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Theoretical analysis of the chemical bond in diatomic hydride molecules

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Iowa State University of Science and Technology
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THEORETICAL ANALYSIS OF THE CHEMICAL BOND
IN DIATOMIC HYDRIDE MOLECULES

by

Edgar Miller Layton, Jr.

A Dissertation Submitted to the
Graduate Faculty in Partial Fulfillment of
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DOCTOR OF PHILOSOPHY

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INTRODUCTION

During the past decade there have appeared an increasing number of publications concerned with the rigorous calculation of molecular electronic energies¹. The impetus for this type of work has come from three main sources: the organization of formal self-consistent-field (SCF) programs for calculating molecular energies (4), the availability of general evaluation formulae for many types of molecular integrals², and the utilization of large computers for the systematic handling of the large number of required arithmetic operations.

As the mechanics of complicated molecular computations have become more and more standardized and automatic, a problem of interpretation has arisen. There are only a limited number of experimental quantities that can be compared with the theoretical calculations, such as molecular dipole moment, various ionization potentials and spectral transitions. While the agreement with experimental values is sometimes encouraging, it is particularly lacking as regards the binding energy. Furthermore, the binding energy represents only the totality of all energy terms in the molecule, and

¹Summary reviews are presented in References 1, 2 and 3.

²Typical integral projects are those of the Tokyo group (5) or the Chicago group (6, 7, 8 and 9).

hence provides little insight as to the detailed nature of chemical binding in the system. The population analysis of Mulliken (10), although in itself not based on the energy, is a noteworthy attempt to fill this gap. By this method, a qualitative estimate is made of relations between the distribution of electrons and binding effects.

Quite recently an energy analysis, based on density matrix properties rather than a particular type of wave function, has been developed by Ruedenberg (11) which is designed to gauge the quality of the various molecular calculations and to trace the energetics of bond formation. It attempts to extract specified physical and "geographical" energy quantities from different molecules in a prescribed manner. It is conjectured that similarities will occur in the more refined calculations for analogous atomic environments. Moreover, it is predicted that a mathematical construct termed interference will reflect bonding ability. The extended partitioning contained in this theory has been designed in the hope of accounting for the energy balance in molecule formation from isolated atoms, as well as bringing out those peculiarities which give the individuality to a particular molecule.

In the present investigation this method of analysis is applied to the linear-combination-of-atomic-orbitals molecular orbital (LCAO MO) calculations of a series of

hydrides, recently published by Ransil (12). The results indicate that it is possible to extract, from calculations of this type, a substantial amount of significant energetic information in addition to the total binding energy. This information provides a quantitative basis for the reasoning about contributory factors to chemical binding.

In spite of a broad variation in electronic parameters, trends can be established. The predicted importance of constructive interference, contractive promotion and sharing penetration is verified. Moreover, sets of valence atomic hybrid orbitals are found which are of consequence for the binding process.

While it is recognized that the wave functions analyzed are far from perfect, they offer the attractive possibility of performing the analysis on a completely analogous series of systems for which equivalent calculations have been executed.

Separate reports present the results of this analysis applied to the water molecule (13) (prototype analysis), the hydrogen molecule ion (14), and some diatomic homonuclear systems (15).

DESCRIPTION OF MOLECULAR SYSTEMS

The molecular systems to be considered are the diatomic hydrides of lithium, boron, nitrogen (for two values of the internuclear distance) and fluorine. The wave functions chosen are the SCF LCAO MO wave functions based on a minimal set of atomic orbitals, recently obtained by Ransil (12).³ The MO's for each hydride are determined by the Hartree-Fock formalism (4) for three approximations concerning the orbital exponents. In the simplest case (denoted by SAO), the orbital exponents (ζ) are chosen by Slater's rules.⁴ In a more refined determination (BAO case), the ζ 's are found by a minimization of the separate atomic energies with respect to their ζ 's (17). In the third approach the ζ 's (BMAO) are specified by minimizing the molecular energy, at an experimental internuclear distance, with respect to all ζ 's. The first approximation is the crudest, but has shown itself to be remarkably effective for many purposes. The second method satisfies the virial theorem separately for each of the combining atoms. The last type of calculation is the most satisfactory of the three and it would satisfy the virial

³For the execution of our analysis, values of all integrals, between all the atomic orbitals involved, are required. We are grateful to Dr. Ransil for providing us with this considerable amount of data.

⁴See, for example, p. 40 of Reference 16.

theorem for the molecule if the calculation were carried out at the theoretically predicted equilibrium distance. Unfortunately, this has not been done and the virial theorem is not satisfied even for this third approach. It is felt that the violation of the virial relationship for all cases presents a serious source of error for the promotion states and therefore precludes a completely satisfactory interpretation of the latter (11). The molecular energy obtained in the last method is, however, an improvement over both the SAO and BAO cases, and some distinct variations do appear in the analytical partitioning, as will be seen later.

Table 1 presents the internuclear distances and ζ values for the hydride systems. The subscripts for the ζ 's refer to the standard AO's: 1s on the hydrogen atom, hereafter referred to as h, and 1s, 2s, 2p σ , 2p π , and 2p $\bar{\pi}$ on the other atom, hereafter denoted by k, s, σ , π , and $\bar{\pi}$ respectively. These entries will be discussed in the text when appropriate.

The significant results for both NH bond lengths are contained in the calculations on the NH' system. The identifying superscript for the particular bond length chosen will be dropped henceforth and the shorter bond length will be implied throughout the analysis.

All wave functions represent $^1\Sigma$ electronic states of the molecule, i.e., a closed-shell configuration. This con-

Table 1. Molecular constants for the hydride systems

System	R_{AB} (Angstrom units)	ζ_h	ζ_k	ζ_s	ζ_σ	ζ_π
LiH	SAO	1.5953 ₅	1.0	2.7	.65	.65
	BAO		1.0	2.6865	.6372	.6372
	BMAO		.9766	2.6909	.7075	.8449
BH	SAO	1.2325	1.0	4.7	1.3	1.3
	BAO		1.0	4.6794	1.3383	1.2106
	BMAO		1.1860	4.6805	1.2955	1.3168
NH'	SAO	1.045 ₅	1.0	6.7	1.95	1.95
	BAO		1.0	6.6652	1.9236	1.9170
	BMAO		1.4096	6.6703	1.9442	2.0959
NH''	SAO	1.1282	1.0	6.7	1.95	1.95
	BAO		1.0	6.6652	1.9236	1.9170
	BMAO		1.3574	6.6707	1.9307	2.0236
HF	SAO	.9171	1.0	8.7	2.6	2.6
	BAO		1.0	8.6501	2.5639	2.5498
	BMAO		1.3163	8.6533	2.5551	2.6693

figuration corresponds to the experimental ground state of each system except NH. Here, the ground state is $^3\Sigma$, so that the calculations represent one of two known excited states. The combining nitrogen atom, in fact, possesses no lone-pair σ electrons. The eight molecular electrons are distributed in the following fashion: two in the nitrogen K-shell, two in a bonding hybrid composed of the nitrogen s, σ and hydrogen h orbitals and two in each of the two nitrogen π orbitals. This circumstance leads to certain deviations in the NH analysis with respect to other members of the series.

NATURE OF THE ANALYSIS

A detailed description of the energy analysis is contained in the original article (11). A supplementary critical discussion of interpretative aspects is found in the report on the water molecule (13). The principal features of the analysis are briefly repeated here for the general diatomic system in order to facilitate an understanding of the details to be presented later.

The transition from isolated atoms to a molecule is considered purely from a conceptual viewpoint⁵. The molecular electronic energy of a diatomic molecule (under the Born-Oppenheimer approximation, excluding magnetic and relativistic effects) may be written⁶

$$E = z_A z_B / R_{AB} + \int d\tau \underline{h} \rho + \frac{1}{2} \iint d\tau_1 d\tau_2 \pi / r_{12} \quad , \quad (3.1)$$

where A and B index the atoms, 1 and 2 index the electrons, ρ and π are the first- and second-order matrices⁷, \underline{h} is the

⁵The allied problem of the kinetic mechanism of molecular formation is another question. An interesting, but formidable, project would be the solution of the SCF equations for selected internuclear distances (ranging from infinite separation to an equilibrium position) and application of the present analysis to the resulting set of wave functions.

⁶Atomic units are employed. The conversion factor for the atomic unit of length is 1 a.u. = 0.5291 Å and for energy is 1 a.u. = 27.2052 eV.

⁷See Reference 11 or 18 for a more complete treatment of density matrices and an expanded discussion of this equation.

one-electron operator including electronic kinetic energy and attractive nuclear-electronic potential energy and r_{12} is the interelectronic distance. The density matrices are given as expansions in terms of atomic orbitals;

$$\rho = \sum_r \sum_s p(r|s) \chi_r(1) \chi_s(1) \quad , \quad (3.2)$$

$$\pi = \sum_r \sum_{\bar{r}} \sum_s \sum_{\bar{s}} p(r\bar{r}|s\bar{s}) \chi_r(1) \chi_{\bar{r}}(1) \chi_s(2) \chi_{\bar{s}}(2) \quad , \quad (3.3)$$

where r , \bar{r} , s and \bar{s} index the AO's (from either atom, in any sequence), and the p 's are bond orders and pair-bond orders. The physical significance of the density matrices is established by the conservation relationships

$$\int d\tau \rho = N, \text{ the number of electrons } \quad , \quad (3.4)$$

$$\iint d\tau_1 d\tau_2 \pi = \frac{1}{2}N(N-1), \text{ the number of} \quad (3.5)$$

electron pairs.

The energy decomposition is effected by partitioning the density matrices, on the basis of considerations concerning physical interactions, and grouping these components with the corresponding integrals over the atomic orbitals. These energy fragments are then further apportioned to the appropriate atom, orbital or orbital pair along with a proportionate fraction of the nuclear-nuclear repulsion energy. All energy components remain separated in kinetic and potential

contributions in order to trace the energetic balance occurring in the molecular formation process. At all steps, conservation restrictions analogous to 3.4 and 3.5 are applied and corresponding electronic populations are determined. To emphasize the molecular role of the atomic orbitals, an initial intra-atomic diagonalization of the bond order matrix is performed which quantitatively defines inner (K-shell), lone-pair and bonding hybrid orbitals. These are labelled the valence atomic orbitals (VAO's).

The electron density is partitioned into three components, viz.,

$$\rho = \rho^{\text{CL}} + \rho^{\text{I}} = \rho^{\text{PR}} + \rho^{\text{T}} + \rho^{\text{I}} \quad (3.6)$$

where the superscript CL refers to the quasiclassical portion, I to the fraction participating in interference, PR to promotion and T to transfer. The interference is sufficiently novel and basic that further comment is warranted. This is that part of the electron density which distinguishes the quantum mechanical interactions in the process of bonding. Interference constitutes a spatial modification in the total electron density of the molecule without addition or deletion of charge density. The interference density between orbital a on atom A and orbital b on atom B is defined as

$$\langle \text{Aa}, \text{Bb} \rangle = (\text{Aa})(\text{Bb}) - \frac{1}{2} S_{\text{Aa}, \text{Bb}} [(\text{Aa})^2 + (\text{Bb})^2] \quad (3.7)$$

This function has the appearance of overlap dependence in both terms. The interference effects are postulated as being crucially associated with bonding behavior⁸

The electron pair-density partitioning is considerably more complex. Although it plays a substantial part in the ultimate analysis, its decomposition will only be intimated. Because of the Hartree-Fock SCF origin of the MO's, the pair density may be written

$$\pi(\underline{x}_1\underline{x}_2) = \rho(\underline{x}_1)\rho(\underline{x}_2) - \frac{1}{2} |\rho(\underline{x}_1|\underline{x}_2)|^2, \quad (3.8)$$

or
$$\pi(\underline{x}_1\underline{x}_2) = \rho(\underline{x}_1)\rho(\underline{x}_2) - \pi_x(\underline{x}_1, \underline{x}_2), \quad (3.9)$$

where the first term represents a coulombic interaction and the second term exhibits exchange character. These equations give the explicit spatial dependence of having one member of the electron pair at point x_1 and the second member at x_2 . Upon substitution of 3.6 into 3.9, and isolation of the various π_x components, energy contributions from the second order density matrix may similarly be incorporated into the orbital and orbital pair decomposition noted above. More accurately, the combined coulombic and exchange fragments are rearranged into interference and interference-free parts. The interference-free parts, furthermore, contain the contri-

⁸See Reference 14 for a lucid explanation of the extremely fundamental nature of interference.

butions attributed to both the intra-atomic and interatomic sharing penetration categories. (See Appendix, especially Equation A.5, ff.)

Since the energy value of interest is that arising from the formation of a molecule, a logical extraction of energy relating to the isolated atomic ground states is desirable. This is easily accomplished so that the total molecular binding energy may be arranged in the form,

$$E_{\text{MB}} = E - E^{\text{G}} = \begin{bmatrix} E^{\text{PRH}} \\ E^{\text{PRC}} \end{bmatrix} + \begin{bmatrix} E^{\text{QCN}} + E^{\text{SPN}} + E^{\text{SIN}} \\ E^{\text{QCT}} + E^{\text{SPT}} + E^{\text{SIT}} \end{bmatrix} \quad (3.10)$$

where the superscripts PRH and PRC denote energy effects attributable to hybridization and contractive (clustering) promotion;⁹ QC, SP, and SI refer to energy terms from quasi-classical electrostatic, sharing penetration and sharing interference both before (N) and after (T) charge transfer. As demonstrated in Reference 13, the promotion and quasi-classical terms may be considered as non-sharing phenomena arising at infinite separation and at the equilibrium inter-nuclear positions, respectively. The penetration and inter-

⁹The hybridization promotion is taken from the bond order density diagonalization, whereas clustering promotion is taken from the observed (14) increased electron density in the neighborhood of the nuclei. Alternatively, promotion may be described as angular (hybridization) and radial (contraction) density rearrangements.

ference terms may similarly be identified primarily with long-range and short-range sharing interactions.

All of the required arithmetic operations were executed on the Iowa State University Cyclone, an electrostatic memory digital computer patterned after the Illiac at the University of Illinois.

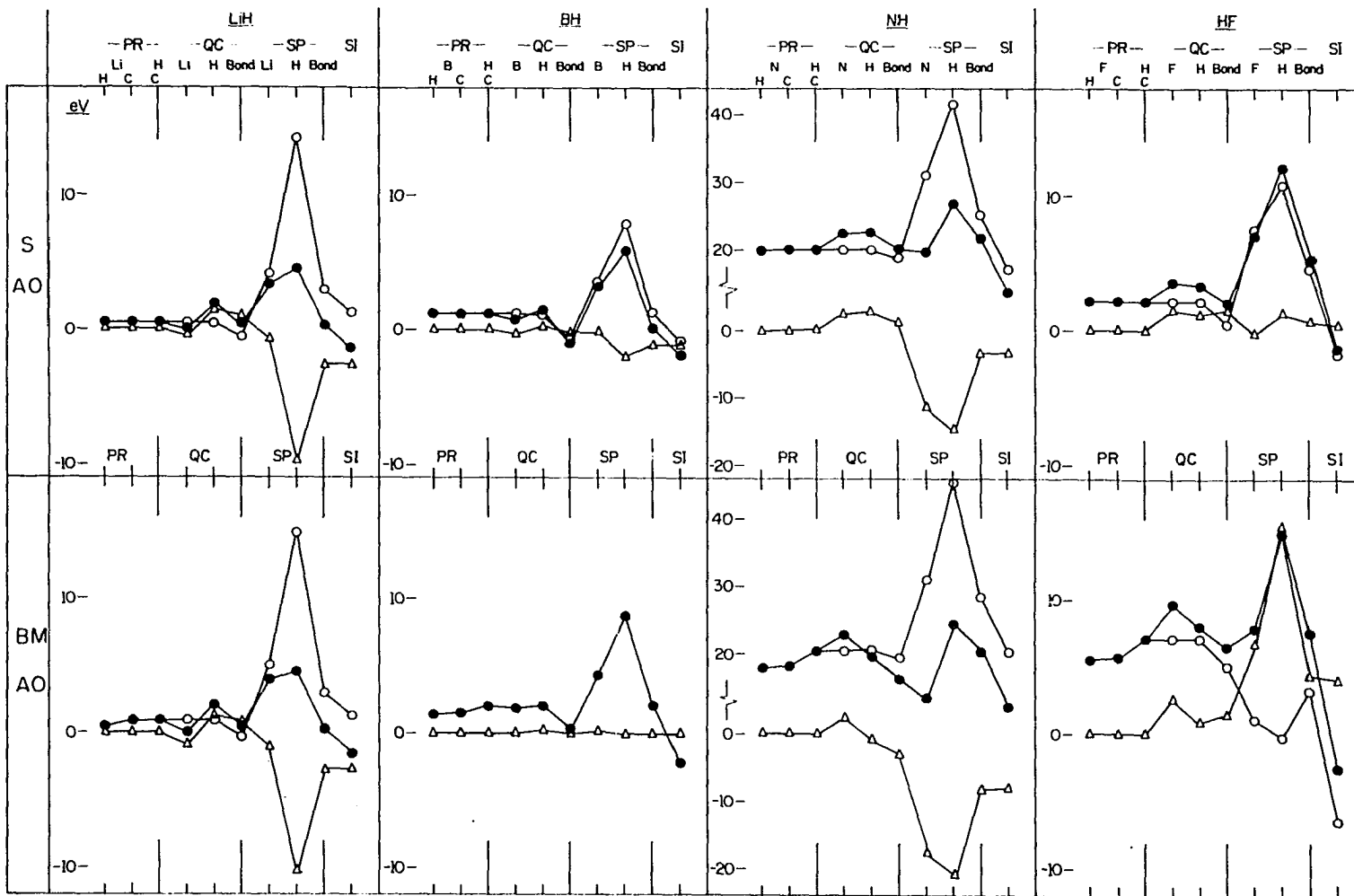
GROSS CHARACTERISTICS OF BINDING ENERGY PARTITIONING

Qualitative Concepts

The approach followed here recognizes five major kinds of energetic interactions in the constitution of the molecular binding energy; promotional effects, quasi-classical effects, sharing penetration effects, sharing interference effects and charge transfer effects. These main divisions are again subjected to a variety of further subdivisions which will be examined in detail in the further course of the discussion. It appears, however, most convenient to first focus attention on the gross effects. For each molecular analysis in the Appendix, they are listed in the first table labelled "Binding Energy Partitioning". A comparative graphical representation of the main features for all molecules, in the SAO and BMAO approximations, is given in Figure 1. (The BAO approximation essentially duplicates the SAO behavior here and throughout the remainder of the analysis except where specific reference is made to the contrary.)

Three curves are given for each system. One represents energetic effects before "charge transfer", a second due to the characteristic charge transfer contributions and the third for the total of these. Each curve is displayed

Figure 1. Theoretical molecular binding energy decomposition, by intra- and interatomic contributions, for SAO and BMAO approximations. PR stands for promotion, QC for quasiclassical, SP for sharing penetration and SI for sharing interference. Subdivisions indicate atomic or bond origin of contribution. Heavy atom indexes the first two promotion contributions, viz., hybridization (H) and contraction (C). Separate plots indicate total (●), neutral (○) and transfer (△) categories.



as a running total.¹⁰

The first three points represent promotion effects on the two atoms. Under the heavy atom symbol, two promotional mechanisms are distinguished: hybridization (denoted by H; hardly to be confused with the symbol for the hydrogen atom) and contraction (denoted by C; expansion being considered as negative contraction) which results from variations in the orbital exponents. The latter is the only kind of promotion for hydrogen and only applies to the BMAO approximation.

The next three points describe all those interactions which, somewhat casually, have been termed "quasiclassical" in the previous discussions of the present analysis (11, 13). In a more careful terminology, this name is a proper description only for the third value, which appears under the "bond" heading. This latter contains those interatomic potential energies which would result from a classical electrostatic energy calculation based on the electron density clouds before electron sharing. In contrast, the first two "quasiclassical" contributions arise entirely from charge transfer. They represent, for each atom, the intra-atomic energy changes resulting from the addition or loss of charge to the promotion state. For this reason, they will subsequently be denoted as intra-atomic charge-addition energies. The arbitrariness

¹⁰Note that the energy scale for NH is interrupted and more condensed, for reasons to be discussed below.

inherent in a definition of transfer, such as is used here, will further be discussed in later sections.

The subsequent three points represent the energetic contributions arising from sharing penetration. This section contains those electron repulsion effects which are specifically a consequence of the sharing of valence electrons between different atoms, as contrasted to those electron repulsions which are incorporated in the quasiclassical energy as shielding effects. These sharing penetration energies again have two intra-atomic portions and an interatomic portion.

The final category provides the interference energy, the most important of all, which is totally interatomic in character.

Quantitative Results

The justification of the present analysis lies in the fact that these enumerated categories exhibit characteristically similar behavior in each of the molecular systems analyzed. The only exception is the BMAO calculation of HF, where the separation of total effect into neutral and transfer parts does not follow the general pattern. A close examination indicates that a miscalculation must have occurred in the automatic calculation of this system, as will be

elaborated upon later, possibly connected with the inversion of some ill-conditioned matrices.

The "neutral plot" (i.e., contributions before transfer) always shows four typical features: a slight energy rise from hybridization and contraction promotion, a somewhat attractive¹¹ (1.0 to 3.0 eV) interatomic quasiclassical energy, a somewhat larger (typically 2 to 4 eV with NH having the extremes of 5 to 8 eV) bond-opposing rise due to sharing penetration and always the result of large intra-atomic effects dominating slightly smaller interatomic effects of opposite sign, and last, the significant energy drop furnished by interference. The last phenomenon must be considered as the source for covalent bonding, analogous to the traditional qualitative resonance stabilization in valence bond theory. It increases regularly with atomic number and so does the binding energy in the optimal BMAO case.

The transfer plot has no promotional contribution and a negligible contribution to interference. The overall effect is negative, indicating the advantage gained by the transfer of charge (excluding the SAO calculation of HF). As seen in

¹¹Here and in the following we denote a negative energy contribution as "attractive" and a positive energy contribution as "repulsive", i.e., attraction and repulsion are used synonymously with binding and anti-binding. This usage must not be confused with the attractive or repulsive quality of forces at the equilibrium or any other distance. Forces are not being discussed in the present investigation.

the next section, charge transfer is very small for the BMAO calculation of BH, relatively small in the SAO calculations of BH and HF, substantial for the SAO calculation of LiH and the BMAO calculations of LiH and HF, and very large for NH. This sequence is reflected in the transfer energies. In all cases, the electron addition energy is positive on the more electronegative partner of the molecule and negative on the other atom. Also, charge transfer invariably provides an attractive interatomic quasiclassical effect. The influence of transfer on the sharing penetration is generally opposite to that of the neutral effect. This is in agreement with the concept that charge transfer tends to suppress the degree of covalent electron sharing.

In all cases (except the disreputable BMAO approximation for HF), the major effects before transfer dominate the total values so that the plot of the totals is similar to, although not identical with, that of the neutral part.

Detailed physical explanations and interpretations for the qualitative behavior of the various aforementioned contributions have been given in the previous expositions of the present analysis (11, 13). The results reported in the preceding paragraphs are in complete agreement with the views and conjectures expressed in those discussions.

ELECTRONIC DISTRIBUTION

The second table of each molecular analysis, entitled "Density Partitioning for Valence AO's", gives information about the distribution of electrons in the individual molecules. The following conclusions can be drawn from the quantitative information contained in its sections.

Hybridization

The four molecules studied form two pairs: the hybrids of lithium and nitrogen show similarities as do those of boron and fluorine. The two sets differ significantly in the composition of the bonding and lone-pair $s-\sigma$ hybrid VAO's which are formed for each heavy atom. The reason is that for boron and fluorine, the total lone-pair occupations are approximately two electrons while in lithium and nitrogen, the lone-pair orbitals are unoccupied. Since the lone-pair orbital is empty in lithium and nitrogen, the bonding orbital hybridizes purely for its own benefit. The $s \rightarrow \sigma$ promotion energy, which must be weighed against binding effects, is entirely determined by the bonding orbital. Under these conditions the optimum binding orbital possesses mainly s character with a small but important admixture of σ character. Its orbital energy is, of course, much lower than that of the

unused lone-pair orbital which primarily has σ character. In boron and fluorine, on the other hand, the promotion energy of the lone-pair orbital cannot be ignored, but must be kept small for two reasons: it contains two electrons, as compared with one in the bonding orbital, and moreover, it does not benefit from energy lowering by binding effects. For these reasons, the composition of the lone-pair and bonding orbitals are reversed; the lone-pair is predominantly s, whereas the bonding orbital has to be content mainly with σ character and a token s admixture.

Contraction and Expansion

This hybridization picture, in conjunction with the ideas of contraction promotion developed in References 11 and 14, explains the changes in orbital exponents of the valence orbitals as given in Table 2. In lithium and nitrogen, the s

Table 2. $\Delta \zeta$ values, BMAO compared to BAO

Orbital	LiH	BH	NH	HF
k	.0044	.0011	.0051	.0032
s	.0703	-.0428	.0206	-.0088
σ	.2077	.1062	.1789	.1195
h	-.0234	.1860	.4096	.3163

and σ orbitals, both being involved only in constructive interference via a bonding orbital, experience a contractive promotion. In boron and fluorine, the σ orbital, the major contributor to the bonding orbital, still contracts whereas the s orbital, primarily associated with the lone-pair orbital, and hence involved in destructive interference, shows expansion.

The hydrogen orbital in BH, where charge transfer is negligible, shows a change in the orbital exponent about identical with that in the H₂ molecule, as discussed in Reference 11, indicating that it is characterized by contractive promotion arising from binding interference. In the other systems, transfer of charge is another effect which influences the hydrogen orbital exponent. In lithium, with additional charge transferred to the hydrogen, electron repulsion causes a considerable expansion sufficient to not only annihilate the bonding contraction but even forcing an expansion, as compared to the free atom. With nitrogen and fluorine, charge transfer is reversed and hence the bonding contraction on hydrogen is reinforced. Nitrogen, with the larger charge transfer, shows the bigger effect.

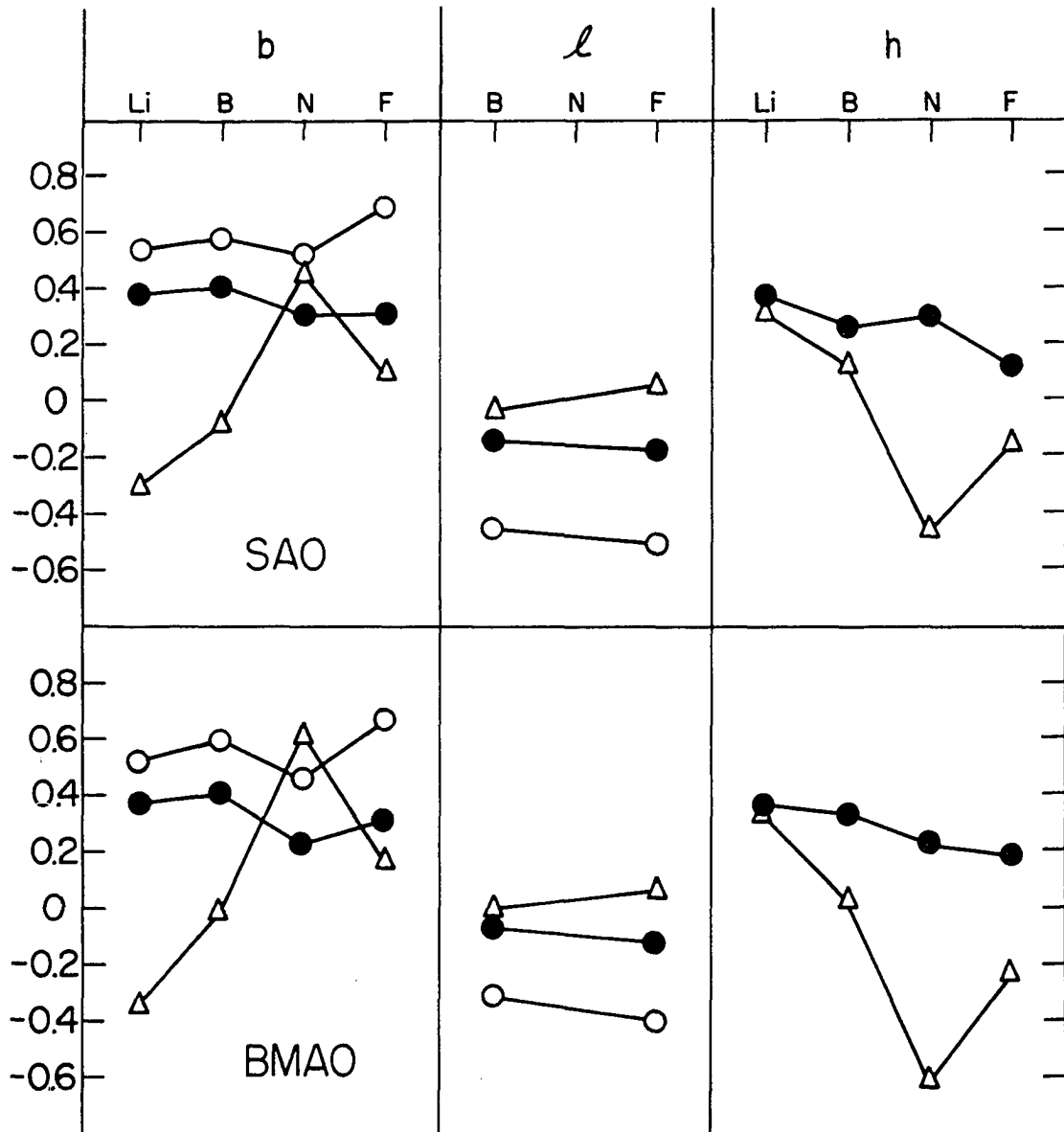
The π orbitals consistently experience an expansive promotion as seen in Table 1. Presumably the presence of the attractive hydrogen nucleus offers the paired π electrons assistance in relieving their repulsion energy.

Transfer Populations, Bond Orders,
and Valence Active Populations

Bonding and transfer properties of the orbital densities are displayed in Figure 2. Corresponding to the well known electronegativity behavior, charge transfer to the heavy atom increases from a negative value in lithium to positive values through fluorine, with that in boron effectively vanishing. The anomalously large nitrogen value is due to its previously mentioned peculiar promotion state where, because of the unoccupied low-energy lone-pair σ orbital, the bonding electrons are considerably less shielded from the nuclear attraction.

The valence active populations of the bonding orbitals follow the behavior of the bond order of these orbitals with the h orbital. These valence active populations are remarkably constant over the series while the bond orders increase slightly. The proper explanation of these trends is not simple. It is a fact that the interference energy, to be discussed below, markedly increases with atomic number. This is a consequence of the increasing steepness of the wave functions near the nuclei leading to an increasingly negative kinetic contribution to the interference energy regardless of overlap. This must be seen as the main reason for the increase in the experimental and theoretical (in the BMAO case) binding

Figure 2. Valence-orbital bond-orders (○), valence activities (●), and charge transfer populations (△) for SAO and BMAO approximations



energy. However, because of the concomitant increase in non-bonded interference repulsions arising from σ and π lone-pair electrons, the shortening of the bond lengths is still less than the shrinkage of the AO's caused by the increase in effective nuclear charge. For this reason, the overlap integral is found to decrease along the series. In spite of these considerable changes along the series, it seems as if there were a tendency to keep the valence active population approximately constant and that therefore the bond order, for the bonding orbital, shows a slight increase with atomic number.

The bond order for the lone-pair orbital is negative, corresponding to a non-bonded repulsion, and also increases in absolute value with atomic number. The conspicuously low value for the bonding orbital bond order in NH presumably reflects the fact that the effectiveness of interference (resonance stabilization) diminishes because there is a strong difference in electronegativities as is evidenced by the large charge transfer. This supposition is supported by the fact that the BMAO calculation, with considerably larger transfer, shows a further decrease in bond order.

It is intriguing that the bond orders for the inner-shell and lone-pair orbitals of all molecular systems, when plotted as a function of overlap, fall remarkably accurately on one curve which passes through the origin and is nearly

linear. These bond orders are negative (anti-binding character) and their overlap integrals have values less than 0.35. The bonding orbitals, on the other hand, with positive bond orders and overlap integrals greater than 0.44, show the different behavior implied above. Except for NH, a reciprocal dependence on overlap is seen; as the bond order decreases from 0.7 to 0.5, the overlap integral increases from 0.45 to 0.7.

PROMOTION

Basic Considerations

In order to find promotion energies, the ground state wave function must be assumed for each participating atom. These were chosen as follows.

The wave function for the hydrogen atom was taken as the $1s$ configuration with an effective charge of $\zeta = 1$.

For the other atoms, a single determinantal wave function corresponding to a ground state atomic configuration was selected. These were $1s^2 2s$ for lithium, $1s^2 2s^2 p\sigma$ for boron, $1s^2 2s^2 2p\sigma 2p\pi 2p\bar{\pi}$ for nitrogen and $1s^2 2s^2 2p\sigma 2p\pi^2 2p\bar{\pi}^2$ for fluorine. In the case of the SAO calculations, the Slater orbital exponents were also used in the ground state wave function. For the BAO and BMAO calculations, the ground state wave functions were assumed to have the BAO orbital exponents.

Mixing of orbitals was thus the only promotion effect for the SAO and BAO calculations and this will be referred to as hybridization promotion. In the case of the BMAO calculation, in addition to hybridization promotion, there were the promotion effects from the changes in orbital exponents. These will be referred to as contractive or expansive promotion.

The choice of the ground state is really impractical for the nitrogen atom, since an excited state of the NH molecule is undergoing analysis. More appropriate would have been a state of the configuration $1s^2 2s^2 2p^2 \bar{2p}^2$. Before this could be done, the computer being used underwent major alterations. The energy differences between the promotion state and ground state in nitrogen are too large to be understood purely as "promotion energies". Only after subtraction of the suitable excitation energy could this interpretation be reasonable. The K-shell is of course unaffected by this excitation and its promotional effects correlate with those of the other atoms.

The promotion energies are given in the intra-atomic tables for the individual molecular analyses. The essential results for all molecules are collected, for comparison, in Figure 3. In the promotional energies, the individualities of the particular isolated atoms become a rather important factor and hence the comparison of different atoms is more complicated than for the characteristically molecular energy effects.

Hybridization

The first observation is that the hybridization promotion energies are remarkably similar in all three

Figure 3. Summary of orbital promotion energy decompositions into kinetic and potential parts for SAO approximation (hybridization only) and BMAO approximation (hybridization and contraction). Negative contributions indicated by solid overscore.

COMPARISON OF PROMOTION ENERGIES

		LiH			BH			NH			HF		
		KIN	POT	TOT	KIN	POT	TOT	KIN	POT	TOT	KIN	POT	TOT
SAO HYBRID	k	.76	.98	.21	1.01	1.94	.93	1.54	2.59	1.05	.53	.80	.27
	s	1.83	3.68	1.85	4.04	10.63	6.59	57.12	56.10	1.01	8.27	13.16	4.89
	σ	1.95	3.06	1.11	2.41	6.86	4.45	49.92	52.22	2.30	10.68	13.47	2.79
	π							51.72	42.86	8.87	.00	.08	.08
TOTAL		.88	.36	.53	.62	1.83	1.22	5.13	25.21	20.07	1.88	.34	2.22
BMAO HYBRID	k	.94	1.22	.27	.40	.81	.41	1.65	2.86	1.20	.79	1.37	.57
	s	1.77	3.54	1.77	4.38	11.03	6.65	54.20	30.37	23.83	8.74	26.21	17.49
	σ	1.78	2.85	1.07	3.18	8.00	4.82	48.29	51.29	3.01	11.87	24.28	12.41
	π							49.99	31.21	18.78	.00	.03	.03
TOTAL		.96	.54	.43	.80	2.22	1.42	4.16	22.09	17.94	2.33	3.26	5.59
BMAO CONTR	k	.65	.63	.01	.28	.24	.04	1.89	1.58	.31	1.58	1.35	.23
	s	1.28	1.19	.10	4.57	4.20	.38	1.77	1.60	.17	2.06	1.92	.14
	σ	1.35	.99	.37	4.24	3.78	.45	.33	.46	.13	9.62	9.58	.04
	π							14.77	14.74	.03	7.32	7.34	.02
TOTAL		3.28	2.81	.48	.06	.18	.12	25.56	25.84	.28	5.50	5.67	.17
h		.63	.64	.01	5.53	5.06	.47	13.43	11.14	2.28	9.97	8.61	1.36
TOTAL		2.65	2.17	.49	5.47	4.88	.59	12.13	14.70	2.56	4.47	2.94	1.53
BMAO HY + CO	k	1.59	1.85	.26	.68	1.05	.37	.24	1.28	1.51	.79	.02	.80
	s	.49	2.35	1.87	8.95	15.23	6.27	52.43	28.77	23.66	10.80	28.13	17.35
	σ	3.13	3.84	.70	7.42	11.78	4.37	47.96	50.83	2.88	21.49	33.86	12.37
	π							35.22	16.47	18.75	7.32	7.31	.01
TOTAL		4.24	3.34	.90	.86	2.39	1.54	29.72	47.94	18.21	3.16	8.93	5.76
h		.63	.64	.01	5.53	5.06	.47	13.43	11.14	2.28	9.97	8.61	1.36
TOTAL		3.61	2.70	.91	4.67	2.67	2.01	16.29	36.80	20.49	6.81	.32	7.12

approximations. For this reason, the BAO values are omitted. In general, removal of electronic charge from an orbital results in a decrease of kinetic energy and an increase in potential energy. The latter tends to be the larger effect (although not twice as large since we are concerned with shielded nuclear attraction for which the virial theorem does not hold) and hence the total energy contributions from that orbital is raised. Addition of charge to an orbital has the opposite effect.

The simplest example is the promotion (approximately 0.35 electron) from the s orbital to the s- σ hybrid orbital in lithium. Due to the nature of the orbitals, the energy decrease provided by the σ contribution does not compensate for the increase of the s contribution. A similar effect is observed in boron. The promotion charge is much smaller (ca. 0.1 electron) since the two lone-pair electrons still mainly occupy the s orbital. Nevertheless, the energy effect is larger than in lithium because of the larger effective nuclear charge of the orbital. Fluorine shows about the same promotion population as boron and the kinetic and potential energy contributions are correspondingly larger. The total orbital contribution to the promotion energy is smaller, however, since the difference between kinetic (proportional to ζ^2) and potential (proportional to ζ) contributions is less.

The values obtained for the nitrogen atom behave differently since here the change in electronic correlation becomes a dominant factor. In the ground state there are two paired s electrons and three unpaired π electrons while in the excited state there are an unpaired electron in the s- σ hybrid and four paired electrons in the π orbitals. Thus, the contribution of the s orbital decreases because of unpairing, the contribution from the σ orbital increases because of depopulation and the contribution from the π orbitals are positive because of pairing.

The non-negligible promotion contributions of the K-shell are due to two circumstances; the K-admixture to the valence hybrid orbitals and the deviation of the q^N 's from 2.000, the latter resulting from our definitions of charge transfer populations. In this context it is interesting to observe that boron and fluorine, where the lone-pair orbital is occupied and therefore has primarily s character, exhibit a not insubstantial k admixture to the lone-pair VAO.

Contraction and Expansion

The total promotional energies from orbital contraction and expansion are so small that the changes in orbital exponent might appear inconsequential to a superficial examination. The separate potential and kinetic

fragments indicate, however, that this would be a serious misjudgment. In all cases, the contraction or expansion gives rise to a substantial reapportioning of the kinetic and the potential energy parts.

The σ orbitals, primarily involved in bonding, always show an increase in kinetic and a slightly smaller decrease in potential energy. The same is shown by the s orbital wherever it is involved in bonding to a significant extent, specifically in lithium and nitrogen. Contrariwise, the s orbital shows a decrease in kinetic and an increase in potential in boron and fluorine where it is involved in anti-binding and, as mentioned earlier, shows an expansive promotion. The k orbital always contributes a not insubstantial decrease in potential and increase in kinetic energy similar to a binding orbital. Perhaps this arises because of the K-admixture to the bonding orbitals; more likely however, constructive interference favors a shift of intra-atomic energy from the potential to the kinetic category not only for those orbitals which produce constructive interference but also for others unless there exist strong opposing factors.

The hydrogen orbitals also show the characteristic shift of energy from potential to kinetic associated with the contractive promotion arising from constructive binding interference. The one exception is in LiH where charge transfer has forced the expansive promotion previously discussed.

The total LiH molecule significantly shows, however, a lowering of the potential and an increase of kinetic energy (considerably larger in absolute magnitude than the calculated binding energy) which must be assigned to an overall contractive promotion. The same is found in all other systems if the subtotal, excluding π orbital contributions, is considered. These results demonstrate the intrinsic connection between potential lowering, contractive promotion and covalent binding which has been repeatedly emphasized (11, 13, 14). There can be no question that the fulfillment of the virial theorem, if the calculations were to be carried out at the theoretical equilibrium internuclear distance, would also be brought about by the appropriate amount of contractive promotion.

For reasons discussed earlier, all π orbitals experience an expansive promotion. Correspondingly, their kinetic energy decreases and their potential energy increases. In fluorine, the effect of the π orbitals is insufficient to upset the total molecular balance established by the bonding σ framework. In nitrogen, the π orbitals do effect a reversal of the σ balance but the significance of this is hard to trace since we are dealing with an excited molecular state and moreover, with an ill-suited atomic reference state.

Total Promotion

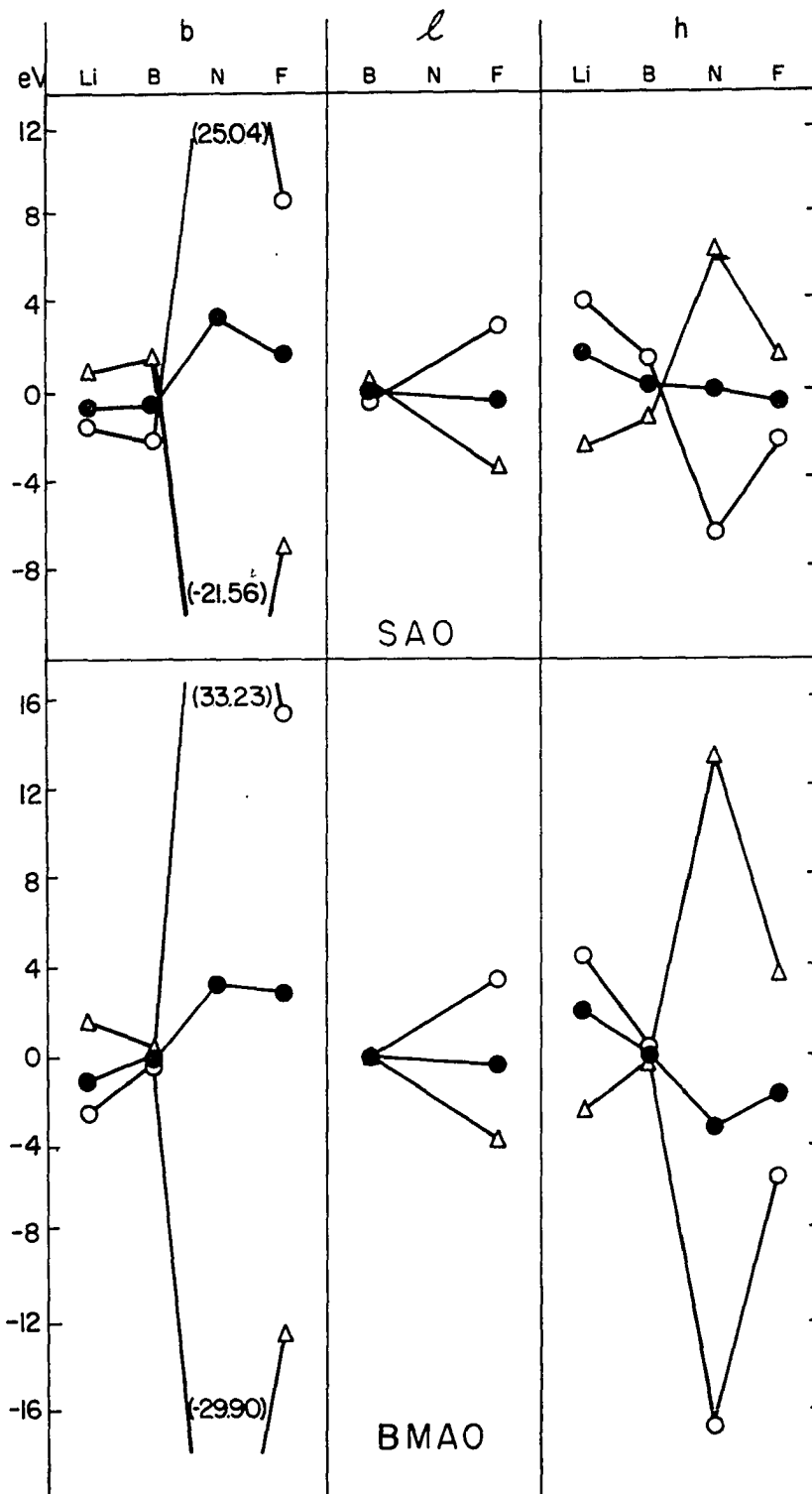
It is interesting to observe that the sum of hybridization and contraction promotion (except for nitrogen with its anomalous hybridization and π expansion) always leads to a positive and regularly increasing kinetic contribution. The potential contribution shows the same negative value for lithium and boron, both of which are free of π electrons. The slightly positive fluorine potential value may be spurious because the potential energies of the hybridization promotion are presumably affected by the suspect behavior of sharing penetration, resulting from the aforementioned miscalculation, in the BMAO analysis for this molecule (see below).

INTRA-ATOMIC CHARGE ADDITION

The contributions discussed in this section are taken from the first column, termed QCT, in the tables of the intra-atomic decompositions in the molecular analyses. In the present method, the charge addition energies displayed in Figure 4 play a role comparable to that played in semi-empirical thinking by the ionization potentials and electron affinity of the promoted state. The numerical values are very different, however, for two reasons. First, the addition energies used here are those calculated for the transferred charge with a one-electron hamiltonian containing an effective potential of the neutral promoted atom. Second, it does not contain the intra-atomic energy changes which charge transfer causes by modifying the sharing situation. As a result, the addition energies always are positive if charge is added and negative if charge is lost.

Within this context the charge addition energies show great regularity. In all cases the bonding orbital contributes the major effect. It closely parallels the charge transfer populations shown in Figure 2. The addition energy is negative for lithium, vanishing for boron, positive for fluorine and exceptionally large and positive for nitrogen. Invariably there is a substantial cancellation between kinetic and potential parts with the kinetic part determining the

Figure 4. Intra-atomic valence-orbital charge-addition energy contributions for SAO and BMAO approximations. ●, total; ○, kinetic; Δ, potential



final value. The effect on the hydrogen is generally opposite to that on the heavy atom. The enormous values for the kinetic and potential energy parts for nitrogen (compared with those for the other atoms) clearly exhibit the unusual character of this molecule in the present series in that here the heavy atom has a low-lying empty orbital. Since there is a very large cancellation between kinetic and potential energy in nitrogen, it is remarkable that the values of the totals still closely reflect the transfer populations.

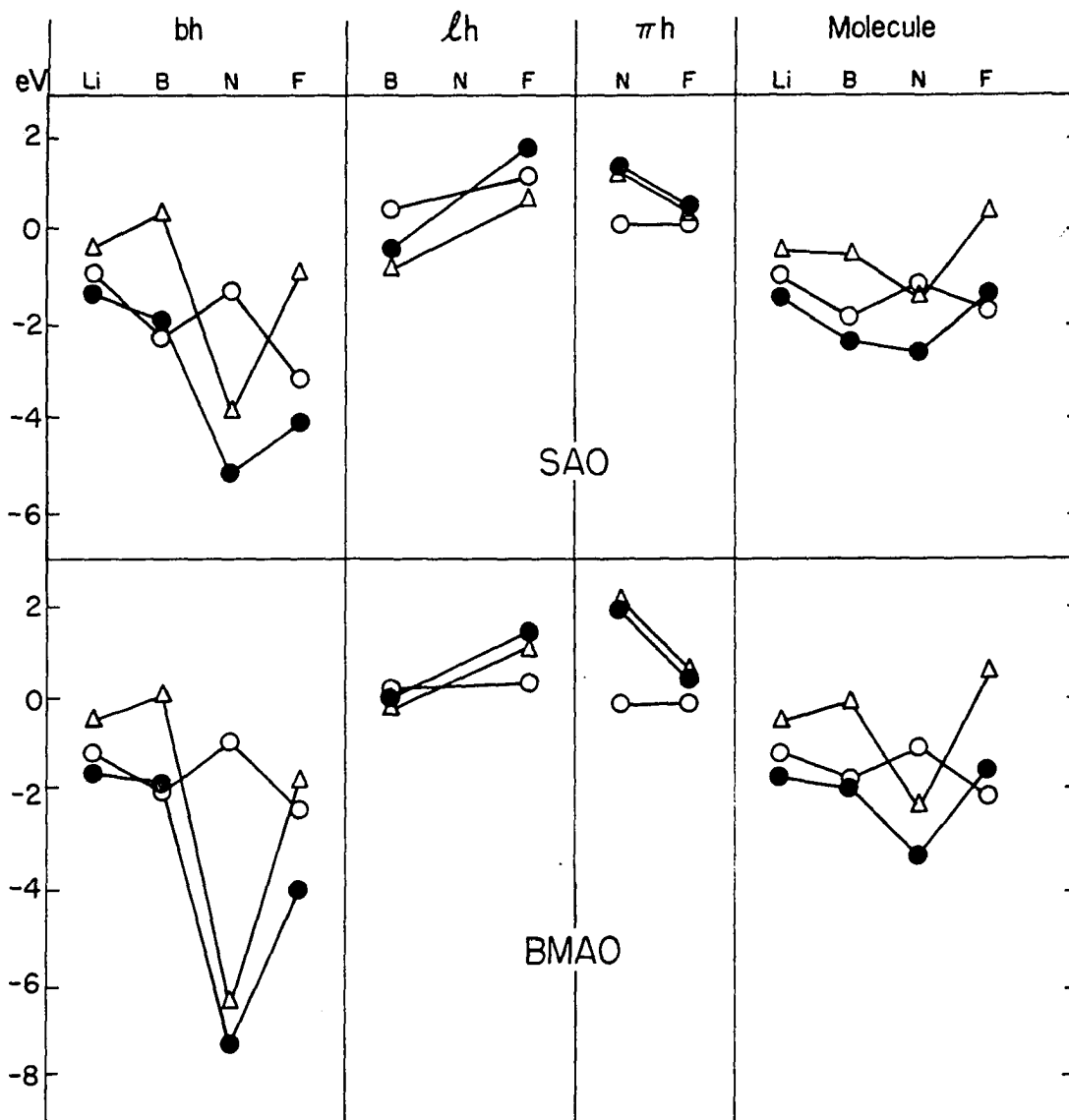
QUASICLASSICAL INTERATOMIC ENERGIES

The interatomic quasiclassical electrostatic energies between orbital pairs are given in the first three columns of the table of interatomic contributions in the molecular analyses. The significant values are plotted in Figure 5. The total interaction "before transfer" is broken down according to interactions between the neutral hydrogen atom and fragments of the neutral heavy atom which are associated with its valence orbitals. Such a neutral orbital fragment consists of the promotion density of that orbital plus an exactly counterbalancing fraction of the positive nucleus. The contribution of one orbital pair to the total transfer energy is the sum of three interactions: the interaction between the neutral orbital fragment of one partner with the transfer density of the other partner, the corresponding interaction between the neutral orbital fragment of the second partner with the transfer density of the first, and the interaction between the transfer densities of the orbitals.

bh Orbital Pair

The interactions between the binding heavy-atom orbital and the hydrogen orbital represents the dominant molecular effect. Consider first the interaction between the

Figure 5. Interatomic quasiclassical energy contributions, and decomposition by valence-orbital pairs, for SAO and BMAO approximations. ●, total; ○, neutral; △, transfer.



neutral hydrogen atom and that part of the neutral heavy atom which we ascribe to the bonding orbital. In all cases, this neutral bonding-orbital fragment is attracted by the neutral hydrogen atom, because the latter attracts the closer, though diffuse, electronic charge of the bonding orbital more strongly than it repels the more distant nuclear fraction associated with the bonding orbital to form the neutral fragment. It is not surprising that the σ type bonding orbitals of boron and fluorine, approaching closer to the hydrogen atom, lead to a stronger shielded nuclear attraction than the s type orbitals of lithium and nitrogen. Thus, hybridization differences explain the saw-tooth appearance of the neutral bh interaction in Figure 5. The slight overall negative slope in the SAO case is presumably caused by the decrease in internuclear distance, although this effect is certainly moderated by the increasing shielding of the orbitals because of their shrinking with atomic number. In the BMAO case, this moderation is accentuated by the contractive promotion previously discussed so that, aside from the hybridization variations, the neutral interatomic interactions essentially remain constant over the series.

Except for nitrogen, the transfer effects of the bh pair are smaller than the neutral effects just discussed. This is so because of the small amounts of charge involved in the transfer process. The quasiclassical transfer energies

are negative except for boron. Their variations follow very closely the absolute values of the transfer populations, because the dominant contribution is the attraction between the transfer populations of the two orbitals. The deviation of boron arises because, here, charge transfer is so small that the other two contributions become important, namely the interaction between the transfer population in the heavy-atom bonding orbital with the neutral hydrogen atom and the interaction of the transfer population on the hydrogen atom with the neutral bonding orbital fragment of the heavy atom. Both are repulsive in lithium and boron and attractive in nitrogen and fluorine; the former because the neutral hydrogen still attracts negative charge, the latter because the interaction of the hydrogen transfer population with the charge in the bonding orbital is dominant over that with the more distant nuclear fraction (see the similar discussion for the neutral quasiclassical energies). The latter contribution is, of course, the smaller effect since it arises from two diffuse charges. In boron, these two positive contributions overcome the attraction between the diminutive transfer populations.

For the reasons stated, the variations in transfer interactions follow a characteristically different pattern than those of the neutral energies. The totals show a rather smooth energy decrease along the series except for the

prominent deviation of the abnormal nitrogen charge transfer.

lh Orbital Pair

Consider now the lone-pair of the heavy atom. The interaction between the neutral lone-pair fragment and the neutral hydrogen atom is positive because the lone-pair orbital cannot sufficiently shield the repulsion between its associated nuclear fraction and the hydrogen atom. This repulsion increases with atomic number for the SAO case and is constant for the BMAO case, that is, it behaves like the absolute value of the quasiclassical neutral attraction found for the bh orbital pair, and indeed, for the same reasons.

In contrast to the situation for the bonding orbital, the transfer portions follow the transfer populations of the heavy atom, with their given signs. The explanation is that the major contribution is now the interaction between the transfer population on hydrogen and the neutral lone-pair fragment of the heavy atom which, because of insufficient shielding, is in turn dominated by the interaction with the positive nuclear fraction of the heavy atom. Thus boron, where electrons move to the hydrogen, exhibits attraction and fluorine, with a positive hole on the hydrogen, displays repulsion. The other two contributions to transfer energy involve, on the heavy atom, only the transfer population of

the lone-pair orbital. Because the transfer populations of the lone-pair are rather small and because the lone-pair orbital is more distant from the hydrogen atom, these contributions are considerably smaller than the one discussed first which involves the heavy atom nucleus.

π h Orbital Pair

For the π orbitals in nitrogen and fluorine, the transfer energies consist only of the interaction between the hydrogen transfer population with the neutral π orbital fragment of the heavy atom. Again, the repulsion of the positive nuclear part of the fragment is insufficiently counterbalanced by the attraction of the π electrons giving positive transfer energy, obviously larger in nitrogen than in fluorine. In fluorine the π quasiclassical energies are lower than those of the σ lone-pair since shielding of the latter is clearly less than that of the former.

Total

Thus, it is evident that the repulsive quasiclassical energy contributions of the σ and π lone-pair orbitals temper the attractive contributions of the bonding orbital. The total molecular values for the quasiclassical energies still

show the principal features of the bh interaction but to a more moderate degree. The neutral values, while remaining remarkably constant over the series, reflect the effect of hybridization. For the transfer values, the influence of the lone-pair interactions is more consequential and in fluorine even leads to a transfer repulsion. It is noteworthy that in both calculations, cancellation of effects from various orbital pairs leaves the total molecular values all negative and confined to a remarkably narrow range.

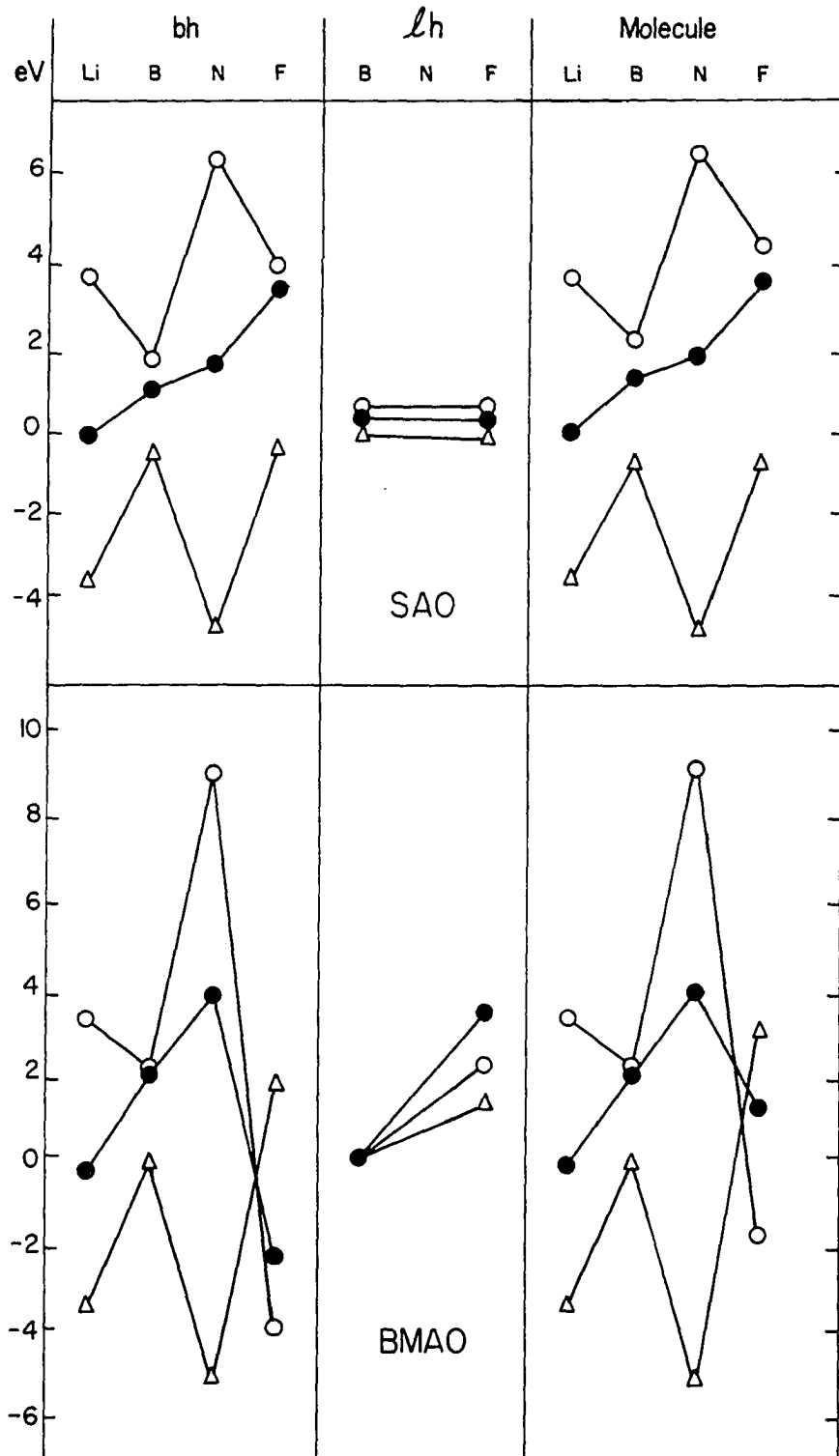
SHARING PENETRATION ENERGIES

The energy values arising from sharing penetration are given in the tables of intra-atomic and interatomic contributions for the molecular analyses. Since penetration is a single phenomenon, both intra- and interatomic contributions must be considered simultaneously and hence the sum of both is given for each orbital pair in Figure 6.¹² In discussing this figure, one must remember that the construction of sharing penetration energies is the most questionable part of the whole analysis. It is therefore gratifying that the results show a reasonable consistency.

In all cases, except one, the sharing penetration energy is positive in complete agreement with the general ideas of the analysis, namely that sharing increases the penetration of electrons from different atoms and hence leads to a net increase of electronic repulsion. The exception is lithium where the sharing penetration energy is slightly negative for which there is no obvious explanation at present. Note that these contributions are very small, however. In

¹²In arriving at these figures, it was necessary to partition the intra-atomic hydrogen contribution according to the heavy atom orbital. For the neutral sharing penetration, this pro-rating was done by use of the interatomic values of the exchange pair-population contributions, which table is given. For the transfer sharing penetration, the separation was carried out according to the orbital charge transfer populations.

Figure 6. Molecular sharing penetration energy contributions and decomposition by valence-orbital pairs for SAO and BMAO approximations. ●, total; ○, neutral; Δ, transfer.



the BMAO case of fluorine, which shows a large negative sharing penetration energy, there appears to have occurred a mechanical computational error. This is indicated, in the table showing the exchange contributions to the pair populations, by the fact that the total interatomic value of the l_h orbital pair (-0.062) is divided into unreasonable neutral (0.193) and transfer (-0.254) portions. Most likely the matrix inversion required for the transfer penetration effects was disturbed by ill-conditioning.

The lone-pair orbital, with the smaller binding interactions, shows the smallest penetration energies, by far. For the b_h orbital pair, the total sharing penetration energy increases very regularly from lithium to fluorine. This increase is entirely attributable to the shrinkage of the heavy atom orbitals whose intra-atomic contributions are the dominant terms. This regularity is not entirely a trivial consequence of the manner in which these numbers were obtained since the total values were calculated by adding together the parts due to transfer and those from neutral penetration, both of which are computed separately. The transfer contributions essentially follow the absolute value of the transfer populations; the neutral contributions seem to reflect the hybridization modulation encountered repeatedly, although it is difficult to trace a theoretical connection between the two.

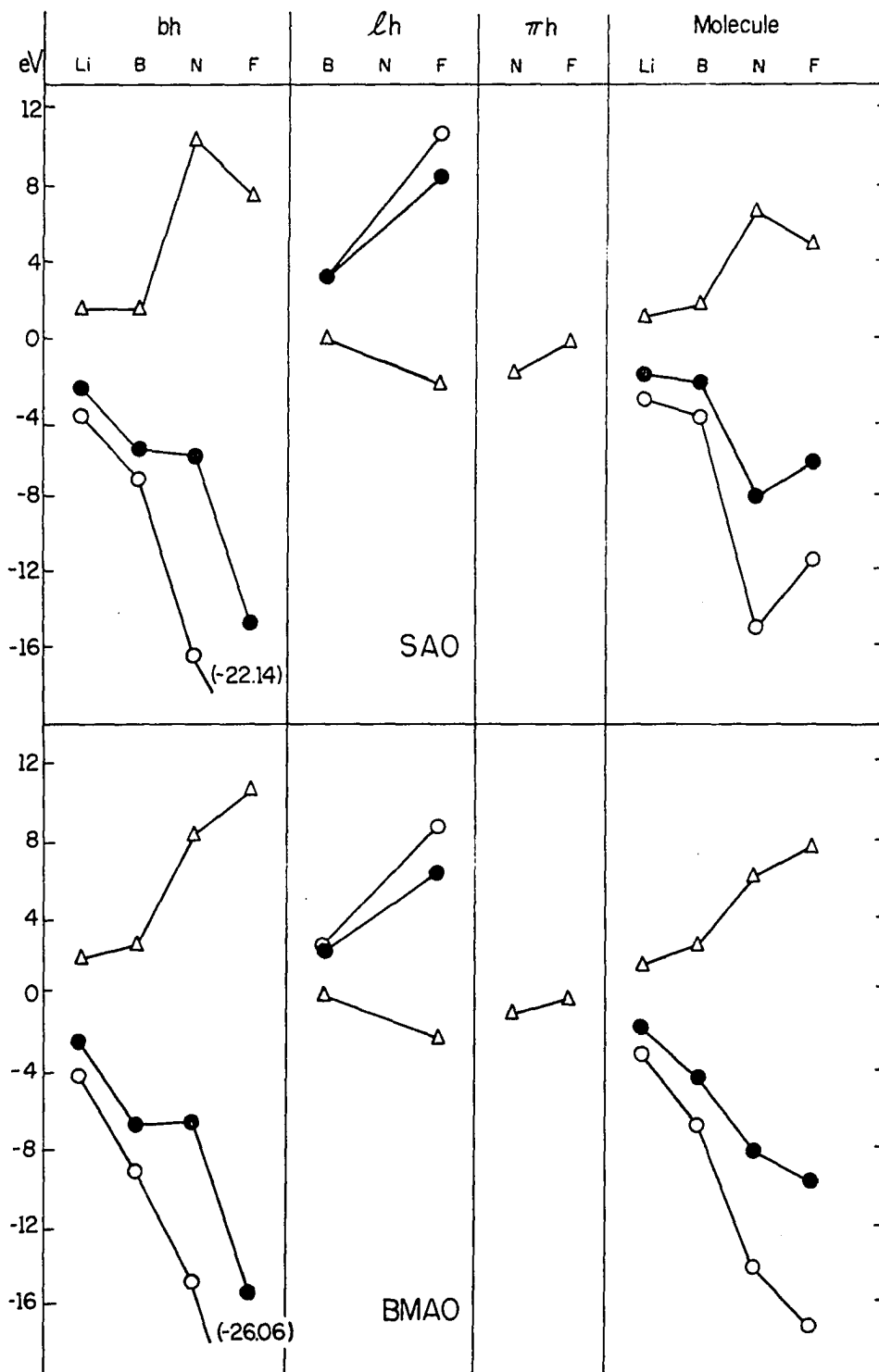
SHARING INTERFERENCE ENERGIES

The interference energies, corresponding to the resonance stabilization operative in the molecule, are also found in the table of interatomic energy contributions in the molecular analyses. The salient features of the "before transfer" interactions are plotted in Figure 7. The modifications from charge transfer are too small to be of consequence. In complete agreement with the basic point of view underlying the present investigation, it is found that the binding bh orbital pair always shows a negative interference energy arising from a negative kinetic part and in spite of a positive potential part, both features being characteristic of constructive interference. The converse holds for the anti-binding lh orbital pair which is characterized by destructive interference.

bh Orbital Pair

The kinetic energy part of the bh pair decreases regularly and rapidly to large negative values. Since we have seen that the bond orders change very little, it is clear that this drop originates in the kinetic resonance integral. In fact, it is a consequence of the increase in gradient of the bonding orbital near the nucleus as the

Figure 7. Molecular sharing interference (neutral) energy and contributions by orbital-pairs for SAO and BMAO approximations. ●, total; ○, kinetic; Δ , potential.



atomic number increases. (The interference energy is proportional to the square of the gradient which, in turn, is proportional to the effective charge of the orbital.) This increase in steepness is not only derived from the increase in effective charge of the s and σ orbitals, but also from the even more drastic increase in effective charge of the orthogonalizing k admixture to the L-shell orbitals. (The variation in overlap integral with atomic number is much less consequential.) On the other hand, the increase of potential interference with atomic number arises from the increase of actual nuclear charge which renders the shift of charge, from the atomic region into the bond region, more costly.

The potential part is smaller than the kinetic part and apparently more susceptible to hybridization effects. One would expect the bonding hybrids of lithium and nitrogen to show stronger relative interference effects because their hybridization is entirely determined by the interactions of the bonding orbital without disturbance from the anti-binding σ lone-pair orbital. In the SAO case, we do indeed find that the boron and fluorine kinetic values lie slightly above the line joining the lithium and nitrogen values. Correspondingly, the line joining the potential values of boron and fluorine is below that joining lithium and nitrogen. (Thus, the equality in lithium and boron potential bh interference

energies, for the SAO case, is explained by the fact that boron has less favorable bonding hybridization but a stronger effective nuclear charge.)

With the exception of nitrogen, the interference effect is accentuated in the BMAO case. This effect of contractive promotion is comparable to the increase in interference energy with atomic number. The deviation of nitrogen is accidental since the somewhat arbitrary SAO ξ sufficiently varies from the BAO ξ (for the s orbital) so that there is actually a slight orbital expansion, in going from the SAO to the BMAO situations. If the BAO values are compared with the BMAO values, the behavior of nitrogen falls in line with that of the other atoms although the not inconsiderable decrease in bond order (see Figure 2) markedly diminishes the effect arising from the orbital contraction. The total interference energy of the bh orbital pair still reflects the difference in hybridization.

lh Orbital Pair

The interference energy of the lh pair is anti-binding due to its positive kinetic part which shows the expected increase from boron to fluorine as a consequence of orbital shrinkage analogous to the decrease of the kinetic part in the bh pair. Similarly, the expansive promotion of this

lone-pair orbital, referred to earlier, is the reason for the BMAO values being smaller than their SAO counterparts. As usual, the potential contributions of destructive interference are negative but they also represent a much smaller fraction of the total interference energy in the lh pair as compared to the bh pair. Such behavior seems to be characteristic of the interaction of a lone-pair orbital on one atom and a bonding orbital on another. As has been discussed in detail in the case of the water molecule (13), where a similar observation has been made, the explanation is presumably that here the destructive interference does not shift charge nearer to the nucleus but rather from one side of the nucleus (the bonding side) to the other side (the lone-pair side)¹³. In fact, the potential energy is negligibly small in the case of boron.

πh Orbital Pair

The interference contributions for the πh orbital pairs arise solely from the exchange part of the second order density. As in other cases (13, 15), they are found to be small and negative and are suspected of being related to the

¹³In the present case this can be directly attributable to the unusually large k admixture to the boron lone-pair orbital.

energy lowering operative in Hund's rules.

Total

Similar to the situation in the case of the quasi-classical interactions, the total molecular effect is a moderated image of the bh interactions. The significant trend is the accentuation of total interference with atomic number upon which there is superimposed modulation which reflects hybridization.

CONCLUSIONS

Following the detailed discussion of the particular molecules and their behavior in the foregoing analysis, it is now appropriate to take a general overview of the results of the investigation.

A first question is what can be said, in view of the detailed analysis, as a general characterization of the electron pair bond in the hydrides considered. The differences between the four molecules have been seen to arise from two properties; the occupation of the σ lone-pair orbital and the electronegativity of the heavy atom.

The σ lone-pair occupancy (zero in LiH and NH, two in BH and HF) determines the hybridization of the lone-pair and bonding orbitals. This in turn is related to the characteristic variations in the neutral quasiclassical interactions favoring the situation with no σ lone-pair electrons. The increase in electronegativity with increasing nuclear charge is of course responsible for the variations in charge transfer along the series, i.e., (Li^+H^-), (B^0H^0), (N^-H^+), (F^-H^+). Associated with this is a corresponding variation of the charge transfer contribution to the binding energy. This effect is abnormally large in NH because of the empty σ lone-pair orbital.

A second effect of the increasing electronegativity

is, however, the regular increase in the interference energy via the kinetic energy of the progressively contracting orbitals. This is the main reason for the increase in binding energy along the series. It must be noted, however, that the anti-binding interference interaction between the lone-pair orbitals and the hydrogen atom rises similarly, and for this reason the increase in binding energy is not accompanied by a corresponding decrease in bond length. More precisely: The actual decrease in bond lengths along the series is slightly less than the shrinkage in orbital diameter due to increasing electronegativity.

As a consequence, the overlap for the various orbital pairs generally remains in the same range, with a slight decrease as atomic charge increases. This must be the reason for the bond orders, and more specifically, the valence active populations, remaining approximately constant and furthermore for the neutral quasiclassical interactions also remaining about constant, aside from the aforementioned hybridization modulation.

In spite of the differences in hybridization, the only trend discernible in the hybridization promotion energies appears to be the steady increase due to increasing the effective charge. The contractive promotion, while small in total, always embodies a substantial reapportionment of the energy from the potential to the kinetic type.

A second question is whether the proposed energetic interactions and the general technique of analysis appear to be justified for these hydride systems. Promotion of isolated atoms has been found expensive to varying degrees. (This is not a trivial observation. The choice of an appropriate reference state is of definite importance, but even a less desirable reference state indicates significant, and justifiable, internal alteration depending upon the molecule which eventually is to be formed.) In all cases the importance of orbital contraction to bonding is evident. Quasiclassical electrostatic interactions are usually of a slightly binding nature. There is an extreme cancellation between repulsive intra-atomic and attractive interatomic sharing penetration effects with a small net repulsion. The predicted importance of constructive interference, kinetic in origin, in forming a bonding situation is emphatically confirmed. Charge transfer effects are seen to improve the binding situation. In all cases, moreover, the observed characteristics and deviations could be understood with the use of only a few variables, such as hybridization, contraction and effective nuclear charge. A pleasant dividend has been the formulation of valence hybrid atomic orbitals which seem to play a fundamental role, not only in determining critical electronic populations, but also in defining the relative contributions to the different energy effects. The

obvious failings which do appear are generally localized (except for the interrelationship mentioned between promotion and sharing penetration) and interpretable. Under the present critical testing, the proposed energetic characteristics of molecular formation have generally been vindicated.

It is, of course, evident that further refinements of the present analysis would lead to a better description of interesting details. For such a closer examination of the method, the wave functions used here are presumably inadequate. Minimization with respect to orbital exponents, at the theoretically deduced equilibrium positions, is indispensable for a proper reapportionment of the kinetic and potential energy. The use of an extended basis to approach the true SCF wave function would also be desirable. The execution of the analysis for such a near-SCF solution as a function of internuclear distance would be worthwhile, before proceeding to more complex wavefunctions incorporating correlation features.

The implied inadequacies in the wave functions and the method of analysis should be kept in mind when judging the reported conclusions.

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APPENDIX: PRESENTATION OF NUMERICAL RESULTS

General Description

Each of the figures, 8 through 22, represents the complete molecular analysis for one of the fifteen hydride calculations. The molecules are arranged in order of increasing molecular weight. For each molecule, the approximations are listed in the order: SAO, BAO, BMAO. The first three parts are the summary binding energy totals; VAO decompositions, bond orders and populations; and the exchange contributions to the pair populations. The last two parts are the detailed decomposition of the energy fragments, by orbital and orbital pair, for each energy mechanism.

Summary Properties

The binding energy partitioning summary contains totals by atom, bond and molecule for the various energy mechanisms. The headings follow the notation of Eq'n 3.10. The entries are sums of the quantities discussed below for the explicit orbital and orbital pair decomposition.

The table of density partitioning shows the AO decomposition, the overlap integrals with the hydrogen 1s

orbital and the populations and bond orders of the orthonormal VAO's. The q 's are the total electronic orbital populations in terms of the valence inactive (p) and valence active (v) fragments, and arising from promotion (N) and charge transfer (T) sources. For review purposes, the following relationships are listed for the diatomic hydride VAO's:

$$q(r) = p(r) + v(r), \quad q(r) = q^N(r) + q^T(r); \quad (\text{A.1})$$

$$\sum_r q(r) = N \quad (\text{sum over all occupied orbitals); \quad (\text{A.2})$$

$$\sum_{r \neq h} q^T(r) = -q^T(h), \quad \sum_{r \neq h} v(r) = v(h); \quad (\text{A.3})$$

$$v(r) = P(r,h)S(r,h). \quad (\text{A.4})$$

The table of exchange contributions to the pair populations lists coefficients, $q_x(Aa,Bb)$, which are used in conjunction with Eq'n 3.9. When a particular AO basis has been chosen (and consequently a particular VAO basis), the pair population between orbitals Aa and Bb is (as is shown in Reference 11)

$$q(Aa,Bb) = q(Aa)q(Bb) - q_x(Aa,Bb). \quad (\text{A.5})$$

Pair populations, as defined in A.5, are an interference-free property of the wave function. In the molecular energy, they

are the coefficients for a limited set of the two-electron integrals, i.e., those particular one- or two-center coulomb integrals having one electron totally in one orbital and the other electron totally in a second orbital, viz.,

$$[Aa^2|Bb^2], \text{ where } A \text{ may equal } B \text{ and } a \text{ may equal } b.$$

The entries in this table are the numerical values of q_x , corresponding to the interference-free parts deriving from promotion (PR), sharing penetration before (SPN) and after (SPT) charge transfer, and their total (TOT). That is,

$$\begin{aligned} q_x(Aa, Bb) &= q_x^{\text{TOT}}(Aa, Bb) \\ &= q_x^{\text{PR}}(Aa, Bb) + q_x^{\text{SPN}}(Aa, Bb) + q_x^{\text{SPT}}(Aa, Bb). \end{aligned} \quad (\text{A.6})$$

Again, the following particular relations are listed for these quantities:

$$\sum_r q_x^{\text{PR}}(r, \bar{r}) = q^{\text{N}}(\bar{r}) \quad (\text{A.7})$$

$$\sum_{r \neq h} q_x^{\text{SPN}}(r, \bar{r} \neq h) = -q_x^{\text{SPN}}(\bar{r}, h) \quad (\text{A.8})$$

$$\sum_r q_x^{\text{SPT}}(r, \bar{r}) = q^{\text{T}}(\bar{r}) \quad (\text{A.9})$$

$$\sum_r \sum_x q_x^{\text{TOT}}(r, \bar{r}) = q(\bar{r}) \quad (\text{A.10})$$

$$\sum_r \sum_x q_x^{\text{PR}}(r, \bar{r}) = N \quad (\text{sum over all occupied orbitals}) \quad (\text{A.11})$$

$$\sum_r \sum_x q_x^{\text{SPN}}(r, \bar{r}) = 0$$

$$\sum_r \sum_x q_x^{\text{SPT}}(r, \bar{r}) = 0 \quad (\text{A.13})$$

$$\sum_r \sum_x q_x^{\text{TOT}}(r, \bar{r}) = N \quad (\text{A.14})$$

Orbital and Orbital Pair Decompositions

The last two sections of each particular figure give the separate intra-atomic and interatomic energy contributions to the molecular binding energy. Under intra-atomic contributions there is an additional division between promotion effects arising in the original AO's and interaction effects occurring in the VAO's. Each of these contributions is further subdivided into kinetic (KIN) and potential (SNA for shielded nuclear attraction, NA for nuclear attraction and OEI for other electronic interactions) contributions.

Formulae for the subdivision of promotion energy into

orbital contributions are developed in detail in Reference 15. The criterion for this orbital partitioning is the difference in orbital electronic population for the promoted atomic valence state with respect to the atomic ground state. The promotion energy terms distributed to the orbitals are obtained from the intra-atomic integrals and coefficients of the density matrices. The total promotion energies are given by Equations A.15 - A.18:

$$\begin{aligned} \text{SAO: } E_{\text{HP}} &= E^{\text{P}} - E^{\text{g}} \\ &= (p^{\text{P}} - p^{\text{g}}) \cdot \underline{1}(\text{SAO}) + (\pi^{\text{P}} - \pi^{\text{g}}) \cdot \underline{2}(\text{SAO}) \end{aligned} \quad (\text{A.15})$$

$$\text{BAO: } E_{\text{HP}} = (p^{\text{P}} - p^{\text{g}}) \cdot \underline{1}(\text{BAO}) + (\pi^{\text{P}} - \pi^{\text{g}}) \cdot \underline{2}(\text{BAO}) \quad (\text{A.16})$$

$$\text{BMAO: } E_{\text{HP}} = (p^{\text{P}} - p^{\text{g}}) \cdot \underline{1}(\text{BAO}) + (\pi^{\text{P}} - \pi^{\text{g}}) \cdot \underline{2}(\text{BAO}) \quad (\text{A.17})$$

$$E_{\text{CP}} = p^{\text{P}} \cdot [\underline{1}(\text{BMAO}) - \underline{1}(\text{BAO})] + \pi^{\text{P}} \cdot [\underline{2}(\text{BMAO}) - \underline{2}(\text{BAO})] \quad (\text{A.18})$$

In these equations, superscripts P and g refer to the promoted and ground states, 1 and 2 denote the one- and two-electron intra-atomic integrals obtained by the specified approximation and HP and CP label hybridization and clustering promotion. Note that clustering promotion is only identified

with the BMAO case. This results from the consideration that only in the BMAO approximation is there an energy minimization with respect to the molecular values of the ζ 's. By definition there is non-zero promotion in the hydrogen atoms only in the sense of contraction.

The remaining intra-atomic contributions, characteristic of the atom in the molecule, are reported for the VAO's. The QCT entries apportion the quasiclassical energy of the transferred charge to the appropriate orbital. Sharing penetration, both neutral and transfer, is separated in a similar fashion, with the fragments appearing only in the OEI rows, re-emphasizing the interpretation (13) that this effect arises from rearrangements within the electron-pair density matrix.

All interatomic contributions are reported for the valence hybrid orbital pairs. In the QCT column, the SNA row is further separated into (left entry) the energy of the charge transferred to the heavy atom orbital in the field of the neutral shielded hydrogen nucleus and (right entry) the energy of the charge transferred to hydrogen in the field ascribed to the neutral heavy atom orbital fragment. The SIN column is similarly decomposed, the left entry showing the energy of the orbital-pair interference density in the field of the shielded heavy atom nucleus and the right entry giving the orbital-pair interference density energy in the field of

the shielded hydrogen nucleus. The SIT column gives the interaction energy of the particular interference density with the charge transferred to the particular heavy atom orbital (left) and with the charge transferred to the hydrogen atom (right). The SPN and SPT entries again illustrate the pair-density origin of this interaction.

The initial summary table may now be recognized as the totals at the bottom of each column of the intra-atomic (atom) and interatomic (bond) contributions with combined SNA entries.

Summarizing Explanation for Figures 8 - 22

The first section, labelled "Binding Energy Partitioning", lists the binding energy fragments by atoms and bond, decomposed in terms of kinetic interactions (KIN) and potential interactions. For the intra-atomic promotion contributions, the latter are subdivided into nuclear attraction (NA) and other electronic interaction (OEI). For all other intra- and interatomic categories the potential contributions are decomposed into shielded nuclear attraction (SNA) and other electronic interaction (OEI). Note that non-zero contraction promotion only occurs for the BMAO cases.

The second section, labelled "Density Partitioning for Valence AO's", gives VAO decompositions in terms of

basis functions; the VAO overlap with the hydrogen is orbital; valence inactive (p), valence active (v), total (q), promoted (q^N), and charge transfer (q^T) populations for these VAO's; and their bond order with the hydrogen 1s orbital.

The third section, entitled "Exchange Contributions to Pair Populations", gives the interference-free intra- and interatomic orbital pair coefficients of $\pi_x(x_1, x_2)$ and their decompositions in terms of contributions due to promotion (PR), sharing penetration before (SPN) and following (SPT) charge transfer.

The last two tables give the detailed partitioning according to orbitals and orbital pairs of the intra- and interatomic summary presented in the first table ("Binding Energy Partitioning") given above. In the SNA rows of the interatomic QCT column, the left entry represents the interaction of the neutral hydrogen with the transfer population of the heavy atom orbital, whereas the right entry represents the interaction of the neutral heavy-atom orbital-fragment with the transfer population on hydrogen. In the SNA rows of the interatomic SIN and SIT columns, the left entry gives the potential interaction of the interference density with the heavy atom while the right entry gives that interaction with the hydrogen atom.

BINDING ENERGY PARTITIONING

		Promotion		Quasi-classical		Sharing Penetration		Sharing Interference		TOTAL
		PRH	PRC	QCN	QCT	SPN	SPT	SIN	SIT	
Li	KIN	.88	-		-2.17					-1.29
	NA	-1.05	-		1.34					.29
	OEI	.69	-		.37	4.65	-1.68			4.03
	TOT	.53	-		-1.46	4.65	-1.68			3.04
H	KIN	-	-		4.21					4.21
	SNA	-	-		-3.16					-3.16
	OEI	-	-		.82	10.15	-8.98			1.99
	TOT	-	-		1.87	10.15	-8.98			3.04
BOND	KIN							-3.03		-3.03
	SNA			-.99	.47			1.32	.00	.80
	OEI				-.91	-11.34	7.09	-.03		-5.19
	TOT			-.99	-.44	-11.34	7.09	-1.74	.00	-7.42
LiH	KIN	.88	-		2.04			-3.03		-.11
	SNA	-1.05	-	-.99	-1.35			1.32	.00	-2.07
	OEI	.69	-		.28	3.46	-3.57	-.03		.83
	TOT	.53	-	-.99	.97	3.46	-3.57	-1.74	.00	-1.34

DENSITY PARTITIONING FOR VALENCE AO'S

	Valence Atomic Orbitals			Overlap $S_{(Li, H)}$	Bondorders and Populations					
	k	s	σ		p	v	q	q^N	q^T	$P_{(Li, H)}$
i	.999617	-.011785	-.025048	.074730	2.010	-.008	2.002	2.008	-.006	-.106
b	.024203	.811232	.584224	.704494	.309	.378	.688	.991	-.303	.537
l	.013435	-.584606	.811206	.178408	.000	.000	.000	.000	.000	.000
h		(unhybridized)		-	.939	.371	1.309	1.000	.309	-

EXCHANGE CONTRIBUTIONS TO PAIRPOPULATIONS

		Li			H
		i	b	l	h
i	PR	2.007	.002	.000	-
	SPN	.000	-.003	.000	-.003
	SPT	.000	.001	.000	-.007
	TOT	2.007	-.001	.000	-.004
b	PR	.002	.989	.000	-
	SPN	-.003	-1.188	.000	1.191
	SPT	.001	.435	.000	-.739
	TOT	-.001	.237	.000	.452
l	PR	.000	.000	.000	-
	SPN	.000	.000	.000	.000
	SPT	.000	.000	.000	.000
	TOT	.000	.000	.000	.000
h	PR	-	-	-	1.000
	SPN	.003	1.191	.000	-1.194
	SPT	-.007	-.739	.000	1.056
	TOT	-.004	.452	.000	.862

Figure 8. Binding energy decomposition and description of electron distribution for LiH, SAO approximation

INTRA-ATOMIC ENERGY CONTRIBUTIONS OF LiH, SAO

Orbital	Promotion			Total	Orbital	Quasi-classical QCT	Sharing Penetration		SP+QC Total																				
	k	s	σ				SPH	SPT																					
Li k	KIN	.77	.08	.00	.76	Li 1	.14	.27	-.01																				
	NA	-1.71	-.89	.00	-1.72																								
	OEI	.66	-3.33	2.99	.72																								
	TOT	-.28	-3.08	2.99	-.21																								
Li s	KIN	.25	-2.02	.00	-1.83	Li b	4.59	-1.67	-1.67																				
	NA	-.89	9.85	.00	9.66																								
	OEI	-3.08	.06	-.00	-3.08																								
	TOT	-3.08	7.91	-.00	1.85																								
Li σ	KIN	.22	.00	1.95	1.95	Li 2	-.02	.00	.00																				
	NA	.22	.00	-9.21	-9.21																								
	OEI	2.99	-.00	-.21	5.95																								
	TOT	2.99	-.00	-7.06	-1.11																								
Total Li	KIN			.88		Total Li	KIN			-2.17				-2.17															
	NA			-1.05			SNA			1.34				1.34															
	OEI			.69			OEI			.37	4.65	-1.68		3.34															
	TOT			.53			TOT			-1.46	4.65	-1.68		2.52															
					Total H																								
					KIN					4.21					4.21														
					SNA					-3.16					-3.16														
					OEI					.82					10.15					-9.98					1.99				
					TOT					1.87					10.15					-3.98					3.84				

INTERATOMIC ENERGY CONTRIBUTIONS OF LiH, SAO

Orbital Pair	Quasiclassical Electrostatic			Sharing			Interference			Totals				
	QCN	QCT	QC(N+T)	SPH	SPT	SP(N+T)	SIN	SIT	SI(N+T)	N	T	N+T		
1 h	KIN						.97		.97	.97		.97		
	SNA	-.04	.22	-.02	-.06		-.11	-.10	.00	.22	-.19	-.24	-.02	
	OEI		-.02	-.02		-.03	.27	.24		-.04	-.07	.05	-.02	
	TOT	-.04	-.04	-.08		-.03	.27	.24		.75	.75	.66	.25	
b h	KIN						-4.21		-4.21	-4.21		-4.21		
	SNA	-.95	.32	.17	-.46		.52	1.00	-.07	.06	1.51	-.58	.48	
	OEI		-.89	-.89		-11.31	7.02	-4.29		.01	-11.30	6.13	-5.17	
	TOT	-.95	-.40	-1.35		-11.31	7.02	-4.29		-2.47	-.01	-2.48	-14.73	6.61
2 h	KIN						.00		.00	.00		.00		
	SNA	.02	.00	.00	.00		.00	.00	.00	.00	.00	.00		
	OEI		.00	.00		.00	.00	.00		.00	.00	.00		
	TOT	.02	.00	.00		.00	.00	.00		.00	.00	.00		
Bond Total	KIN						-3.03		-3.03	-3.03		-3.03		
	SNA	-.99	.32	.15	-.52		.42	.90	-.07	.27	1.32	-.33	.47	
	OEI		-.91	-.91		-11.34	7.09	-4.25		-.03	-11.37	6.18	-5.19	
	TOT	-.99	-.44	-1.43		-11.34	7.09	-4.25		-1.74	.00	-1.74	-14.07	6.65

Figure 8 (Continued)

BINDING ENERGY PARTITIONING

		Promotion		Quasi-classical		Sharing Penetration		Sharing Interference		TOTAL
		PRH	PRC	QCN	QCT	SPN	SPT	SIN	SIT	
Li	KIN	1.02	-		-2.10					-1.08
	NA	-1.22	-		1.33					.11
	OEI	.70	-		.37	4.56	-1.64			3.99
	TOT	.50	-		- .40	4.56	-1.64			3.02
H	KIN	-	-		4.27					4.27
	SNA	-	-		-3.20					-3.20
	OEI	-	-		.84	10.16	-9.03			1.96
	TOT	-	-		1.91	10.16	-9.03			3.03
BOND	KIN							-2.95		-2.95
	SNA			-.96	.43			1.25	.01	.74
	OEI				-.92	-11.22	7.03	-.03		-5.15
	TOT			-.96	-.49	-11.22	7.03	-1.72	.01	-7.36
LiH	KIN	1.02	-		2.17			-2.95		.24
	SNA	-1.22	-	-.96	-1.44			1.25	.01	-2.35
	OEI	.70	-		.29	3.50	-3.64	-.03		.80
	TOT	.50	-	-.96	1.02	3.50	-3.64	-1.72	.01	-1.31

DENSITY PARTITIONING FOR VALENCE AO'S

	Valence Atomic Orbitals			Overlap	Bondorders and Populations					
	k	s	σ	S(Li, H)	p	v	q	q^N	q^T	P(Li, H)
i	.999593	-.013973	-.024866	.074658	2.010	-.008	2.002	2.009	-.007	-.107
b	.025640	.812773	.582007	.700009	.308	.376	.684	.991	-.307	.538
l	.012078	-.582413	.812803	.179878	.000	.000	.000	.000	.000	.000
h	(unhybridized)			-	.946	.368	1.314	1.000	.314	-

EXCHANGE CONTRIBUTIONS TO PAIRPOPULATIONS

		Li			H
		i	b	l	h
i	PR	2.007	.002	.000	-
	SPN	.000	-.003	.000	-.003
	SPT	.000	.001	.000	-.008
	TOT	2.007	-.001	.000	-.004
b	PR	.002	.989	.000	-
	SPN	-.003	-1.188	.000	1.191
	SPT	.001	.433	.000	-.741
	TOT	-.001	.234	.000	.451
l	PR	.000	.000	.000	-
	SPN	.000	.000	.000	.000
	SPT	.000	.000	.000	.000
	TOT	.000	.000	.000	.000
h	PR	-	-	-	1.000
	SPN	.003	1.191	.000	-1.195
	SPT	-.008	-.741	.000	1.062
	TOT	-.004	.451	.000	.868

Figure 9. Binding energy decomposition and description of electron distribution for LiH, BAO approximation

INTRA-ATOMIC ENERGY CONTRIBUTIONS OF LiH, BAO

Orbital	Promotion				Total	Orbital	Quasi-classical QCT	Sharing		SP+QC Total
	k	s	σ					Penetration SPN	SPT	
KIN	.77	.14	.00		.76	KIN	-.64			-.64
Li k NA	-1.72	-.15	.00		-1.71	Li k SNA	.78			.78
OEI	.67	-2.91	2.91		1.74	OEI	.01	.06	-.01	.06
TOT	-.28	-2.93	2.91		-.21	TOT	.14	.06	-.01	.19
KIN	.14	-1.88	.00		-1.62	KIN	-1.46			-1.46
Li s NA	-.15	9.57	.00		9.25	Li s SNA	.55			.55
OEI	-2.91	.00	-.00		-5.82	OEI	.36	4.52	-1.63	3.25
TOT	-2.93	7.74	-.00		1.81	TOT	-.55	4.52	-1.63	2.32
KIN	.00	.00	1.86		1.86	KIN	.00			.00
Li σ NA	.00	.00	-8.76		-8.76	Li σ SNA	.00			.00
OEI	2.91	-.00	-.01		5.79	OEI	.00	-.00	.00	-.00
TOT	2.91	-.00	-6.91		-1.11	TOT	.00	-.00	.00	-.00
Total Li KIN					1.02	Total Li KIN	-2.10			-2.10
NA					-1.22	NA	1.33			1.33
OEI					.70	OEI	.37	4.56	-1.64	3.29
TOT					.50	TOT	-.40	4.56	-1.64	2.52
Total H KIN						Total H KIN	4.27			4.27
SNA						SNA	-3.20			-3.20
OEI						OEI	.84	10.16	-9.83	1.96
TOT						TOT	1.91	10.16	-9.83	3.03

INTERATOMIC ENERGY CONTRIBUTIONS OF LiH, BAO

Orbital Pair Li H	Quasiclassical Electrostatic				Sharing					Interference			Totals		
	QCN	QCT	QC(N+T)		SPN	SPT	SP(N+T)	SIN	SIT	SI(N+T)	N	T	N+T		
KIN															
1 h SNA	-.04	.00	-.02	-.26				-.10	-.10	.00	.02	-.18	-.24	-.00	
OEI				-.22	-.03	.07	.04	-.04		.02		-.07	.05	-.02	
TOT	-.04	-.04	-.08	-.08	-.03	.07	.04	.73		.02		.75	.66	.71	
KIN															
b h SNA	-.92	.31	.14	-.47				-3.92				-3.92	-3.92	-3.92	
OEI				-.91	-11.19	6.96	-4.23	.46	.99	-.07	.06	1.44	.53	.44	
TOT	-.92	-.45	-1.37	-1.37	-11.19	6.96	-4.23	-2.45		-.01	-.01	-11.13	6.05	-5.12	
KIN															
l h SNA	.00	.00	.00	.00				.00	.00	.00	.00	.00	.00	.00	
OEI				.00	.00	.00	.00	.00	.00	.00	.00	.00	.00	.00	
TOT	.00	.00	.00	.00	.00	.00	.00	.00	.00	.00	.00	.00	.00	.00	
Bond KIN															
Total SNA	-.96	.31	.12	-.53				-2.95				-2.95	-2.95	-2.95	
OEI				-.92	-11.22	7.03	-4.19	.56	.99	-.27	.08	1.20	.50	.74	
TOT	-.96	-.49	-1.45	-1.45	-11.22	7.03	-4.19	-1.72		.01	-.01	-11.25	6.10	-5.15	
												-13.98	6.54	-7.36	

Figure 9 (Continued)

BINDING ENERGY PARTITIONING

		Promotion		Quasi-classical		Sharing Penetration		Sharing Interference		TOTAL
		PRH	PRC	QCN	QCT	SPN	SPT	SIN	SIT	
Li	KIN	.96	3.28		-3.35					.89
	NA	-1.34	-5.87		1.90					-5.30
	OEI	.80	3.06		.55	5.28	-1.76			7.93
	TOT	.43	.48		-.90	5.28	-1.76			3.51
H	KIN	.00	-.63		4.60					3.97
	SNA	.00	.64		-3.53					-2.89
	OEI	.00	.00		1.04	9.87	-9.22			1.69
	TOT	.00	.01		2.11	9.87	-9.22			2.77
BOND	KIN							-3.21		-3.21
	SNA			-1.17	.78			1.51	.00	1.13
	OEI				-1.25	-11.88	7.56	-.03		-5.61
	TOT			-1.17	-.48	-11.88	7.56	-1.75	.00	-7.69
LiH	KIN	.96	2.65		1.25			-3.21		1.65
	SNA	-1.34	-5.23	-1.17	-.85			1.51	.00	-7.06
	OEI	.80	3.06		.34	3.27	-3.42	-.03		4.01
	TOT	.43	.43	-1.17	.73	3.27	-3.42	-1.75	.00	-1.41

DENSITY PARTITIONING FOR VALENCE AO'S

	Valence Atomic Orbitals			Overlap $S_{(Li,H)}$	Bond orders and Populations					
	k	s	σ		p	v	q	q^N	q^T	$P_{(Li,H)}$
i	.999610	-.009977	-.026071	.077872	2.011	-.009	2.002	2.011	-.008	-.114
b	.023080	.821135	.570267	.720442	.271	.372	.643	.989	-.346	.517
l	.015734	-.570646	.821045	.182277	.000	.000	.000	.000	.000	.000
h	(unhybridized)			-	.991	.363	1.354	1.000	.354	-

EXCHANGE CONTRIBUTIONS TO PAIR POPULATIONS

		Li			H
		i	b	l	h
i	PR	2.007	.003	.000	-
	SPN	.000	-.005	.000	.005
	SPT	.001	.001	.000	-.009
	TOT	2.008	-.001	.000	-.005
b	PR	.003	.986	.000	-
	SPN	-.005	-1.179	.000	1.184
	SPT	.001	.400	.000	-.747
	TOT	-.001	.207	.000	.437
l	PR	.000	.000	.000	-
	SPN	.000	.000	.000	.000
	SPT	.000	.000	.000	.000
	TOT	.000	.000	.000	.000
h	PR	-	-	-	1.000
	SPN	.005	1.184	.000	-1.189
	SPT	-.009	-.747	.000	1.111
	TOT	-.005	.437	.000	.922

Figure 10. Binding energy decomposition and description of electron distribution for LiH, BMAO approximation

INTRA-ATOMIC ENERGY CONTRIBUTIONS OF LIH, BMAO

Orbital	Promotion σ									Orbital	Quasi-classical QCT	Sharing Penetration SPT		SP+QC Total		
	PHH ^k	PRC	PRH ^a	PRC	PRH ^c	PRC	PRH	Total PRC	PR(H+C)			SPN	SPT			
Li ^k	KIN	.94	.65	.02	.00	.00	.00	.94	.65	1.59	Li ^k	KIN	-.81		-.81	
	NA	-2.11	-.72	-.03	-.01	.00	.00	-2.11	-.72	-2.83		SNA	.97		.97	
	OEI	.81	.06	-2.81	.62	2.79	.89	.89	.09	.98		OEI	.02	.09	-.02	.09
	TOT	-.36	-.02	-2.82	.62	2.79	.89	-.27	.01	-.26		TOT	.17	.09	-.02	.25
Li ^a	KIN	.02	.00	-1.82	1.28	.00	.00	-1.77	1.28	-.48	Li ^b	KIN	-2.54		-2.54	
	NA	-.03	-.01	9.23	-2.40	.00	.00	9.17	-2.41	6.77		SNA	.93		.93	
	OEI	-2.81	.62	.86	-.01	-.00	-.00	-5.63	1.22	-4.41		OEI	.54	5.19	-1.75	3.98
	TOT	-2.82	.62	7.47	-1.13	-.00	-.00	1.77	1.10	1.87		TOT	-1.08	5.19	-1.75	2.36
Li ^c	KIN	.00	.00	.00	.00	1.78	1.35	1.78	1.35	3.14	Li ^l	KIN	.00		.00	
	NA	.00	.00	.00	.00	-8.40	-2.74	-8.40	-2.74	-11.14		SNA	.00		.00	
	OEI	2.79	.89	-.00	-.00	-.01	-.01	5.55	1.75	7.30		OEI	.00	-.00	.00	-.00
	TOT	2.79	.89	-.00	-.00	-6.62	-1.39	-1.07	.57	-.70		TOT	.00	-.00	.00	-.00
Total Li										Total Li						
KIN										KIN	-5.55		-5.55			
NA										NA	1.90		1.90			
OEI										OEI	.55	5.28	-1.76	4.87		
TOT										TOT	-.90	5.28	-1.76	2.61		
Total H										Total H						
KIN										KIN	4.60		4.60			
NA										NA	-3.53		-3.53			
OEI										OEI	1.84	9.87	-9.22	1.69		
TOT										TOT	2.11	9.87	-9.22	2.76		

INTERATOMIC ENERGY CONTRIBUTIONS OF LIH, BMAO

Orbital Pair	Quasiclassical Electrostatic				Sharing				Interference			Totals			
	QCN	QCT	QC(N+T)		Penetration SPT		SP(N+T)		SIN	SIT		SI(N+T)	N	T	N+T
i h	KIN	-.04	.00	-.03	-.07				1.06			1.06	1.06		1.06
	SNA							-.14	-.11	.01	.02	-.22	-.29	-.08	-.29
	OEI					-.04	.08	.04	-.05			-.05	-.09	.06	-.03
	TOT	-.04		-.06	-.10	-.04	.08	.04	.77		.03	.00	-.09	.05	.75
b h	KIN	-1.13	.43	.38	-.32				-4.27			-4.27	-4.27		-4.27
	SNA							.89	.87	-.07	.05	1.74	.63	.79	1.42
	OEI					-11.84	7.47	-4.37	.01			-.01	-11.85	6.25	-5.58
	TOT	-1.13		-.42	-1.55	-11.84	7.47	-4.37	-2.50		-.02	-2.52	-15.47	7.03	-8.44
l h	KIN	.00	.00	.00	.00				.00	.00	.00	.00	.00	.00	.00
	SNA								.00	.00	.00	.00	.00	.00	.00
	OEI					.00	.00	.00	.00	.00	.00	.00	.00	.00	.00
	TOT	.00		.00	.00	.00	.00	.00	.00	.00	.00	.00	.00	.00	.00
Bond Total	KIN	-1.17	.43	.35	-.39				-3.21			-3.21	-3.21		-3.21
	SNA								1.52	.76	-.07	.07	1.55	.78	1.13
	OEI					-11.88	7.56	-4.33	-.03			-.03	-11.92	6.38	-5.61
	TOT	-1.17		-.48	-1.64	-11.88	7.56	-4.33	-1.73		.00	-1.72	-14.78	7.09	-7.69

Figure 10 (Continued)

BINDING ENERGY PARTITIONING

		Promotion		Quasi-classical		Sharing Penetration		Sharing Interference		TOTAL
		PRH	PRC	QCN	QCT	SPN	SPT	SIN	SIT	
B	KIN	- .62	-		-2.33					- 2.95
	SNA	.40	-		1.92					2.32
	OEI	1.43	-		.10	4.20	.18			5.91
	TOT	1.22	-		-.31	4.20	.18			5.29
H	KIN	-	-		1.65					1.65
	SNA	-	-		-1.24					- 1.24
	OEI	-	-		.12	4.42	-1.83			2.65
	TOT	-	-		.54	4.42	-1.83			3.06
BOND	KIN							-4.00		- 4.00
	SNA			-1.85	-.36			1.37	.13	-.11
	OEI				-.18	-6.60	.85	-.14		- 6.06
	TOT			-1.85	-.54	-6.60	.85	-2.17	.13	-10.17
BH	KIN	- .62	-		-.68			-4.00		- 5.30
	SNA	.40	-	-1.85	.32			1.37	.13	-.97
	OEI	1.43	-		.04	2.02	-.86	-.14		2.50
	TOT	1.22	-	-1.85	-.31	2.02	-.86	-2.17	.13	- 1.82

DENSITY PARTITIONING FOR VALENCE AO'S

	Valence Atomic Orbitals			Overlap S(B, H)	Bondorders and Populations					
	k	s	σ		p	v	q	q ^N	q ^T	P(B, H)
i	.977686	-.178557	.067140	.000000	2.000	.000	2.000	2.000	.000	.000
l	.203437	.895130	-.333546	.313669	2.140	-.141	2.049	2.080	-.032	-.451
b	.016173	.392245	.916701	.702931	.428	.403	.830	.920	-.090	.573
h		(unhybridized)		-	.860	.261	1.121	1.000	.121	-

EXCHANGE CONTRIBUTIONS TO PAIRPOPULATIONS

		B			H
		i	l	b	h
i	PR	2.000	.000	.000	-
	SPN	.000	.000	.000	.000
	SPT	.000	.000	.000	.000
	TOT	2.000	.000	.000	.000
l	PR	.000	2.080	.000	-
	SPN	.000	-.001	-.018	.019
	SPT	.000	.060	.004	-.096
	TOT	.000	2.140	-.014	-.077
b	PR	.000	.000	.920	-
	SPN	.000	-.018	-.483	.501
	SPT	.000	.004	-.087	-.006
	TOT	.000	-.014	.350	.495
h	PR	-	-	-	1.000
	SPN	.000	.019	.501	-.520
	SPT	.000	-.096	-.006	.223
	TOT	.000	-.077	.495	.703

Figure 11. Binding energy decomposition and description of electron distribution for BH, SAO approximation

INTRA-ATOMIC ENERGY CONTRIBUTIONS OF BH, SAO

Orbital	Promotion				Orbital	Quasi-classical QCT	Sharing Penetration		SP-QC Total
	k	s	o	Total			SPN	SPT	
B k	KIN	.97	-.62	.02	1.01	KIN	.00		.00
	NA	-2.07	.63	.02	-2.11	SNA	.00		.00
	OEI	.01	-1.71	1.91	-.17	OEI	.00	-.02	.00
	TOT	-1.09	-1.67	1.91	-.93	TOT	.00	-.02	.00
B s	KIN	-.68	-2.31	.00	-4.04	KIN	-.31		-.31
	NA	.63	10.46	.02	11.77	SNA	.44		.44
	OEI	-1.71	-.03	-.96	-1.14	OEI	.02	.35	-.46
	TOT	-1.67	7.62	-.96	6.59	TOT	.16	.35	-.46
B o	KIN	.02	.02	2.41	2.41	KIN	-2.03		-2.03
	NA	.00	.00	-9.26	-9.26	SNA	1.48		1.48
	OEI	1.91	-.96	2.97	2.40	OEI	.08	3.85	.63
	TOT	1.91	-.96	-3.88	-4.45	TOT	-.47	3.85	.63
Total B	KIN			-.62		KIN	-2.33		-2.33
	NA			.48		SNA	1.92		1.92
	OEI			1.43		OEI	.10	4.20	.18
	TOT			1.22		TOT	-.31	4.20	.18
Total H	KIN					KIN	1.65		1.65
	NA					SNA	-1.24		-1.24
	OEI					OEI	.12	4.42	-1.89
	TOT					TOT	.54	4.42	-1.89

INTERATOMIC ENERGY CONTRIBUTIONS OF BH, SAO

Orbital Pair B H	Quasiclassical Electrostatic			Sharing			Interference			Totals		
	QCN	QCT	QC(N+T)	SPN	SPT	SP(N+T)	SIN	SIT	SI(N+T)	N	T	N+T
i h	KIN						.00		.00	.00	.00	.00
	SNA	-.04	.02	-.03	-.07		.00	.00	.00	.00	.00	.00
	OEI		.02			.08	.02	.08		.02	-.03	.23
	TOT	-.04	-.03	-.07		.08	.08	.08		.02	-.12	.12
l h	KIN						3.26		3.26	3.26		3.26
	SNA	.45	.02	-.02	-.36		1.07	-.90	.02	.03	.21	.62
	OEI		-.03			-.04	.77	.73		-.07	-.11	.74
	TOT	.45	-.04	-.39		-.04	.77	.73		3.36	3.40	3.77
b h	KIN						-7.26		-7.26	-7.26		-7.26
	SNA	-2.26	.25	.22	-1.79		2.01	-.50	-.01	.10	1.60	-.75
	OEI		-.14		-.14	-6.56	.08	-6.47		.05	-6.51	-.06
	TOT	-2.26	.33	-1.93		-6.56	.08	-6.47		-5.70	-.09	-5.62
Bond Total	KIN						-4.00		-4.00	-4.00		-4.00
	SNA	-1.85	.26	-.62	-2.22		3.37	-1.40	.00	.13	2.11	.12
	OEI		-.18		-.18	-6.60	.05	-5.74		-.14	-6.74	.68
	TOT	-1.85	-.54	-2.39		-6.60	.05	-5.74		-2.17	-2.03	-10.62

Figure 11 (Continued)

BINDING ENERGY PARTITIONING

		Promotion		Quasi-classical		Sharing Penetration		Sharing Interference		TOTAL
		PRH	PRC	QCN	QCT	SPN	SPT	SIN	SIT	
B	KIN	-1.13	-		-1.97					- 3.10
	SNA	1.71	-		1.06					3.37
	OEI	.65	-		.08	4.18	.04			4.95
	TOT	1.23	-		-.23	4.18	.04			5.22
H	KIN	-	-		1.47					1.47
	SNA	-	-		-1.10					- 1.10
	OEI	-	-		.10	4.59	-1.80			2.89
	TOT	-	-		.47	4.59	-1.80			3.26
BOND	KIN							-4.07		- 4.07
	SNA			-1.90	-.31			2.26	.11	.15
	OEI				-.14	-7.02	1.10	-.13		- 6.13
	TOT			-1.90	-.45	-7.02	1.10	-1.74	.11	-10.10
BH	KIN	-1.13	-		-.50			-4.07		- 5.70
	SNA	1.71	-	-1.90	.25			2.26	.11	2.42
	OEI	.65	-		.04	1.75	-.66	-.13		1.65
	TOT	1.23	-	-1.90	-.21	1.75	-.66	-1.74	.11	-1.62

DENSITY PARTITIONING FOR VALENCE AO'S

	Valence Atomic Orbitals			Overlap $S_{(B,H)}$	Bond orders and Populations					
	k	s	σ		p	v	q	q^N	q^T	$P_{(B,H)}$
i	.972426	-.217607	.083356	.000000	2.000	.000	2.000	2.000	.000	.000
l	.232611	.880182	-.413729	.281115	2.148	-.109	2.039	2.062	-.023	-.386
b	.016743	.421711	.906576	.727660	.440	.413	.853	.938	-.086	.568
h	(unhybridized)			-	.804	.305	1.108	1.000	.108	-

EXCHANGE CONTRIBUTIONS TO PAIR POPULATIONS

		B			H
		i	l	b	h
i	PR	2.000	.000	.000	-
	SPN	.000	.000	.000	.000
	SPT	.000	.000	.000	.000
	TOT	2.000	.000	.000	.000
l	PR	.000	2.085	-.023	-
	SPN	.000	.000	.009	-.009
	SPT	.000	.026	.003	-.051
	TOT	.000	2.110	-.011	-.060
b	PR	.000	-.023	.961	-
	SPN	.000	.009	-.558	.549
	SPT	.000	.003	-.036	-.052
	TOT	.000	-.011	.368	.496
h	PR	-	-	-	1.000
	SPN	.000	-.009	.549	-.540
	SPT	.000	-.051	-.052	.211
	TOT	.000	-.060	.496	.672

Figure 12. Binding energy decomposition and description of electron distribution for BH, BAO approximation

INTRA-ATOMIC ENERGY CONTRIBUTIONS OF BH, BAO

Orbital	Promotion				Orbital	Quasi-classical QCT	Sharing Penetration		SP*QC Total
	k	s	σ	Total			SPN	SPT	
B k	KIN	.90	-.40	.00	.92	KIN	.00		.00
	MA	-1.93	.42	.00	-1.95	SMA	.00		.00
	OEI	.02	-2.36	2.33	.17	OEI	.00	-.00	.00
TOT	-1.01	-2.33	2.33	-.06	TOT	.00	-.00	.00	-.02
B s	KIN	-.40	-3.99	.00	-4.80	KIN	-.22		-.22
	MA	.42	14.16	.00	15.03	SMA	.35		.35
	OEI	-2.36	-.55	-.92	-2.96	OEI	.01	.13	-.20
TOT	-2.33	9.62	-.92	7.27	TOT	.15	.13	-.22	.27
B σ	KIN	.00	.00	2.75	2.75	KIN	-1.75		-1.75
	MA	.00	.00	-11.36	-11.36	SMA	1.31		1.31
	OEI	2.33	-.92	3.09	3.43	OEI	.06	4.06	.24
TOT	2.33	-.92	-5.53	-5.18	TOT	-.38	4.06	.24	3.92
Total B	KIN				-1.13	KIN	-1.97		-1.97
	MA				1.71	SMA	1.66		1.66
	OEI				.65	OEI	.08	4.18	.04
	TOT				1.23	TOT	-.23	4.18	.04
Total H	KIN				1.47	KIN	1.47		1.47
	MA				-1.10	SMA	-1.10		-1.10
	OEI				.12	OEI	.12	4.59	-1.00
	TOT				.47	TOT	.47	4.59	-1.00

INTERATOMIC ENERGY CONTRIBUTIONS OF BH, BAO

Orbital Pair B H	Quasiclassical Electrostatic				Sharing					Interference			Totals	
	QCN	QCT	QC(N+T)	QC(N-T)	SPN	Penetration SPT	SP(N+T)	SIN	SIT	SI(N+T)	N	T	N+T	
i h	KIN							.00		.00	.00	.00	.00	
	SMA	-.04	.00	-.03	-.07	.00	.00	.00	.31	.00	.00	.00	.00	
	OEI		.00	.00	.00	.00	.00	.00	-.10	.00	.00	.00	.00	
TOT	-.04	-.03	-.07	.00	.00	.00	.00	.22	.00	.00	.00	.00	.00	
f h	KIN							2.66		2.66	2.66	2.66	2.66	
	SMA	.48	.00	-.73	-.24	.16	.41	.57	1.30	-.78	.02	.03	.56	
	OEI		-.02	-.02	-.02	.16	.41	.57	.27	.00	.00	.00	.00	
TOT	.48	-.74	-.26	.16	.41	.57	3.10	.05	.00	3.15	3.74	-.28	3.46	
b h	KIN							-6.73		-6.73	-6.73	-6.73	-6.73	
	SMA	-2.34	.25	-.20	-1.90	-7.18	.69	-6.49	1.80	-.36	-.02	.00	1.49	
	OEI		-.12	-.12	-.12	-7.18	.69	-6.49	.04	.00	.00	.00	.00	
TOT	-2.34	.32	-2.02	-7.18	.69	-6.49	-5.25	.06	.00	-5.15	-14.77	1.07	-13.70	
Bond Total	KIN							-4.07		-4.07	-4.07	-4.07	-4.07	
	SMA	-1.90	.25	-.56	-2.21	-7.02	1.10	-5.92	3.41	-1.15	-.00	.11	2.36	
	OEI		-.14	-.14	-.14	-7.02	1.10	-5.92	.13	.00	.00	.00	.00	
	TOT	-1.90	-.45	-2.35	-7.02	1.10	-5.92	-1.94	.11	.00	-1.83	-10.06	.76	-10.10

Figure 12 (Continued)

BINDING ENERGY PARTITIONING

		Promotion		Quasi-classical		Sharing Penetration		Sharing Interference		TOTAL
		PRH	PRC	QCN	QCT	SPN	SPT	SIN	SIT	
B	KIN	- .80	- .06		- .50					- 1.36
	SNA	1.27	-1.53		.33					.77
	OEI	.25	1.77		.00	3.27	16			6.15
	TOT	1.42	.14		- .10	3.27	16			5.57
H	KIN	.00	5.53		.45					5.98
	SNA	.00	-5.06		- .27					- 5.35
	OEI	.00	.00		.01	4.09	- 27			4.43
	TOT	.00	.47		.17	4.09	- 27			5.06
BOND	KIN							-6.21		- 6.21
	SNA			-1.76	- .07			2.62	.02	.80
	OEI				- .01	-6.60	.00	- .08		- 6.69
	TOT			-1.76	- .08	-6.60	.00	-4.37	.02	-12.79
BH	KIN	- .80	5.47		- .05			-6.21		- 2.29
	SNA	1.27	-6.05	-1.76	.03			2.62	.02	- 3.78
	OEI	.25	1.77		.00	2.06	- 11	- .08		3.83
	TOT	1.42	.59	-1.76	- .02	2.06	- 11	-4.37	.02	-2.16

DENSITY PARTITIONING FOR VALENCE AO'S

	Atomic Orbitals			Overlap	Bondorders and Populations					
	σ	π	σ^*	$S_{(B,H)}$	p	v	q	q^N	q^T	$P_{(B,H)}$
i	.973727	-.212751	.081189	.000000	2.000	.000	2.000	2.000	.000	.000
l	.227053	.889038	-.417105	.232642	2.103	-.074	2.029	2.032	-.004	-.309
b	.017290	.424581	.705225	.686640	.542	.496	.948	.968	-.020	.592
h		(unhybridized)		-	.692	.332	1.024	1.000	.024	-

EXCHANGE CONTRIBUTIONS TO PAIR POPULATIONS

		B			H
		i	l	b	h
i	PR	2.000	.000	.000	-
	SPN	.000	.000	.000	.000
	SPT	.000	.000	.000	.000
	TOT	2.000	.000	.000	.000
l	PR	.000	2.077	-.044	-
	SPN	.000	-.002	.036	-.034
	SPT	.000	.003	.000	-.007
	TOT	.000	2.077	-.008	-.041
b	PR	.000	-.044	1.012	-
	SPN	.000	.036	-.536	.499
	SPT	.000	.000	-.024	.004
	TOT	.000	-.008	.452	.503
h	PR	-	-	-	1.000
	SPN	.000	-.034	.499	-.465
	SPT	.000	-.007	.004	.027
	TOT	.000	-.041	.503	.561

Figure 13. Binding energy decomposition and description of electron distribution for BH, BMAO approximation

INTRA-ATOMIC ENERGY CONTRIBUTIONS OF BH, BMAU

Orbital	Promotion								Total PRC	PR(H+C)	Orbital	Quasi-classical QCT	Sharing Penetration SPT		SP+QC Total	
	PRH ^k	PRC	PRH ^s	PRC	PRH ^o	PRC	PRH	PRC					SPN	SPT		
B k	KIN	.40	-.28	.09	-.00	.00	.00	.40	.28	.68	B i	KIN	.00			.00
	SMA	-.86	-.30	-.09	-.00	.00	.00	-.86	-.30	-1.16		SMA	.00			.00
	OEI	-.02	.04	-2.76	-1.02	2.66	1.62	.05	.06	.11		OEI	.00	-.00	.00	-.00
	TOT	-.48	.02	-2.77	-1.02	2.66	1.62	-.41	.04	-.37		TOT	.00	-.00	.00	-.00
B s	KIN	.09	-.00	-4.56	-4.57	.00	.00	-4.38	-4.57	-8.96	B l	KIN	-.04			-.04
	SMA	-.09	.00	16.17	7.09	.00	.00	15.99	7.09	23.07		SMA	.06			.06
	OEI	-2.76	-1.02	-1.16	-.32	-.68	.31	-4.96	-2.99	-7.85		OEI	.00	-.00	-.02	-.03
	TOT	-2.77	-1.02	10.46	2.20	-.68	.31	6.65	-.38	6.27		TOT	.02	-.00	-.02	-.01
B o	KIN	.00	.00	.00	.00	3.18	4.24	3.18	4.24	7.42	B b	KIN	-.46			-.46
	SMA	-.00	-.00	-.00	-.00	-13.15	-8.38	-13.15	-8.38	-21.53		SMA	.34			.34
	OEI	2.66	1.62	-.68	.31	2.97	.22	5.15	4.60	9.75		OEI	.00	3.97	.18	4.16
	TOT	2.66	1.62	-.68	.31	-7.00	-3.93	-4.92	.45	-4.36		TOT	-.12	3.97	.18	4.03
Total B											Total B	KIN	-.50			-.50
												SMA	.39			-.39
												OEI	.00	3.97	.16	4.14
												TOT	-.10	3.97	.16	4.03
Total H											Total H	KIN	.45			.45
												SMA	-.29			-.29
												OEI	.01	4.69	-.27	4.43
												TOT	.17	4.69	-.27	4.59

INTERATOMIC ENERGY CONTRIBUTIONS OF BH, BMAU

Orbital Pair B H	Quasiclassical Electrostatic			Sharing				Interference			Totals	
	QCEN	QCT	QC(N+T)	SPN	SPT	SP(N+T)	SIN	SIT	SI(N+T)	N	T	N+T
i h	KIN						.00		.00	.00	.00	.00
	SMA	-.03	.00	-.01	-.04		.19	.00	.00	.00	.19	-.16
	OEI		.00		.00	.00	-.07			-.07	-.07	-.01
	TOT	-.03		-.01	-.04	.00	.12		.00	.12	.09	-.01
l h	KIN						2.42			2.42	2.42	2.42
	SMA	.22	.00	-.17	-.05		.60	-.63	.00	.01	-.02	.19
	OEI		-.00		-.00	.35	.06	.41		-.05	.29	-.06
	TOT	.22		-.17	-.05	.35	.06	.41		2.34	2.90	-.10
b h	KIN						-9.33			-9.33	-9.33	-9.33
	SMA	-1.94	.04	.06	-1.84		2.12	.33	-.00	.01	2.46	.11
	OEI		-.01		-.01	-6.95	-.06	-7.01		.04	-6.91	-.06
	TOT	-1.94		.10	-1.85	-6.95	-.06	-7.01		-6.83	-15.73	.05
Bond Total	KIN						-6.91			-6.91	-6.91	-6.91
	SMA	-1.76	.04	-.11	-1.83		2.92	-.30	-.00	.02	2.63	-.05
	OEI		-.01		-.01	-6.60	.00	-6.60		-.08	-6.68	-.01
	TOT	-1.76		-.08	-1.84	-6.60	.00	-6.60		-4.37	-12.73	-.06

Figure 13 (Continued)

Figure 14. Binding energy decomposition and description of electron distribution for NH^+ , SAO approximation

BINDING ENERGY PARTITIONING

		Promotion		Quasi-classical		Sharing Penetration		Sharing Interference		TOTAL
		PRH	PRC	QCN	QCT	SPN	SPT	SIN	SIT	
N	KIN	- 5.13	-		27.22					22.09
	NA	17.24	-		-26.86					- 9.62
	OEI	7.97	-		2.06	12.26	-12.71			9.58
	TOT	20.07	-		2.42	12.26	-12.71			22.04
H	KIN	-	-		- 6.26					- 6.26
	SNA	-	-		4.70					4.70
	OEI	-	-		1.80	10.62	- 3.36			9.06
	TOT	-	-		24	10.62	- 3.36			7.49
BOND	KIN							-14.93		-14.93
	SNA			-1.17	1.38			7.12	.12	7.44
	OEI				- 2.80	-16.51	11.31	- .31		- 8.30
	TOT			-1.17	- 1.43	-16.51	11.31	- 8.12	.12	-15.80
NH	KIN	- 5.13	-		20.26			-14.93		.90
	SNA	17.24	-	-1.17	-20.78			7.12	.12	2.52
	OEI	7.97	-		1.06	6.37	- 4.76	- .31		10.34
	TOT	20.07	-	-1.17	1.23	6.37	- 4.76	- 8.12	.12	13.73

DENSITY PARTITIONING FOR VALENCE AO'S

	Atomic Orbitals			Overlap		Bondorders and Populations				
	k	s	σ	$S_{(N,H)}$	p	v	q	q^N	q^T	$P_{(N,H)}$
i	.999821	-.018267	-.004915	.052271	2.004	-.002	2.001	1.398	.004	-.045
b	.018866	.982294	.186324	.590041	1.153	.307	1.459	1.002	.457	.520
l	.001423	-.186453	.982463	.292040	.000	.000	.000	.000	.000	.000
π		(unhybridized)		0	2.000	.000	2.000	2.000	.000	.000
h		(unhybridized)		-	.235	.304	.540	1.000	-.460	-

EXCHANGE CONTRIBUTIONS TO PAIRPOPULATIONS

		N				H
		i	b	l	π	h
i	PR	2.003	-.005	.000	.000	-
	SPN	.000	.005	.000	.000	-.005
	SPT	.000	.000	.000	.000	.004
	TOT	2.003	.000	.000	.000	-.001
b	PR	-.005	1.008	.000	.000	-
	SPN	.005	-1.260	.000	.000	1.255
	SPT	.000	1.317	.000	.000	-.860
	TOT	.000	1.065	.000	.000	.395
l	PR	.000	.000	.000	.000	-
	SPN	.000	.000	.000	.000	.000
	SPT	.000	.000	.000	.000	.000
	TOT	.000	.000	.000	.000	.000
π	PR	.000	.000	.000	2.000	-
	SPN	.000	.000	.000	.000	.000
	SPT	.000	.000	.000	.000	.000
	TOT	.000	.000	.000	2.000	.000
h	PR	-	-	-	-	1.000
	SPN	-.005	1.255	.000	.000	-1.249
	SPT	.004	-.860	.000	.000	.396
	TOT	-.001	.395	.000	.000	.146

INTRAMOLECULAR ENERGY CONTRIBUTIONS OF MH⁺, SAO

Orbital	Promotion						Total	Orbital	Quasi-classical QCT	Sharing Penetration		SP+QC Total
	k	s	σ	π	π̄	π̄				SPM	SPT	
KIN	-1.56	2.92	.00	.00	.00	.00	-1.54	KIN	2.18			2.18
NA	3.25	-3.05	.00	.00	.00	.00	3.24	SMA	-3.26			-3.26
OEI	-1.31	-26.79	-25.29	26.14	26.14	-65	-65	OEI	.02	.11	.01	.14
TOT	1.38	-26.92	-25.29	26.14	26.14	-1.05	-1.05	TOT	-1.06	.11	.01	-.94
KIN	2.92	-62.94	.00	.00	.00	.00	-57.12	KIN	25.84			25.84
NA	-3.05	212.23	.00	.00	.00	.00	206.15	SMA	-23.68			-23.68
OEI	-26.79	-17.64	-17.96	-7.72	-7.72	-150.05	-150.05	OEI	2.84	12.16	-12.72	1.48
TOT	-26.92	131.66	-17.96	-7.72	-7.72	-1.01	-1.01	TOT	3.48	12.16	-12.72	2.91
KIN	.00	.00	-49.92	.00	.00	.00	-49.92	KIN	.00			.00
NA	.00	.00	179.20	.00	.00	.00	179.20	SMA	.00			.00
OEI	-25.29	-17.96	1.70	-8.35	-8.35	-126.98	-126.98	OEI	.00	-.00	.00	-.00
TOT	-25.29	-17.96	130.98	-8.35	-8.35	2.30	2.30	TOT	.00	-.00	.00	-.00
KIN	.00	.00	.00	51.72	.00	.00	51.72	KIN	.00			.00
NA	.00	.00	.00	-185.68	.00	.00	-185.68	SMA	.00			.00
OEI	26.14	-7.72	-8.35	28.49	27.51	142.82	142.82	OEI	.00	-.00	.00	-.00
TOT	26.14	-7.72	-8.35	-113.46	27.51	8.87	8.87	TOT	.00	-.00	.00	-.00
KIN	.00	.00	.00	.00	51.72	.00	51.72	KIN	.00			.00
NA	.00	.00	.00	.00	-185.68	.00	-185.68	SMA	.00			.00
OEI	26.14	-7.72	-8.35	27.51	20.49	142.82	142.82	OEI	.00	-.00	.00	-.00
TOT	26.14	-7.72	-8.35	27.51	-113.46	8.87	8.87	TOT	.00	-.00	.00	-.00
Total								Total				
M KIN							-5.13	M KIN	27.22			27.22
NA							17.24	SMA	-26.86			-26.86
OEI							7.97	OEI	2.86	12.26	-12.71	1.61
TOT							20.07	TOT	2.42	12.26	-12.71	1.97
Total								Total				
H KIN							-6.26	H KIN	-6.26			-6.26
NA							4.70	SMA	4.70			4.70
OEI							1.00	OEI	1.00	10.62	-3.36	9.06
TOT							2.44	TOT	2.44	10.62	-3.36	7.49

INTERATOMIC ENERGY CONTRIBUTIONS OF MH⁺, SAO

Orbital Pair	Quasiclassical Electrostatic				Sharing				Interference				Totals	
	QCN	QCT	QC(M+T)	QC(N+T)	SPM	SP2	SP(N+T)	SIM	SIT	SI(N+T)	M	T	N+T	
KIN								1.50			1.50			1.50
SMA	-.04	-.00	.02	-.02	.07	-.05	.02	-.02	-.03	-.02	-.00	-.06	-.09	.00
OEI		-.02		-.02				-.01				-.01	-.06	-.07
TOT	-.04	-.00	.02	-.05	.07	-.05	.02	1.44		-.02		1.42	1.47	-.07
KIN								-16.43				-16.43	-16.43	-16.43
SMA	-1.32	-.96	-.11	-2.39	-16.58	11.36	-5.21	10.10	.27	.21	-.08	-16.43	9.05	-.93
OEI		-2.78		-2.78				-.03				-16.54	8.38	-7.96
TOT	-1.32	-3.85		-5.17	-16.58	11.36	-5.21	-6.02		.13		-5.89	-23.92	7.65
KIN								.00				.00	.00	.00
SMA	.00	.00	.00	.00	.00	.00	.00	.00	.00	.00	.00	.00	.00	.00
OEI		.00		.00				.00				.00	.00	.00
TOT	.00	.00	.00	.00	.00	.00	.00	.00	.00	.00	.00	.00	.00	.00
KIN								.00				.00	.00	.00
SMA	.10	.00	1.21	1.30	.00	.00	.00	-1.60	.00	.00	.00	-1.60	-1.51	1.21
OEI		.00		.00	.00	.00	.00	-.17				-.17	-.17	.00
TOT	.10	.00	1.21	1.30	.00	.00	.00	-1.77	.00	.00	.00	-1.77	-1.67	1.21
KIN								.00				.00	.00	.00
SMA	.10	.00	1.21	1.30	.00	.00	.00	-1.60	.00	.00	.00	-1.60	-1.51	1.21
OEI		.00		.00	.00	.00	.00	-.17				-.17	-.17	.00
TOT	.10	.00	1.21	1.30	.00	.00	.00	-1.77	.00	.00	.00	-1.77	-1.67	1.21
Bond								-14.93				-14.93	-14.93	-14.93
Total								6.88	.24	.20	-.08	-14.93	7.24	5.95
KIN								-.31				-.31	-16.81	8.51
SMA	-1.17	-.96	2.34	-.20	-16.51	11.31	-5.19	-8.12				-8.00	-25.80	10.00
OEI		-2.80		-2.80										
TOT	-1.17	-1.43	2.60	-2.60	-16.51	11.31	-5.19	-8.12		.12		-8.00	-25.80	10.00

Figure 14 (Continued)

Figure 15. Binding energy decomposition and description of electron distribution for NH^+ , BAO approximation

BINDING ENERGY PARTITIONING

		Promotion		Quasi-classical		Sharing Penetration		Sharing Interference		TOTAL
		PRH	PRC	QCN	QCT	SPN	SPT	SIN	SIT	
N	KIN	- 3.82	-		27.98					24.16
	NA	16.29	-		-28.02					-11.73
	OEI	7.10	-		2.42	11.92	-12.99			8.46
	TOT	11.57	-		2.38	11.92	-12.99			20.89
H	KIN	-	-		- 6.84					- 6.84
	SNA	-	-		5.13					5.13
	OEI	-	-		2.15	10.48	- 3.04			9.59
	TOT	-	-		.44	10.48	- 3.04			7.88
BOND	KIN							-13.64		-13.64
	SNA			-1.18	1.56			6.30	.12	6.81
	OEI			-1.18	- 3.34	-16.28	11.36	- .27		- 8.53
	TOT			-1.18	- 1.77	-16.28	11.36	- 7.60	.12	-15.36
NH	KIN	- 3.82	-		21.14			-13.64		3.68
	SNA	16.29	-	-1.18	-21.33			6.30	.12	.21
	OEI	7.10	-		1.23	6.12	- 4.67	- .27		9.52
	TOT	11.57	-	-1.18	1.05	6.12	- 4.67	- 7.60	.12	13.41

DENSITY PARTITIONING FOR VALENCE AO'S

	Valence Atomic Orbitals			Overlap	Bondorders and Populations					
	k	s	σ	$S_{(N,H)}$	p	v	q	q^N	q^T	$P_{(N,H)}$
i	.779739	-.022175	-.005484	.050326	2.003	-.002	2.001	1.998	.004	-.041
b	.022811	.981612	.188480	.597723	1.206	.296	1.502	1.002	.499	.495
l	.001205	-.188556	.982062	.297275	.000	.000	.000	.000	.000	.000
π		(unhybridized)		0	2.000	.000	2.000	2.000	.000	.000
h		(unhybridized)		-	.204	.294	.497	1.000	-.503	-

EXCHANGE CONTRIBUTIONS TO PAIRPOPULATIONS

		N				H
		i	b	l	π	h
i	PR	2.003	-.005	.000	.000	-
	SPN	.000	.005	.000	.000	-.005
	SPT	.000	.000	.000	.000	.004
	TOT	2.003	.000	.000	.000	-.001
b	PR	-.005	1.007	.000	.000	-
	SPN	.005	-1.243	.000	.000	1.238
	SPT	.000	1.363	.000	.000	-.864
	TOT	.000	1.127	.000	.000	.374
l	PR	.000	.000	.000	.000	-
	SPN	.000	.000	.000	.000	.000
	SPT	.000	.000	.000	.000	.000
	TOT	.000	.000	.000	.000	.000
π	PR	.000	.000	.000	2.000	-
	SPN	.000	.000	.000	.000	.000
	SPT	.000	.000	.000	.000	.000
	TOT	.000	.000	.000	2.000	.000
h	PR	-	-	-	-	1.000
	SPN	-.005	1.238	.000	.000	-1.233
	SPT	.004	-.864	.000	.000	.357
	TOT	-.001	.374	.000	.000	.124

INTRA-ATOMIC ENERGY CONTRIBUTIONS OF NH', BAO

Orbital	Promotion						Total	Orbital	Quasi-classical QCI	Sharing Penetration SPT		SP+QC Total
	k	s	σ	π	π'	π''				SPT	SPT'	
N k	KIN	-1.68	3.48	.00	.00	.00	-1.66	KIN	2.13			2.13
	NA	3.53	-3.65	.00	.00	.00	3.51	SNA	-3.22			-3.22
	OEI	-.30	-26.44	-24.85	25.70	25.70	-.66	OEI	.02	.09	.01	.12
	TOT	1.55	-26.62	-24.85	25.70	25.70	1.19	TOT	-1.05	.09	.01	-.95
N s	KIN	3.48	-60.86	.00	.00	.00	-53.93	KIN	25.84			25.84
	NA	-3.65	269.12	.00	.00	.00	261.82	SNA	-24.81			-24.81
	OEI	-26.44	-17.53	-17.70	-.77	-.77	-152.69	OEI	2.42	11.94	-13.00	1.24
	TOT	-26.62	130.71	-17.70	-.77	-.77	-4.81	TOT	3.43	11.94	-13.00	2.27
N σ	KIN	.00	.00	-48.21	.00	.00	-48.21	KIN	.00			.00
	NA	.00	.00	176.22	.00	.00	176.22	SNA	.00			.00
	OEI	-24.85	-17.70	1.67	-8.19	-8.19	-124.80	OEI	.00	-.00	.00	-.00
	TOT	-24.85	-17.70	129.49	-8.19	-8.19	3.22	TOT	.00	-.00	.00	-.00
N π	KIN	.00	.00	.00	49.99	.00	49.99	KIN	.00			.00
	NA	.00	.00	.00	-182.53	.00	-182.53	SNA	.00			.00
	OEI	25.70	-.77	-8.19	20.12	27.04	142.63	OEI	.00	-.00	.00	-.00
	TOT	25.70	-.77	-8.19	-112.44	27.04	18.09	TOT	.00	-.00	.00	-.00
N π'	KIN	.00	.00	.00	49.99	.00	49.99	KIN	.00			.00
	NA	.00	.00	.00	-182.53	.00	-182.53	SNA	.00			.00
	OEI	25.70	-.77	-8.19	27.04	27.04	142.63	OEI	.00	-.00	.00	-.00
	TOT	25.70	-.77	-8.19	27.04	-112.44	18.09	TOT	.00	-.00	.00	-.00
Total N	KIN						-3.82	KIN	27.98			27.98
	NA						16.29	SNA	-28.02			-28.02
	OEI						7.10	OEI	2.42	11.92	-12.99	1.36
	TOT						19.57	TOT	2.38	11.92	-12.99	1.32
Total H	KIN						-6.84	KIN				-6.84
	NA						5.13	SNA				5.13
	OEI						2.15	OEI	12.48	-3.24		9.59
	TOT						.44	TOT	12.48	-3.24		7.88

INTERATOMIC ENERGY CONTRIBUTIONS OF NH', BAO

Orbital Pair N H	Quasi-classical Electrostatic			Sharing				Interference			Totals		
	QCN	QCT	QC(N+T)	SPN	Penetration SPT	SP(N+T)	SIN	Interference SII	SI(N+T)	M	T	N+T	
i m	KIN						1.29			1.29			1.29
	SNA	-.05	-.00	.03	-.02		.09	-.02	-.02	.04	.02	.00	.02
	OEI		-.02	-.02	.07	-.05	.02	-.01		-.01	.06	-.07	-.01
	TOT	-.05	-.02	-.04	.07	-.05	.02	1.35	-.02	1.33	1.37	-.07	1.30
b h	KIN						-14.93			-14.93			-14.93
	SNA	-1.34	-1.06	-.11	-2.52		9.04	.26	.22	7.96	-1.04		6.92
	OEI		-3.31	-3.31	-16.35	11.41	-4.94	.83		.03	-16.32	8.09	-8.23
	TOT	-1.34	-4.49	-5.83	-16.35	11.41	-4.94	-5.62	.14	-5.47	-23.29	7.85	-16.24
f h	KIN						.00			.00	.00		.00
	SNA	.00	.00	.00	.00		.00	.00	.00	.00	.00	.00	.00
	OEI	.00	.00	.00	.00	.00	.00	.00	.00	.00	.00	.00	.00
	TOT	.00	.00	.00	.00	.00	.00	.00	.00	.00	.00	.00	.00
rr h	KIN						.00			.00	.00		.00
	SNA	.10	.02	1.36	1.46		-1.53	.00	.00	-.00	-1.42	1.36	-.06
	OEI		.00	.00	.00	.00	-.15		.00	-.15	-.15	.02	-.15
	TOT	.10	1.36	1.46	.00	.00	-.00	-1.67	.00	-1.67	-1.57	1.36	-.21
π h	KIN						.00			.00	.00		.00
	SNA	.10	.00	1.36	1.46		-1.53	.00	.00	-.00	-1.42	1.36	-.06
	OEI		.00	.00	.00	.00	-.15		.00	-.15	-.15	.02	-.15
	TOT	.10	1.36	1.46	.00	.00	-.00	-1.67	.00	-1.67	-1.57	1.36	-.21
Bond Total	KIN						-13.64			-13.64			-13.64
	SNA	-1.18	-1.07	2.63	-.39		6.07	.23	.20	6.42	5.13	1.69	6.81
	OEI		-3.34	-3.34	-16.28	11.36	-4.93	-.27		-.27	-16.55	8.22	-8.53
	TOT	-1.18	-1.77	-2.95	-16.28	11.36	-4.93	-7.60	.12	-7.48	-25.06	9.71	-15.36

Figure 15 (Continued)

Figure 16. Binding energy decomposition and description of electron distribution for NH^+ , BMAO approximation

BINDING ENERGY PARTITIONING

		Promotion		Quasi-classical		Sharing Penetration		Sharing Interference		TOTAL
		PRH	PRC	QCN	QCT	SPN	SPT	SIN	SIT	
N	KIN	- 4.16	-25.56		35.04					5.32
	SNA	16.61	50.96		-36.32					31.25
	OEI	5.48	-25.12		3.70	11.66	-14.53			-12.80
	TOT	17.94	.28		2.42	11.66	-14.53			17.75
H	KIN	.00	13.43		-16.72					- 3.29
	SNA	.00	-11.14		8.90					- 2.24
	OEI	.00	.00		4.59	14.34	- 3.23			15.69
	TOT	.00	2.28		- 3.24	14.34	- 3.23			10.15
BOND	KIN							-14.29		-14.29
	SNA			-1.07	3.13			6.21	.11	8.37
	OEI				- 5.42	-16.95	12.58	- .11		- 9.90
	TOT			-1.07	- 2.29	-16.95	12.58	- 8.20	.11	-15.82
NH	KIN	- 4.16	-12.13		18.32			-14.29		-12.26
	SNA	16.61	32.82	-1.07	-24.29			6.21	.11	37.38
	OEI	5.46	-25.12		2.87	9.05	- 5.18	- .11		-13.01
	TOT	17.94	2.56	-1.07	- 3.11	9.05	- 5.18	- 8.20	.11	12.08

DENSITY PARTITIONING FOR VALENCE AO'S

	Valence Atomic Orbitals			Overlap S(N, H)	Bondorders and Populations					
	k	s	σ		p	v	q	q^N	q^T	$P_{(N, H)}$
i	.999761	-.021121	-.005638	.037489	2.002	-.001	2.001	1.998	.003	-.030
b	.021798	.982665	.184102	.505593	1.387	.231	1.618	1.002	.616	.457
l	.001652	-.164180	.982891	.312673	.000	.000	.000	.000	.000	.000
π		(unhybridized)		0	2.000	.000	2.000	2.000	.000	.000
h		(unhybridized)		-	.151	.230	.381	1.000	-.619	-

EXCHANGE CONTRIBUTIONS TO PAIRPOPULATIONS

		N				H
		i	b	l	π	h
i	PR	2.002	-.004	.000	.000	-
	SPN	.000	.004	.000	.000	-.004
	SPT	.000	.000	.000	.000	.003
	TOT	2.001	.000	.000	.000	-.001
b	PR	-.004	1.006	.000	.000	-
	SPN	.004	-1.204	.000	.000	1.200
	SPT	.000	1.507	.000	.000	-.891
	TOT	.000	1.309	.000	.000	.309
l	PR	.000	.000	.000	.000	-
	SPN	.000	.000	.000	.000	.000
	SPT	.000	.000	.000	.000	.000
	TOT	.000	.000	.000	.000	.000
π	PR	.000	.000	.000	2.000	-
	SPN	.000	.000	.000	.000	.000
	SPT	.000	.000	.000	.000	.000
	TOT	.000	.000	.000	2.000	.000
h	PR	-	-	-	-	1.000
	SPN	-.004	1.200	.000	.000	-1.197
	SPT	.003	-.891	.000	.000	.270
	TOT	-.001	.309	.000	.000	.073

Figure 16 (Continued)

INTRA-ATOMIC ENERGY CONTRIBUTIONS OF NH⁺, BMAU

Orbital	Promotion												Total PRC	PR(H+C)	Orbital	Quasi-classical			SP+QC Total	
	PRH ^k	PRC	PRH ^a	PRC	PRH ^o	PRC	PRH ^r	PRC	PRH ^w	PRC	PRH	PRC				QCT	SPN	SPT		
KIN	-1.67	1.95	3.30	-.05	.00	.00	.00	.00	.00	.00	.00	-1.65	1.99	.23	KIN	1.81			1.81	
NA	3.91	-1.94	-3.46	-.06	.00	.00	.00	.00	.00	.00	.00	3.49	-1.97	1.52	SMA	-2.74			-2.74	
OEI	-.28	.21	-26.47	.25	-24.89	.08	25.70	-3.84	25.70	-3.84	.63	-.39	-.24	.02	OEI	.02	.06	.01	.09	
TOT	1.36	.12	-26.64	-.25	-24.89	.08	25.70	-3.84	25.70	-3.84	1.20	.31	1.51	TOT	-.91	.06	.01	-.84		
KIN	3.30	.05	-28.77	1.69	.00	.00	.00	.00	.00	.00	-54.28	1.77	-52.43	KIN	33.23			33.23		
NA	-3.46	-.06	288.77	-2.32	.00	.00	.00	.00	.00	.00	281.97	-2.60	199.27	SMA	-33.53			-33.53		
OEI	-26.47	.25	-17.95	.07	-17.70	-.00	-.92	-.59	-.92	-.59	-171.50	1.00	-170.51	OEI	3.68	11.68	-14.54	.75		
TOT	-26.64	.25	130.06	-.75	-17.70	-.00	-.92	-.59	-.92	-.59	-23.93	.17	-23.66	TOT	3.32	11.68	-14.54	.39		
KIN	.00	.00	.00	.00	-48.29	.33	.00	.00	.00	.00	-48.29	.33	-47.95	KIN	.00			.00		
NA	.00	.00	.00	.00	176.32	-.78	.00	.00	.00	.00	176.32	-.98	175.74	SMA	.00			.00		
OEI	-24.89	.08	-17.70	-.00	1.67	-.00	-8.22	-.00	-8.22	-.00	-129.03	.12	-128.91	OEI	.00	-.00	.00	-.00		
TOT	-24.89	.08	-17.70	-.00	129.70	-.25	-8.22	-.00	-8.22	-.00	3.01	-.15	2.86	TOT	.00	-.00	.00	-.00		
KIN	.00	.00	.00	.00	.00	.00	49.99	-14.77	.00	.00	49.99	-14.77	35.21	KIN	.00			.00		
NA	.00	.00	.00	.00	.00	.00	-182.53	28.05	.00	.00	-182.53	28.05	-154.48	SMA	.00			.00		
OEI	25.70	-3.84	-.92	-.59	-8.22	-.00	19.92	-1.41	27.04	-2.76	151.32	-13.31	138.01	OEI	.00	-.00	.00	-.00		
TOT	25.70	-3.84	-.92	-.59	-8.22	-.00	27.04	-2.76	11.86	27.04	18.78	-.03	18.74	TOT	.00	-.00	.00	-.00		
KIN	.00	.00	.00	.00	.00	.00	49.99	-14.77	.00	.00	49.99	-14.77	35.21	KIN	.00			.00		
NA	.00	.00	.00	.00	.00	.00	-182.53	28.05	.00	.00	-182.53	28.05	-154.48	SMA	.00			.00		
OEI	25.70	-3.84	-.92	-.59	-8.22	-.00	27.04	-2.76	11.86	27.04	18.78	-.03	18.74	OEI	.00	-.00	.00	-.00		
TOT	25.70	-3.84	-.92	-.59	-8.22	-.00	27.04	-2.76	-112.63	11.96	18.78	-.03	18.74	TOT	.00	-.00	.00	-.00		
Total															Total					
KIN															KIN	35.04			35.04	
NA													-4.16	-25.96	-29.72	SMA	-36.32			-36.32
OEI													16.61	50.96	67.57	OEI	3.70	11.66	-14.53	.83
TOT													5.48	-25.12	-19.63	TOT	2.42	11.66	-14.53	-.46
													17.94	.28	18.21					
Total																Total				
KIN													.00	13.43	13.43	KIN	-16.72			-16.72
NA													.00	-11.14	-11.14	SMA	8.98			8.98
OEI													.00	.00	.00	OEI	4.59	14.34	-3.23	15.69
TOT													.00	2.28	2.28	TOT	-3.24	14.34	-3.23	7.87

INTERATOMIC ENERGY CONTRIBUTIONS OF NH⁺, BMAU

Orbital Pair	Quasi-classical Electrostatic			Sharing						Totals						
	QCN	QCT	QC(H+T)	Penetration		SP(H+T)		Interference		SI(H+T)		N	T	N+T		
1 h	KIN	-.03	-.00	.02	-.01	-.02	.05	-.04	.01	.06	-.02	-.01	-.01	.73	.02	.02
	SMA						.05	-.04	.01	-.02	-.01	-.01	-.01	.02	.00	.02
	OEI						.05	-.04	.01	.77				.05	-.07	-.02
	TOT													.75	-.07	.73
b h	KIN	-.88	-.66	-.37	-1.91	-17.01	12.63	-4.38	7.29	-.97	.19	-.05	8.39	-15.03	7.38	-9.92
	SMA					-17.01	12.63	-4.38	.83	.97	.19	-.05	8.39	7.38	-9.92	6.49
	OEI					-17.01	12.63	-4.38	-.67				-.03	-16.97	7.23	-9.74
	TOT								-6.73		.14		-6.60	-24.62	6.33	-18.28
f h	KIN	.00	.00	.00	.00	.00	.00	.00	.00	.00	.00	.00	.00	.00	.00	.00
	SMA															
	OEI															
	TOT															
w h	KIN	-.09	.00	2.07	1.98	.00	.00	.00	-1.05	.00	.00	.00	-1.05	-.00	-1.14	2.07
	SMA								-.07	.00	.00	.00	-.07	-.07	-.07	.93
	OEI								-1.12		.00	.00	-1.12	-1.21	2.07	-.07
	TOT													-1.21	2.07	.96
w̄ h	KIN	-.09	.00	2.07	1.98	.00	.00	.00	-1.05	.00	.00	.00	-1.05	-.00	-1.14	2.07
	SMA								-.07	.00	.00	.00	-.07	-.07	-.07	.93
	OEI								-1.12		.00	.00	-1.12	-1.21	2.07	-.07
	TOT													-1.21	2.07	.96
Bond	KIN	-1.07	-.66	3.79	2.05				-14.29	.95	.17	-.06	-14.29	-14.29		-14.29
	SMA								6.32				6.32	5.13	3.24	8.37
	OEI								-.11				-.11	-17.86	7.17	-9.98
	TOT								-16.95	12.58	-4.37	-.11	-16.95	-26.23	10.41	-15.82

Figure 17. Binding energy decomposition and description of electron distribution for NH^+ , SAO approximation

BINDING ENERGY PARTITIONING

		Promotion		Quasi-classical		Sharing Penetration		Sharing Interference		TOTAL
		PRH	PRC	QCN	QCT	SPN	SPT	SIN	SIT	
N	KIN	- 5.49	-		27.95					22.46
	NA	17.44	-		-27.47					-10.03
	OEI	7.63	-		2.16	12.19	-12.82			9.15
	TOT	19.57	-		2.64	12.19	-12.82			21.57
H	KIN	-	-		- 6.43					- 6.43
	SNA	-	-		4.83					4.83
	OEI	-	-		1.90	10.64	- 3.33			9.22
	TOT	-	-		.29	10.64	- 3.33			7.61
BOND	KIN							-14.95		-14.95
	SNA			-1.03	1.23			7.12	.15	7.47
	OEI				- 2.78	-15.58	10.76	- .24		- 7.85
	TOT			-1.03	- 1.55	-15.58	10.76	- 8.07	.15	-15.32
NH	KIN	- 5.49	-		21.52			-14.95		1.08
	SNA	17.44	-	-1.03	-21.41			7.12	.15	2.27
	OEI	7.63	-		1.28	7.25	- 5.39	- .24		10.52
	TOT	19.57	-	-1.03	1.39	7.25	- 5.39	- 8.07	.15	13.86

DENSITY PARTITIONING FOR VALENCE AO'S

	Valence Atomic Orbitals			Overlap	Bondorders and Populations					
	k	s	σ	$S_{(N,H)}$	p	v	q	q^N	q^T	$P_{(N,H)}$
i	.799855	-.016544	-.004081	.045305	2.003	-.002	2.001	1.396	.003	-.042
b	.016988	.786442	.163227	.534668	1.186	.286	1.472	1.002	.470	.535
l	.001325	-.163273	.986580	.292164	.000	.000	.000	.000	.000	.000
π		(unhybridized)		0	2.000	.000	2.000	2.000	.000	.000
h		(unhybridized)		-	.243	.254	.527	1.000	-.473	-

EXCHANGE CONTRIBUTIONS TO PAIRPOPULATIONS

		N				H
		i	b	l	π	h
i	PR	2.002	-.004	.000	.000	-
	SPN	.000	.005	.000	.000	-.005
	SPT	.000	.000	.000	.000	.003
	TOT	2.002	.000	.000	.000	-.001
b	PR	-.004	1.007	.000	.000	-
	SPN	.005	-1.261	.000	.000	1.256
	SPT	.000	1.338	.000	.000	-.868
	TOT	.000	1.084	.000	.000	.389
l	PR	.000	.000	.000	.000	-
	SPN	.000	.000	.000	.000	.000
	SPT	.000	.000	.000	.000	.000
	TOT	.000	.000	.000	.000	.000
π	PR	.000	.000	.000	2.000	-
	SPN	.000	.000	.000	.000	.000
	SPT	.000	.000	.000	.000	.000
	TOT	.000	.000	.000	2.000	.000
h	PR	-	-	-	-	1.000
	SPN	-.005	1.256	.000	.000	-1.252
	SPT	.003	-.868	.000	.000	.391
	TOT	-.001	.389	.000	.000	.139

INTRA-ATOMIC ENERGY CONTRIBUTIONS OF NH₃, SAO

Orbital	Promotion						Total	Orbital	Quasi-classical qct	Sharing Penetration SPT		SP+QC Total
	k	s	σ	π	π*	π*				SPT	SPT	
N k	KIN	-1.44	2.65	.02	.02	.02	-1.43	KIN	1.90			1.90
	NA	3.01	-2.77	.02	.02	.02	3.02	SNA	-2.85			-2.85
	OEI	-.26	-26.61	-25.50	26.15	26.15	-5.7	OEI	.02	.10	.01	.13
	TOT	1.31	-26.73	-25.52	26.15	26.15	1.02	TOT	-.92	.10	.01	-.81
N s	KIN	2.65	-62.45	.02	.02	.02	-57.17	KIN	26.05			26.05
	NA	-3.77	216.60	.02	.02	.02	209.88	SNA	-24.62			-24.62
	OEI	-26.61	-17.73	-17.96	-.61	-.61	-157.92	OEI	2.14	12.09	-12.93	1.30
	TOT	-26.73	132.41	-17.96	-.61	-.61	-9.99	TOT	3.56	12.09	-12.93	2.82
N σ	KIN	.02	.02	-52.34	.02	.02	-52.34	KIN	.02			.02
	NA	.02	.02	180.71	.02	.02	182.71	SNA	.02			.02
	OEI	-25.50	-17.96	1.71	-8.50	-8.50	-128.04	OEI	.02	-.02	.02	-.02
	TOT	-25.50	-17.96	132.38	-8.50	-8.50	2.33	TOT	.02	-.02	.02	-.02
N π	KIN	.02	.02	.02	51.72	.02	51.72	KIN	.02			.02
	NA	.02	.02	.02	-185.68	.02	-185.68	SNA	.02			.02
	OEI	26.15	-.61	-8.50	20.45	27.51	147.07	OEI	.02	-.02	.02	-.02
	TOT	26.15	-.61	-8.50	-113.52	27.51	13.12	TOT	.02	-.02	.02	-.02
N π*	KIN	.02	.02	.02	51.72	.02	51.72	KIN	.02			.02
	NA	.02	.02	.02	-185.68	.02	-185.68	SNA	.02			.02
	OEI	26.15	-.61	-8.50	27.51	20.45	147.07	OEI	.02	-.02	.02	-.02
	TOT	26.15	-.61	-8.50	-113.52	27.51	13.12	TOT	.02	-.02	.02	-.02
Total N	KIN						-5.49	KIN	27.95			27.95
	NA						17.44	SNA	-27.47			-27.47
	OEI						7.63	OEI	2.16	12.19	-12.92	1.52
	TOT						19.57	TOT	2.64	12.19	-12.92	2.82
Total H	KIN						-6.43	KIN	-6.43			-6.43
	NA						4.83	SNA	4.83			4.83
	OEI						1.92	OEI	1.92	10.64	-3.33	9.22
	TOT						2.64	TOT	.29	12.64	-3.33	7.61

INTERATOMIC ENERGY CONTRIBUTIONS OF NH₃, SAO

Orbital Pair N H	Quasi-classical Electrostatic				Sharing				Interference			Totals		
	QC(N)	QC(T)	QC(N+T)	QC(N+T)	SPN	Penetration SPT	SP(N+T)	SIN	SIT	SI(N+T)	N	T	N+T	
1 h	KIN	-.03	-.02	.02	-.02			1.19			1.19	1.19		1.19
	SNA				-.02			-.01	-.02		-.02	-.02		-.02
	TOT	-.03	-.02	.02	-.02	.05	-.04	.21	-.23	-.01	-.02	-.01	-.02	-.02
b h	KIN	-.99	-.73	-.12	-1.84			-16.14			-16.14	-16.14		-16.14
	SNA				-2.77			9.63	.47	.22	12.27	9.11	-.68	8.43
	TOT	-.99	-3.61	-4.61	-4.61	-15.64	12.32	-4.84	-.04	.22	-.05	12.27	-15.68	8.03
2 h	KIN	.02	.02	.02	.02			.02			.02	.02		.02
	SNA				.02			.02	.02	.02	.02	.02		.02
	TOT	.02	.02	.02	.02	.02	.02	.02	.02	.02	.02	.02	.02	.02
π h	KIN	.02	.02	1.03	1.03			1.47			1.47	1.47		1.47
	SNA				.02			-.14	.02	.02	-.14	-.14		-.14
	TOT	.02	1.03	1.03	1.03	.02	.02	.22	-.14	.02	1.47	1.03		1.03
π* h	KIN	.02	.02	1.03	1.03			1.47			1.47	1.47		1.47
	SNA				.02			-.14	.02	.02	-.14	-.14		-.14
	TOT	.02	1.03	1.03	1.03	.02	.02	.22	-.14	.02	1.47	1.03		1.03
Bond Total	KIN							-14.95			-14.95	-14.95		-14.95
	SNA	1.03	-.73	1.96	-.21			6.57	.45	.21	7.27	6.09	1.38	7.47
	OEI				-2.78			-.24			-.24	-15.83	7.97	-7.95
	TOT	1.03	-1.95	-2.98	-2.98	-15.58	12.76	-4.82	-8.07	.15	-7.92	-24.68	9.36	-15.32

Figure 17 (Continued)

BINDING ENERGY PARTITIONING

		Promotion		Quasi-classical		Sharing Penetration		Sharing Interference		TOTAL
		PRH	PRC	QCN	QCT	SPN	SPT	SIN	SIT	
N	KIN	- 4.20	-		28.69					24.49
	NA	16.48	-		-28.63					-12.15
	OEI	6.78	-		2.52	11.85	-13.09			8.06
	TOT	19.06	-		2.58	11.85	-13.09			20.40
H	KIN	-	-		- 7.91					- 7.01
	SNA	-	-		5.25					5.25
	OEI	-	-		2.25	10.50	- 3.00			9.75
	TOT	-	-		.50	10.50	- 3.00			8.00
BOND	KIN							-13.69		-13.69
	SNA			-1.04	1.40			6.33	.15	6.85
	OEI				- 3.30	-15.37	10.80	- .21		- 8.08
	TOT			-1.04	- 1.90	-15.37	10.80	- 7.57	.15	-14.92
NH	KIN	- 4.20	-		21.68			-13.69		3.79
	SNA	16.48	-	-1.04	-21.98			6.33	.15	- .05
	OEI	6.78	-		1.47	6.98	- 5.29	- .21		9.73
	TOT	19.06	-	-1.04	1.17	6.98	- 5.29	- 7.57	.15	13.47

DENSITY PARTITIONING FOR VALENCE AO'S

	Valence Atomic Orbitals			Overlap	Bondorders and Populations					
	k	s	σ	S(N, H)	P	v	q	q ^N	q ^T	P(N, H)
i	.999784	-.020294	-.004537	.043615	2.003	-.002	2.001	1.998	.003	-.035
b	.020765	.986065	.165060	.542155	1.238	.276	1.514	1.002	.512	.510
l	.001124	-.165118	.986273	.298061	.000	.000	.000	.000	.000	.000
π		(unhybridized)		0	2.000	.000	2.000	2.000	.000	.000
h		(unhybridized)		-	.210	.275	.485	1.000	-.515	-

EXCHANGE CONTRIBUTIONS TO PAIR POPULATIONS

		N				H
		i	b	l	π	h
i	PR	2.002	-.004	.000	.000	-
	SPN	.000	.004	.000	.000	-.004
	SPT	.000	.000	.000	.000	-.003
	TOT	2.002	.000	.000	.000	-.001
b	PR	-.004	1.006	.000	.000	-
	SPN	.004	-1.244	.000	.000	1.239
	SPT	.000	1.384	.000	.000	-.871
	TOT	.000	1.146	.000	.000	.368
l	PR	.000	.000	.000	.000	-
	SPN	.000	.000	.000	.000	.000
	SPT	.000	.000	.000	.000	.000
	TOT	.000	.000	.000	.000	.000
π	PR	.000	.000	.000	2.000	-
	SPN	.000	.000	.000	.000	.000
	SPT	.000	.000	.000	.000	.000
	TOT	.000	.000	.000	2.000	.000
h	PR	-	-	-	-	1.000
	SPN	-.004	1.239	.000	.000	-1.235
	SPT	.003	-.871	.000	.000	.353
	TOT	-.001	.368	.000	.000	.118

INTRAMOLECULAR ENERGY CONTRIBUTIONS OF NH⁺, BAO

Orbital	Promotion						Total	Orbital	Quasi-classical QCT	Sharing Penetration SPT		SP+QC Total
	k	s	σ	π	π*	π*				SPN	SIT	
N k	KIN -1.54	3.19	.00	.00	.00	.00	-1.52	KIN 1.86				1.86
	NA 3.23	-3.35	.00	.00	.00	.00	3.21	SNA -2.80				-2.80
	OEI -.25	-26.26	-25.06	25.71	25.71	.00	-5.5	OEI .22	.22	.21	.21	.11
	TOT 1.44	-26.42	-25.06	25.71	25.71	.00	1.12	TOT -.92	.28	.21	.21	-.33
N s	KIN 3.19	-60.39	.00	.00	.00	.00	-54.23	KIN 26.83				26.83
	NA -3.35	207.46	.00	.00	.00	.00	207.79	SNA -25.83				-25.83
	OEI -26.26	-17.62	-17.70	-5.6	-5.6	.00	-161.65	OEI 2.50	11.77	-13.12	-13.12	1.17
	TOT -26.42	129.45	-17.70	-6.6	-6.6	.00	-14.93	TOT 3.50	11.77	-13.12	-13.12	2.17
N σ	KIN .00	.00	-48.62	.00	.00	.00	-48.62	KIN .00				.00
	NA .00	.00	177.54	.00	.00	.00	177.54	SNA .00				.00
	OEI -25.06	-17.70	1.65	-8.34	-8.34	.00	-125.87	OEI .00	-1.00	.00	.00	-.00
	TOT -25.06	-17.70	130.60	-8.34	-8.34	.00	3.25	TOT .00	-1.00	.00	.00	-.00
N π	KIN .00	.00	.00	49.99	.00	.00	49.99	KIN .00				.00
	NA .00	.00	.00	-182.53	.00	.00	-182.53	SNA .00				.00
	OEI 25.71	-6.6	-8.34	20.26	27.24	.00	147.46	OEI .00	-1.00	.00	.00	-.00
	TOT 25.71	-6.6	-8.34	-112.48	27.24	.00	14.91	TOT .00	-1.00	.00	.00	-.00
N π*	KIN .00	.00	.00	.00	49.99	.00	49.99	KIN .00				.00
	NA .00	.00	.00	.00	-182.53	.00	-182.53	SNA .00				.00
	OEI 25.71	-6.6	-8.34	27.24	27.24	.00	147.46	OEI .00	-1.00	.00	.00	-.00
	TOT 25.71	-6.6	-8.34	27.24	-112.48	.00	14.91	TOT .00	-1.00	.00	.00	-.00
Total	N KIN						-4.20	Total	N KIN	28.69		28.69
	NA						16.48		SNA	-28.63		-28.63
	OEI						6.78		OEI	2.50	11.35	-13.23
	TOT						19.26		TOT	2.58	11.55	-13.09
												1.14
	H KIN						-7.01	Total	H KIN	-7.01		-7.01
	NA						5.25		SNA	2.25	10.50	-3.20
	OEI						6.78		OEI	2.50	-3.20	5.75
	TOT						5.02		TOT	.50	10.50	-3.20
												2.80

INTERMOLECULAR ENERGY CONTRIBUTIONS OF NH⁺, BAO

Orbital Pair	Quasiclassical Electrostatic				Sharing						Totals				
	QCEN	QCT	QC(N+T)	QC(N+T)	Penetration SPT		Sharing SP(N+T)		Interference SIT		SI(N+T)		N	T	N+T
1 h	KIN -.03	.00	.02	.02	.25	-.24	.21	1.03	-.02	-.21	-.02	1.23	1.23	.02	1.03
	SNA .00				.05	-.24	.21	.05	.01	.01	.01	.02	-.02	.02	-.02
	OEI -.03	-.00	-.03	-.03	.05	-.24	.21	1.02	-.02	-.21	-.02	1.04	1.08	-.06	1.22
	TOT -.03	-.00	-.03	-.03	.05	-.24	.21	1.02	-.02	-.21	-.02	1.04	1.08	-.06	1.22
b h	KIN -1.21	-.91	-.13	-1.95	-15.42	10.24	-4.58	-14.72	.44	.22	-.26	-14.72	-14.72	-7.6	-14.72
	SNA -1.21				-15.42	10.24	-4.58	2.66	.03	.22	-.26	9.27	8.09	7.56	7.56
	OEI -1.01	-3.28	-3.28	-5.23	-15.42	10.24	-4.58	-5.59	.03	.22	-.26	-15.19	-15.19	7.56	-7.52
	TOT -1.01	-4.21	-5.23	-5.23	-15.42	10.24	-4.58	-5.59	.03	.22	-.26	-5.42	-22.02	6.82	-15.23
l h	KIN .00	.00	.00	.00	.00	.00	.00	.00	.00	.00	.00	.00	.00	.00	.00
	SNA .00	.00	.00	.00	.00	.00	.00	.00	.00	.00	.00	.00	.00	.00	.00
	OEI .00	.00	.00	.00	.00	.00	.00	.00	.00	.00	.00	.00	.00	.00	.00
	TOT .00	.00	.00	.00	.00	.00	.00	.00	.00	.00	.00	.00	.00	.00	.00
w h	KIN .01	.00	1.16	1.16	.00	.00	.00	-1.40	.00	.00	.00	-1.40	-1.39	1.16	-.23
	SNA .01	.00	.00	.00	.00	.00	.00	-.12	.00	.00	.00	-.12	-.12	.02	-.12
	OEI .01	1.16	1.16	1.16	.00	.00	.00	-1.52	.00	.00	.00	-1.52	-1.51	1.16	-.36
	TOT .01	1.16	1.16	1.16	.00	.00	.00	-1.52	.00	.00	.00	-1.52	-1.51	1.16	-.36
w h	KIN .01	.00	1.16	1.16	.00	.00	.00	-1.40	.00	.00	.00	-1.40	-1.39	1.16	-.23
	SNA .01	.00	.00	.00	.00	.00	.00	-.12	.00	.00	.00	-.12	-.12	.02	-.12
	OEI .01	1.16	1.16	1.16	.00	.00	.00	-1.52	.00	.00	.00	-1.52	-1.51	1.16	-.36
	TOT .01	1.16	1.16	1.16	.00	.00	.00	-1.52	.00	.00	.00	-1.52	-1.51	1.16	-.36
Bond	KIN							-13.69				-13.69	-13.69		-13.69
Total	SNA	-1.04	-.81	2.21	.37	-15.37	10.82	-4.57	5.91	.42	-.26	6.49	5.12	7.55	6.35
	OEI		-3.30	-3.30		-15.37	10.82	-4.57	5.91	-.21	-.26	6.49	5.12	7.55	6.35
	TOT	-1.04	-1.70	-2.93		-15.37	10.82	-4.57	5.91	-.21	-.26	6.49	5.12	7.55	6.35
										.15		-7.42	-25.57	9.25	-14.92

Figure 18 (Continued)

Figure 19. Binding energy decomposition and description of electron distribution for NH^n , BMAO approximation

BINDING ENERGY PARTITIONING

		Promotion		Quasi-classical		Sharing Penetration		Sharing Interference		TOTAL
		PRH	PRC	QCN	QCT	SPN	SPT	SIN	SIT	
N	KIN	- 4.71	-28.69		36.26					2.87
	SNA	16.98	56.58		-37.75					35.82
	OEI	4.94	-27.48		4.03	11.40	-14.74			-21.84
	TOT	17.21	.42		2.54	11.40	-14.74			16.84
H	KIN	.00	11.46		-16.29					- 4.83
	SNA	.00	- 9.72		9.00					- .72
	OEI	.00	.00		4.87	13.70	- 2.87			15.70
	TOT	.00	1.74		- 2.42	13.70	- 2.87			10.16
BOND	KIN							-13.15		-13.15
	SNA			-.88	2.68			5.87	.14	7.80
	OEI				- 5.56	-15.63	11.83	- .08		- 9.44
	TOT			-.88	- 2.88	-15.63	11.83	- 7.36	.14	-14.78
NH	KIN	- 4.71	-17.23		19.97			-13.15		-15.11
	SNA	16.98	46.86	-.88	-26.07			5.87	.14	42.30
	OEI	4.94	-27.48		3.34	9.47	- 5.78	- .08		-15.58
	TOT	17.21	2.15	-.88	- 2.76	9.47	- 5.78	- 7.36	.14	12.22

DENSITY PARTITIONING FOR VALENCE AO'S

	Valence Atomic Orbitals			Overlap	Bondorders and Populations					
	k	s	σ	$S_{(N,H)}$	p	v	q	q^N	q^T	$P_{(N,H)}$
i	.999816	-.018633	-.004580	.032278	2.001	-.001	2.001	1.998	.003	-.026
b	.019140	.986018	.165536	.462178	1.440	.209	1.649	1.002	.647	.452
l	.001431	-.165593	.986193	.308842	.000	.000	.000	.000	.000	.000
π		(unhybridized)		0	2.000	.000	2.000	2.000	.000	.000
h		(unhybridized)		-	.142	.208	.350	1.000	-.650	-

EXCHANGE CONTRIBUTIONS TO PAIRPOPULATIONS

		N				H
		i	b	l	π	h
i	PR	2.001	-.003	.000	.000	-
	SPN	.000	.003	.000	.000	-.003
	SPT	.000	.000	.000	.000	.003
	TOT	2.001	.000	.000	.000	-.001
b	PR	-.003	1.005	.000	.000	-
	SPN	.003	-1.194	.000	.000	1.190
	SPT	.000	1.548	.000	.000	-.901
	TOT	.000	1.360	.000	.000	.289
l	PR	.000	.000	.000	.000	-
	SPN	.000	.000	.000	.000	.000
	SPT	.000	.000	.000	.000	.000
	TOT	.000	.000	.000	.000	.000
π	PR	.000	.000	.000	2.000	-
	SPN	.000	.000	.000	.000	.000
	SPT	.000	.000	.000	.000	.000
	TOT	.000	.000	.000	2.000	.000
h	PR	-	-	-	-	1.000
	SPN	-.003	1.190	.000	.000	-1.187
	SPT	.003	-.901	.000	.000	.249
	TOT	-.001	.289	.000	.000	.062

Figure 19 (Continued)

INTRA-ATOMIC ENERGY CONTRIBUTIONS OF NH⁺, BH₃

Orbital	Promotion														Orbital	Quasi-classical QCT	Sharing Penetration		SP+QC Total	
	PH ^k	PRC	PH ^a	PRC	PH ^σ	PRC	PH ^π	PRC	PH ^{π'}	PRC	PH	Total PRC	PR(R+C)	SPN			SPT			
KIN	-1.50	1.99	2.91	.02	.00	.00	.00	.00	.00	.00	.00	-1.49	2.02	.53	KIN	1.60			1.60	
NA	3.15	-2.89	-3.06	-.02	.00	.00	.00	.00	.00	.00	.00	3.13	-2.11	1.03	SNA	-2.42			-2.42	
ORI	-.25	.24	-26.35	.09	-25.06	.04	25.71	-4.10	25.71	-4.10	25.71	-4.10	-.57	-.42	-.14	OEI	.02	.05	.08	.08
TOT	1.40	.14	-26.49	.09	-25.06	.04	25.71	-4.10	25.71	-4.10	1.08	.33	1.41		TOT	-.80	.05	.08	-.75	
KIN	2.91	.02	-60.40	-.36	.00	.00	.00	.00	.00	.00	-54.59	.57	-54.01	KIN	34.66			34.66		
NA	-3.06	-.02	207.51	-.05	.00	.00	.00	.00	.00	.00	201.40	-.36	200.54	SNA	-35.32			-35.32		
ORI	-26.35	.09	-18.09	.10	-17.70	-.00	-.87	-.69	-.87	-.69	-136.68	.39	-136.28	OEI	4.01	11.35	-14.74	.62		
TOT	-26.49	.09	129.02	-.19	-17.70	-.00	-.87	-.69	-.87	-.69	-39.96	.10	-39.76	TOT	3.35	11.35	-14.74	-.04		
KIN	.00	.00	.00	.00	-48.61	.16	.00	.00	.00	.00	-48.61	.16	-48.46	KIN	.00			.00		
NA	.00	.00	.00	.00	177.51	-.28	.00	.00	.00	.00	177.51	-.28	177.23	SNA	.00			.00		
ORI	-25.06	.04	-17.70	-.00	1.67	-.00	-8.34	-.01	-8.34	-.01	-125.87	.14	-125.73	OEI	.00	-.00	.00	-.00		
TOT	-25.06	.04	-17.70	-.00	130.57	-.12	-8.34	-.01	-8.34	-.01	3.05	.02	3.05	TOT	.00	-.00	.00	-.00		
KIN	.00	.00	.00	.00	.00	.00	49.99	-15.71	.00	.00	49.99	-15.71	34.27	KIN	.00			.00		
NA	.00	.00	.00	.00	.00	.00	-182.53	29.92	.00	.00	-182.53	29.92	-152.62	SNA	.00			.00		
ORI	25.71	-4.10	-.87	-.69	-8.34	-.01	19.86	-1.50	27.04	-2.94	159.02	-14.22	144.80	OEI	.00	-.00	.00	-.00		
TOT	25.71	-4.10	-.87	-.69	-8.34	-.01	-112.69	12.70	27.04	-2.94	26.48	-.02	26.46	TOT	.00	-.00	.00	-.00		
KIN	.00	.00	.00	.00	.00	.00	49.99	-15.71	.00	.00	49.99	-15.71	34.27	KIN	.00			.00		
NA	.00	.00	.00	.00	.00	.00	-182.53	29.92	.00	.00	-182.53	29.92	-152.62	SNA	.00			.00		
ORI	25.71	-4.10	-.87	-.69	-8.34	-.01	19.86	-1.50	27.04	-2.94	159.02	-14.22	144.80	OEI	.00	-.00	.00	-.00		
TOT	25.71	-4.10	-.87	-.69	-8.34	-.01	-112.69	12.70	27.04	-2.94	26.48	-.02	26.46	TOT	.00	-.00	.00	-.00		
Total															Total					
M KIN															M KIN	36.26			35.26	
MA															SMA	-37.75			-37.75	
ORI															OEI	4.03	11.40	-14.74	.70	
TOT															TOT	2.54	11.40	-14.74	-.79	
Total															Total					
H KIN												.00	11.46	11.46	H KIN	-16.29			-16.29	
NA												.00	-9.72	-9.72	SNA	9.00			9.00	
ORI												.00	.00	.00	OEI	4.87	13.70	-2.87	15.70	
TOT												.00	1.74	1.74	TOT	-2.42	13.70	-2.87	8.42	

INTERATOMIC ENERGY CONTRIBUTIONS OF NH⁺, BH₃

Orbital Pair	Quasi-classical Electrostatic				Sharing						Totals		
	QCN	QCT	QC(M+T)		Penetration		Interference		SI(M+T)		M	T	M+T
KIN													
SNA	-.02	-.00	.02	-.00									
OEI				-.02	.04	-.04	.01	.04	-.01	-.01	-.01	.55	-.55
TOT	-.02			-.02	.04	-.04	.01	.57		-.02		.01	-.01
KIN													
SNA	-.68	-.54	-.16	-1.58									
OEI				-5.54	-15.67	11.00	-3.81	6.75	.25	.18	-.02	-13.71	13.71
TOT	-.68			-6.43	-15.67	11.00	-3.81	5.97		.16	-.02	7.85	-7.85
KIN													
SNA	.00	.00	.00	.00									
OEI				.00	.00	.00	.00	.00	.00	.00	.00	.00	.00
TOT	.00			.00	.00	.00	.00	.00	.00	.00	.00	.00	.00
KIN													
SNA	-.09	.00	1.78	1.69									
OEI				.00	.00	.00	.00	-.93	.00	.00	.00	-.00	.00
TOT	-.09			1.78	.00	.00	.00	-.98	.00	.00	-.00	-1.02	1.78
KIN													
SNA	-.09	.00	1.78	1.69									
OEI				.00	.00	.00	.00	-.93	.00	.00	.00	-.00	.00
TOT	-.09			1.78	.00	.00	.00	-.98	.00	.00	-.00	-1.02	1.78
Bond KIN													
Total SNA	-.08	-.54	3.22	1.80	-15.63	11.00	-3.80	4.93	.04	.17	-.05	-13.15	13.15
OEI				-5.56				-.08				6.00	-6.00
TOT	-.08			-3.75	-15.63	11.00	-3.80	-7.36		.14	-.05	-7.23	-23.87

Figure 20. Binding energy decomposition and description of electron distribution for HF, SAO approximation

BINDING ENERGY PARTITIONING

		Promotion		Quasi-classical		Sharing Penetration		Sharing Interference		TOTAL
		PRH	PRC	QCN	QCT	SPN	SPT	SIN	SIT	
F	KIN	1.88	-		11.90					13.78
	SNA	.45	-		-10.70					-10.25
	OEI	-.11	-		.31	7.01	-1.78			5.44
	TOT	2.22	-		1.51	7.01	-1.78			8.97
H	KIN	-	-		-2.09					-2.09
	SNA	-	-		1.57					1.57
	OEI	-	-		.20	3.33	1.52			5.06
	TOT	-	-		-.32	3.33	1.52			4.53
BOND	KIN							-11.39		-11.39
	SNA			-1.72	.68			6.19	-.29	4.84
	OEI				-.34	-6.14	-.61	-1.14		-8.23
	TOT			-1.72	.33	-6.14	-.61	-6.34	-.29	-14.78
HF	KIN	1.88	-		2.81			-11.39		-.30
	SNA	.45	-	-1.72	-8.45			6.19	-.29	-3.82
	OEI	-.11	-		.17	4.23	-.87	-1.14		2.25
	TOT	2.22	-	-1.72	1.52	4.20	-.87	-6.34	-.29	-1.28

DENSITY PARTITIONING FOR VALENCE AO'S

	Valence Atomic Orbitals			Overlap $S_{(F,H)}$	Bondorders and Populations					
	k	s	π		p	v	q	q^N	q^T	$P_{(F,H)}$
i	.991435	-.128805	.021585	.000000	2.000	.000	2.000	2.000	.000	.000
l	.128347	.939356	-.943460	.343668	2.234	-.175	2.059	2.003	.056	-.509
b	.024157	.343268	.938919	.444080	.789	.306	1.095	.927	.098	.688
π		(unhybridized)		0	2.000	.000	2.000	2.000	.000	.000
h		(unhybridized)		-	.716	.131	.646	1.000	-.154	-

EXCHANGE CONTRIBUTIONS TO PAIRPOPULATIONS

		F				H
		i	l	b	π	h
i	PR	2.000	.000	.000	.000	-
	SPN	.000	.000	.000	.000	.000
	SPT	.000	.000	.000	.000	.000
	TOT	2.000	.000	.000	.000	.000
l	PR	.000	2.063	-.060	.000	-
	SPN	.000	-.004	.043	.000	-.039
	SPT	.000	.100	.004	.000	-.048
	TOT	.000	2.159	-.013	.000	-.087
b	PR	.000	-.060	1.057	.000	-
	SPN	.000	.043	-.474	.000	.431
	SPT	.000	.004	.021	.000	.073
	TOT	.000	-.013	.604	.000	.504
π	PR	.000	.000	.000	2.000	-
	SPN	.000	.000	.000	.000	.000
	SPT	.000	.000	.000	.000	.000
	TOT	.000	.000	.000	2.000	.000
h	PR	-	-	-	-	1.000
	SPN	.000	-.039	.431	.000	-.392
	SPT	.000	-.048	.073	.000	-.179
	TOT	.000	-.087	.504	.000	.429

INTRA-ATOMIC ENERGY CONTRIBUTIONS OF HP, SAO

Orbital	Promotion						Total	Orbital	Quasi-classical QCT	Sharing Penetration SPT		SP+QC Total
	k	s	σ	π	π̄							
P k	KIN	.55	2.27	.00	.00	.00	-1.53	KIN	.00			.00
	NA	1.14	-2.35	.00	.00	.00	1.12	SNA	.00			.00
	OEI	-.17	-3.79	4.09	-.02	-.02	-3.32	OEI	.00	-.00	.00	-.00
	TOT	.42	-3.87	4.09	-.02	-.02	.27	TOT	.00	-.00	.00	-.00
P s	KIN	2.27	-12.79	.00	.00	.00	-8.27	KIN	3.10			3.10
	NA	-2.35	40.97	.00	.00	.00	36.29	SNA	-3.47			-3.47
	OEI	-3.79	-3.22	.14	-3.01	-3.31	-23.13	OEI	.11	.19	-1.42	-1.13
	TOT	-3.87	24.95	.14	-3.01	-3.31	4.89	TOT	-.27	.19	-1.42	-1.50
F σ	KIN	.00	.00	10.68	.00	.00	10.68	KIN	8.00			8.00
	NA	.00	.00	-36.96	.00	.00	-36.96	SNA	-7.23			-7.23
	OEI	4.09	.14	3.16	2.88	2.88	23.49	OEI	1.78	6.83	-.35	6.68
	TOT	4.09	.14	-23.12	2.92	2.88	-2.79	TOT	1.78	6.83	-.35	8.25
P π	KIN	.00	.00	.00	.00	.00	.00	KIN	.00			.00
	NA	.00	.00	.00	.00	.00	.00	SNA	.00			.00
	OEI	-.02	-3.01	2.88	-.02	.00	-.02	OEI	.00	-.00	.00	-.00
	TOT	-.02	-3.01	2.88	-.02	.00	-.02	TOT	.00	-.00	.00	-.00
P π̄	KIN	.00	.00	.00	.00	.00	.00	KIN	.00			.00
	NA	.00	.00	.00	.00	.00	.00	SNA	.00			.00
	OEI	-.02	-3.01	2.88	-.02	-.02	-.02	OEI	.00	-.00	.00	-.00
	TOT	-.02	-3.01	2.88	.00	-.02	-.02	TOT	.00	-.00	.00	-.02
Total P	KIN						1.88	Total P KIN	11.90			11.90
	NA						.45	SNA	-10.70			-10.70
	OEI						-1.11	OEI	.31	7.01	-1.78	5.55
	TOT						2.22	TOT	1.51	7.01	-1.78	6.75
Total H	KIN							Total H KIN	-2.09			-2.09
	NA							SNA	1.57			1.57
	OEI							OEI	.20	3.33	1.52	5.06
	TOT							TOT	-.32	3.33	1.52	4.53

INTERATOMIC ENERGY CONTRIBUTIONS OF HP, SAO

Orbital Pair P H	Quasiclassical Electrostatic			Penetration			Sharing			Interference			Totals		
	QCN	QCT	QC(N+T)	SPN	SPT	SP(N+T)	SIN	SIT	SI(N+T)	M	T	N+T			
i h	KIN						.12	.00	.00	.00	.00	.00	.00	.00	
	SNA	-.05	.02	.01	-.04			.12	.00	.12	.07	.01	.08		
	OEI		.00	.00	-.00	.00	.00	-.10	.00	-.10	-.00	-.10	-.10		
	TOT	-.05	.01	.01	-.04	.00	.00	.00	.00	.00	.00	.00	-.01		
f h	KIN						10.75			10.75	10.75	10.75	10.75		
	SNA	1.12	-.04	.75	1.83			-1.40	-.78	-.11	-.02	-2.31	-1.06	.58	-.48
	OEI		-.10		-.10	.63	.57	1.22				-.12	.51	.47	.98
	TOT	1.12	.61		1.73	.63	.57	1.22				8.32	10.20	1.05	11.25
b h	KIN						-22.14			-22.14	-22.14	-22.14	-22.14		
	SNA	-3.13	-.44	-.27	-3.84			9.72	-2.43	.07	-.25	7.11	4.14	-.87	3.27
	OEI		-.24		-.24	-6.77	-1.17	-7.95				.15	-6.62	-1.42	-8.03
	TOT	-3.13	-.95		-4.08	-6.77	-1.17	-7.95	-14.72		-.16	-14.88	-24.62	-2.28	-26.91
π h	KIN						.49	.00	.00	.00	.00	.00	.00	.00	
	SNA	.17	.02	.33	.52				.00	.00	.00	.49	.66	.33	.98
	OEI		.00		.00	.00	.00	.00	.00	.00	.00	-.54	-.54	-.02	-.54
	TOT	.17	.33		.50	.00	.00	.00	.00	.00	.00	-.05	-.12	.33	.44
π̄ h	KIN						.49	.00	.00	.00	.00	.00	.00	.00	
	SNA	.17	.02	.33	.50				.00	.00	.00	.49	.66	.33	.98
	OEI		.00		.00	.00	.00	.00	.00	.00	.00	-.54	-.54	-.02	-.54
	TOT	.17	.33		.50	.00	.00	.00	.00	.00	.00	-.05	-.12	.33	.44
Bond Total	KIN						-11.39			-11.39	-11.39	-11.39	-11.39		
	SNA	1.72	-.48	1.16	-1.25			9.40	-3.21	-.04	-.25	5.89	4.47	.38	4.84
	OEI		-.34		-.34	-6.14	-.61	-6.75				-1.14	-7.28	-.95	-8.23
	TOT	1.72	.33		-1.39	-6.14	-.61	-6.75	-6.34		-.29	-6.64	-14.21	-.57	-14.78

Figure 20 (Continued)

Figure 21. Binding energy decomposition and description of electron distribution for HF, BAO approximation

BINDING ENERGY PARTITIONING

		Promotion		Quasi-classical		Sharing Penetration		Sharing Interference		TOTAL
		PRH	PRC	QCN	QCT	SPN	SPT	SIN	SIT	
F	KIN	2.79	-		16.38					19.17
	SNA	.17	-		-14.98					-14.81
	OEI	-.56	-		.62	6.64	-2.75			3.95
	TOT	2.41	-		2.02	6.64	-2.75			8.32
H	KIN	-	-		-2.98					-2.98
	SNA	-	-		2.24					2.24
	OEI	-	-		.41	3.33	2.01			5.75
	TOT	-	-		-.34	3.33	2.01			5.00
BOND	KIN							-10.75		-10.75
	SNA			-1.83	.98			5.71	-.41	-4.44
	OEI				-.70	-6.90	-.64	-1.04		-8.37
	TOT			-1.83	.28	-6.00	-.64	-6.07	-.41	-14.67
HF	KIN	2.79	-		13.40			-10.75		5.44
	SNA	.17	-	-1.83	-11.76			5.71	-.41	-8.12
	OEI	-.56	-		.33	3.37	-1.38	-1.04		1.32
	TOT	2.41	-	-1.83	1.96	3.37	-1.38	-6.07	-.41	-1.36

DENSITY PARTITIONING FOR VALENCE AO'S

	Valence Atomic Orbitals			Overlap $S_{(F,H)}$	Bond orders and Populations					
	k	s	σ		p	v	q	c^N	q^T	$p_{(F,H)}$
i	.991851	-.126137	.017920	.000000	2.000	.000	2.000	2.000	.000	.000
l	.124571	.930657	-.344036	.346572	2.233	-.171	2.062	1.364	.078	-.492
b	.026719	.343464	.938786	.454322	.850	.307	1.157	1.016	.141	.675
π		(unhybridized)		0	2.000	.000	2.000	2.000	.000	.000
h		(unhybridized)		-	.645	.136	.781	1.000	-.219	-

EXCHANGE CONTRIBUTIONS TO PAIR POPULATIONS

		F				H
		i	l	b	π	h
i	PR	2.000	.000	.000	.000	-
	SPN	.000	.000	.000	.000	.000
	SPT	.000	.000	.000	.000	.000
	TOT	2.000	.000	.000	.000	.000
l	PR	.000	2.004	-.020	.000	-
	SPN	.000	.000	.001	.000	-.001
	SPT	.000	.158	.006	.000	-.085
	TOT	.000	2.162	-.013	.000	-.087
b	PR	.000	-.020	1.037	.000	-
	SPN	.000	.001	-.395	.000	.394
	SPT	.000	.006	.032	.000	.102
	TOT	.000	-.013	.674	.000	.496
π	PR	.000	.000	.000	2.000	-
	SPN	.000	.000	.000	.000	.000
	SPT	.000	.000	.000	.000	.000
	TOT	.000	.000	.000	2.000	.000
h	PR	-	-	-	-	1.000
	SPN	.000	-.001	.394	.000	-.392
	SPT	.000	-.085	.102	.000	-.236
	TOT	.000	-.087	.496	.000	.372

INTRA-ATOMIC ENERGY CONTRIBUTIONS OF HF, BAO

Orbital	Promotion			Total	Orbital	Sharing			SP+QC
	k	s	σ			Quasi-classical QCT	Penetration SPN	SPT	
P k	KIN	-.97	3.04	.00	.00	.00	.00	.00	.00
	NA	2.02	-3.17	.00	.00	.00	.00	.00	.00
	OEI	-.20	-4.22	4.50	-.23	-.03	-.43	-.00	-.00
	TOT	.85	-4.35	4.50	-.23	-.23	.61	-.00	-.00
P e	KIN	3.04	-13.91	.00	.00	.00	.00	.00	.00
	NA	-3.17	45.40	.00	.00	.00	.00	.00	.00
	OEI	-4.22	-5.62	.15	-3.33	-3.33	-29.67	.00	.00
	TOT	-4.35	27.86	.15	-3.33	-3.33	5.57	.00	.00
P o	KIN	.00	.00	11.59	.00	.00	.00	.00	.00
	NA	.00	.00	-40.91	.00	.00	.00	.00	.00
	OEI	4.50	.15	3.40	3.17	3.17	25.75	.00	.00
	TOT	4.50	.15	-25.92	3.17	3.17	-3.57	.00	.00
P π	KIN	.00	.00	.00	.00	.00	.00	.00	.00
	NA	.00	.00	.00	.00	.00	.00	.00	.00
	OEI	-.03	-3.33	3.17	-.10	.00	-.10	.00	.00
	TOT	-.03	-3.33	3.17	-.10	.00	-.10	.00	.00
P $\bar{\pi}$	KIN	.00	.00	.00	.00	.00	.00	.00	.00
	NA	.00	.00	.00	.00	.00	.00	.00	.00
	OEI	-.03	-3.33	3.17	.00	-.10	-.10	.00	.00
	TOT	-.03	-3.33	3.17	.00	-.10	-.10	.00	.00
Total P	KIN						2.79		
	NA						.17		
	OEI						-.56		
	TOT						2.41		
Total H	KIN						16.38		16.38
	NA						-14.96		-14.96
	OEI						.62	6.64	-2.75
	TOT						2.04	6.64	-2.75
Total	KIN						-2.98		-2.98
	NA						2.24		2.24
	OEI						.41	3.33	2.01
	TOT						-3.34	3.33	2.01

INTRASATOMIC ENERGY CONTRIBUTIONS OF HF, BAO

Orbital Pair	Quasiclassical Electrostatic				Sharing					Totals			
	QCN	QCT	QC(N+T)		SPN	Penetration SPT	SP(N+T)	SIN	Interference SIT	SI(N+T)	N	T	N+T
1 h	KIN							.00	.00	.00	.00	.00	.00
	SNA	-.05	.00	.01	-.04			.10	.00	.00	.10	.05	.05
	OEI		.00	.01	-.04	.00	.00	.00	-.29	.00	-.29	-.09	.00
	TOT	-.05	.00	.01	-.04	.00	.00	.00	.01	.00	.01	-.04	.01
f h	KIN							10.30			10.30	10.30	10.30
	SNA	1.12	-.06	1.09	2.15			-1.34	-.76	-.15	-2.28	-.98	.85
	OEI		-.20	.00	-.20	.10	1.01	1.19	-.11		-.11	.27	.81
	TOT	1.12	.82	1.94	1.94	.10	1.01	1.19	8.10	-.18	7.92	9.39	1.66
b h	KIN							-21.05			-21.05	-21.05	-21.05
	SNA	-3.27	-.64	-.39	-4.30			9.21	-2.39	.10	-3.33	6.58	3.55
	OEI		-.50	-.50	-.50	-6.17	-1.65	-7.82	.15		-.15	-6.82	-2.15
	TOT	-3.27	-1.52	-4.79	-4.79	-6.17	-1.65	-7.82	-14.06	-.23	-14.31	-23.52	-3.41
w h	KIN							.45	.00	.00	.45	.00	.45
	SNA	.18	.00	.48	.67			.45	.00	.00	.45	.63	.48
	OEI		.00	.00	.00	.00	.00	.00	.00	.00	-.50	-.50	.00
	TOT	.18	.48	.67	.67	.00	.00	.00	-.05	.00	-.05	.13	.48
w \bar{h}	KIN							.45	.00	.00	.45	.00	.45
	SNA	.18	.00	.48	.67			.45	.00	.00	.45	.63	.48
	OEI		.00	.00	.00	.00	.00	.00	.00	.00	-.50	-.50	.00
	TOT	.18	.48	.67	.67	.00	.00	.00	-.05	.00	-.05	.13	.48
Bond Total	KIN							-10.75			-10.75	-10.75	-10.75
	SNA	-1.83	-.70	1.68	-.85			8.86	-3.15	-.05	-3.36	5.30	3.88
	OEI		-.70	-.70	-.70	-6.02	-.64	-6.63	-1.04		-1.04	-7.83	-1.34
	TOT	-1.83	.28	-1.55	-1.55	-6.02	-.64	-6.63	-6.07	-.41	-6.49	-13.90	-.77

Figure 21 (Continued)

Figure 22. Binding energy decomposition and description of electron distribution for HF, BMAO approximation

BINDING ENERGY PARTITIONING

		Promotion		Quasi-classical		Sharing Penetration		Sharing Interference		TOTAL
		PRH	PRC	QCN	QCT	SPN	SPT	SIN	SIT	
F	KIN	2.33	-5.50		19.03					15.87
	NA	.59	10.75		-17.14					-5.80
	OEI	2.67	-5.08		.71	-3.92	5.29			-1.33
	TOT	5.59	.17		2.60	-3.92	5.29			9.72
H	KIN	.00	9.97		-5.41					4.56
	SNA	.00	-8.61		3.08					-5.53
	OEI	.00	.00		.57	-1.35	6.69			7.94
	TOT	.00	1.36		-1.74	-1.35	6.69			6.97
BOND	KIN							-17.36		-17.36
	SNA			-2.07	1.37			8.37	-36	7.33
	OEI				.85	3.48	-11.07		.77	-9.21
	TOT			-2.07	.54	3.48	-11.07	-9.76	-36	-19.25
HF	KIN	2.33	4.47		13.62			-17.36		3.06
	SNA	.59	2.14	-2.07	-12.67			8.37	-36	-4.00
	OEI	2.67	-5.08		.45	-1.79	2.91		.77	-1.61
	TOT	5.59	1.53	-2.07	1.40	-1.79	2.91	-9.76	-36	-2.55

DENSITY PARTITIONING FOR VALENCE AO'S

	Valence Atomic Orbitals			Overlap $S_{(F,H)}$	Bondorders and Populations					
	k	s	σ		p	v	q	q^N	q^T	$P_{(F,H)}$
i	.991632	-.127929	.022622	.000000	2.000	.000	2.000	2.000	.000	.000
l	.127041	.422591	-.346008	.299000	2.166	-.120	2.046	1.982	.064	-.401
b	.022248	.345987	.037359	.467125	.873	.310	1.184	1.018	.166	.665
π	(unhybridized)			0	2.000	.000	2.000	2.000	.000	.000
h	(unhybridized)			-	.580	.191	.771	1.000	-.230	-

EXCHANGE CONTRIBUTIONS TO PAIRPOPULATIONS

		F				H
		i	l	b	π	h
i	PR	2.000	.000	.000	.000	-
	SPN	.000	.000	.000	.000	.000
	SPT	.000	.000	.000	.000	.000
	TOT	2.000	.000	.000	.000	.000
l	PR	.000	1.502	.479	.000	-
	SPN	.000	.308	-.501	.000	.193
	SPT	.000	.306	.013	.000	-.254
	TOT	.000	2.117	-.009	.000	-.062
b	PR	.000	.479	.539	.000	-
	SPN	.000	-.501	.814	.000	-.313
	SPT	.000	.013	-.649	.000	.802
	TOT	.000	-.009	.704	.000	.489
π	PR	.000	.000	.000	2.000	-
	SPN	.000	.000	.000	.000	.000
	SPT	.000	.000	.000	.000	.000
	TOT	.000	.000	.000	2.000	.000
h	PR	-	-	-	-	1.000
	SPN	.000	.193	-.313	.000	.120
	SPT	.000	-.254	.802	.000	-.777
	TOT	.000	-.062	.489	.000	.343

Figure 22 (Continued)

INTRA-ATOMIC ENERGY CONTRIBUTIONS OF HP, BMAO

Orbital	Promotion												Total PRC	PR(H+C)	Orbital	Quasi-classical QCT		Sharing Penetration SPN SPT		SP+QC Total
	PRH ^k	PRC	PRH ^s	PRC	PRH ^o	PRC	PRH ^r	PRC	PRH ^v	PRC	PRH ^w	PRC				PRH	PRC	PR(H+C)	QCT	
KIN	-0.03	1.51	2.78	-0.01	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	-0.79	1.58	.78	KIN	.00			.00
NA	1.72	-1.57	-2.89	-0.02	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	1.69	-1.60	.09	SMA	.00			.00
OBI	-1.13	.09	-4.28	-0.21	4.52	1.75	-0.03	-1.38	-0.03	-1.38	-0.03	-1.38	-0.32	-.25	-.07	OBI	.00	-.00	.00	-.00
TOT	.77	.03	-4.39	-0.21	4.52	1.75	-0.03	-1.38	-0.03	-1.38	-0.03	-1.38	.57	-.23	-.00	TOT	.00	-.00	.00	-.00
KIN	2.79	-0.01	-14.26	-1.97	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	-8.74	-2.06	-10.80	KIN	3.45			3.45
NA	-2.89	.02	46.53	2.78	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	40.78	2.84	43.62	SMA	-3.99			-3.99
OBI	-4.28	-.21	.46	-0.03	-2.00	.42	-3.33	-.52	-3.33	-.52	-3.33	-.52	-14.56	-.92	-15.48	OBI	.12	2.18	-4.32	-1.96
TOT	-4.39	-.21	32.73	.78	-2.00	.42	-3.33	-.52	-3.33	-.52	-3.33	-.52	17.49	-.14	17.34	TOT	-3.36	2.18	-4.32	-2.49
KIN	.00	.00	.00	.00	11.97	9.62	.00	.00	.00	.00	.00	.00	11.97	9.62	21.49	KIN	15.57			15.57
NA	.00	.00	.00	.00	-31.88	-16.59	.00	.00	.00	.00	.00	.00	-41.98	-16.59	-58.47	SMA	-13.15			-13.15
OBI	4.52	1.75	-2.00	.42	7.97	-3.6	3.24	.31	3.24	.31	3.24	.31	17.60	7.01	24.62	OBI	.54	-6.11	9.61	4.04
TOT	4.52	1.75	-2.00	.42	-22.05	-6.67	3.24	.31	3.24	.31	3.24	.31	-12.41	.04	-12.37	TOT	2.99	-6.11	9.61	6.45
KIN	.00	.00	.00	.00	.00	.00	.00	-7.32	.00	.00	.00	.00	.00	-7.32	-7.32	KIN	.00			.00
NA	.00	.00	.00	.00	.00	.00	.00	13.05	.00	.00	.00	.00	.00	13.05	13.05	SMA	.00			.00
OBI	-0.03	-1.38	-3.33	-.52	3.24	.31	-0.03	-.50	.00	-1.00	-0.03	-0.50	-0.03	-5.71	-5.74	OBI	.00	-.00	.00	-.00
TOT	-0.03	-1.38	-3.33	-.52	3.24	.31	-0.03	-.50	.00	-1.00	-0.03	-0.50	-0.03	-5.71	-5.74	TOT	.00	-.00	.00	-.00
KIN	.00	.00	.00	.00	.00	.00	.00	-7.32	.00	.00	.00	.00	-7.32	-7.32	-7.32	KIN	.00			.00
NA	.00	.00	.00	.00	.00	.00	.00	13.05	.00	.00	.00	.00	13.05	13.05	13.05	SMA	.00			.00
OBI	-0.03	-1.38	-3.33	-.52	3.24	.31	-0.03	-.50	.00	-1.00	-0.03	-0.50	-0.03	-5.71	-5.74	OBI	.00	-.00	.00	-.00
TOT	-0.03	-1.38	-3.33	-.52	3.24	.31	-0.03	-.50	.00	-1.00	-0.03	-0.50	-0.03	-5.71	-5.74	TOT	.00	-.00	.00	-.00
Total P													2.55	-5.50	-5.16	Total P	19.03			19.03
KIN													.59	10.75	11.34	KIN	-17.14			-17.14
NA													2.67	-9.09	-2.41	NA	.71	-3.92	5.29	2.08
OBI													5.99	.17	5.76	OBI	2.60	-3.92	5.29	3.96
TOT																TOT				
Total H													.00	9.97	9.97	Total H	-5.41			-5.41
KIN													.00	-8.61	-8.61	KIN	3.08			3.08
NA													.00	.00	.00	NA	.59	-1.35	2.69	7.94
OBI													.00	.00	.00	OBI	-1.74	-1.35	2.69	5.61
TOT													.00	1.36	1.36	TOT				

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INTERATOMIC ENERGY CONTRIBUTIONS OF HP, BMAO

Orbital Pair F H	Quasiclassical Electrostatic				Sharing				Interference				Totale		
	QCM	QCT	QC(H+T)	QC(N+T)	SPN	Penetration SPT	SP(N+T)	SIN	SIT	Interference SIT	SI(N+T)	N	T	N+T	
KIN			.01	-.03				.00	.00	.00	.00	.00	.00	.00	
SMA	-.04	.00	.00	-.03	.00	.00	.00	.00	.00	.00	.00	.00	.00	.00	
OBI		.00	.00	-.03	.00	.00	.00	.00	.00	.00	.00	.00	.00	.00	
TOT	-.04	.00	.01	-.03	.00	.00	.00	.00	.00	.00	.00	.00	.00	.00	
KIN			1.29	1.65				8.70	.00	.00	8.70	8.70	.00	8.70	
SMA	.37	-.02	.00	-.18	-2.22	3.13	.91	-1.35	-.86	-.09	-.05	-2.36	-1.84	1.13	
OBI		.18	.00	-.18	-2.22	3.13	.91	-1.11			-.11	-2.33	2.95	.63	
TOT	.37	-.02	1.29	1.47	-2.22	3.13	.91	6.38		-1.14	-.11	4.94	4.08	8.61	
KIN			-.60	-3.36				-26.06	.00	.00	-26.06	-26.06	.00	-26.06	
SMA	-2.30	-.46	.00	-.67	5.69	-14.28	-8.51	11.32	-.86	.07	-.29	8.16	-1.28	6.88	
OBI		.67	.00	-.67	5.69	-14.28	-8.51	11.32	.12		.12	9.91	-14.97	-9.06	
TOT	-2.30	-.46	-.60	-3.36	5.69	-14.28	-8.51	-15.48		-.22	-.15	-12.09	-16.15	-28.24	
KIN			.58	.53				.00	.00	.00	.00	.00	.00	.00	
SMA	-.05	.00	.00	.53	.00	.00	.00	.00	.00	.00	.00	-.03	.58	.55	
OBI		.00	.00	.53	.00	.00	.00	-.36	.00	.00	-.36	-.36	.00	-.36	
TOT	-.05	.00	.58	.53	.00	.00	.00	-.33	.00	.00	-.33	-.39	.58	.20	
KIN			.58	.53				.00	.00	.00	.00	.00	.00	.00	
SMA	-.05	.00	.00	.53	.00	.00	.00	.00	.00	.00	.00	-.03	.58	.55	
OBI		.00	.00	.53	.00	.00	.00	-.36	.00	.00	-.36	-.36	.00	-.36	
TOT	-.05	.00	.58	.53	.00	.00	.00	-.33	.00	.00	-.33	-.39	.58	.20	
Bond KIN			1.88	-.68				-17.36			-17.36	-17.36		-17.36	
Total SMA	-2.07	-.49	.00	-.68	3.48	-11.07	-7.59	10.05	-1.72	-.02	-.34	8.01	6.30	7.33	
OBI		.54	.00	-.68	3.48	-11.07	-7.59	9.76			-.77	2.71	-11.92	-9.21	
TOT	-2.07	-.49	.54	-1.54	3.48	-11.07	-7.59	-9.76		-.06	-.34	-10.12	-8.35	-19.25	