-1.62457366E-01 -5.65499135E-02 1.97702799E-02

THE ELLIPTICITY IS 1.87281

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EIGENVECTORS OF THE HESSIAN
    5.09151191E-01    0.00000000E+00    8.60677097E-01
    8.60677097E-01    0.00000000E+00   -5.09151191E-01
    0.00000000E+00    1.00000000E+00    0.00000000E+00

EIGENVALUES OF THE STRESSIAN
   -6.83077814E-02   -6.77567601E-02   -6.47921043E-03

THE TRACE OF THE STRESSIAN IS  -0.14254375

EIGENVECTORS OF THE STRESSIAN
    0.00000000E+00    5.56830915E-01    8.30625868E-01
    0.00000000E+00    8.30625868E-01   -5.56830915E-01
    1.00000000E+00    0.00000000E+00    0.00000000E+00

VALUES
RHO         1.2618468000E-01
GRAD        8.2305189803E-17
DEL2       -1.9923699953E-01
G(X)        4.6367251041E-02
K(X)        9.6176500922E-02
L(X)        4.9809249882E-02

COMPONENTS OF THE DIVERGENCE OF THE STRESSIAN
    8.01048857E-02   -4.80802494E-02    2.84811774E-13

MAGNITUDE OF THE DIVERGENCE OF THE STRESSIAN        0.093426

SEARCHING BETWEEN ATOMS    1   3
NUMBER OF PERFORMED NEWTON ITERATION STEPS :    6

COORDINATES OF CRITICAL POINT
         X =   3.73375050E+00
         Y =   2.22008455E-01
         Z =  -3.35153950E-19
         R =   3.74034497E+00

VECTORS FROM NUCLEI TO CRITICAL POINT
LENGTHS AND ANGLES MADE WITH PROJECTIONS ONTO YZ/XZ/XY PLANES OF MCS

NUCLEUS        LENGTH        YZ ANGLE        XZ ANGLE        XY ANGLE
  B    1   9.53650464E-01  6.91816484E+01  2.08183516E+01  0.00000000E+00
  B    2   3.99421065E+00  6.91943382E+01  2.08056618E+01  0.00000000E+00
  H    3   1.27142449E+00  6.77577726E+01  2.22422274E+01  0.00000000E+00
  B    4   4.08206091E+00  4.79567821E+01  6.08753216E+00  4.13945998E+01
  B    5   4.08206091E+00  4.79567821E+01  6.08753216E+00  4.13945998E+01
  H    6   2.91051993E+00  2.27419382E+01  4.32212623E+01  3.81499372E+01
  H    7   2.91051993E+00  2.27419382E+01  4.32212623E+01  3.81499372E+01
  H    8   5.22797694E+00  4.57534819E+01  4.42465181E+01  0.00000000E+00
  B    9   6.38212982E+00  7.49824796E+01  5.19231707E+00  1.40516579E+01
  B   10   6.38212982E+00  7.49824796E+01  5.19231707E+00  1.40516579E+01
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  H    11   5.30637973E+00  2.64801691E+01  1.35480685E+00  6.34797258E+01
  H    12   5.30637973E+00  2.64801691E+01  1.35480685E+00  6.34797258E+01
  H    13   5.83710636E+00  5.29051635E+01  2.35373541E+01  2.68714525E+01
  H    14   5.83710636E+00  5.29051635E+01  2.35373541E+01  2.68714525E+01
  H    15   8.28177263E+00  6.84462191E+01  3.24262235E-01  2.15510954E+01
  H    16   8.28177263E+00  6.84462191E+01  3.24262235E-01  2.15510954E+01

EIGENVALUES OF THE HESSIAN
   -4.27293821E-01   -3.97559820E-01    5.70559040E-01

THE ELLIPTICITY IS      0.07479

EIGENVECTORS OF THE HESSIAN
    0.00000000E+00    3.74064280E-01   -9.27402779E-01
    0.00000000E+00   -9.27402779E-01   -3.74064280E-01
    1.00000000E+00    0.00000000E+00    0.00000000E+00

EIGENVALUES OF THE STRESSIAN
   -1.40838005E-01   -1.35859890E-01   -8.77453258E-02

THE TRACE OF THE STRESSIAN IS  -0.36444322

EIGENVECTORS OF THE STRESSIAN
    3.53368314E-01    0.00000000E+00    9.35484278E-01
   -9.35484278E-01    0.00000000E+00    3.53368314E-01
    0.00000000E+00    1.00000000E+00    0.00000000E+00

VALUES
RHO        1.8726999512E-01
GRAD       4.0609675207E-17
DEL2      -2.5429460089E-01
G(X)       1.5043478533E-01
K(X)       2.1400843555E-01
L(X)       6.3573650222E-02

COMPONENTS OF THE DIVERGENCE OF THE STRESSIAN
    5.98411407E-01    2.31365050E-01    4.12580017E-14

MAGNITUDE OF THE DIVERGENCE OF THE STRESSIAN        0.641581

SEARCHING BETWEEN ATOMS    2   8
NUMBER OF PERFORMED NEWTON ITERATION STEPS :    6

COORDINATES OF CRITICAL POINT
         X =  -7.38687359E-03
         Y =   2.59356866E+00
         Z =   1.30404105E-18
         R =   2.59357918E+00

VECTORS FROM NUCLEI TO CRITICAL POINT
LENGTHS AND ANGLES MADE WITH PROJECTIONS ONTO YZ/XZ/XY PLANES OF MCS
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NUCLEUS		LENGTH	YZ ANGLE	XZ ANGLE	XY ANGLE
B	1	3.93291811E+00	4.64346627E+01	4.35653373E+01	0.00000000E+00
B	2	9.52847866E-01	4.44185200E-01	8.95558148E+01	0.00000000E+00
H	3	5.26873116E+00	6.89749266E+01	2.10250734E+01	0.00000000E+00
B	4	3.95655998E+00	1.03322998E+01	4.51382598E+01	4.30170168E+01
B	5	3.95655998E+00	1.03322998E+01	4.51382598E+01	4.30170168E+01
H	6	5.39691619E+00	2.89940305E+01	5.39736112E+01	1.94590452E+01
H	7	5.39691619E+00	2.89940305E+01	5.39736112E+01	1.94590452E+01
H	8	1.27625059E+00	1.74832854E-01	8.98251671E+01	0.00000000E+00
B	9	4.11941437E+00	3.60290642E+01	4.57179638E+01	2.20960354E+01
B	10	4.11941437E+00	3.60290642E+01	4.57179638E+01	2.20960354E+01
H	11	5.42950690E+00	1.46706069E+01	2.44364453E+01	6.09841081E+01
H	12	5.42950690E+00	1.46706069E+01	2.44364453E+01	6.09841081E+01
H	13	5.46917311E+00	9.62842288E+00	5.92981410E+01	2.88421053E+01
H	14	5.46917311E+00	9.62842288E+00	5.92981410E+01	2.88421053E+01
H	15	5.50930840E+00	4.59768310E+01	2.49581912E+01	3.35169528E+01
H	16	5.50930840E+00	4.59768310E+01	2.49581912E+01	3.35169528E+01

EIGENVALUES OF THE HESSIAN

-3.91456887E-01	-3.84276775E-01	5.91821653E-01

THE ELLIPTICITY IS 0.01868

EIGENVECTORS OF THE HESSIAN

0.00000000E+00	9.99990856E-01	-4.27643220E-03
0.00000000E+00	4.27643220E-03	9.99990856E-01
1.00000000E+00	0.00000000E+00	0.00000000E+00

EIGENVALUES OF THE STRESSIAN

-1.36304165E-01	-1.36074791E-01	-8.46435471E-02

THE TRACE OF THE STRESSIAN IS -0.35702250

EIGENVECTORS OF THE STRESSIAN

9.99971732E-01	0.00000000E+00	-7.51903642E-03
-7.51903642E-03	0.00000000E+00	-9.99971732E-01
0.00000000E+00	1.00000000E+00	0.00000000E+00

VALUES

RHO	1.8129777167E-01
GRAD	1.5488761465E-16
DEL2	-1.8391200848E-01
G(X)	1.5552225087E-01
K(X)	2.0150025298E-01
L(X)	4.5978002119E-02

COMPONENTS OF THE DIVERGENCE OF THE STRESSIAN

-5.58878613E-03	6.20630997E-01	3.45802918E-13

MAGNITUDE OF THE DIVERGENCE OF THE STRESSIAN 0.620656

2-4 Bond
NUMBER OF PERFORMED NEWTON ITERATION STEPS : 5

COORDINATES OF CRITICAL POINT
X = 2.17911909E-01
Y = 9.08930599E-01
Z = 1.00608502E+00
R = 1.37326163E+00

VECTORS FROM NUCLEI TO CRITICAL POINT
LENGTHS AND ANGLES MADE WITH PROJECTIONS ONTO YZ/XZ/XY PLANES OF MCS

NUCLEUS		LENGTH	YZ ANGLE	XZ ANGLE	XY ANGLE
B	1	2.99204368E+00	6.12996221E+01	2.00512880E+01	1.96487778E+01
B	2	1.26303265E+00	9.93499213E+00	3.54093389E+01	5.28031311E+01
H	3	4.80370156E+00	7.76565940E+01	2.45372774E+00	1.20895096E+01
B	4	2.08693500E+00	1.34196015E+01	3.24513777E+01	5.42236717E+01
B	5	3.90101320E+00	7.13206459E+00	1.66818777E+01	7.17745403E+01
H	6	3.67767034E+00	4.05457141E+01	4.67815925E+01	1.24331811E+01
H	7	4.55637827E+00	3.16473793E+01	3.60299328E+01	3.79806811E+01
H	8	3.13553233E+00	4.19179908E+00	7.07866731E+01	1.87152916E+01
B	9	2.98461399E+00	6.25389017E+01	2.50666635E+01	1.04916401E+01
B	10	3.89151323E+00	4.28856465E+01	1.89617913E+01	4.10503934E+01
H	11	3.95466200E+00	1.69023990E+01	8.16210164E+00	7.11219564E+01
H	12	5.89465967E+00	1.12479812E+01	5.46564745E+00	7.74630391E+01
H	13	3.61551535E+00	1.83804107E+01	5.65869611E+01	2.68368613E+01
H	14	4.86717888E+00	1.35465001E+01	3.83206560E+01	4.84839975E+01
H	15	4.69943125E+00	6.29890394E+01	7.82788820E+00	2.56744866E+01
H	16	5.85895053E+00	4.56105621E+01	6.27170759E+00	4.37052676E+01

EIGENVALUES OF THE HESSIAN
-1.67426629E-01 -4.78898016E-02 2.83207930E-02

THE ELLIPTICITY IS 2.49608

EIGENVECTORS OF THE HESSIAN
1.51018887E-01 9.77923123E-01 1.44428739E-01
8.41066755E-01 -5.03413728E-02 -5.38583754E-01
5.19422766E-01 -2.02810530E-01 8.30101126E-01

EIGENVALUES OF THE STRESSIAN
-7.22936218E-02 -6.93484749E-02 -9.51464732E-03

THE TRACE OF THE STRESSIAN IS -0.15115674

EIGENVECTORS OF THE STRESSIAN
-9.12237826E-01 3.56248936E-01 2.02259352E-01
1.81274814E-01 7.93790502E-01 -5.80548086E-01
3.67371190E-01 4.92933397E-01 7.88704681E-01

VALUES
RHO 1.2465558058E-01

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GRAD        5.9285935503E-17
DEL2       -1.8699563806E-01
G(X)        5.2203917244E-02
K(X)        9.8952826758E-02
L(X)        4.6748909514E-02

COMPONENTS OF THE DIVERGENCE OF THE STRESSIAN
    1.90089279E-02   -6.67738230E-02    1.01956381E-01

MAGNITUDE OF THE DIVERGENCE OF THE STRESSIAN        0.123350



SEARCHING BETWEEN ATOMS    2   9
NUMBER OF PERFORMED NEWTON ITERATION STEPS :    6

COORDINATES OF CRITICAL POINT
         X =  -1.09381897E+00
         Y =   5.42788593E-01
         Z =   9.79091496E-01
         R =   1.56514521E+00

VECTORS FROM NUCLEI TO CRITICAL POINT
LENGTHS AND ANGLES MADE WITH PROJECTIONS ONTO YZ/XZ/XY PLANES OF MCS

NUCLEUS         LENGTH         YZ ANGLE         XZ ANGLE         XY ANGLE
  B     1   4.10942372E+00   7.33040060E+01   9.23805324E+00   1.37835826E+01
  B     2   1.83318796E+00   3.66321914E+01   3.67936766E+01   3.22823715E+01
  H     3   6.08580889E+00   8.06173085E+01   1.51107020E+00   9.25804084E+00
  B     4   2.59860530E+00   4.37224958E+01   1.68597474E+01   4.14484208E+01
  B     5   4.16220004E+00   2.55639951E+01   1.04324226E+01   6.20973190E+01
  H     6   4.44215201E+00   5.64572493E+01   3.13932207E+01   1.06217757E+01
  H     7   5.17435143E+00   4.56868654E+01   2.65639993E+01   3.24580654E+01
  H     8   3.63312559E+00   1.73353093E+01   6.63120682E+01   1.56339290E+01
  B     9   1.70849326E+00   5.14735245E+01   3.17233365E+01   1.95057373E+01
  B    10   2.99793120E+00   2.64769132E+01   1.74371168E+01   5.75078796E+01
  H    11   4.50578175E+00   3.31136925E+01   2.48445369E+00   5.67687684E+01
  H    12   6.23675129E+00   2.32459902E+01   1.79464082E+00   6.66766295E+01
  H    13   3.13282503E+00   3.14121996E+00   5.78286737E+01   3.19801556E+01
  H    14   4.48856346E+00   2.19187341E+00   3.62132765E+01   5.36988531E+01
  H    15   3.54927470E+00   5.41006748E+01   4.42612018E+00   3.55393590E+01
  H    16   4.95091150E+00   3.55010785E+01   3.17151973E+00   5.43136482E+01

EIGENVALUES OF THE HESSIAN
   -1.31863501E-01   -7.47293706E-03    4.65461153E-02

THE ELLIPTICITY IS      16.64547

EIGENVECTORS OF THE HESSIAN
   -4.46148755E-01    4.09807414E-01    7.95618735E-01
    7.95952822E-01   -2.24740013E-01    5.62095215E-01
    4.09158151E-01    8.84053059E-01   -2.25919890E-01
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EIGENVALUES OF THE STRESSIAN
   -5.02222294E-02   -4.20996884E-02    2.38215554E-03

THE TRACE OF THE STRESSIAN IS  -0.08993976

EIGENVECTORS OF THE STRESSIAN
    1.39112261E-01    7.10072411E-01   -6.90249918E-01
   -7.25069315E-01   -4.01711067E-01   -5.59377070E-01
   -6.74479256E-01    5.78295245E-01    4.58968782E-01

VALUES
RHO         1.0680479036E-01
GRAD        6.5467140175E-17
DEL2       -9.2790323143E-02
G(X)        3.3371090728E-02
K(X)        5.6568671514E-02
L(X)        2.3197580786E-02

COMPONENTS OF THE DIVERGENCE OF THE STRESSIAN
    1.97997016E-02    4.80140090E-03    6.81953866E-03

MAGNITUDE OF THE DIVERGENCE OF THE STRESSIAN        0.021485


(3,-3)  BETWEEN ATOMS    9  10
NUMBER OF PERFORMED NEWTON ITERATION STEPS :    4

COORDINATES OF CRITICAL POINT
         X =  -2.45610400E+00
         Y =  -4.53891194E-01
         Z =  -4.20522952E-15
         R =   2.49769175E+00

VECTORS FROM NUCLEI TO CRITICAL POINT
LENGTHS AND ANGLES MADE WITH PROJECTIONS ONTO YZ/XZ/XY PLANES OF MCS

NUCLEUS         LENGTH          YZ ANGLE          XZ ANGLE          XY ANGLE
  B    1   5.30917027E+00  8.63610647E+01  3.63893529E+00  0.00000000E+00
  B    2   3.22799724E+00  4.95414405E+01  4.04585595E+01  0.00000000E+00
  H    3   7.45700490E+00  8.10728800E+01  8.92712002E+00  0.00000000E+00
  B    4   4.16173907E+00  4.93675197E+01  3.34743967E+00  4.04347336E+01
  B    5   4.16173907E+00  4.93675197E+01  3.34743967E+00  4.04347336E+01
  H    6   5.53342883E+00  6.62472052E+01  1.37719349E+01  1.89603896E+01
  H    7   5.53342883E+00  6.62472052E+01  1.37719349E+01  1.89603896E+01
  H    8   4.96704933E+00  2.94858286E+01  6.05141714E+01  0.00000000E+00
  B    9   1.55288842E+00  9.48124906E-01  3.63018082E+00  8.62477255E+01
  B   10   1.55288842E+00  9.48124906E-01  3.63018082E+00  8.62477255E+01
  H   11   6.14877051E+00  3.84536221E+01  7.48859171E+00  5.05510221E+01
  H   12   6.14877051E+00  3.84536221E+01  7.48859171E+00  5.05510221E+01
  H   13   3.47176953E+00  2.62211248E+01  2.84726842E+01  4.94583758E+01
  H   14   3.47176953E+00  2.62211248E+01  2.84726842E+01  4.94583758E+01
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  H    15   3.47356262E+00  2.58182730E+01  1.20097024E+01  6.11399378E+01
  H    16   3.47356262E+00  2.58182730E+01  1.20097024E+01  6.11399378E+01

EIGENVALUES OF THE HESSIAN
   -2.59572980E-01   -1.92299305E-01   -7.59341966E-03

THE ELLIPTICITY IS      0.34984

EIGENVECTORS OF THE HESSIAN
    7.68069340E-01   -6.40366683E-01    0.00000000E+00
   -6.40366683E-01   -7.68069340E-01    0.00000000E+00
    0.00000000E+00    0.00000000E+00    1.00000000E+00

EIGENVALUES OF THE STRESSIAN
   -8.65130137E-02   -7.76727178E-02   -5.31635884E-03

THE TRACE OF THE STRESSIAN IS  -0.16950209

EIGENVECTORS OF THE STRESSIAN
   -7.46458026E-01    6.65432502E-01    0.00000000E+00
   -6.65432502E-01   -7.46458026E-01    0.00000000E+00
    0.00000000E+00    0.00000000E+00    1.00000000E+00

VALUES
RHO         1.6980610970E-01
GRAD        7.8223157467E-17
DEL2       -4.5946570424E-01
G(X)        2.7317832149E-02
K(X)        1.4218425821E-01
L(X)        1.1486642606E-01

COMPONENTS OF THE DIVERGENCE OF THE STRESSIAN
   -1.33718714E-02   -1.59018823E-02   -3.15812499E-12

MAGNITUDE OF THE DIVERGENCE OF THE STRESSIAN        0.020777


(3,-1) btw non-nuclear attractor and atom 9
NUMBER OF PERFORMED NEWTON ITERATION STEPS :    6

COORDINATES OF CRITICAL POINT
         X =  -2.45839407E+00
         Y =  -4.63370629E-01
         Z =   3.87414898E-01
         R =   2.53150233E+00

VECTORS FROM NUCLEI TO CRITICAL POINT
LENGTHS AND ANGLES MADE WITH PROJECTIONS ONTO YZ/XZ/XY PLANES OF MCS

NUCLEUS        LENGTH         YZ ANGLE         XZ ANGLE         XY ANGLE
  B    1   5.32617410E+00  8.44001917E+01  3.72948699E+00  4.17126035E+00
  B    2   3.25900490E+00  4.89676352E+01  4.02131280E+01  6.82719231E+00
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  H     3   7.47079557E+00  8.05291622E+01  8.98410296E+00  2.97253474E+00
  B     4   3.92401440E+00  5.36548673E+01  3.68917577E+00  3.60963284E+01
  B     5   4.42501656E+00  4.55831591E+01  3.27100230E+00  4.42302506E+01
  H     6   5.41979554E+00  6.92127530E+01  1.39632742E+01  1.50846129E+01
  H     7   5.67100541E+00  6.33152564E+01  1.33330454E+01  2.26652922E+01
  H     8   4.99148621E+00  2.93574984E+01  6.02403211E+01  4.45149695E+00
  B     9   1.16746937E+00  1.37359497E+00  5.29815849E+00  8.45256920E+01
  B    10   1.94017384E+00  8.26488858E-01  3.18518318E+00  8.67091209E+01
  H    11   5.85759000E+00  4.07822139E+01  7.95676053E+00  4.81107910E+01
  H    12   6.45516697E+00  3.63501203E+01  7.21605253E+00  5.27076787E+01
  H    13   3.18351534E+00  2.88528957E+01  3.11264716E+01  4.49953008E+01
  H    14   3.77137388E+00  2.40380735E+01  2.58714309E+01  5.33492112E+01
  H    15   3.14093109E+00  2.87449468E+01  1.34814894E+01  5.76940671E+01
  H    16   3.81834328E+00  2.33029603E+01  1.10561795E+01  6.39200488E+01

EIGENVALUES OF THE HESSIAN
   -2.77498680E-01   -2.03658623E-01    3.01365440E-02

THE ELLIPTICITY IS      0.36257

EIGENVECTORS OF THE HESSIAN
    7.40649547E-01   -6.71885599E-01   -2.82671264E-03
   -6.71630392E-01   -7.40237829E-01   -3.09930992E-02
   -1.87313774E-02   -2.48535310E-02    9.99515601E-01

EIGENVALUES OF THE STRESSIAN
   -1.00032664E-01   -8.89015748E-02   -2.43922015E-02

THE TRACE OF THE STRESSIAN IS  -0.21332644

EIGENVECTORS OF THE STRESSIAN
   -7.90551362E-01    6.11821127E-01   -2.65226734E-02
   -6.11591417E-01   -7.90991242E-01   -1.69939530E-02
   -3.13764619E-02    2.78644672E-03    9.99503754E-01

VALUES
RHO         1.6945469295E-01
GRAD        5.7245874707E-17
DEL2       -4.5102075907E-01
G(X)        5.0285625112E-02
K(X)        1.6304081488E-01
L(X)        1.1275518977E-01

COMPONENTS OF THE DIVERGENCE OF THE STRESSIAN
   -2.04100347E-02   -3.04939274E-02   -2.24056322E-01

MAGNITUDE OF THE DIVERGENCE OF THE STRESSIAN        0.227041


SEARCHING BETWEEN ATOMS    4  11
NUMBER OF PERFORMED NEWTON ITERATION STEPS :    5
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COORDINATES OF CRITICAL POINT

X =	9.97710605E-01
Y =	1.23300481E-02
Z =	3.57699307E+00
R =	3.71355058E+00

VECTORS FROM NUCLEI TO CRITICAL POINT
LENGTHS AND ANGLES MADE WITH PROJECTIONS ONTO YZ/XZ/XY PLANES OF MCS

NUCLEUS		LENGTH	YZ ANGLE	XZ ANGLE	XY ANGLE
B	1	4.02670154E+00	2.72648837E+01	1.83948089E+00	6.26626925E+01
B	2	4.05488046E+00	1.42439999E+01	2.36779224E+01	6.19022223E+01
H	3	5.34628413E+00	4.70445737E+01	7.42554877E+00	4.19946750E+01
B	4	9.52678351E-01	1.80675236E+01	1.35505005E+01	6.71267484E+01
B	5	6.28713424E+00	2.69358456E+00	2.03462354E+00	8.66234337E+01
H	6	2.99015464E+00	3.25972626E+01	3.66165236E+01	3.65116857E+01
H	7	5.88771568E+00	1.58786876E+01	1.76329673E+01	6.59089561E+01
H	8	5.35659603E+00	1.08573460E+01	4.60657966E+01	4.18954569E+01
B	9	3.99972923E+00	5.89911461E+01	5.27757010E+00	3.04570747E+01
B	10	6.17809750E+00	3.37026282E+01	3.41391382E+00	5.60776552E+01
H	11	1.27299761E+00	1.68964935E+01	1.52641085E+01	6.69114526E+01
H	12	8.33997068E+00	2.54266459E+00	2.30304278E+00	8.65683641E+01
H	13	3.01116415E+00	3.96116411E+01	4.47888037E+01	1.81636659E+01
H	14	6.84222590E+00	1.62954162E+01	1.80615353E+01	6.52817791E+01
H	15	5.00191287E+00	8.31891184E+01	2.93999362E+00	6.13823839E+00
H	16	8.27925926E+00	3.68617565E+01	1.77570147E+00	5.30809486E+01

EIGENVALUES OF THE HESSIAN

-4.34601024E-01	-4.23878879E-01	5.74728147E-01

THE ELLIPTICITY IS 0.02530

EIGENVECTORS OF THE HESSIAN

-9.17330198E-01	2.65853192E-01	2.96356859E-01
-1.91427867E-01	-9.47213589E-01	2.57180459E-01
3.49085491E-01	1.79188440E-01	9.19799339E-01

EIGENVALUES OF THE STRESSIAN

-1.38827246E-01	-1.38112438E-01	-9.00193643E-02

THE TRACE OF THE STRESSIAN IS -0.36695905

EIGENVECTORS OF THE STRESSIAN

5.48024733E-01	-7.79075268E-01	3.04484184E-01
-8.35900820E-01	-4.96750756E-01	2.33470567E-01
3.06383960E-02	3.82466224E-01	9.23461356E-01

VALUES

RHO	1.8960591820E-01
GRAD	9.5366413231E-17
DEL2	-2.8375175506E-01

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G(X)        1.4801055445E-01
K(X)        2.1894849322E-01
L(X)        7.0937938765E-02

COMPONENTS OF THE DIVERGENCE OF THE STRESSIAN
    1.98531797E-01    1.57434892E-01    6.00045772E-01

MAGNITUDE OF THE DIVERGENCE OF THE STRESSIAN        0.651349


SEARCHING BETWEEN ATOMS    9  15
NUMBER OF PERFORMED NEWTON ITERATION STEPS :    5

COORDINATES OF CRITICAL POINT
         X =  -3.06935471E+00
         Y =  -9.25853457E-02
         Z =   2.20686063E+00
         R =   3.78150026E+00

VECTORS FROM NUCLEI TO CRITICAL POINT
LENGTHS AND ANGLES MADE WITH PROJECTIONS ONTO YZ/XZ/XY PLANES OF MCS

NUCLEUS        LENGTH         YZ ANGLE         XZ ANGLE         XY ANGLE
  B    1   6.31024734E+00   6.95281124E+01   2.20999634E-01   2.04705867E+01
  B    2   4.15880050E+00   4.75645892E+01   2.46319149E+01   3.20492718E+01
  H    3   8.31762175E+00   7.36174434E+01   5.49064772E+00   1.53861770E+01
  B    4   3.80544548E+00   8.23531536E+01   1.78143294E+00   7.43403272E+00
  B    5   6.18940093E+00   3.75435981E+01   1.09517327E+00   5.24347435E+01
  H    6   5.93498452E+00   7.30760765E+01   1.64290775E+01   3.95128773E+00
  H    7   7.14806397E+00   5.25924307E+01   1.35816148E+01   3.40735585E+01
  H    8   5.47015999E+00   3.39898784E+01   4.64161433E+01   2.37931693E+01
  B    9   9.53654773E-01   4.20668930E+01   1.60074962E+01   4.35703172E+01
  B   10   3.81943780E+00   9.63018199E+00   3.94815606E+00   7.95775957E+01
  H   11   5.13211512E+00   5.98332234E+01   4.91889695E+00   2.96795908E+01
  H   12   8.26144719E+00   3.24850485E+01   3.05337362E+00   5.73357980E+01
  H   13   2.97702217E+00   4.61585697E+01   4.26356091E+01   8.33313024E+00
  H   14   5.67029452E+00   2.22517087E+01   2.08310819E+01   5.87027807E+01
  H   15   1.27966924E+00   4.46645162E+01   1.64074724E+01   4.07484073E+01
  H   16   5.33778605E+00   9.70205613E+00   3.88292261E+00   7.95357878E+01

EIGENVALUES OF THE HESSIAN
   -4.27900921E-01   -3.81647269E-01    5.89126535E-01

THE ELLIPTICITY IS      0.12119

EIGENVECTORS OF THE HESSIAN
    8.28172686E-02    7.14588171E-01    6.94625832E-01
   -8.82964126E-01    3.75802541E-01   -2.81330415E-01
    4.62077539E-01    5.90030674E-01   -6.62078659E-01

EIGENVALUES OF THE STRESSIAN
   -1.41949361E-01   -1.30483375E-01   -8.56957021E-02
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THE TRACE OF THE STRESSIAN IS -0.35812844

EIGENVECTORS OF THE STRESSIAN

7.41541910E-01	2.92791829E-02	6.70267354E-01
3.01723959E-01	-9.06869676E-01	-2.94193886E-01
5.99231381E-01	4.20392816E-01	-6.81316103E-01

VALUES

RHO	1.8321214125E-01
GRAD	1.4724726891E-16
DEL2	-2.2042165542E-01
G(X)	1.5151151223E-01
K(X)	2.0661692608E-01
L(X)	5.5105413855E-02

COMPONENTS OF THE DIVERGENCE OF THE STRESSIAN

-4.26276651E-01	1.71422528E-01	4.24874150E-01

MAGNITUDE OF THE DIVERGENCE OF THE STRESSIAN 0.625792

SEARCHING BETWEEN ATOMS 1 6
NUMBER OF PERFORMED NEWTON ITERATION STEPS : 6

COORDINATES OF CRITICAL POINT

X =	2.58870255E+00
Y =	-6.79457960E-01
Z =	7.70324424E-01
R =	2.78503927E+00

VECTORS FROM NUCLEI TO CRITICAL POINT
LENGTHS AND ANGLES MADE WITH PROJECTIONS ONTO YZ/XZ/XY PLANES OF MCS

NUCLEUS		LENGTH	YZ ANGLE	XZ ANGLE	XY ANGLE
B	1	9.87008719E-01	1.48920236E+01	3.47458455E+01	5.13030460E+01
B	2	3.56063800E+00	4.66382620E+01	4.06643734E+01	1.24944177E+01
H	3	2.81005573E+00	5.57175835E+01	2.94763946E+01	1.59102561E+01
B	4	2.73841763E+00	4.35418684E+01	9.85241870E+00	4.47799391E+01
B	5	3.97694005E+00	2.83169031E+01	6.76645297E+00	6.07407673E+01
H	6	1.49937203E+00	7.60298847E-01	4.67282386E+01	4.32616545E+01
H	7	2.79069044E+00	4.08482077E-01	2.30289798E+01	6.69669760E+01
H	8	5.29614808E+00	2.94010531E+01	5.92019536E+01	8.36333512E+00
B	9	5.08955636E+00	8.04560740E+01	3.64866127E+00	8.80689279E+00
B	10	5.53879393E+00	6.49818592E+01	3.35237443E+00	2.47615501E+01
H	11	4.28573457E+00	1.65528365E+01	1.38638493E+01	6.81444565E+01
H	12	5.74435327E+00	1.22722493E+01	1.02982304E+01	7.38745905E+01
H	13	4.22600544E+00	5.61782345E+01	1.97719813E+01	2.62330207E+01
H	14	5.09789737E+00	4.35262000E+01	1.62854058E+01	4.19619120E+01
H	15	7.00447966E+00	6.94231764E+01	7.78117138E+00	1.89255325E+01
H	16	7.64437740E+00	5.90742400E+01	7.12628585E+00	2.99159640E+01

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EIGENVALUES OF THE HESSIAN
   -2.23241472E-01   -1.15458814E-01    4.89348982E-01

THE ELLIPTICITY IS      0.93352

EIGENVECTORS OF THE HESSIAN
   -5.87595763E-01    7.86859982E-01   -1.88633474E-01
   -5.68493686E-01   -5.67349565E-01   -5.95759515E-01
   -5.75800441E-01   -2.42828828E-01    7.80697133E-01

EIGENVALUES OF THE STRESSIAN
   -1.08256703E-01   -1.01464606E-01   -5.05003348E-02

THE TRACE OF THE STRESSIAN IS  -0.26022164

EIGENVECTORS OF THE STRESSIAN
    9.68501228E-01   -1.17282471E-01   -2.19659267E-01
   -2.30944789E-01   -7.52927626E-01   -6.16250350E-01
    9.31121665E-02   -6.47568384E-01    7.56297106E-01

VALUES
RHO         1.2543925263E-01
GRAD        4.6547515373E-17
DEL2        1.5064869573E-01
G(X)        1.4894190888E-01
K(X)        1.1127973494E-01
L(X)       -3.7662173932E-02

COMPONENTS OF THE DIVERGENCE OF THE STRESSIAN
   -9.75447821E-02   -2.13801155E-01    3.05837832E-01

MAGNITUDE OF THE DIVERGENCE OF THE STRESSIAN        0.385698

SEARCHING BETWEEN ATOMS    4    6
NUMBER OF PERFORMED NEWTON ITERATION STEPS :   10

COORDINATES OF CRITICAL POINT
         X =   1.46140336E+00
         Y =  -3.19791284E-01
         Z =   1.73539686E+00
         R =   2.29119368E+00

VECTORS FROM NUCLEI TO CRITICAL POINT
LENGTHS AND ANGLES MADE WITH PROJECTIONS ONTO YZ/XZ/XY PLANES OF MCS

NUCLEUS         LENGTH         YZ ANGLE         XZ ANGLE         XY ANGLE
  B    1   2.22706173E+00   3.83220514E+01   5.22640080E+00   5.11902744E+01
  B    2   2.99850328E+00   2.91683646E+01   4.08317341E+01   3.53629788E+01
  H    3   3.99437301E+00   5.97126093E+01   1.48403228E+01   2.57509627E+01
  B    4   1.23172385E+00   3.80489654E+01   5.07260347E+00   5.14904905E+01
  B    5   4.50045129E+00   9.71131298E+00   1.38663800E+00   8.01882876E+01
  H    6   1.85106787E+00   3.82977046E+01   5.16351791E+01   1.93473049E+00
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  H     7   3.98831646E+00  1.67166515E+01  2.13403206E+01  6.23636588E+01
  H     8   4.76793339E+00  1.79913089E+01  6.14864825E+01  2.13443651E+01
  B     9   3.89641016E+00  8.72160312E+01  5.26097804E-01  2.73373055E+00
  B    10   5.09297704E+00  4.98316596E+01  4.02491680E-01  4.01654723E+01
  H    11   3.08705974E+00  1.73941369E+00  1.24828879E+01  7.73926212E+01
  H    12   6.51834010E+00  8.23681189E-01  5.87547980E+00  8.40666625E+01
  H    13   3.11414987E+00  4.99420781E+01  3.50680249E+01  1.68544039E+01
  H    14   5.29263899E+00  2.67662922E+01  1.97587324E+01  5.57282949E+01
  H    15   5.61625962E+00  7.52150231E+01  6.01652302E+00  1.34545087E+01
  H    16   7.25670201E+00  4.84447253E+01  4.65299416E+00  4.11751766E+01

EIGENVALUES OF THE HESSIAN
   -1.52154056E-01   -1.61088193E-02    8.18426811E-02

THE ELLIPTICITY IS      8.44539

EIGENVECTORS OF THE HESSIAN
    6.05937994E-01   -2.12060723E-01    7.66726416E-01
    6.03550393E-01   -5.05325560E-01   -6.16743870E-01
    5.18233607E-01    8.36466573E-01   -1.78206623E-01

EIGENVALUES OF THE STRESSIAN
   -6.34184323E-02   -5.98742976E-02   -1.39424958E-02

THE TRACE OF THE STRESSIAN IS  -0.13723523

EIGENVECTORS OF THE STRESSIAN
   -7.50001759E-01    1.60495550E-02    6.61241086E-01
   -7.61766976E-02    9.90957569E-01   -1.10454548E-01
   -6.57034605E-01   -1.33212267E-01   -7.41997317E-01

VALUES
RHO         1.0817737805E-01
GRAD        2.2079425200E-17
DEL2       -8.6420194265E-02
G(X)        5.7815088582E-02
K(X)        7.9420137148E-02
L(X)        2.1605048566E-02



SEARCHING BETWEEN ATOMS    4  13
NUMBER OF PERFORMED NEWTON ITERATION STEPS :    8

COORDINATES OF CRITICAL POINT
          X =  -1.67114630E-01
          Y =  -7.33037335E-01
          Z =   2.48132904E+00
          R =   2.59273308E+00

VECTORS FROM NUCLEI TO CRITICAL POINT
LENGTHS AND ANGLES MADE WITH PROJECTIONS ONTO YZ/XZ/XY PLANES OF MCS
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NUCLEUS		LENGTH	YZ ANGLE	XZ ANGLE	XY ANGLE
B	1	3.94886543E+00	4.96507194E+01	8.97610987E+00	3.89296018E+01
B	2	3.43799137E+00	2.78614358E+00	4.36663311E+01	4.61981604E+01
H	3	5.83119765E+00	6.05493075E+01	1.42595374E+01	2.51839927E+01
B	4	1.03726384E+00	5.69433690E+01	3.02248158E+01	1.21264352E+01
B	5	5.27888196E+00	9.47905895E+00	5.67660782E+00	7.89241330E+01
H	6	3.04127972E+00	6.58782678E+01	1.99589159E+01	1.29864504E+01
H	7	5.20519130E+00	3.22258884E+01	1.15042818E+01	5.52961868E+01
H	8	5.23139674E+00	1.70698526E+00	6.16244177E+01	2.83147478E+01
B	9	2.47652475E+00	6.60498514E+01	8.76713138E+00	2.21010189E+01
B	10	4.63821550E+00	2.92070089E+01	4.66803136E+00	6.03496134E+01
H	11	2.94296697E+00	3.14342142E+01	2.15399068E+01	5.03725009E+01
H	12	7.46904869E+00	1.18581774E+01	8.31786488E+00	7.54452783E+01
H	13	1.57735683E+00	2.85986149E+01	6.07311821E+01	5.71182132E+00
H	14	5.35482684E+00	8.10575719E+00	1.48898443E+01	7.29560736E+01
H	15	3.97139225E+00	7.31949053E+01	1.46126647E+01	8.11817472E+00
H	16	6.77984214E+00	3.41076063E+01	8.49821663E+00	5.45568627E+01

EIGENVALUES OF THE HESSIAN

-2.25229557E-01	-7.40984049E-02	2.77710497E-01

THE ELLIPTICITY IS 2.03960

EIGENVECTORS OF THE HESSIAN

-3.91397160E-01	5.51752747E-01	7.36462605E-01
3.78876366E-01	-6.32707964E-01	6.75376437E-01
8.38606560E-01	5.43368695E-01	3.85940251E-02

EIGENVALUES OF THE STRESSIAN

-9.73072433E-02	-8.87917050E-02	-4.56869363E-02

THE TRACE OF THE STRESSIAN IS -0.23178588

EIGENVECTORS OF THE STRESSIAN

-2.53530091E-02	6.27008094E-01	-7.78600074E-01
2.60548040E-01	-7.47787533E-01	-6.10678740E-01
-9.65127942E-01	-2.18345267E-01	-1.44407066E-01

VALUES

RHO	1.3002207852E-01
GRAD	5.9995872871E-17
DEL2	-2.1617464247E-02
G(X)	1.1319075927E-01
K(X)	1.1859512534E-01
L(X)	5.4043660619E-03

COMPONENTS OF THE DIVERGENCE OF THE STRESSIAN

-2.90742970E-01	-1.62802388E-01	-6.80256162E-02

MAGNITUDE OF THE DIVERGENCE OF THE STRESSIAN 0.340093

9-13 Bond
NUMBER OF PERFORMED NEWTON ITERATION STEPS : 3

COORDINATES OF CRITICAL POINT
X = -1.32333302E+00
Y = -2.25029197E-01
Z = 1.83842254E+00
R = 2.27632288E+00

VECTORS FROM NUCLEI TO CRITICAL POINT
LENGTHS AND ANGLES MADE WITH PROJECTIONS ONTO YZ/XZ/XY PLANES OF MCS

NUCLEUS		LENGTH	YZ ANGLE	XZ ANGLE	XY ANGLE
B	1	4.55461300E+00	6.61504180E+01	1.36004893E+00	2.38059107E+01
B	2	2.93464438E+00	2.68036701E+01	3.94776175E+01	3.87890579E+01
H	3	6.56529478E+00	7.17179508E+01	8.12858822E+00	1.62614774E+01
B	4	2.20094691E+00	6.69733600E+01	3.68216780E-01	2.30233532E+01
B	5	4.96924987E+00	2.40556241E+01	1.63087211E-01	6.59437523E+01
H	6	4.22519436E+00	6.85272548E+01	2.14650052E+01	5.49639963E-01
H	7	5.57435189E+00	4.48587278E+01	1.61030820E+01	4.07174554E+01
H	8	4.67643160E+00	1.62940404E+01	6.11200983E+01	2.31490912E+01
B	9	1.15156309E+00	7.40219675E+01	6.50892975E+00	1.45274778E+01
B	10	3.56666206E+00	1.80830542E+01	2.09748003E+00	7.17872901E+01
H	11	4.00439611E+00	4.22231230E+01	8.21961759E+00	4.66022517E+01
H	12	7.13797461E+00	2.21481165E+01	4.60033727E+00	6.73289824E+01
H	13	2.08571451E+00	1.10898703E+01	6.45931439E+01	2.25512892E+01
H	14	4.87355724E+00	4.72184667E+00	2.27415157E+01	6.67189427E+01
H	15	2.94821129E+00	6.38116012E+01	9.64411657E+00	2.40975143E+01
H	16	5.57341729E+00	2.83382954E+01	5.08413279E+00	6.11264660E+01

EIGENVALUES OF THE HESSIAN
-1.26065936E-01 -1.10759877E-02 8.21501337E-02

THE ELLIPTICITY IS 10.38191

EIGENVECTORS OF THE HESSIAN
-2.62603097E-01 3.23296093E-01 -9.09131041E-01
5.40382779E-01 8.29856144E-01 1.39015226E-01
7.99391059E-01 -4.54772929E-01 -3.92626434E-01

EIGENVALUES OF THE STRESSIAN
-7.71634253E-02 -6.99072886E-02 -1.99840928E-02

THE TRACE OF THE STRESSIAN IS -0.16705481

EIGENVECTORS OF THE STRESSIAN
2.44910099E-01 9.26448180E-02 9.65109310E-01
-4.41438798E-01 8.96916834E-01 2.59225797E-02
-8.63221195E-01 -4.32385396E-01 2.60561008E-01

VALUES

RHO 1.1114319771E-01
GRAD 7.7287722784E-17
DEL2 -5.4991789902E-02
G(X) 7.6653429634E-02
K(X) 9.0401377109E-02
L(X) 1.3747947476E-02

COMPONENTS OF THE DIVERGENCE OF THE STRESSIAN
1.72059324E-01 2.22818392E-02 4.65924357E-02

MAGNITUDE OF THE DIVERGENCE OF THE STRESSIAN 0.179643

1-2-4-6 Ring
NUMBER OF PERFORMED NEWTON ITERATION STEPS : 11

COORDINATES OF CRITICAL POINT
X = 1.53301153E+00
Y = -5.65382657E-03
Z = 1.27472691E+00
R = 1.99376153E+00

VECTORS FROM NUCLEI TO CRITICAL POINT
LENGTHS AND ANGLES MADE WITH PROJECTIONS ONTO YZ/XZ/XY PLANES OF MCS

NUCLEUS		LENGTH	YZ ANGLE	XZ ANGLE	XY ANGLE
B	1	1.83076727E+00	4.56589558E+01	3.48449516E+00	4.41293167E+01
B	2	2.58567143E+00	3.63621625E+01	3.95492382E+01	2.95377225E+01
H	3	3.67905017E+00	6.66429297E+01	1.11099635E+01	2.02723263E+01
B	4	1.66177176E+00	2.99950804E+01	7.09421251E+00	5.90055821E+01
B	5	4.06504528E+00	1.17924636E+01	2.89390725E+00	7.78476973E+01
H	6	2.13251565E+00	3.02898442E+01	5.58837718E+01	1.42011642E+01
H	7	3.70336360E+00	1.68840050E+01	2.84721978E+01	5.60661841E+01
H	8	4.36222585E+00	2.07330793E+01	6.26747547E+01	1.69908736E+01
B	9	3.98831649E+00	8.35946773E+01	5.03330777E+00	3.95135089E+00
B	10	4.87931649E+00	5.43202712E+01	4.11242825E+00	3.53681733E+01
H	11	3.49511285E+00	2.71099415E+00	5.79870214E+00	8.35949305E+01
H	12	6.03535806E+00	1.56956390E+00	3.35424990E+00	8.62959262E+01
H	13	3.50875242E+00	4.44049166E+01	3.68314594E+01	2.28689651E+01
H	14	5.07581234E+00	2.89272076E+01	2.44809320E+01	5.04365267E+01
H	15	5.78534574E+00	7.19911741E+01	2.71988047E+00	1.77882499E+01
H	16	6.99870478E+00	5.18256221E+01	2.24806971E+00	3.80836194E+01

EIGENVALUES OF THE HESSIAN
-1.45633911E-01 1.48779273E-02 5.08552359E-02

EIGENVECTORS OF THE HESSIAN
-5.81017518E-01 2.85757978E-01 -7.62076782E-01
-6.47061909E-01 -7.30144618E-01 2.19544354E-01
-4.93689711E-01 6.20669973E-01 6.09129916E-01

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EIGENVALUES OF THE STRESSIAN
   -4.96907414E-02   -4.44306791E-02   -4.11219402E-04

THE TRACE OF THE STRESSIAN IS  -0.09453264

EIGENVECTORS OF THE STRESSIAN
    4.34986268E-01    6.69046937E-01   -6.02630188E-01
    8.20979911E-01   -5.69571630E-01   -3.97510230E-02
    3.69836358E-01    4.77456129E-01    7.97029932E-01

VALUES
RHO         1.0710928719E-01
GRAD        5.9704862718E-16
DEL2       -7.9900747748E-02
G(X)        3.7278726508E-02
K(X)        5.7253913445E-02
L(X)        1.9975186937E-02

COMPONENTS OF THE DIVERGENCE OF THE STRESSIAN
   -4.66593232E-05    1.16797225E-02   -2.22869008E-02

MAGNITUDE OF THE DIVERGENCE OF THE STRESSIAN        0.025162


2-4-13-9 Ring
NUMBER OF PERFORMED NEWTON ITERATION STEPS :    4

COORDINATES OF CRITICAL POINT
         X =  -1.00804581E+00
         Y =   4.87786668E-01
         Z =   1.15260406E+00
         R =   1.60704334E+00

VECTORS FROM NUCLEI TO CRITICAL POINT
LENGTHS AND ANGLES MADE WITH PROJECTIONS ONTO YZ/XZ/XY PLANES OF MCS

NUCLEUS         LENGTH         YZ ANGLE         XZ ANGLE         XY ANGLE
  B    1   4.06445730E+00   7.13225314E+01   8.55625665E+00   1.64740644E+01
  B    2   1.91676175E+00   3.17295818E+01   3.69785468E+01   3.69651260E+01
  H    3   6.03365154E+00   7.87938847E+01   2.04669140E+00   1.10128574E+01
  B    4   2.40941744E+00   4.52217015E+01   1.68564729E+01   3.99341898E+01
  B    5   4.27198444E+00   2.36001492E+01   9.41285249E+00   6.43756831E+01
  H    6   4.31269978E+00   5.69929180E+01   3.15868909E+01   8.60518187E+00
  H    7   5.18540299E+00   4.42240795E+01   2.58258343E+01   3.46805291E+01
  H    8   3.70946626E+00   1.55874209E+01   6.57453410E+01   1.81026053E+01
  B    9   1.70056919E+00   5.67622824E+01   2.97307664E+01   1.34988037E+01
  B   10   3.16797254E+00   2.66783823E+01   1.54390298E+01   5.85354271E+01
  H   11   4.31171588E+00   3.34354789E+01   1.86490487E+00   5.64985711E+01
  H   12   6.36248837E+00   2.19253790E+01   1.26368358E+00   6.80344262E+01
  H   13   2.99301360E+00   1.64456297E+00   6.01836152E+01   2.97616592E+01
  H   14   4.59585283E+00   1.07092421E+00   3.44045801E+01   5.55739570E+01
  H   15   3.51923082E+00   5.72815399E+01   3.56629653E+00   3.24742302E+01
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  H    16   5.13912099E+00  3.51795718E+01  2.44133467E+00  5.47101208E+01

EIGENVALUES OF THE HESSIAN
   -1.31578855E-01    8.44173771E-03    4.38951817E-02

EIGENVECTORS OF THE HESSIAN
   -3.73268223E-01    4.21476288E-01    8.26455427E-01
    7.87100677E-01   -3.27665915E-01    5.22596950E-01
    4.91063496E-01    8.45572461E-01   -2.09436998E-01

EIGENVALUES OF THE STRESSIAN
   -4.99656031E-02   -3.57087608E-02   -3.04617560E-04

THE TRACE OF THE STRESSIAN IS  -0.08597898

EIGENVECTORS OF THE STRESSIAN
   -1.82514533E-01    6.68440196E-01   -7.21024375E-01
    7.46082347E-01   -3.83460354E-01   -5.44352173E-01
    6.40351135E-01    6.37295740E-01    4.28724343E-01

VALUES
RHO         1.0675049840E-01
GRAD        4.1930458984E-17
DEL2       -7.9241935192E-02
G(X)        3.3084248835E-02
K(X)        5.2894732633E-02
L(X)        1.9810483798E-02

COMPONENTS OF THE DIVERGENCE OF THE STRESSIAN
    3.09259300E-02    1.02085067E-02    8.87130752E-03

MAGNITUDE OF THE DIVERGENCE OF THE STRESSIAN        0.033754


2-9-10 Ring
NUMBER OF PERFORMED NEWTON ITERATION STEPS :    3

COORDINATES OF CRITICAL POINT
          X =  -1.30450018E+00
          Y =   6.01713700E-01
          Z =   6.69814603E-16
          R =   1.43658627E+00

VECTORS FROM NUCLEI TO CRITICAL POINT
LENGTHS AND ANGLES MADE WITH PROJECTIONS ONTO YZ/XZ/XY PLANES OF MCS

NUCLEUS         LENGTH         YZ ANGLE         XZ ANGLE         XY ANGLE
  B    1   4.20867059E+00  8.01684584E+01  9.83154161E+00  0.00000000E+00
  B    2   1.66772779E+00  5.14626424E+01  3.85373576E+01  0.00000000E+00
  H    3   6.21590055E+00  8.90638336E+01  9.36166437E-01  0.00000000E+00
  B    4   3.46022892E+00  3.54468155E+01  1.35821615E+01  5.12671421E+01
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  B     5   3.46022892E+00  3.54468155E+01  1.35821615E+01  5.12671421E+01
  H     6   4.91683962E+00  5.27362220E+01  2.88555318E+01  2.14481957E+01
  H     7   4.91683962E+00  5.27362220E+01  2.88555318E+01  2.14481957E+01
  H     8   3.51466788E+00  2.15891897E+01  6.84108103E+01  0.00000000E+00
  B     9   2.14130614E+00  3.17224031E+01  2.65548994E+01  4.63567888E+01
  B    10   2.14130614E+00  3.17224031E+01  2.65548994E+01  4.63567888E+01
  H    11   5.45426586E+00  2.93358720E+01  2.67173239E+00  6.05186094E+01
  H    12   5.45426586E+00  2.93358720E+01  2.67173239E+00  6.05186094E+01
  H    13   3.80197153E+00  5.77179591E+00  4.54780189E+01  4.39422946E+01
  H    14   3.80197153E+00  5.77179591E+00  4.54780189E+01  4.39422946E+01
  H    15   4.05764760E+00  4.10439312E+01  4.70506761E+00  4.85672111E+01
  H    16   4.05764760E+00  4.10439312E+01  4.70506761E+00  4.85672111E+01

EIGENVALUES OF THE HESSIAN
   -1.30471986E-01    2.09349634E-02    7.53467601E-02

EIGENVECTORS OF THE HESSIAN
    6.33375522E-01    0.00000000E+00    7.73844589E-01
   -7.73844589E-01    0.00000000E+00    6.33375522E-01
    0.00000000E+00    1.00000000E+00    0.00000000E+00

EIGENVALUES OF THE STRESSIAN
   -4.63071834E-02   -3.09729000E-02   -9.71300140E-03

THE TRACE OF THE STRESSIAN IS  -0.08699308

EIGENVECTORS OF THE STRESSIAN
    6.38806102E-01    0.00000000E+00   -7.69367769E-01
   -7.69367769E-01    0.00000000E+00   -6.38806102E-01
    0.00000000E+00    1.00000000E+00    0.00000000E+00

VALUES
RHO         1.0324756065E-01
GRAD        6.9019755924E-17
DEL2       -3.4190262971E-02
G(X)        3.9222759505E-02
K(X)        4.7770325248E-02
L(X)        8.5475657428E-03

COMPONENTS OF THE DIVERGENCE OF THE STRESSIAN
   -3.46289221E-02   -2.27332038E-02    1.20760734E-12

MAGNITUDE OF THE DIVERGENCE OF THE STRESSIAN        0.041424


CRITICAL POINTS
 1.10054963E+00  9.05150686E-01  1.35635635E-16  B    1  B    2
 3.73375050E+00  2.22008455E-01 -3.35153950E-19  B    1  H    3
-7.38687359E-03  2.59356866E+00  1.30404105E-18  B    2  H    8
 2.17911909E-01  9.08930599E-01  1.00608502E+00  B    2  B    4
 2.17911909E-01  9.08930599E-01 -1.00608502E+00  B    2  B    5
-1.09381897E+00  5.42788593E-01  9.79091496E-01  B    2  B    9
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-1.09381897E+00	5.42788593E-01	-9.79091496E-01	B	2	B	10	
-2.45610400E+00	-4.53891194E-01	-4.20522952E-15	B	9	B	10	attr
-2.45839407E+00	-4.63370629E-01	3.87414898E-01	attr		B	9	
-2.45839407E+00	-4.63370629E-01	-3.87414898E-01	attr		B	10	
9.97710605E-01	1.23300481E-02	3.57699307E+00	B	4	H	11	
9.97710605E-01	1.23300481E-02	-3.57699307E+00	B	5	H	12	
-3.06935471E+00	-9.25853457E-02	2.20686063E+00	B	9	H	15	
-3.06935471E+00	-9.25853457E-02	-2.20686063E+00	B	10	H	16	
2.58870255E+00	-6.79457960E-01	7.70324424E-01	B	1	H	6	
2.58870255E+00	-6.79457960E-01	-7.70324424E-01	B	1	H	7	
1.46140336E+00	-3.19791284E-01	1.73539686E+00	B	4	H	6	
1.46140336E+00	-3.19791284E-01	-1.73539686E+00	B	5	H	7	
-1.67114630E-01	-7.33037335E-01	2.48132904E+00	B	4	H	13	
-1.67114630E-01	-7.33037335E-01	-2.48132904E+00	B	5	H	14	
-1.32333302E+00	-2.25029197E-01	1.83842254E+00	B	9	H	13	
-1.32333302E+00	-2.25029197E-01	-1.83842254E+00	B	10	H	14	
1.53301153E+00	-5.65382657E-03	1.27472691E+00	1-2-4-6 ring				
1.53301153E+00	-5.65382657E-03	-1.27472691E+00	1-2-5-7 ring				
-1.00804581E+00	4.87786668E-01	1.15260406E+00	2-4-13-9 ring				
-1.00804581E+00	4.87786668E-01	-1.15260406E+00	2-5-14-10 ring				
-1.30450018E+00	6.01713700E-01	6.69814603E-16	2-9-10 ring				

B6H6(2-)

SADDLE
B6H6(2-) OPTIMIZATION USING VD SET(Renormalized); d=0.75, p=1.0725

B	1	0.00000000	0.00000000	-2.33569172
B	2	2.33569172	0.00000000	0.00000000
B	3	-2.33569172	0.00000000	0.00000000
B	4	0.00000000	2.33569172	0.00000000
B	5	0.00000000	-2.33569172	0.00000000
B	6	0.00000000	0.00000000	2.33569172
H	7	0.00000000	0.00000000	-4.63095754
H	8	4.63095754	0.00000000	0.00000000
H	9	-4.63095754	0.00000000	0.00000000
H	10	0.00000000	4.63095754	0.00000000
H	11	0.00000000	-4.63095754	0.00000000
H	12	0.00000000	0.00000000	4.63095754

SEARCHING BETWEEN ATOMS 1 7
NUMBER OF PERFORMED NEWTON ITERATION STEPS : 6

COORDINATES OF CRITICAL POINT
X = 1.90111760E-10
Y = 7.06271497E-10
Z = -3.29694296E+00
R = 3.29694296E+00

VECTORS FROM NUCLEI TO CRITICAL POINT
LENGTHS AND ANGLES MADE WITH PROJECTIONS ONTO YZ/XZ/XY PLANES OF MCS

NUCLEUS		LENGTH	YZ ANGLE	XZ ANGLE	XY ANGLE
B	1	9.61251238E-01	0.00000000E+00	0.00000000E+00	9.00000000E+01
B	2	4.04045649E+00	3.53153460E+01	0.00000000E+00	5.46846540E+01
B	3	4.04045649E+00	3.53153460E+01	0.00000000E+00	5.46846540E+01
B	4	4.04045649E+00	0.00000000E+00	3.53153460E+01	5.46846540E+01
B	5	4.04045649E+00	0.00000000E+00	3.53153460E+01	5.46846540E+01
B	6	5.63263468E+00	0.00000000E+00	0.00000000E+00	9.00000000E+01
H	7	1.33401458E+00	0.00000000E+00	0.00000000E+00	9.00000000E+01
H	8	5.68468122E+00	5.45515873E+01	0.00000000E+00	3.54484127E+01
H	9	5.68468122E+00	5.45515873E+01	0.00000000E+00	3.54484127E+01
H	10	5.68468122E+00	0.00000000E+00	5.45515873E+01	3.54484127E+01
H	11	5.68468122E+00	0.00000000E+00	5.45515873E+01	3.54484127E+01
H	12	7.92790050E+00	0.00000000E+00	0.00000000E+00	9.00000000E+01

EIGENVALUES OF THE HESSIAN

-3.11412808E-01	-3.11412767E-01	6.02784939E-01

THE ELLIPTICITY IS 0.00000

EIGENVECTORS OF THE HESSIAN

-2.63582567E-06	1.00000000E+00	6.31528417E-10
-1.00000000E+00	-2.63582567E-06	7.61147756E-10
7.61149420E-10	-6.31526410E-10	1.00000000E+00

EIGENVALUES OF THE STRESSIAN

-1.17500143E-01	-1.17500134E-01	-6.73315292E-02

THE TRACE OF THE STRESSIAN IS -0.30233181

EIGENVECTORS OF THE STRESSIAN

-1.00000000E+00	-3.23047793E-06	-1.61511259E-09
3.23047793E-06	-1.00000000E+00	-1.29684228E-09
-1.61510840E-09	-1.29684750E-09	1.00000000E+00

VALUES

RHO	1.5310409467E-01
GRAD	8.3270205693E-17
DEL2	-2.0040636310E-02
G(X)	1.4866082372E-01
K(X)	1.5367098279E-01
L(X)	5.0101590776E-03

COMPONENTS OF THE DIVERGENCE OF THE STRESSIAN

-7.99779931E-11	-2.44498764E-11	-5.06984500E-01

MAGNITUDE OF THE DIVERGENCE OF THE STRESSIAN 0.506985

SEARCHING BETWEEN ATOMS 1 2
NUMBER OF PERFORMED NEWTON ITERATION STEPS : 3

COORDINATES OF CRITICAL POINT

X =	1.18716482E+00
Y =	2.04904328E-09
Z =	-1.18716372E+00
R =	1.67890381E+00

VECTORS FROM NUCLEI TO CRITICAL POINT
LENGTHS AND ANGLES MADE WITH PROJECTIONS ONTO YZ/XZ/XY PLANES OF MCS

NUCLEUS		LENGTH	YZ ANGLE	XZ ANGLE	XY ANGLE
B	1	1.65181018E+00	4.59476953E+01	0.00000000E+00	4.40523047E+01
B	2	1.65180863E+00	4.40523038E+01	0.00000000E+00	4.59476962E+01
B	3	3.71750937E+00	7.13767521E+01	0.00000000E+00	1.86232479E+01
B	4	2.87648637E+00	2.43754084E+01	5.42912805E+01	2.43753844E+01
B	5	2.87648637E+00	2.43754084E+01	5.42912805E+01	2.43753844E+01
B	6	3.71750868E+00	1.86232693E+01	0.00000000E+00	7.13767307E+01
H	7	3.64267431E+00	1.90203973E+01	0.00000000E+00	7.09796027E+01
H	8	3.64267292E+00	7.09796134E+01	0.00000000E+00	1.90203866E+01
H	9	5.93800518E+00	7.84673476E+01	0.00000000E+00	1.15326524E+01
H	10	4.92589949E+00	1.39458449E+01	7.00724323E+01	1.39458317E+01
H	11	4.92589949E+00	1.39458448E+01	7.00724323E+01	1.39458317E+01
H	12	5.93800432E+00	1.15326649E+01	0.00000000E+00	7.84673351E+01

EIGENVALUES OF THE HESSIAN

-1.45844380E-01	-4.45209363E-02	2.11906998E-02

THE ELLIPTICITY IS 2.27586

EIGENVECTORS OF THE HESSIAN

-7.07106803E-01	3.34041725E-09	-7.07106759E-01
-2.16473735E-09	-1.00000000E+00	-2.55932604E-09
7.07106759E-01	2.79016438E-10	-7.07106803E-01

EIGENVALUES OF THE STRESSIAN

-6.42897944E-02	-6.00668637E-02	-2.45823794E-03

THE TRACE OF THE STRESSIAN IS -0.12681490

EIGENVECTORS OF THE STRESSIAN

-4.50137985E-09	-7.07106719E-01	7.07106844E-01
-1.00000000E+00	7.15154351E-09	7.85629740E-10
5.61242942E-09	7.07106844E-01	7.07106719E-01

VALUES

RHO	1.2509513417E-01
GRAD	4.3662532430E-17
DEL2	-1.6917461602E-01
G(X)	4.2260621023E-02
K(X)	8.4554275028E-02
L(X)	4.2293654005E-02

COMPONENTS OF THE DIVERGENCE OF THE STRESSIAN

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    4.83600955E-03    1.54496435E-10   -4.83621869E-03

MAGNITUDE OF THE DIVERGENCE OF THE STRESSIAN        0.006839


STARTING COORDINATES
1.000000-1.000000 1.000000
NUMBER OF PERFORMED NEWTON ITERATION STEPS :    7

COORDINATES OF CRITICAL POINT
         X =   8.98235840E-01
         Y =  -8.98235581E-01
         Z =   8.98235522E-01
         R =   1.55578978E+00

VECTORS FROM NUCLEI TO CRITICAL POINT
LENGTHS AND ANGLES MADE WITH PROJECTIONS ONTO YZ/XZ/XY PLANES OF MCS

NUCLEUS        LENGTH         YZ ANGLE         XZ ANGLE         XY ANGLE
  B    1   3.47446977E+00  1.49825340E+01  1.49825296E+01  6.85549388E+01
  B    2   1.91831531E+00  4.85325844E+01  2.79202341E+01  2.79202321E+01
  B    3   3.47446999E+00  6.85549442E+01  1.49825286E+01  1.49825276E+01
  B    4   3.47446981E+00  1.49825338E+01  6.85549398E+01  1.49825284E+01
  B    5   1.91831562E+00  2.79202378E+01  4.85325854E+01  2.79202271E+01
  B    6   1.91831569E+00  2.79202367E+01  2.79202279E+01  4.85325856E+01
  H    7   5.67323811E+00  9.10989541E+00  9.10989276E+00  7.70611848E+01
  H    8   3.94295137E+00  7.12058493E+01  1.31680496E+01  1.31680487E+01
  H    9   5.67323837E+00  7.70611878E+01  9.10989234E+00  9.10989173E+00
  H   10   5.67323816E+00  9.10989533E+00  7.70611854E+01  9.10989207E+00
  H   11   3.94295167E+00  1.31680524E+01  7.12058480E+01  1.31680477E+01
  H   12   3.94295174E+00  1.31680522E+01  1.31680483E+01  7.12058477E+01

EIGENVALUES OF THE HESSIAN
   -1.35652101E-01    4.62454655E-02    4.62454827E-02

EIGENVECTORS OF THE HESSIAN
    5.77350271E-01    8.14872151E-01    5.14785525E-02
   -5.77350269E-01    4.52017813E-01   -6.79960708E-01
    5.77350267E-01   -3.62854343E-01   -7.31439262E-01

EIGENVALUES OF THE STRESSIAN
   -5.38736219E-02   -2.18528313E-02   -2.18528135E-02

THE TRACE OF THE STRESSIAN IS  -0.09757927

EIGENVECTORS OF THE STRESSIAN
    5.77350232E-01    5.83024522E-02    8.14412385E-01
   -5.77350284E-01   -6.76150573E-01    4.57697555E-01
    5.77350291E-01   -7.34453011E-01   -3.56714753E-01

VALUES
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```
RHO          1.1592836213E-01
GRAD         4.1233906303E-17
DEL2        -4.3161152644E-02
G(X)         4.3394489264E-02
K(X)         5.4184777425E-02
L(X)         1.0790288161E-02

COMPONENTS OF THE DIVERGENCE OF THE STRESSIAN
    1.02638406E-02   -1.02638734E-02    1.02638806E-02

MAGNITUDE OF THE DIVERGENCE OF THE STRESSIAN        0.017778



STARTING COORDINATES
0.000000 0.000000 0.000000
NUMBER OF PERFORMED NEWTON ITERATION STEPS :    1

COORDINATES OF CRITICAL POINT
          X =   2.56031172E-12
          Y =  -2.58139969E-13
          Z =  -3.30662485E-12
          R =   4.18994036E-12

VECTORS FROM NUCLEI TO CRITICAL POINT
LENGTHS AND ANGLES MADE WITH PROJECTIONS ONTO YZ/XZ/XY PLANES OF MCS

NUCLEUS          LENGTH          YZ ANGLE          XZ ANGLE          XY ANGLE
  B     1   2.33569172E+00  0.00000000E+00  0.00000000E+00  9.00000000E+01
  B     2   2.33569172E+00  9.00000000E+01  0.00000000E+00  0.00000000E+00
  B     3   2.33569172E+00  9.00000000E+01  0.00000000E+00  0.00000000E+00
  B     4   2.33569172E+00  0.00000000E+00  9.00000000E+01  0.00000000E+00
  B     5   2.33569172E+00  0.00000000E+00  9.00000000E+01  0.00000000E+00
  B     6   2.33569172E+00  0.00000000E+00  0.00000000E+00  9.00000000E+01
  H     7   4.63095754E+00  0.00000000E+00  0.00000000E+00  9.00000000E+01
  H     8   4.63095754E+00  9.00000000E+01  0.00000000E+00  0.00000000E+00
  H     9   4.63095754E+00  9.00000000E+01  0.00000000E+00  0.00000000E+00
  H    10   4.63095754E+00  0.00000000E+00  9.00000000E+01  0.00000000E+00
  H    11   4.63095754E+00  0.00000000E+00  9.00000000E+01  0.00000000E+00
  H    12   4.63095754E+00  0.00000000E+00  0.00000000E+00  9.00000000E+01

EIGENVALUES OF THE HESSIAN
    8.33710342E-02    8.33710610E-02    8.33710684E-02

EIGENVECTORS OF THE HESSIAN
    9.99999357E-01   -6.37074153E-04    9.38491479E-04
   -6.29507771E-04   -9.99967475E-01   -8.04063299E-03
   -9.43583434E-04   -8.04003703E-03    9.99967233E-01

EIGENVALUES OF THE STRESSIAN
   -2.65436806E-02   -2.65436799E-02   -2.65436735E-02
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THE TRACE OF THE STRESSIAN IS  -0.07963103

EIGENVECTORS OF THE STRESSIAN
   -5.73576279E-04    1.28524500E-03    9.99999010E-01
   -9.99781292E-01    2.09047300E-02   -6.00319127E-04
    2.09054808E-02    9.99780646E-01   -1.27297345E-03

VALUES
RHO         6.4205563001E-02
GRAD        2.5625558875E-17
DEL2        2.5011316369E-01
G(X)        7.1079662453E-02
K(X)        8.5513715303E-03
L(X)       -6.2528290923E-02

COMPONENTS OF THE DIVERGENCE OF THE STRESSIAN
    2.29730690E-14    2.60865088E-13    1.85266919E-12

MAGNITUDE OF THE DIVERGENCE OF THE STRESSIAN        0.000000

CRITICAL POINTS
 1.90111760E-10  7.06271497E-10 -3.29694296E+00  B    1  H    7
 3.29694294E+00 -2.29825066E-10  1.84086656E-10  B    2  H    8
-3.29694294E+00  2.29471319E-10 -1.83237296E-10  B    3  H    9
 2.44768782E-10  3.29694296E+00  4.14380540E-11  B    4  H   10
-2.50455268E-10 -3.29694296E+00 -3.83858950E-11  B    5  H   11
-1.87540653E-10 -7.05899446E-10  3.29694296E+00  B    6  H   12
 1.18716482E+00  2.04904328E-09 -1.18716372E+00  B    1  B    2
-1.18716482E+00  2.17661984E-09 -1.18716372E+00  B    1  B    3
-1.23017901E-09  1.18716431E+00 -1.18716418E+00  B    1  B    4
-9.76785490E-10 -1.18716431E+00 -1.18716418E+00  B    1  B    5
 1.18716469E+00  1.18716386E+00 -8.48730293E-10  B    2  B    4
-1.18716469E+00  1.18716386E+00 -3.04553520E-09  B    3  B    4
-1.18716469E+00 -1.18716386E+00  8.01671722E-10  B    3  B    5
 1.18716469E+00 -1.18716386E+00  2.99847645E-09  B    2  B    5
 1.18716482E+00 -2.17622837E-09  1.18716372E+00  B    2  B    6
-1.18716482E+00 -2.04865176E-09  1.18716373E+00  B    3  B    6
 9.75453402E-10  1.18716431E+00  1.18716419E+00  B    4  B    6
 1.22884687E-09 -1.18716431E+00  1.18716418E+00  B    5  B    6
 8.98235843E-01  8.98235580E-01  8.98235521E-01  2-4-6 Ring
 8.98235840E-01 -8.98235581E-01  8.98235522E-01  2-5-6 Ring
-8.98235839E-01 -8.98235582E-01  8.98235522E-01  3-5-6 Ring
-8.98235842E-01  8.98235581E-01  8.98235520E-01  3-4-6 Ring
 8.98235839E-01  8.98235583E-01 -8.98235522E-01  1-2-4 Ring
 8.98235842E-01 -8.98235581E-01 -8.98235520E-01  1-2-5 Ring
-8.98235843E-01 -8.98235580E-01 -8.98235521E-01  1-3-5 Ring
-8.98235840E-01  8.98235582E-01 -8.98235522E-01  1-3-4 Ring
 2.56031172E-12 -2.58139969E-13 -3.30662485E-12  Cage
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B7H7(2-)

SADDLE
B7H7 2- OPTIMIZATION USING VD SET ON H & 9S/5P+1D ON B

B	1	0.82777604	2.54763270	0.00000000
B	2	-2.16714582	1.57452360	0.00000000
B	3	-2.16714582	-1.57452360	0.00000000
B	4	0.82777604	-2.54763270	0.00000000
B	5	2.67873955	0.00000000	0.00000000
B	6	0.00000000	0.00000000	-2.24056705
B	7	0.00000000	0.00000000	2.24056705
H	8	1.53721263	4.73105400	0.00000000
H	9	-4.02447491	2.92395217	0.00000000
H	10	-4.02447491	-2.92395217	0.00000000
H	11	1.53721263	-4.73105400	0.00000000
H	12	4.97452456	0.00000000	0.00000000
H	13	0.00000000	0.00000000	-4.53698226
H	14	0.00000000	0.00000000	4.53698226

SEARCHING BETWEEN ATOMS 7 14
NUMBER OF PERFORMED NEWTON ITERATION STEPS : 6

COORDINATES OF CRITICAL POINT
X = 3.05178418E-11
Y = -1.47143907E-11
Z = 3.19995675E+00
R = 3.19995675E+00

VECTORS FROM NUCLEI TO CRITICAL POINT
LENGTHS AND ANGLES MADE WITH PROJECTIONS ONTO YZ/XZ/XY PLANES OF MCS

NUCLEUS		LENGTH	YZ ANGLE	XZ ANGLE	XY ANGLE
B	1	4.17317251E+00	1.14408701E+01	3.76241202E+01	5.00667120E+01
B	2	4.17317251E+00	3.12855871E+01	2.21663251E+01	5.00667120E+01
B	3	4.17317251E+00	3.12855871E+01	2.21663251E+01	5.00667120E+01
B	4	4.17317251E+00	1.14408701E+01	3.76241202E+01	5.00667120E+01
B	5	4.17317251E+00	3.99332880E+01	0.00000000E+00	5.00667120E+01
B	6	5.44052380E+00	0.00000000E+00	0.00000000E+00	9.00000000E+01
B	7	9.59389702E-01	0.00000000E+00	0.00000000E+00	9.00000000E+01
H	8	5.91486414E+00	1.50635211E+01	5.31165864E+01	3.27519148E+01
H	9	5.91486414E+00	4.28749262E+01	2.96262189E+01	3.27519148E+01
H	10	5.91486414E+00	4.28749262E+01	2.96262189E+01	3.27519148E+01
H	11	5.91486414E+00	1.50635211E+01	5.31165864E+01	3.27519148E+01
H	12	5.91486414E+00	5.72480852E+01	0.00000000E+00	3.27519148E+01
H	13	7.73693901E+00	0.00000000E+00	0.00000000E+00	9.00000000E+01
H	14	1.33702551E+00	0.00000000E+00	0.00000000E+00	9.00000000E+01

EIGENVALUES OF THE HESSIAN
-3.31020010E-01 -3.31020010E-01 5.92906708E-01

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THE ELLIPTICITY IS      0.00000

EIGENVECTORS OF THE HESSIAN
   -9.99345845E-01   -3.61646609E-02   -1.76655402E-11
    3.61646609E-02   -9.99345845E-01   -1.99694796E-12
   -1.75817653E-11   -2.63450992E-12    1.00000000E+00

EIGENVALUES OF THE STRESSIAN
   -1.19933152E-01   -1.19933152E-01   -7.12528048E-02

THE TRACE OF THE STRESSIAN IS  -0.31111911

EIGENVECTORS OF THE STRESSIAN
   -1.85820647E-02    9.99827339E-01   -2.89643904E-11
   -9.99827339E-01   -1.85820647E-02    4.59930586E-11
    4.54468992E-11    2.98140353E-11    1.00000000E+00

VALUES
RHO        1.5817579195E-01
GRAD       9.0238305158E-17
DEL2      -6.9133312631E-02
G(X)       1.4691789020E-01
K(X)       1.6420121835E-01
L(X)       1.7283328158E-02

COMPONENTS OF THE DIVERGENCE OF THE STRESSIAN
    9.07957196E-12   -5.57255428E-12    5.28530881E-01

MAGNITUDE OF THE DIVERGENCE OF THE STRESSIAN        0.528531

SEARCHING BETWEEN ATOMS    1   7
NUMBER OF PERFORMED NEWTON ITERATION STEPS :    4

COORDINATES OF CRITICAL POINT
         X =   4.04450557E-01
         Y =   1.24477084E+00
         Z =   1.17938310E+00
         R =   1.76181134E+00

VECTORS FROM NUCLEI TO CRITICAL POINT
LENGTHS AND ANGLES MADE WITH PROJECTIONS ONTO YZ/XZ/XY PLANES OF MCS

NUCLEUS        LENGTH        YZ ANGLE        XZ ANGLE        XY ANGLE
  B    1   1.80764985E+00  1.35436189E+01  4.61163557E+01  4.07258222E+01
  B    2   2.84829586E+00  6.45358362E+01  6.64815181E+00  2.44605256E+01
  B    3   3.99405478E+00  4.00799610E+01  4.49000956E+01  1.71746074E+01
  B    4   3.99405478E+00  6.08414446E+00  7.17158222E+01  1.71746074E+01
  B    5   2.84829587E+00  5.29845860E+01  2.59140913E+01  2.44605255E+01
  B    6   3.66184294E+00  6.34125681E+00  1.98726189E+01  6.90579383E+01
  B    7   1.68497658E+00  1.38885081E+01  4.76247603E+01  3.90347426E+01
  H    8   3.85074859E+00  1.71075769E+01  6.48707413E+01  1.78348104E+01
  H    9   4.88118584E+00  6.51411553E+01  2.01214316E+01  1.39820646E+01
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  H    10   6.19552878E+00  4.56315915E+01  4.22881806E+01  1.09738152E+01
  H    11   6.19552879E+00  1.05349584E+01  7.46958506E+01  1.09738152E+01
  H    12   4.88118585E+00  6.94331685E+01  1.47744161E+01  1.39820646E+01
  H    13   5.86428747E+00  3.95473801E+00  1.22549988E+01  7.71037421E+01
  H    14   3.60367963E+00  6.44403480E+00  2.02072299E+01  6.87036099E+01

EIGENVALUES OF THE HESSIAN
   -1.26087912E-01   -1.56256570E-02    4.76703734E-02

THE ELLIPTICITY IS      7.06929

EIGENVECTORS OF THE HESSIAN
   -2.05885274E-01    9.51056518E-01    2.30440346E-01
   -6.33649732E-01   -3.09016988E-01    7.09222475E-01
   -7.45720639E-01   -1.89967386E-10   -6.66258755E-01

EIGENVALUES OF THE STRESSIAN
   -4.93515331E-02   -4.86592833E-02    2.30020035E-03

THE TRACE OF THE STRESSIAN IS  -0.09571062

EIGENVECTORS OF THE STRESSIAN
    9.51056507E-01   -1.93882105E-01   -2.40626787E-01
   -3.09017024E-01   -5.96707593E-01   -7.40573107E-01
   -4.22975891E-08   -7.78684646E-01    6.27415510E-01

VALUES
RHO         1.0645429647E-01
GRAD        3.7670370058E-17
DEL2       -9.4043195915E-02
G(X)        3.6099908529E-02
K(X)        5.9610707507E-02
L(X)        2.3510798979E-02

COMPONENTS OF THE DIVERGENCE OF THE STRESSIAN
    4.27203313E-03    1.31479673E-02   -5.90183229E-03

MAGNITUDE OF THE DIVERGENCE OF THE STRESSIAN        0.015032


3-4-7 Ring
NUMBER OF PERFORMED NEWTON ITERATION STEPS :    7

COORDINATES OF CRITICAL POINT
          X =  -4.03169638E-01
          Y =  -1.24082851E+00
          Z =   1.13248328E+00
          R =   1.72763408E+00

VECTORS FROM NUCLEI TO CRITICAL POINT
LENGTHS AND ANGLES MADE WITH PROJECTIONS ONTO YZ/XZ/XY PLANES OF MCS
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NUCLEUS		LENGTH	YZ ANGLE	XZ ANGLE	XY ANGLE
B	1	4.14127806E+00	1.72917931E+01	6.61780268E+01	1.58703961E+01
B	2	3.51003388E+00	3.01690139E+01	5.33298490E+01	1.88227588E+01
B	3	2.12261225E+00	5.62057441E+01	9.04497013E+00	3.22444648E+01
B	4	2.12261226E+00	3.54449285E+01	3.79997804E+01	3.22444646E+01
B	5	3.51003390E+00	6.14054284E+01	2.07020910E+01	1.88227587E+01
B	6	3.61658259E+00	6.40052668E+00	2.00655020E+01	6.88537004E+01
B	7	1.71173912E+00	1.36229947E+01	4.64599867E+01	4.03416369E+01
H	8	6.38051585E+00	1.77046613E+01	6.93831571E+01	1.02236438E+01
H	9	5.63398335E+00	3.99980164E+01	4.76654293E+01	1.15959887E+01
H	10	4.15081624E+00	6.07425054E+01	2.39219753E+01	1.58329687E+01
H	11	4.15081627E+00	2.78701966E+01	5.72302833E+01	1.58329686E+01
H	12	5.63398337E+00	7.26517680E+01	1.27231299E+01	1.15959887E+01
H	13	5.81764906E+00	3.97384727E+00	1.23150447E+01	7.70404474E+01
H	14	3.64593122E+00	6.34879162E+00	1.98971268E+01	6.90319892E+01

EIGENVALUES OF THE HESSIAN

-1.23957457E-01	1.71479490E-02	6.74918215E-02

EIGENVECTORS OF THE HESSIAN

-2.16423198E-01	9.51056514E-01	-2.20573134E-01
-6.66082100E-01	-3.09017002E-01	-6.78854277E-01
7.13789630E-01	-2.72244051E-09	-7.00360167E-01

EIGENVALUES OF THE STRESSIAN

-4.68939479E-02	-3.03897482E-02	-6.96477759E-03

THE TRACE OF THE STRESSIAN IS -0.08424847

EIGENVECTORS OF THE STRESSIAN

2.15320043E-01	9.51056512E-01	-2.21650151E-01
6.62686958E-01	-3.09017007E-01	-6.82168957E-01
-7.17274895E-01	-1.52495205E-08	-6.96790302E-01

VALUES

RHO	1.0421330140E-01
GRAD	5.5592829820E-17
DEL2	-3.9317686372E-02
G(X)	3.7209526077E-02
K(X)	4.7038947670E-02
L(X)	9.8294215929E-03

COMPONENTS OF THE DIVERGENCE OF THE STRESSIAN

-1.06000775E-02	-3.26236851E-02	-1.70706869E-02

MAGNITUDE OF THE DIVERGENCE OF THE STRESSIAN 0.038315

CAGE
0.000000 0.000000 0.000000
NUMBER OF PERFORMED NEWTON ITERATION STEPS : 1

COORDINATES OF CRITICAL POINT

X =	-1.26328315E-09
Y =	-6.07672990E-11
Z =	5.43924972E-12
R =	1.26475554E-09

VECTORS FROM NUCLEI TO CRITICAL POINT
LENGTHS AND ANGLES MADE WITH PROJECTIONS ONTO YZ/XZ/XY PLANES OF MCS

NUCLEUS		LENGTH	YZ ANGLE	XZ ANGLE	XY ANGLE
B	1	2.67873954E+00	1.80000000E+01	7.20000000E+01	0.00000000E+00
B	2	2.67873955E+00	5.40000000E+01	3.60000000E+01	0.00000000E+00
B	3	2.67873955E+00	5.40000000E+01	3.60000000E+01	0.00000000E+00
B	4	2.67873954E+00	1.80000000E+01	7.20000000E+01	0.00000000E+00
B	5	2.67873955E+00	9.00000000E+01	0.00000000E+00	0.00000000E+00
B	6	2.24056705E+00	0.00000000E+00	0.00000000E+00	9.00000000E+01
B	7	2.24056705E+00	0.00000000E+00	0.00000000E+00	9.00000000E+01
H	8	4.97452456E+00	1.80000000E+01	7.20000000E+01	0.00000000E+00
H	9	4.97452456E+00	5.40000000E+01	3.60000000E+01	0.00000000E+00
H	10	4.97452456E+00	5.40000000E+01	3.60000000E+01	0.00000000E+00
H	11	4.97452456E+00	1.80000000E+01	7.20000000E+01	0.00000000E+00
H	12	4.97452456E+00	9.00000000E+01	0.00000000E+00	0.00000000E+00
H	13	4.53698226E+00	0.00000000E+00	0.00000000E+00	9.00000000E+01
H	14	4.53698226E+00	0.00000000E+00	0.00000000E+00	9.00000000E+01

EIGENVALUES OF THE HESSIAN

5.80263183E-02	5.80263188E-02	8.32636120E-02

EIGENVECTORS OF THE HESSIAN

9.99775006E-01	-2.12117368E-02	-6.99418488E-12
2.12117368E-02	9.99775006E-01	1.47980233E-12
6.96122206E-12	-1.62782819E-12	1.00000000E+00

EIGENVALUES OF THE STRESSIAN

-1.95146177E-02	-1.95146177E-02	-1.86601135E-02

THE TRACE OF THE STRESSIAN IS -0.05768935

EIGENVECTORS OF THE STRESSIAN

1.45662507E-01	9.89334339E-01	5.16423145E-11
9.89334339E-01	-1.45662507E-01	-1.09268934E-11
3.28800185E-12	-5.26831537E-11	1.00000000E+00

VALUES

RHO	4.8523040836E-02
GRAD	6.0953988825E-18
DEL2	1.9931624901E-01
G(X)	5.3759205579E-02
K(X)	3.9301433249E-03
L(X)	-4.9829062254E-02

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COMPONENTS OF THE DIVERGENCE OF THE STRESSIAN
   -8.42319828E-12    6.91087834E-12    2.63275707E-13

MAGNITUDE OF THE DIVERGENCE OF THE STRESSIAN        0.000000


SEARCHING BETWEEN ATOMS    1   2
NUMBER OF PERFORMED NEWTON ITERATION STEPS :    9

COORDINATES OF CRITICAL POINT
         X =  -3.22857638E-01
         Y =   2.20095531E+00
         Z =  -8.93387032E-13
         R =   2.22450923E+00

VECTORS FROM NUCLEI TO CRITICAL POINT
LENGTHS AND ANGLES MADE WITH PROJECTIONS ONTO YZ/XZ/XY PLANES OF MCS

NUCLEUS        LENGTH         YZ ANGLE         XZ ANGLE         XY ANGLE
  B     1   1.20172504E+00   7.32328356E+01   1.67671644E+01   0.00000000E+00
  B     2   1.94777195E+00   7.12394087E+01   1.87605913E+01   0.00000000E+00
  B     3   4.20186148E+00   2.60351015E+01   6.39648985E+01   0.00000000E+00
  B     4   4.88600511E+00   1.36208502E+01   7.63791498E+01   0.00000000E+00
  B     5   3.72206797E+00   5.37488431E+01   3.62511569E+01   0.00000000E+00
  B     6   3.15730614E+00   5.86917142E+00   4.41947264E+01   4.52060527E+01
  B     7   3.15730614E+00   5.86917142E+00   4.41947264E+01   4.52060527E+01
  H     8   3.14026444E+00   3.63224688E+01   5.36775312E+01   0.00000000E+00
  H     9   3.77156398E+00   7.89481742E+01   1.10518258E+01   0.00000000E+00
  H    10   6.32191799E+00   3.58398219E+01   5.41601781E+01   0.00000000E+00
  H    11   7.17722889E+00   1.50203876E+01   7.49796124E+01   0.00000000E+00
  H    12   5.73641547E+00   6.74381022E+01   2.25618978E+01   0.00000000E+00
  H    13   5.05298420E+00   3.66337774E+00   2.58219093E+01   6.38810137E+01
  H    14   5.05298420E+00   3.66337774E+00   2.58219093E+01   6.38810137E+01

EIGENVALUES OF THE HESSIAN
   -1.89564811E-01   -1.27651630E-01    2.31375176E-02

THE ELLIPTICITY IS      0.48502

EIGENVECTORS OF THE HESSIAN
    3.25593454E-01    0.00000000E+00    9.45509864E-01
   -9.45509864E-01    0.00000000E+00    3.25593454E-01
    0.00000000E+00    1.00000000E+00    0.00000000E+00

EIGENVALUES OF THE STRESSIAN
   -8.96451713E-02   -8.57235914E-02   -1.83682918E-02

THE TRACE OF THE STRESSIAN IS  -0.19373705

EIGENVECTORS OF THE STRESSIAN
    0.00000000E+00   -3.45345339E-01    9.38475677E-01
    0.00000000E+00    9.38475677E-01    3.45345339E-01
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    1.00000000E+00     0.00000000E+00     0.00000000E+00

VALUES
RHO          1.4816538107E-01
GRAD         3.9667462456E-17
DEL2        -2.9407892293E-01
G(X)         6.0108661854E-02
K(X)         1.3362839259E-01
L(X)         7.3519730732E-02

 COMPONENTS OF THE DIVERGENCE OF THE STRESSIAN
    -1.60597767E-01    -3.60859233E-02    -1.24393647E-13

 MAGNITUDE OF THE DIVERGENCE OF THE STRESSIAN         0.164602


 STARTING COORDINATES
-0.700000 2.000000 0.000000
 NUMBER OF PERFORMED NEWTON ITERATION STEPS :     6

 COORDINATES OF CRITICAL POINT
          X =  -6.76656725E-01
          Y =   2.08253532E+00
          Z =  -8.56593484E-13
          R =   2.18970721E+00

 VECTORS FROM NUCLEI TO CRITICAL POINT
 LENGTHS AND ANGLES MADE WITH PROJECTIONS ONTO YZ/XZ/XY PLANES OF MCS

 NUCLEUS         LENGTH          YZ ANGLE          XZ ANGLE          XY ANGLE
   B     1   1.57468521E+00   7.28209367E+01   1.71790633E+01   0.00000000E+00
   B     2   1.57468525E+00   7.11790634E+01   1.88209366E+01   0.00000000E+00
   B     3   3.94913125E+00   2.21740878E+01   6.78259122E+01   0.00000000E+00
   B     4   4.86844675E+00   1.79999998E+01   7.20000002E+01   0.00000000E+00
   B     5   3.94913123E+00   5.81740874E+01   3.18259126E+01   0.00000000E+00
   B     6   3.13288340E+00   1.24733384E+01   4.16619513E+01   4.56577304E+01
   B     7   3.13288340E+00   1.24733384E+01   4.16619513E+01   4.56577304E+01
   H     8   3.45193696E+00   3.98919015E+01   5.01080985E+01   0.00000000E+00
   H     9   3.45193698E+00   7.58919019E+01   1.41080981E+01   0.00000000E+00
   H    10   6.02269072E+00   3.37704885E+01   5.62295115E+01   0.00000000E+00
   H    11   7.16423177E+00   1.79999999E+01   7.20000001E+01   0.00000000E+00
   H    12   6.02269070E+00   6.97704883E+01   2.02295117E+01   0.00000000E+00
   H    13   5.03775999E+00   7.71912622E+00   2.44176646E+01   6.42364089E+01
   H    14   5.03775999E+00   7.71912622E+00   2.44176646E+01   6.42364089E+01

 EIGENVALUES OF THE HESSIAN
    -1.86301986E-01    -1.24045565E-01    -6.07966677E-03

 THE ELLIPTICITY IS       0.50188

 EIGENVECTORS OF THE HESSIAN
     3.09016995E-01     0.00000000E+00     9.51056516E-01
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  -9.51056516E-01     0.00000000E+00     3.09016995E-01
   0.00000000E+00     1.00000000E+00     0.00000000E+00

EIGENVALUES OF THE STRESSIAN
   -7.86354538E-02   -7.36220800E-02   -6.13087783E-03

THE TRACE OF THE STRESSIAN IS  -0.15838841

EIGENVECTORS OF THE STRESSIAN
    0.00000000E+00     3.09016996E-01     9.51056516E-01
    0.00000000E+00    -9.51056516E-01     3.09016996E-01
    1.00000000E+00     0.00000000E+00     0.00000000E+00

 VALUES
 RHO          1.4842449275E-01
 GRAD         4.7854916600E-17
 DEL2        -3.1642721724E-01
 G(X)         3.9640803667E-02
 K(X)         1.1874760798E-01
 L(X)         7.9106804310E-02

 COMPONENTS OF THE DIVERGENCE OF THE STRESSIAN
    -3.33628675E-03     1.02680211E-02     3.89023512E-14

 MAGNITUDE OF THE DIVERGENCE OF THE STRESSIAN        0.010796

 STARTING COORDINATES
-1.000000 1.800000 0.000000
 NUMBER OF PERFORMED NEWTON ITERATION STEPS :    7

 COORDINATES OF CRITICAL POINT
          X =  -1.03249177E+00
          Y =   1.97038120E+00
          Z =  -4.13564599E-13
          R =   2.22450924E+00

 VECTORS FROM NUCLEI TO CRITICAL POINT
 LENGTHS AND ANGLES MADE WITH PROJECTIONS ONTO YZ/XZ/XY PLANES OF MCS

 NUCLEUS         LENGTH          YZ ANGLE          XZ ANGLE          XY ANGLE
   B     1   1.94777197E+00   7.27605914E+01   1.72394086E+01   0.00000000E+00
   B     2   1.20172503E+00   7.07671645E+01   1.92328355E+01   0.00000000E+00
   B     3   3.72206796E+00   1.77488429E+01   7.22511571E+01   0.00000000E+00
   B     4   4.88600511E+00   2.23791499E+01   6.76208501E+01   0.00000000E+00
   B     5   4.20186149E+00   6.20351017E+01   2.79648983E+01   0.00000000E+00
   B     6   3.15730614E+00   1.90877998E+01   3.86139874E+01   4.52060527E+01
   B     7   3.15730614E+00   1.90877998E+01   3.86139874E+01   4.52060527E+01
   H     8   3.77156400E+00   4.29481742E+01   4.70518258E+01   0.00000000E+00
   H     9   3.14026443E+00   7.23224687E+01   1.76775313E+01   0.00000000E+00
   H    10   5.73641545E+00   3.14381022E+01   5.85618978E+01   0.00000000E+00
   H    11   7.17722889E+00   2.09796126E+01   6.90203874E+01   0.00000000E+00
   H    12   6.32191801E+00   7.18398219E+01   1.81601781E+01   0.00000000E+00
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 H   13   5.05298420E+00  1.17904604E+01  2.29510190E+01  6.38810137E+01
 H   14   5.05298420E+00  1.17904604E+01  2.29510190E+01  6.38810137E+01

EIGENVALUES OF THE HESSIAN
  -1.89564811E-01   -1.27651630E-01    2.31375216E-02

THE ELLIPTICITY IS      0.48502

EIGENVECTORS OF THE HESSIAN
    2.92346116E-01    0.00000000E+00   -9.56312579E-01
   -9.56312579E-01    0.00000000E+00   -2.92346116E-01
    0.00000000E+00    1.00000000E+00    0.00000000E+00

EIGENVALUES OF THE STRESSIAN
   -8.96451721E-02   -8.57235922E-02   -1.83682930E-02

THE TRACE OF THE STRESSIAN IS  -0.19373706

EIGENVECTORS OF THE STRESSIAN
    0.00000000E+00    2.72231912E-01    9.62231670E-01
    0.00000000E+00   -9.62231670E-01    2.72231912E-01
    1.00000000E+00    0.00000000E+00    0.00000000E+00

VALUES
RHO         1.4816538098E-01
GRAD        8.9125629451E-17
DEL2       -2.9407891915E-01
G(X)        6.0108663777E-02
K(X)        1.3362839356E-01
L(X)        7.3519729787E-02

COMPONENTS OF THE DIVERGENCE OF THE STRESSIAN
    1.51137106E-01    6.52028773E-02    1.21206072E-12

MAGNITUDE OF THE DIVERGENCE OF THE STRESSIAN        0.164602

CRITICAL POINTS
-3.22857638E-01  2.20095531E+00 -8.93387032E-13  B    1  B    2
-6.76656725E-01  2.08253532E+00 -8.56593484E-13
-1.03249177E+00  1.97038120E+00 -4.13564599E-13
 3.05178418E-11 -1.47143907E-11  3.19995675E+00  B    7  H   14
 4.04450557E-01  1.24477084E+00  1.17938310E+00  B    1  B    7
-1.05886532E+00  7.69310694E-01  1.17938310E+00  B    2  B    7
-1.05886532E+00 -7.69310694E-01  1.17938309E+00  B    3  B    7
 4.04450556E-01 -1.24477084E+00  1.17938310E+00  B    4  B    7
 1.30882952E+00  1.28853336E-09  1.17938309E+00  B    5  B    7
-4.03169638E-01 -1.24082851E+00  1.13248328E+00  3-4-7 Ring
 1.05551179E+00 -7.66874189E-01  1.13248327E+00  4-5-7 Ring
-1.30468431E+00 -1.94211133E-09  1.13248328E+00  2-3-7 Ring
 1.05551179E+00  7.66874190E-01  1.13248327E+00  1-5-7 Ring
-4.03169635E-01  1.24082851E+00  1.13248328E+00  1-2-7 Ring
-1.26328315E-09 -6.07672990E-11  5.43924972E-12  Cage
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B12H12(2-)

SADDLE
B12H12 OPTIMIZATION USING VD SET(Renormalized) d=0.75, p=1.0725
B12H12(2-)

B	1	0.00000000	0.00000000	3.23340418
B	2	0.00000000	2.89204464	1.44602225
B	3	2.75049790	0.89369094	1.44602225
B	4	1.69990119	-2.33971327	1.44602225
B	5	-1.69990119	-2.33971327	1.44602225
B	6	-2.75049790	0.89369094	1.44602225
B	7	0.00000000	0.00000000	-3.23340418
B	8	0.00000000	-2.89204464	-1.44602225
B	9	2.75049790	-0.89369094	-1.44602225
B	10	1.69990119	2.33971327	-1.44602225
B	11	-1.69990119	2.33971327	-1.44602225
B	12	-2.75049790	-0.89369094	-1.44602225
H	13	0.00000000	0.00000000	5.50293878
H	14	0.00000000	4.92197813	2.46098894
H	15	4.68107937	1.52097489	2.46098894
H	16	2.89306616	-3.98196395	2.46098894
H	17	-2.89306616	-3.98196395	2.46098894
H	18	-4.68107937	1.52097489	2.46098894
H	19	0.00000000	0.00000000	-5.50293878
H	20	0.00000000	-4.92197813	-2.46098894
H	21	4.68107937	-1.52097489	-2.46098894
H	22	2.89306616	3.98196395	-2.46098894
H	23	-2.89306616	3.98196395	-2.46098894
H	24	-4.68107937	-1.52097489	-2.46098894

SEARCHING BETWEEN ATOMS 1 2
NUMBER OF PERFORMED NEWTON ITERATION STEPS : 3

COORDINATES OF CRITICAL POINT
X = 2.70182614E-09
Y = 1.42077990E+00
Z = 2.29887015E+00
R = 2.70248395E+00

VECTORS FROM NUCLEI TO CRITICAL POINT
LENGTHS AND ANGLES MADE WITH PROJECTIONS ONTO YZ/XZ/XY PLANES OF MCS

NUCLEUS		LENGTH	YZ ANGLE	XZ ANGLE	XY ANGLE
B	1	1.70057913E+00	0.00000000E+00	5.66646291E+01	3.33353709E+01
B	2	1.70057916E+00	0.00000000E+00	5.99004207E+01	3.00995793E+01
B	3	2.92752643E+00	6.99727175E+01	1.03724300E+01	1.69370175E+01
B	4	4.21406247E+00	2.37901348E+01	6.31722938E+01	1.16762521E+01
B	5	4.21406247E+00	2.37901349E+01	6.31722937E+01	1.16762521E+01
B	6	2.92752644E+00	6.99727175E+01	1.03724300E+01	1.69370175E+01
B	7	5.71180137E+00	0.00000000E+00	1.44032381E+01	7.55967619E+01

B	8	5.71180135E+00	0.00000000E+00	4.90317115E+01	4.09682885E+01
B	9	5.19097612E+00	3.19960910E+01	2.64786486E+01	4.61721365E+01
B	10	4.21406237E+00	2.37901354E+01	1.25953209E+01	6.27060468E+01
B	11	4.21406238E+00	2.37901354E+01	1.25953209E+01	6.27060468E+01
B	12	5.19097612E+00	3.19960910E+01	2.64786486E+01	4.61721365E+01
H	13	3.50494954E+00	0.00000000E+00	2.39139310E+01	6.60860690E+01
H	14	3.50494958E+00	0.00000000E+00	8.73488812E+01	2.65111875E+00
H	15	4.68495737E+00	8.76685884E+01	1.22545140E+00	1.98306543E+00
H	16	6.13072226E+00	2.81574707E+01	6.17944068E+01	1.51528722E+00
H	17	6.13072226E+00	2.81574707E+01	6.17944067E+01	1.51528722E+00
H	18	4.68495738E+00	8.76685884E+01	1.22545140E+00	1.98306543E+00
H	19	7.93012220E+00	0.00000000E+00	1.03209771E+01	7.96790229E+01
H	20	7.93012220E+00	0.00000000E+00	5.31139727E+01	3.68860273E+01
H	21	7.29538785E+00	3.99149022E+01	2.37805624E+01	4.07264039E+01
H	22	6.13072215E+00	2.81574712E+01	2.46933870E+01	5.09316364E+01
H	23	6.13072215E+00	2.81574713E+01	2.46933870E+01	5.09316363E+01
H	24	7.29538785E+00	3.99149022E+01	2.37805624E+01	4.07264039E+01

EIGENVALUES OF THE HESSIAN

-1.54414472E-01	-4.07235785E-02	3.37691577E-02

THE ELLIPTICITY IS 2.79177

EIGENVECTORS OF THE HESSIAN

-2.26142922E-09	1.00000000E+00	1.10465950E-09
-5.25731116E-01	-2.12858321E-09	8.50650806E-01
-8.50650806E-01	-1.34293272E-09	-5.25731116E-01

EIGENVALUES OF THE STRESSIAN

-5.49475736E-02	-5.46012313E-02	2.10785592E-03

THE TRACE OF THE STRESSIAN IS -0.10744095

EIGENVECTORS OF THE STRESSIAN

1.00000000E+00	2.27148087E-08	-5.14999366E-10
1.15037972E-08	-5.25731120E-01	-8.50650803E-01
1.95931215E-08	-8.50650803E-01	5.25731120E-01

VALUES

RHO	1.1789177283E-01
GRAD	9.1575848532E-17
DEL2	-1.6136889292E-01
G(X)	3.3549362849E-02
K(X)	7.3891586079E-02
L(X)	4.0342223230E-02

COMPONENTS OF THE DIVERGENCE OF THE STRESSIAN

1.99298108E-10	-5.51101655E-04	-8.91705696E-04

MAGNITUDE OF THE DIVERGENCE OF THE STRESSIAN 0.001048

SEARCHING BETWEEN ATOMS 1 13
NUMBER OF PERFORMED NEWTON ITERATION STEPS : 6

COORDINATES OF CRITICAL POINT
X = -4.18863135E-10
Y = -2.69050368E-10
Z = 4.19091652E+00
R = 4.19091652E+00

VECTORS FROM NUCLEI TO CRITICAL POINT
LENGTHS AND ANGLES MADE WITH PROJECTIONS ONTO YZ/XZ/XY PLANES OF MCS

NUCLEUS		LENGTH	YZ ANGLE	XZ ANGLE	XY ANGLE
B	1	9.57512343E-01	0.00000000E+00	0.00000000E+00	9.00000000E+01
B	2	3.98727561E+00	0.00000000E+00	4.64953472E+01	4.35046528E+01
B	3	3.98727561E+00	4.36157715E+01	1.29520614E+01	4.35046528E+01
B	4	3.98727561E+00	2.52349721E+01	3.59298978E+01	4.35046528E+01
B	5	3.98727561E+00	2.52349721E+01	3.59298978E+01	4.35046528E+01
B	6	3.98727561E+00	4.36157715E+01	1.29520614E+01	4.35046528E+01
B	7	7.42432070E+00	0.00000000E+00	0.00000000E+00	9.00000000E+01
B	8	6.33553478E+00	0.00000000E+00	2.71601977E+01	6.28398023E+01
B	9	6.33553478E+00	2.57304712E+01	8.10919220E+00	6.28398023E+01
B	10	6.33553478E+00	1.55638568E+01	2.16724556E+01	6.28398022E+01
B	11	6.33553478E+00	1.55638568E+01	2.16724556E+01	6.28398022E+01
B	12	6.33553478E+00	2.57304712E+01	8.10919220E+00	6.28398023E+01
H	13	1.31202226E+00	0.00000000E+00	0.00000000E+00	9.00000000E+01
H	14	5.21713697E+00	0.00000000E+00	7.06349557E+01	1.93650443E+01
H	15	5.21713697E+00	6.37989941E+01	1.69498406E+01	1.93650443E+01
H	16	5.21713697E+00	3.36784434E+01	4.97512853E+01	1.93650443E+01
H	17	5.21713697E+00	3.36784434E+01	4.97512853E+01	1.93650443E+01
H	18	5.21713697E+00	6.37989941E+01	1.69498406E+01	1.93650443E+01
H	19	9.69385530E+00	0.00000000E+00	0.00000000E+00	9.00000000E+01
H	20	8.27488459E+00	0.00000000E+00	3.64990372E+01	5.35009628E+01
H	21	8.27488459E+00	3.44507229E+01	1.05915378E+01	5.35009629E+01
H	22	8.27488459E+00	2.04640818E+01	2.87645121E+01	5.35009628E+01
H	23	8.27488459E+00	2.04640818E+01	2.87645121E+01	5.35009628E+01
H	24	8.27488459E+00	3.44507229E+01	1.05915378E+01	5.35009629E+01

EIGENVALUES OF THE HESSIAN
-3.46658051E-01 -3.46658050E-01 6.03376890E-01

THE ELLIPTICITY IS 0.00000

EIGENVECTORS OF THE HESSIAN
-5.34740345E-03 9.99985703E-01 -6.62335846E-11
-9.99985703E-01 -5.34740345E-03 -1.32251014E-10
-1.32603301E-10 6.55254381E-11 1.00000000E+00

EIGENVALUES OF THE STRESSIAN
-1.27566338E-01 -1.27566337E-01 -7.32682815E-02

THE TRACE OF THE STRESSIAN IS -0.32840096

EIGENVECTORS OF THE STRESSIAN

-9.99996360E-01	2.69803623E-03	8.46475103E-10
-2.69803623E-03	-9.99996360E-01	3.30536435E-10
8.47363821E-10	3.28251412E-10	1.00000000E+00

VALUES

RHO	1.6567247580E-01
GRAD	1.2001494860E-16
DEL2	-8.9939211822E-02
G(X)	1.5295807671E-01
K(X)	1.7544287967E-01
L(X)	2.2484802955E-02

COMPONENTS OF THE DIVERGENCE OF THE STRESSIAN

-3.18852417E-10	-2.64922140E-10	5.57553236E-01

MAGNITUDE OF THE DIVERGENCE OF THE STRESSIAN 0.557553

STARTING COORDINATES

0.000000-1.601500 2.096000

NUMBER OF PERFORMED NEWTON ITERATION STEPS : 2

COORDINATES OF CRITICAL POINT

X =	1.26391486E-09
Y =	-1.60153686E+00
Z =	2.09643893E+00
R =	2.63817673E+00

VECTORS FROM NUCLEI TO CRITICAL POINT

LENGTHS AND ANGLES MADE WITH PROJECTIONS ONTO YZ/XZ/XY PLANES OF MCS

NUCLEUS		LENGTH	YZ ANGLE	XZ ANGLE	XY ANGLE
B	1	1.96408001E+00	0.00000000E+00	5.46282432E+01	3.53717568E+01
B	2	4.54040929E+00	0.00000000E+00	8.17640075E+01	8.23599250E+00
B	3	3.77020454E+00	4.68474640E+01	4.14394534E+01	9.93407630E+00
B	4	1.96408002E+00	5.99392616E+01	2.20761317E+01	1.93389486E+01
B	5	1.96408002E+00	5.99392616E+01	2.20761317E+01	1.93389486E+01
B	6	3.77020455E+00	4.68474640E+01	4.14394534E+01	9.93407629E+00
B	7	5.56526260E+00	0.00000000E+00	1.67247245E+01	7.32752755E+01
B	8	3.77020444E+00	0.00000000E+00	2.00165276E+01	6.99834724E+01
B	9	4.54040920E+00	3.72851308E+01	8.96894750E+00	5.12795751E+01
B	10	5.56526260E+00	1.77851496E+01	4.50876466E+01	3.95336153E+01
B	11	5.56526260E+00	1.77851496E+01	4.50876465E+01	3.95336153E+01
B	12	4.54040920E+00	3.72851308E+01	8.96894750E+00	5.12795751E+01
H	13	3.76419468E+00	0.00000000E+00	2.51801634E+01	6.48198366E+01
H	14	6.53369302E+00	0.00000000E+00	8.68014981E+01	3.19850194E+00
H	15	5.63874812E+00	5.61154731E+01	3.36253318E+01	3.70680773E+00
H	16	3.76419469E+00	5.02261024E+01	3.92264378E+01	5.55762087E+00
H	17	3.76419469E+00	5.02261024E+01	3.92264378E+01	5.55762087E+00
H	18	5.63874812E+00	5.61154731E+01	3.36253318E+01	3.70680773E+00
H	19	7.76630297E+00	0.00000000E+00	1.19006988E+01	7.80993012E+01
H	20	5.63874800E+00	0.00000000E+00	3.60762542E+01	5.39237458E+01

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  H    21    6.53369291E+00  4.57623479E+01  7.06488324E-01  4.42289380E+01
  H    22    7.76630297E+00  2.18708221E+01  4.59669805E+01  3.59317233E+01
  H    23    7.76630297E+00  2.18708221E+01  4.59669805E+01  3.59317233E+01
  H    24    6.53369291E+00  4.57623479E+01  7.06488323E-01  4.42289380E+01

EIGENVALUES OF THE HESSIAN
   -1.42118189E-01    4.61033205E-02    4.61033229E-02

EIGENVECTORS OF THE HESSIAN
    7.75975466E-10    9.98734458E-01   -5.02939541E-02
   -6.07062007E-01   -3.99663147E-02   -7.93648797E-01
    7.94654466E-01   -3.05315493E-02   -6.06293745E-01

EIGENVALUES OF THE STRESSIAN
   -4.78104527E-02   -1.55705381E-02   -1.55705375E-02

THE TRACE OF THE STRESSIAN IS  -0.07895153

EIGENVECTORS OF THE STRESSIAN
   -1.13780872E-09    9.99570729E-01    2.92977268E-02
   -6.07062004E-01    2.32815688E-02   -7.94313346E-01
    7.94654468E-01    1.77855376E-02   -6.06801410E-01

VALUES
RHO         1.0973095815E-01
GRAD        2.2234353998E-17
DEL2       -4.9911545712E-02
G(X)        3.3236820931E-02
K(X)        4.5714707359E-02
L(X)        1.2477886428E-02

COMPONENTS OF THE DIVERGENCE OF THE STRESSIAN
   -7.24468951E-11   -3.89949163E-03    5.10450083E-03

MAGNITUDE OF THE DIVERGENCE OF THE STRESSIAN        0.006424



STARTING COORDINATES
0.000000 0.000000 0.000000
NUMBER OF PERFORMED NEWTON ITERATION STEPS :    1

COORDINATES OF CRITICAL POINT
         X =   4.58481793E-14
         Y =   3.61668322E-14
         Z =  -3.89315865E-15
         R =   5.85256523E-14

VECTORS FROM NUCLEI TO CRITICAL POINT
LENGTHS AND ANGLES MADE WITH PROJECTIONS ONTO YZ/XZ/XY PLANES OF MCS
```

NUCLEUS		LENGTH	YZ ANGLE	XZ ANGLE	XY ANGLE
B	1	3.23340418E+00	0.00000000E+00	0.00000000E+00	9.00000000E+01
B	2	3.23340417E+00	0.00000000E+00	6.34349499E+01	2.65650501E+01
B	3	3.23340417E+00	5.82825265E+01	1.60450573E+01	2.65650501E+01
B	4	3.23340418E+00	3.17174747E+01	4.63530736E+01	2.65650500E+01
B	5	3.23340418E+00	3.17174747E+01	4.63530736E+01	2.65650500E+01
B	6	3.23340417E+00	5.82825265E+01	1.60450573E+01	2.65650501E+01
B	7	3.23340418E+00	0.00000000E+00	0.00000000E+00	9.00000000E+01
B	8	3.23340417E+00	0.00000000E+00	6.34349499E+01	2.65650501E+01
B	9	3.23340417E+00	5.82825265E+01	1.60450573E+01	2.65650501E+01
B	10	3.23340418E+00	3.17174747E+01	4.63530736E+01	2.65650500E+01
B	11	3.23340418E+00	3.17174747E+01	4.63530736E+01	2.65650500E+01
B	12	3.23340417E+00	5.82825265E+01	1.60450573E+01	2.65650501E+01
H	13	5.50293878E+00	0.00000000E+00	0.00000000E+00	9.00000000E+01
H	14	5.50293879E+00	0.00000000E+00	6.34349500E+01	2.65650500E+01
H	15	5.50293878E+00	5.82825265E+01	1.60450573E+01	2.65650500E+01
H	16	5.50293878E+00	3.17174748E+01	4.63530735E+01	2.65650500E+01
H	17	5.50293878E+00	3.17174748E+01	4.63530735E+01	2.65650500E+01
H	18	5.50293878E+00	5.82825265E+01	1.60450573E+01	2.65650500E+01
H	19	5.50293878E+00	0.00000000E+00	0.00000000E+00	9.00000000E+01
H	20	5.50293879E+00	0.00000000E+00	6.34349500E+01	2.65650500E+01
H	21	5.50293878E+00	5.82825265E+01	1.60450573E+01	2.65650500E+01
H	22	5.50293878E+00	3.17174748E+01	4.63530735E+01	2.65650500E+01
H	23	5.50293878E+00	3.17174748E+01	4.63530735E+01	2.65650500E+01
H	24	5.50293878E+00	5.82825265E+01	1.60450573E+01	2.65650500E+01

EIGENVALUES OF THE HESSIAN

2.81590419E-02	2.81590428E-02	2.81590431E-02

EIGENVECTORS OF THE HESSIAN

-2.10447990E-01	9.28128320E-01	3.07065896E-01
-6.90934738E-01	8.10011982E-02	-7.18364805E-01
6.91607426E-01	3.63340924E-01	-6.24229559E-01

EIGENVALUES OF THE STRESSIAN

-5.30905824E-03	-5.30905812E-03	-5.30905792E-03

THE TRACE OF THE STRESSIAN IS -0.01592717

EIGENVECTORS OF THE STRESSIAN

7.35519095E-01	6.68384591E-01	-1.10786731E-01
-6.74217663E-01	7.38185638E-01	-2.26386211E-02
6.66498682E-02	9.13455089E-02	9.93586329E-01

VALUES

RHO	1.3586552480E-02
GRAD	1.1388197849E-17
DEL2	8.4477127874E-02
G(X)	1.8523228125E-02
K(X)	-2.5960538436E-03
L(X)	-2.1119281968E-02

COMPONENTS OF THE DIVERGENCE OF THE STRESSIAN
-4.12885906E-14 4.60621719E-14 2.83183909E-14

MAGNITUDE OF THE DIVERGENCE OF THE STRESSIAN 0.000000

CRITICAL POINTS

2.70182614E-09	1.42077990E+00	2.29887015E+00	B	1	B	2
1.35124200E+00	4.39045150E-01	2.29887014E+00	B	1	B	3
8.35113491E-01	-1.14943510E+00	2.29887015E+00	B	1	B	4
-8.35113490E-01	-1.14943510E+00	2.29887015E+00	B	1	B	5
-1.35124201E+00	4.39045149E-01	2.29887014E+00	B	1	B	6
1.35124205E+00	1.85982508E+00	1.42077974E+00	B	2	B	3
2.18635553E+00	-7.10389992E-01	1.42077973E+00	B	3	B	4
9.37610652E-09	-2.29887027E+00	1.42077973E+00	B	4	B	5
-2.18635553E+00	-7.10389987E-01	1.42077973E+00	B	5	B	6
-1.35124205E+00	1.85982509E+00	1.42077973E+00	B	2	B	6
8.35113493E-01	2.57021501E+00	-9.18447640E-09	B	2	B	10
2.18635547E+00	1.58848024E+00	5.23014110E-11	B	3	B	10
2.70248399E+00	7.91079028E-10	1.38521541E-08	B	3	B	9
2.18635547E+00	-1.58848024E+00	6.39409850E-09	B	4	B	9
8.35113493E-01	-2.57021501E+00	9.36104544E-10	B	4	B	8
-8.35113493E-01	-2.57021501E+00	9.18306144E-09	B	5	B	8
-2.18635547E+00	-1.58848024E+00	-5.08395404E-11	B	5	B	12
-2.70248399E+00	-7.90760057E-10	-1.38521342E-08	B	6	B	12
-2.18635547E+00	1.58848024E+00	-6.39687372E-09	B	6	B	11
-8.35113493E-01	2.57021501E+00	-9.38055768E-10	B	2	B	11
1.35124205E+00	-1.85982509E+00	-1.42077973E+00	B	8	B	9
2.18635553E+00	7.10389987E-01	-1.42077973E+00	B	9	B	10
-9.37734201E-09	2.29887027E+00	-1.42077973E+00	B	10	B	11
-2.18635553E+00	7.10389992E-01	-1.42077973E+00	B	11	B	12
-1.35124205E+00	-1.85982508E+00	-1.42077974E+00	B	8	B	12
-2.70420474E-09	-1.42077990E+00	-2.29887015E+00	B	7	B	8
1.35124201E+00	-4.39045149E-01	-2.29887014E+00	B	7	B	9
8.35113490E-01	1.14943510E+00	-2.29887015E+00	B	7	B	10
-8.35113491E-01	1.14943510E+00	-2.29887015E+00	B	7	B	11
-1.35124200E+00	-4.39045150E-01	-2.29887014E+00	B	7	B	12
-4.18863135E-10	-2.69050368E-10	4.19091652E+00	B	1	H	13
3.27293522E-10	3.74846973E+00	1.87423478E+00	B	2	H	14
3.56500656E+00	1.15834085E+00	1.87423477E+00	B	3	H	15
2.20329523E+00	-3.03257572E+00	1.87423478E+00	B	4	H	16
-2.20329523E+00	-3.03257572E+00	1.87423478E+00	B	5	H	17
-3.56500656E+00	1.15834085E+00	1.87423477E+00	B	6	H	18
4.18716741E-10	2.68997408E-10	-4.19091652E+00	B	7	H	19
-3.26531644E-10	-3.74846973E+00	-1.87423478E+00	B	8	H	20
3.56500656E+00	-1.15834085E+00	-1.87423477E+00	B	9	H	21
2.20329523E+00	3.03257572E+00	-1.87423478E+00	B	10	H	22
-2.20329523E+00	3.03257572E+00	-1.87423478E+00	B	11	H	23
-3.56500656E+00	-1.15834085E+00	-1.87423477E+00	B	12	H	24
1.26391486E-09	-1.60153686E+00	2.09643893E+00				
-1.52315206E+00	-4.94902117E-01	2.09643892E+00				
1.52315206E+00	-4.94902120E-01	2.09643892E+00				

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-9.41359752E-01  1.29567052E+00  2.09643892E+00
 9.41359748E-01  1.29567052E+00  2.09643893E+00
 3.81487126E-09 -2.59134104E+00  4.94902285E-01
-1.52315206E+00 -2.09643893E+00 -4.94902258E-01
-2.46451177E+00 -8.00768437E-01  4.94902273E-01
-2.46451177E+00  8.00768427E-01 -4.94902281E-01
-1.52315205E+00  2.09643893E+00  4.94902269E-01
-3.81688775E-09  2.59134104E+00 -4.94902285E-01
 1.52315206E+00  2.09643893E+00  4.94902258E-01
 2.46451177E+00  8.00768437E-01 -4.94902273E-01
 2.46451177E+00 -8.00768427E-01  4.94902281E-01
 1.52315205E+00 -2.09643893E+00 -4.94902269E-01
-1.26431437E-09  1.60153686E+00 -2.09643893E+00
 1.52315206E+00  4.94902117E-01 -2.09643892E+00
-1.52315206E+00  4.94902120E-01 -2.09643892E+00
 9.41359752E-01 -1.29567052E+00 -2.09643892E+00
-9.41359748E-01 -1.29567052E+00 -2.09643893E+00
 4.58481793E-14  3.61668322E-14 -3.89315865E-15
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C2B3H5

```
SADDLE
C2B3H5 1,5-dicarbapentaborane(5) 9s/5p + 1d on B, C
       C    1          0.00000000     0.00000000     2.10213119
       B    2          0.00000000     2.06718430     0.00000000
       B    3         -1.79023412    -1.03359215     0.00000000
       B    4          1.79023412    -1.03359215     0.00000000
       C    5          0.00000000     0.00000000    -2.10213119
       H    6          0.00000000     0.00000000     4.12035855
       H    7          0.00000000     0.00000000    -4.12035855
       H    8          0.00000000     4.29422638     0.00000000
       H    9         -3.71890913    -2.14711319     0.00000000
       H   10          3.71890913    -2.14711319     0.00000000

SEARCHING BETWEEN ATOMS    1   2
NUMBER OF PERFORMED NEWTON ITERATION STEPS :    8

COORDINATES OF CRITICAL POINT
         X =   1.87272359E-17
         Y =   1.46474106E+00
         Z =   7.42225183E-01
         R =   1.64206108E+00

VECTORS FROM NUCLEI TO CRITICAL POINT
LENGTHS 'AND ANGLES MADE WITH PROJECTIONS ONTO YZ/XZ/XY PLANES OF MCS

NUCLEUS        LENGTH         YZ ANGLE         XZ ANGLE         XY ANGLE
  C    1   1.99870226E+00  0.00000000E+00  4.71255224E+01  4.28744776E+01
  B    2   9.55947737E-01  0.00000000E+00  3.90652636E+01  5.09347364E+01
  B    3   3.16188318E+00  3.44851323E+01  5.21986804E+01  1.35763852E+01
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  B     4   3.16188318E+00  3.44851323E+01  5.21986804E+01  1.35763852E+01
  C     5   3.19934830E+00  0.00000000E+00  2.72468360E+01  6.27531640E+01
  H     6   3.68201730E+00  0.00000000E+00  2.34413042E+01  6.65586958E+01
  H     7   5.07840398E+00  0.00000000E+00  1.67637148E+01  7.32362852E+01
  H     8   2.92521544E+00  0.00000000E+00  7.53014473E+01  1.46985527E+01
  H     9   5.23704826E+00  4.52443133E+01  4.36042819E+01  8.14772681E+00
  H    10   5.23704826E+00  4.52443133E+01  4.36042819E+01  8.14772681E+00

EIGENVALUES OF THE HESSIAN
   -2.94823635E-01   -2.92707295E-01    6.18077341E-01

THE ELLIPTICITY IS       0.00723

EIGENVECTORS OF THE HESSIAN
    1.00000000E+00    1.20320301E-17    1.05197339E-17
    1.59823199E-17   -7.52833767E-01   -6.58210695E-01
    0.00000000E+00   -6.58210695E-01    7.52833767E-01

EIGENVALUES OF THE STRESSIAN
   -1.49725598E-01   -1.33550045E-01   -7.44616066E-02

THE TRACE OF THE STRESSIAN IS  -0.35773725

EIGENVECTORS OF THE STRESSIAN
   -2.69523669E-19    1.00000000E+00    3.22076176E-19
    6.41766551E-01    4.19971512E-19   -7.66900055E-01
    7.66900055E-01    0.00000000E+00    6.41766551E-01

VALUES
RHO         1.6848115646E-01
GRAD        7.9867661918E-17
DEL2        3.0546411009E-02
G(X)        1.8268692594E-01
K(X)        1.7505032319E-01
L(X)       -7.6366027522E-03

COMPONENTS OF THE DIVERGENCE OF THE STRESSIAN
   -7.04924406E-13   -3.50363873E-01    4.49332826E-01

MAGNITUDE OF THE DIVERGENCE OF THE STRESSIAN        0.569785


SEARCHING BETWEEN ATOMS    1   6
NUMBER OF PERFORMED NEWTON ITERATION STEPS :    5

COORDINATES OF CRITICAL POINT
         X =   2.43344822E-19
         Y =  -5.70853206E-11
         Z =   3.32632144E+00
         R =   3.32632144E+00

VECTORS FROM NUCLEI TO CRITICAL POINT
```

LENGTHS 'AND ANGLES MADE WITH PROJECTIONS ONTO YZ/XZ/XY PLANES OF MCS

NUCLEUS		LENGTH	YZ ANGLE	XZ ANGLE	XY ANGLE
C	1	1.22419025E+00	0.00000000E+00	0.00000000E+00	9.00000000E+01
B	2	3.91633314E+00	0.00000000E+00	3.18594045E+01	5.81405955E+01
B	3	3.91633314E+00	2.72014205E+01	1.53026904E+01	5.81405955E+01
B	4	3.91633314E+00	2.72014205E+01	1.53026904E+01	5.81405955E+01
C	5	5.42845263E+00	0.00000000E+00	0.00000000E+00	9.00000000E+01
H	6	7.94037107E-01	0.00000000E+00	0.00000000E+00	9.00000000E+01
H	7	7.44667999E+00	0.00000000E+00	0.00000000E+00	9.00000000E+01
H	8	5.43183160E+00	0.00000000E+00	5.22385227E+01	3.77614773E+01
H	9	5.43183160E+00	4.32081693E+01	2.32836539E+01	3.77614774E+01
H	10	5.43183160E+00	4.32081693E+01	2.32836539E+01	3.77614774E+01

EIGENVALUES OF THE HESSIAN

-7.34351285E-01	-7.34351285E-01	2.81972209E-01

THE ELLIPTICITY IS 0.00000

EIGENVECTORS OF THE HESSIAN

-3.58554281E-09	1.00000000E+00	5.79614765E-19
-1.00000000E+00	-3.58554281E-09	1.61653283E-10
1.61653283E-10	0.00000000E+00	1.00000000E+00

EIGENVALUES OF THE STRESSIAN

-2.28197405E-01	-2.28197405E-01	6.38313871E-02

THE TRACE OF THE STRESSIAN IS -0.39256342

EIGENVECTORS OF THE STRESSIAN

1.00000000E+00	-1.36319505E-07	1.19773162E-18
-1.36319505E-07	-1.00000000E+00	8.78620871E-12
0.00000000E+00	8.78620871E-12	1.00000000E+00

VALUES

RHO	2.9333196071E-01
GRAD	2.3680085477E-16
DEL2	-1.1867303605E+00
G(X)	4.7940416436E-02
K(X)	3.4462300655E-01
L(X)	2.9668259012E-01

COMPONENTS OF THE DIVERGENCE OF THE STRESSIAN

2.72957094E-19	7.30075696E-12	1.51483131E-02

MAGNITUDE OF THE DIVERGENCE OF THE STRESSIAN 0.015148

SEARCHING BETWEEN ATOMS 2 8
NUMBER OF PERFORMED NEWTON ITERATION STEPS : 6

COORDINATES OF CRITICAL POINT

```
          X =  -8.83335577E-19
          Y =   3.01728191E+00
          Z =   1.43530899E-18
          R =   3.01728191E+00

VECTORS FROM NUCLEI TO CRITICAL POINT
LENGTHS 'AND ANGLES MADE WITH PROJECTIONS ONTO YZ/XZ/XY PLANES OF MCS

NUCLEUS          LENGTH          YZ ANGLE          XZ ANGLE          XY ANGLE
  C     1   3.67735580E+00  0.00000000E+00  5.51351899E+01  3.48648101E+01
  B     2   9.50097613E-01  0.00000000E+00  9.00000000E+01  0.00000000E+00
  B     3   4.42882816E+00  2.38424443E+01  6.61575557E+01  0.00000000E+00
  B     4   4.42882816E+00  2.38424443E+01  6.61575557E+01  0.00000000E+00
  C     5   3.67735580E+00  0.00000000E+00  5.51351899E+01  3.48648101E+01
  H     6   5.10698979E+00  0.00000000E+00  3.62148052E+01  5.37851948E+01
  H     7   5.10698979E+00  0.00000000E+00  3.62148052E+01  5.37851948E+01
  H     8   1.27694447E+00  0.00000000E+00  9.00000000E+01  0.00000000E+00
  H     9   6.36406017E+00  3.57578667E+01  5.42421333E+01  0.00000000E+00
  H    10   6.36406017E+00  3.57578667E+01  5.42421333E+01  0.00000000E+00

EIGENVALUES OF THE HESSIAN
   -4.55408536E-01   -3.86142349E-01    5.97663218E-01

THE ELLIPTICITY IS      0.17938

EIGENVECTORS OF THE HESSIAN
    1.00000000E+00    0.00000000E+00   -2.81830742E-17
   -2.81830742E-17    0.00000000E+00   -1.00000000E+00
    0.00000000E+00    1.00000000E+00    0.00000000E+00

EIGENVALUES OF THE STRESSIAN
   -1.44205193E-01   -1.24409603E-01   -9.06018247E-02

THE TRACE OF THE STRESSIAN IS  -0.35921662

EIGENVECTORS OF THE STRESSIAN
    0.00000000E+00    1.00000000E+00    3.40843324E-17
    0.00000000E+00    3.40843324E-17   -1.00000000E+00
    1.00000000E+00    0.00000000E+00    0.00000000E+00

VALUES
RHO        1.8540585174E-01
GRAD       1.3909041362E-17
DEL2      -2.4388766587E-01
G(X)       1.4912235181E-01
K(X)       2.1009426828E-01
L(X)       6.0971916468E-02

COMPONENTS OF THE DIVERGENCE OF THE STRESSIAN
    2.80623972E-14    6.40873469E-01   -6.44243066E-13

MAGNITUDE OF THE DIVERGENCE OF THE STRESSIAN        0.640873
```

SEARCHING BETWEEN ATOMS 2 3
NUMBER OF PERFORMED NEWTON ITERATION STEPS : 5

COORDINATES OF CRITICAL POINT
X = -7.13790147E-01
Y = 4.12106927E-01
Z = -6.05852400E-17
R = 8.24213864E-01

VECTORS FROM NUCLEI TO CRITICAL POINT
LENGTHS 'AND ANGLES MADE WITH PROJECTIONS ONTO YZ/XZ/XY PLANES OF MCS

NUCLEUS		LENGTH	YZ ANGLE	XZ ANGLE	XY ANGLE
C	1	2.25793800E+00	1.84287289E+01	1.05162696E+01	6.85906050E+01
B	2	1.80243654E+00	2.33292311E+01	6.66707689E+01	0.00000000E+00
B	3	1.80243653E+00	3.66707690E+01	5.33292310E+01	0.00000000E+00
B	4	2.89139817E+00	6.00000001E+01	2.99999999E+01	0.00000000E+00
C	5	2.25793800E+00	1.84287289E+01	1.05162696E+01	6.85906050E+01
H	6	4.20198561E+00	9.78024477E+00	5.62829264E+00	7.86881668E+01
H	7	4.20198561E+00	9.78024477E+00	5.62829264E+00	7.86881668E+01
H	8	3.94719493E+00	1.04183874E+01	7.95816126E+01	0.00000000E+00
H	9	3.94719492E+00	4.95816126E+01	4.04183874E+01	0.00000000E+00
H	10	5.11844024E+00	6.00000000E+01	3.00000000E+01	0.00000000E+00

EIGENVALUES OF THE HESSIAN
-8.18565905E-02 7.87543889E-02 1.79639622E-01

EIGENVECTORS OF THE HESSIAN
8.66025404E-01 4.99999999E-01 0.00000000E+00
-4.99999999E-01 8.66025404E-01 0.00000000E+00
0.00000000E+00 0.00000000E+00 1.00000000E+00

EIGENVALUES OF THE STRESSIAN
-5.31433685E-02 -5.00237823E-02 -2.12261783E-02

THE TRACE OF THE STRESSIAN IS -0.12439333

EIGENVECTORS OF THE STRESSIAN
8.66025403E-01 0.00000000E+00 5.00000002E-01
-5.00000002E-01 0.00000000E+00 8.66025403E-01
0.00000000E+00 1.00000000E+00 0.00000000E+00

VALUES
RHO 1.0031750220E-01
GRAD 4.4020412428E-17
DEL2 1.7653742064E-01
G(X) 8.4263842137E-02
K(X) 4.0129486976E-02
L(X) -4.4134355161E-02

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COMPONENTS OF THE DIVERGENCE OF THE STRESSIAN
    4.61394390E-04   -2.66385803E-04    5.83721483E-13

MAGNITUDE OF THE DIVERGENCE OF THE STRESSIAN        0.000533


STARTING COORDINATES
0.000000 0.000000 0.000000
NUMBER OF PERFORMED NEWTON ITERATION STEPS :    1

COORDINATES OF CRITICAL POINT
         X =  -7.75257164E-17
         Y =  -1.77055278E-09
         Z =  -5.34393430E-18
         R =   1.77055278E-09

VECTORS FROM NUCLEI TO CRITICAL POINT
LENGTHS 'AND ANGLES MADE WITH PROJECTIONS ONTO YZ/XZ/XY PLANES OF MCS

NUCLEUS        LENGTH         YZ ANGLE         XZ ANGLE         XY ANGLE
  C     1   2.10213119E+00  0.00000000E+00  0.00000000E+00  9.00000000E+01
  B     2   2.06718430E+00  0.00000000E+00  9.00000000E+01  0.00000000E+00
  B     3   2.06718430E+00  6.00000001E+01  2.99999999E+01  0.00000000E+00
  B     4   2.06718430E+00  6.00000001E+01  2.99999999E+01  0.00000000E+00
  C     5   2.10213119E+00  0.00000000E+00  0.00000000E+00  9.00000000E+01
  H     6   4.12035855E+00  0.00000000E+00  0.00000000E+00  9.00000000E+01
  H     7   4.12035855E+00  0.00000000E+00  0.00000000E+00  9.00000000E+01
  H     8   4.29422638E+00  0.00000000E+00  9.00000000E+01  0.00000000E+00
  H     9   4.29422638E+00  6.00000000E+01  3.00000000E+01  0.00000000E+00
  H    10   4.29422638E+00  6.00000000E+01  3.00000000E+01  0.00000000E+00

EIGENVALUES OF THE HESSIAN
    7.35263255E-02    7.35263264E-02    2.46656839E-01

EIGENVECTORS OF THE HESSIAN
    1.00000000E+00    1.80244300E-08    0.00000000E+00
    1.80244300E-08   -1.00000000E+00    0.00000000E+00
    0.00000000E+00    0.00000000E+00    1.00000000E+00

EIGENVALUES OF THE STRESSIAN
   -4.61051158E-02   -4.61051157E-02   -4.50664937E-02

THE TRACE OF THE STRESSIAN IS  -0.13727673

EIGENVECTORS OF THE STRESSIAN
    9.76782386E-08    1.00000000E+00    0.00000000E+00
   -1.00000000E+00    9.76782386E-08    0.00000000E+00
    0.00000000E+00    0.00000000E+00    1.00000000E+00

VALUES
RHO        9.0755576195E-02
GRAD       7.5740093603E-18
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```
DEL2        3.9370949067E-01
G(X)        1.1785204894E-01
K(X)        1.9424676267E-02
L(X)       -9.8427372669E-02

COMPONENTS OF THE DIVERGENCE OF THE STRESSIAN
    1.02952403E-13   -1.52214936E-10   -3.61115241E-14

MAGNITUDE OF THE DIVERGENCE OF THE STRESSIAN        0.000000


CRITICAL POINTS
 1.87272359E-17  1.46474106E+00  7.42225183E-01  C    1  B    2
-1.26850297E+00 -7.32370533E-01  7.42225186E-01  C    1  B    3
 1.26850297E+00 -7.32370533E-01  7.42225186E-01  C    1  B    4
 1.86867691E-17  1.46474106E+00 -7.42225183E-01  B    2  C    5
-1.26850297E+00 -7.32370533E-01 -7.42225186E-01  B    3  C    5
 1.26850297E+00 -7.32370533E-01 -7.42225186E-01  B    4  C    5
 2.43344822E-19 -5.70853206E-11  3.32632144E+00  C    1  H    6
-2.83440701E-19 -5.70853204E-11 -3.32632144E+00  C    5  H    7
-8.83335577E-19  3.01728191E+00  1.43530899E-18  B    2  H    8
-2.61304279E+00 -1.50864096E+00  9.62442530E-19  B    3  H    9
 2.61304279E+00 -1.50864096E+00  9.62442530E-19  B    4  H   10
-7.13790147E-01  4.12106927E-01 -6.05852400E-17  B    2  B    3 Ring
 1.86373285E-16 -8.24213862E-01  1.50833835E-16  B    3  B    4 Ring
 7.13790147E-01  4.12106927E-01 -5.93610112E-17  B    2  B    4 Ring
-7.75257164E-17 -1.77055278E-09 -5.34393430E-18                 Cage
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C2B4H6

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 SADDLE
C2B4H6 OPTIMIZATION USING VD SET(Renormalized); d=0.75, p=1.0725

       B    1        -2.29337481     0.00000000     0.00000000
       B    2         0.00000000    -2.29337481     0.00000000
       B    3         2.29337481     0.00000000     0.00000000
       B    4         0.00000000     2.29337481     0.00000000
       C    5         0.00000000     0.00000000    -2.04619646
       C    6         0.00000000     0.00000000     2.04619646
       H    7        -4.50801835     0.00000000     0.00000000
       H    8         0.00000000    -4.50801835     0.00000000
       H    9         4.50801835     0.00000000     0.00000000
       H   10         0.00000000     4.50801835     0.00000000
       H   11         0.00000000     0.00000000    -4.05778910
       H   12         0.00000000     0.00000000     4.05778910

 SEARCHING BETWEEN ATOMS    1   5
 NUMBER OF PERFORMED NEWTON ITERATION STEPS :    9
```

COORDINATES OF CRITICAL POINT
X = -1.53078077E+00
Y = -2.36670351E-12
Z = -6.55355620E-01
R = 1.66516688E+00

VECTORS FROM NUCLEI TO CRITICAL POINT
LENGTHS AND ANGLES MADE WITH PROJECTIONS ONTO YZ/XZ/XY PLANES OF MCS

NUCLEUS		LENGTH	YZ ANGLE	XZ ANGLE	XY ANGLE
B	1	1.00550518E+00	4.93250015E+01	0.00000000E+00	4.06749985E+01
B	2	2.83413986E+00	3.26919317E+01	5.40174585E+01	1.33698606E+01
B	3	3.87990423E+00	8.02755349E+01	0.00000000E+00	9.72446513E+00
B	4	2.83413986E+00	3.26919317E+01	5.40174585E+01	1.33698606E+01
C	5	2.06826691E+00	4.77422593E+01	0.00000000E+00	4.22577407E+01
C	6	3.10510441E+00	2.95371970E+01	0.00000000E+00	6.04628030E+01
H	7	3.04851351E+00	7.75859119E+01	0.00000000E+00	1.24140881E+01
H	8	4.80572681E+00	1.85742073E+01	6.97268336E+01	7.83783162E+00
H	9	6.07425598E+00	8.38062631E+01	0.00000000E+00	6.19373685E+00
H	10	4.80572681E+00	1.85742073E+01	6.97268336E+01	7.83783162E+00
H	11	3.73093063E+00	2.42233438E+01	0.00000000E+00	6.57766562E+01
H	12	4.95550430E+00	1.79932617E+01	0.00000000E+00	7.20067383E+01

EIGENVALUES OF THE HESSIAN
-2.07684763E-01 -8.25063605E-02 3.77505717E-01

THE ELLIPTICITY IS 1.51720

EIGENVECTORS OF THE HESSIAN
-7.03737198E-01 2.57780478E-12 -7.10460383E-01
-3.47545986E-12 -1.00000000E+00 -1.86099668E-13
-7.10460383E-01 2.33821129E-12 7.03737198E-01

EIGENVALUES OF THE STRESSIAN
-1.25828246E-01 -1.18794909E-01 -5.88652963E-02

THE TRACE OF THE STRESSIAN IS -0.30348845

EIGENVECTORS OF THE STRESSIAN
5.07183184E-12 6.05605989E-01 7.95764655E-01
1.00000000E+00 -3.07159897E-12 -4.03607287E-12
0.00000000E+00 7.95764655E-01 -6.05605989E-01

VALUES
RHO 1.4450790976E-01
GRAD 5.3016544898E-17
DEL2 8.7314593702E-02
G(X) 1.6265854974E-01
K(X) 1.4082990132E-01
L(X) -2.1828648426E-02

COMPONENTS OF THE DIVERGENCE OF THE STRESSIAN

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    3.12433583E-01   -3.78721848E-14   -2.85611289E-01

MAGNITUDE OF THE DIVERGENCE OF THE STRESSIAN        0.423307


SEARCHING BETWEEN ATOMS    1   2
NUMBER OF PERFORMED NEWTON ITERATION STEPS :   11

COORDINATES OF CRITICAL POINT
         X =  -1.09501230E+00
         Y =  -1.09501230E+00
         Z =  -6.76617222E-15
         R =   1.54858124E+00

VECTORS FROM NUCLEI TO CRITICAL POINT
LENGTHS AND ANGLES MADE WITH PROJECTIONS ONTO YZ/XZ/XY PLANES OF MCS

NUCLEUS         LENGTH         YZ ANGLE         XZ ANGLE         XY ANGLE
  B     1   1.62330670E+00   4.75802705E+01   4.24197295E+01   0.00000000E+00
  B     2   1.62330670E+00   4.24197295E+01   4.75802705E+01   0.00000000E+00
  B     3   3.56092953E+00   7.20909192E+01   1.79090808E+01   0.00000000E+00
  B     4   3.56092953E+00   1.79090809E+01   7.20909191E+01   0.00000000E+00
  C     5   2.56613013E+00   2.52594159E+01   2.52594159E+01   5.28812121E+01
  C     6   2.56613013E+00   2.52594159E+01   2.52594159E+01   5.28812121E+01
  H     7   3.58436357E+00   7.22119332E+01   1.77880668E+01   0.00000000E+00
  H     8   3.58436358E+00   1.77880668E+01   7.22119332E+01   0.00000000E+00
  H     9   5.70902832E+00   7.89419399E+01   1.10580601E+01   0.00000000E+00
  H    10   5.70902832E+00   1.10580601E+01   7.89419399E+01   0.00000000E+00
  H    11   4.34324260E+00   1.46029163E+01   1.46029163E+01   6.91115566E+01
  H    12   4.34324260E+00   1.46029163E+01   1.46029163E+01   6.91115566E+01

EIGENVALUES OF THE HESSIAN
   -1.38773222E-01   -2.36992734E-03    1.32792524E-02

THE ELLIPTICITY IS     57.55590

EIGENVECTORS OF THE HESSIAN
   -7.07106781E-01    0.00000000E+00    7.07106781E-01
   -7.07106781E-01    0.00000000E+00   -7.07106781E-01
    0.00000000E+00    1.00000000E+00    0.00000000E+00

EIGENVALUES OF THE STRESSIAN
   -7.40942983E-02   -6.95612793E-02   -1.16013351E-02

THE TRACE OF THE STRESSIAN IS  -0.15525691

EIGENVECTORS OF THE STRESSIAN
    0.00000000E+00   -7.07106781E-01    7.07106781E-01
    0.00000000E+00   -7.07106781E-01   -7.07106781E-01
    1.00000000E+00    0.00000000E+00    0.00000000E+00

VALUES
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RHO          1.2973497634E-01
GRAD         7.3340994713E-17
DEL2        -1.2786389669E-01
G(X)         6.1645469259E-02
K(X)         9.3611443431E-02
L(X)         3.1965974172E-02

COMPONENTS OF THE DIVERGENCE OF THE STRESSIAN
   -4.86462958E-03   -4.86462965E-03   -3.00183014E-13

MAGNITUDE OF THE DIVERGENCE OF THE STRESSIAN        0.006880


STARTING COORDINATES
1.000000 1.000000 1.000000
NUMBER OF PERFORMED NEWTON ITERATION STEPS :   18

COORDINATES OF CRITICAL POINT
         X =   1.08383200E+00
         Y =   1.08383200E+00
         Z =  -1.51189554E-01
         R =   1.54020839E+00

VECTORS FROM NUCLEI TO CRITICAL POINT
LENGTHS AND ANGLES MADE WITH PROJECTIONS ONTO YZ/XZ/XY PLANES OF MCS

NUCLEUS         LENGTH         YZ ANGLE         XZ ANGLE         XY ANGLE
  B     1   3.55008111E+00  7.20459667E+01  1.77760819E+01  2.44082987E+00
  B     2   3.55008111E+00  1.77760819E+01  7.20459667E+01  2.44082987E+00
  B     3   1.63111738E+00  4.78629768E+01  4.16418396E+01  5.31842516E+00
  B     4   1.63111738E+00  4.16418396E+01  4.78629768E+01  5.31842516E+00
  C     5   2.43730072E+00  2.64032113E+01  2.64032113E+01  5.10324536E+01
  C     6   2.67915824E+00  2.38624289E+01  2.38624289E+01  5.51025924E+01
  H     7   5.69792422E+00  7.89271464E+01  1.09653454E+01  1.52047304E+00
  H     8   5.69792422E+00  1.09653454E+01  7.89271464E+01  1.52047304E+00
  H     9   3.59480212E+00  7.22767828E+01  1.75477049E+01  2.41044678E+00
  H    10   3.59480212E+00  1.75477049E+01  7.22767828E+01  2.41044678E+00
  H    11   4.19653472E+00  1.49673356E+01  1.49673356E+01  6.85772422E+01
  H    12   4.47938443E+00  1.40022519E+01  1.40022519E+01  6.99900602E+01

EIGENVALUES OF THE HESSIAN
   -1.40640666E-01    4.68654325E-03    1.53691702E-02

EIGENVECTORS OF THE HESSIAN
   -6.92532071E-01   -1.42826225E-01    7.07106781E-01
   -6.92532071E-01   -1.42826224E-01   -7.07106781E-01
    2.01986783E-01   -9.79388247E-01   -5.42956593E-10

EIGENVALUES OF THE STRESSIAN
   -7.35245262E-02   -6.81619081E-02   -1.24640118E-02

THE TRACE OF THE STRESSIAN IS  -0.15415045
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 EIGENVECTORS OF THE STRESSIAN
    -2.59019997E-01   -6.57957933E-01    7.07106781E-01
    -2.59019997E-01   -6.57957933E-01   -7.07106781E-01
     9.30493032E-01   -3.66309592E-01    3.15095834E-11

 VALUES
 RHO         1.2972129025E-01
 GRAD        6.2338392969E-16
 DEL2       -1.2058495267E-01
 G(X)        6.2002103967E-02
 K(X)        9.2148342136E-02
 L(X)        3.0146238169E-02

 COMPONENTS OF THE DIVERGENCE OF THE STRESSIAN
     3.36010803E-03    3.36010809E-03   -1.55205474E-02

 MAGNITUDE OF THE DIVERGENCE OF THE STRESSIAN        0.016232


CAGE POINT
 NUMBER OF PERFORMED NEWTON ITERATION STEPS :    9

 COORDINATES OF CRITICAL POINT
          X =   2.43484309E-14
          Y =   4.37899556E-15
          Z =   2.77750885E-16
          R =   2.47406312E-14

 VECTORS FROM NUCLEI TO CRITICAL POINT
 LENGTHS AND ANGLES MADE WITH PROJECTIONS ONTO YZ/XZ/XY PLANES OF MCS

 NUCLEUS         LENGTH         YZ ANGLE         XZ ANGLE         XY ANGLE
   B    1   2.29337481E+00  9.00000000E+01  0.00000000E+00  0.00000000E+00
   B    2   2.29337481E+00  0.00000000E+00  9.00000000E+01  0.00000000E+00
   B    3   2.29337481E+00  9.00000000E+01  0.00000000E+00  0.00000000E+00
   B    4   2.29337481E+00  0.00000000E+00  9.00000000E+01  0.00000000E+00
   C    5   2.04619646E+00  0.00000000E+00  0.00000000E+00  9.00000000E+01
   C    6   2.04619646E+00  0.00000000E+00  0.00000000E+00  9.00000000E+01
   H    7   4.50801835E+00  9.00000000E+01  0.00000000E+00  0.00000000E+00
   H    8   4.50801835E+00  0.00000000E+00  9.00000000E+01  0.00000000E+00
   H    9   4.50801835E+00  9.00000000E+01  0.00000000E+00  0.00000000E+00
   H   10   4.50801835E+00  0.00000000E+00  9.00000000E+01  0.00000000E+00
   H   11   4.05778910E+00  0.00000000E+00  0.00000000E+00  9.00000000E+01
   H   12   4.05778910E+00  0.00000000E+00  0.00000000E+00  9.00000000E+01

 EIGENVALUES OF THE HESSIAN
     9.02323337E-02    9.02323337E-02    2.47763484E-01

 EIGENVECTORS OF THE HESSIAN
    -9.99962694E-01   -8.63774131E-03    0.00000000E+00
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    8.63774131E-03   -9.99962694E-01    0.00000000E+00
    0.00000000E+00    0.00000000E+00    1.00000000E+00

EIGENVALUES OF THE STRESSIAN
   -4.19213326E-02   -3.98720054E-02   -3.98720054E-02

THE TRACE OF THE STRESSIAN IS  -0.12166534

EIGENVECTORS OF THE STRESSIAN
    0.00000000E+00   -8.62676655E-03   -9.99962789E-01
    0.00000000E+00   -9.99962789E-01    8.62676655E-03
    1.00000000E+00    0.00000000E+00    0.00000000E+00

VALUES
RHO         7.8029161581E-02
GRAD        9.6854799924E-17
DEL2        4.2822815102E-01
G(X)        1.1436119059E-01
K(X)        7.3041528377E-03
L(X)       -1.0705703776E-01

COMPONENTS OF THE DIVERGENCE OF THE STRESSIAN
   -1.29231546E-14    3.34504286E-13    3.77284313E-14

MAGNITUDE OF THE DIVERGENCE OF THE STRESSIAN        0.000000


SEARCHING BETWEEN ATOMS    1   7
NUMBER OF PERFORMED NEWTON ITERATION STEPS :    6

COORDINATES OF CRITICAL POINT
         X =  -3.24465823E+00
         Y =  -8.08026747E-14
         Z =  -4.27335488E-19
         R =   3.24465823E+00

VECTORS FROM NUCLEI TO CRITICAL POINT
LENGTHS AND ANGLES MADE WITH PROJECTIONS ONTO YZ/XZ/XY PLANES OF MCS

NUCLEUS         LENGTH         YZ ANGLE         XZ ANGLE         XY ANGLE
  B    1   9.51283422E-01  9.00000000E+01  0.00000000E+00  0.00000000E+00
  B    2   3.97333299E+00  5.47467370E+01  3.52532630E+01  0.00000000E+00
  B    3   5.53803304E+00  9.00000000E+01  0.00000000E+00  0.00000000E+00
  B    4   3.97333299E+00  5.47467370E+01  3.52532630E+01  0.00000000E+00
  C    5   3.83597797E+00  5.77630164E+01  0.00000000E+00  3.22369836E+01
  C    6   3.83597797E+00  5.77630164E+01  0.00000000E+00  3.22369836E+01
  H    7   1.26336012E+00  9.00000000E+01  0.00000000E+00  0.00000000E+00
  H    8   5.55428092E+00  3.57445532E+01  5.42554468E+01  0.00000000E+00
  H    9   7.75267658E+00  9.00000000E+01  0.00000000E+00  0.00000000E+00
  H   10   5.55428092E+00  3.57445532E+01  5.42554468E+01  0.00000000E+00
  H   11   5.19552302E+00  3.86462622E+01  0.00000000E+00  5.13537378E+01
  H   12   5.19552302E+00  3.86462622E+01  0.00000000E+00  5.13537378E+01
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EIGENVALUES OF THE HESSIAN
   -4.28490090E-01   -3.96238469E-01    5.96447110E-01

THE ELLIPTICITY IS      0.08139

EIGENVECTORS OF THE HESSIAN
    0.00000000E+00    1.15359025E-13    1.00000000E+00
    0.00000000E+00    1.00000000E+00   -1.15248002E-13
    1.00000000E+00    0.00000000E+00    0.00000000E+00

EIGENVALUES OF THE STRESSIAN
   -1.36825327E-01   -1.32018153E-01   -8.96749215E-02

THE TRACE OF THE STRESSIAN IS  -0.35851840

EIGENVECTORS OF THE STRESSIAN
   -5.50924830E-13    0.00000000E+00    1.00000000E+00
    1.00000000E+00    0.00000000E+00    5.51035852E-13
    0.00000000E+00    1.00000000E+00    0.00000000E+00

VALUES
RHO         1.8573227336E-01
GRAD        6.2502255075E-17
DEL2       -2.2828144899E-01
G(X)        1.5072401953E-01
K(X)        2.0779438178E-01
L(X)        5.7070362248E-02

COMPONENTS OF THE DIVERGENCE OF THE STRESSIAN
   -6.41797297E-01    1.16336238E-12    3.95922484E-19

MAGNITUDE OF THE DIVERGENCE OF THE STRESSIAN        0.641797


SEARCHING BETWEEN ATOMS    6  12
NUMBER OF PERFORMED NEWTON ITERATION STEPS :    5

COORDINATES OF CRITICAL POINT
         X =  -6.08154996E-15
         Y =  -5.08729991E-16
         Z =   3.27322768E+00
         R =   3.27322768E+00

VECTORS FROM NUCLEI TO CRITICAL POINT
LENGTHS AND ANGLES MADE WITH PROJECTIONS ONTO YZ/XZ/XY PLANES OF MCS

NUCLEUS        LENGTH         YZ ANGLE         XZ ANGLE         XY ANGLE
  B    1   3.99669707E+00  3.50168645E+01  0.00000000E+00  5.49831355E+01
  B    2   3.99669707E+00  0.00000000E+00  3.50168645E+01  5.49831355E+01
  B    3   3.99669707E+00  3.50168645E+01  0.00000000E+00  5.49831355E+01
  B    4   3.99669707E+00  0.00000000E+00  3.50168645E+01  5.49831355E+01
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  C     5    5.31942414E+00  0.00000000E+00  0.00000000E+00  9.00000000E+01
  C     6    1.22703122E+00  0.00000000E+00  0.00000000E+00  9.00000000E+01
  H     7    5.57101866E+00  5.40169684E+01  0.00000000E+00  3.59830316E+01
  H     8    5.57101866E+00  0.00000000E+00  5.40169684E+01  3.59830316E+01
  H     9    5.57101866E+00  5.40169684E+01  0.00000000E+00  3.59830316E+01
  H    10    5.57101866E+00  0.00000000E+00  5.40169684E+01  3.59830316E+01
  H    11    7.33101678E+00  0.00000000E+00  0.00000000E+00  9.00000000E+01
  H    12    7.84561418E-01  0.00000000E+00  0.00000000E+00  9.00000000E+01

EIGENVALUES OF THE HESSIAN
   -7.39952872E-01   -7.39952872E-01    2.96990582E-01

THE ELLIPTICITY IS      0.00000

EIGENVECTORS OF THE HESSIAN
   -9.96349584E-01    8.53668938E-02    0.00000000E+00
   -8.53668938E-02   -9.96349584E-01    0.00000000E+00
    0.00000000E+00    0.00000000E+00    1.00000000E+00

EIGENVALUES OF THE STRESSIAN
   -2.36117848E-01   -2.36117848E-01    6.70426749E-02

THE TRACE OF THE STRESSIAN IS  -0.40519302

EIGENVECTORS OF THE STRESSIAN
    8.05314382E-02   -9.96752069E-01    0.00000000E+00
   -9.96752069E-01   -8.05314382E-02    0.00000000E+00
    0.00000000E+00    0.00000000E+00    1.00000000E+00

VALUES
RHO        2.9693012501E-01
GRAD       5.3777152674E-16
DEL2      -1.1829151610E+00
G(X)       5.4732115283E-02
K(X)       3.5046090554E-01
L(X)       2.9572879026E-01

COMPONENTS OF THE DIVERGENCE OF THE STRESSIAN
    2.01476718E-14    1.69684832E-15   -1.33982379E-02

MAGNITUDE OF THE DIVERGENCE OF THE STRESSIAN        0.013398

CRITICAL POINTS
-1.53078077E+00 -2.36670351E-12 -6.55355620E-01  B    1  C    5
-9.47087843E-12 -1.53078077E+00 -6.55355620E-01  B    2  C    5
 1.53078077E+00  2.36372938E-12 -6.55355620E-01  B    3  C    5
 9.45172833E-12  1.53078077E+00 -6.55355620E-01  B    4  C    5
-1.53078077E+00 -2.36641355E-12  6.55355620E-01  B    1  C    6
-9.47090793E-12 -1.53078077E+00  6.55355620E-01  B    2  C    6
 1.53078077E+00  2.36370115E-12  6.55355620E-01  B    3  C    6
 9.45173011E-12  1.53078077E+00  6.55355620E-01  B    4  C    6
-1.09501230E+00 -1.09501230E+00 -6.76617222E-15  B    1  B    2
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1.09501230E+00	-1.09501230E+00	-1.02557785E-14	B	2	B	3	
1.09501230E+00	1.09501230E+00	7.77702253E-15	B	3	B	4	
-1.09501230E+00	1.09501230E+00	3.99777517E-15	B	1	B	4	
1.08383200E+00	1.08383200E+00	-1.51189554E-01	3-4-5 Ring				
1.08383200E+00	-1.08383200E+00	-1.51189554E-01	2-3-5 Ring				
-1.08383200E+00	-1.08383200E+00	-1.51189554E-01	1-2-5 Ring				
-1.08383200E+00	1.08383200E+00	-1.51189554E-01	1-4-5 Ring				
1.08383200E+00	1.08383200E+00	1.51189554E-01	3-4-6 Ring				
2.43484309E-14	4.37899556E-15	2.77750885E-16	Cage				
1.08383200E+00	-1.08383200E+00	1.51189554E-01	2-3-6 Ring				
-1.08383200E+00	-1.08383200E+00	1.51189554E-01	1-2-6 Ring				
-1.08383200E+00	1.08383200E+00	1.51189554E-01	1-4-6 Ring				
-3.24465823E+00	-8.08026747E-14	-4.27335488E-19	B	1	H	7	
-2.67926030E-13	-3.24465823E+00	3.39340249E-19	B	2	H	8	
3.24465823E+00	8.08117219E-14	-3.26810012E-19	B	3	H	9	
2.68016767E-13	3.24465823E+00	-8.53978143E-19	B	4	H	10	
-6.08154996E-15	-5.08729991E-16	-3.27322768E+00	C	5	H	11	
-6.08154996E-15	-5.08729991E-16	3.27322768E+00	C	6	H	12	