1971

Even-tempered atomic orbitals in quantum chemical ab initio calculations: light atoms, heavy atoms, triatomic alkali ions

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Recommended Citation

Raffenetti, Richard Charles, "Even-tempered atomic orbitals in quantum chemical ab initio calculations: light atoms, heavy atoms, triatomic alkali ions " (1971). *Retrospective Theses and Dissertations*. 4909.
https://lib.dr.iastate.edu/rtd/4909

71-26,883

RAFFENETTI, Richard Charles, 1942-
EVEN-TEMPERED ATOMIC ORBITALS IN QUANTUM
CHEMICAL *AB INITIO* CALCULATIONS: LIGHT
ATOMS, HEAVY ATOMS, TRIATOMIC ALKALI IONS.

Iowa State University, Ph.D., 1971
Chemistry, physical

University Microfilms, A XEROX Company, Ann Arbor, Michigan

Even-tempered atomic orbitals in quantum chemical *ab initio* calculations: Light atoms, heavy atoms, triatomic alkali ions

by

Richard Charles Raffenetti

A Dissertation Submitted to the
Graduate Faculty in Partial Fulfillment of
The Requirements for the Degree of
DOCTOR OF PHILOSOPHY

Major Subject: Physical Chemistry

Approved:

Signature was redacted for privacy.

In Charge of Major Work

Signature was redacted for privacy.

Head of Major Department

Signature was redacted for privacy.

Dean of Graduate College

Iowa State University
Of Science and Technology
Ames, Iowa

1971

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INTRODUCTION

One aim of theoretical chemistry is to apply the laws of quantum physics to atoms and molecules and thereby, to form complete and accurate mathematical descriptions of these systems. An important intermediate step in this quest is the determination of rigorous solutions for the Schroedinger equation which describe electronic motion in the field of stationary nuclei. Recent advances in computer technology have put this goal within reach for small systems, i.e. those with, perhaps, up to a dozen electrons. As a result, theoretical chemists have indeed been able to make important contributions to the field of chemistry, not only with general theory but also with concrete accurate calculations.

Such calculations on systems with many electrons have been limited in number for several reasons. Usually very accurate techniques are difficult to extend to larger systems because of the mathematical complexities. Secondly, a large problem generates immense quantities of intermediate information which must be handled over and over. This information increases approximately as the fourth power of the number of electrons, causing a rapid explosion of data while the speed of calculation remains essentially constant. Computing machinery belonging to the current prototype has progressed so that the technical limit with respect to calculation speed is very close. New prototypes (1) are being developed which promise to alleviate this bind, but there certainly will always be calculations on some molecules which will tax the new limit. Consequently the concerned theoretician must continue to look for improvements in his mathematical techniques which will facilitate the treatment of larger systems. It is the purpose of this investigation to point out one avenue of approach toward this goal.

Notable attempts at simplification exist, based on parametrization with the help of experimental data. Such data fitting techniques were originally devised in the face of a complete inability to obtain accurate ab initio results (2,3). More recently, these semi-empirical techniques have been used in order to defeat the data handling and data generation problems encountered with large systems (4,5). On the other hand, there are methods employing mathematical approximations rather than experimental data which are called non-empirical or semi-quantitative. Typically, they can be trusted only after repeated verification of success for similar systems.

The theory used for calculations contained in this work is a first principle or ab initio theory. Characteristic of ab initio theories is the assumption of some form for the wavefunction Ψ which is to form a solution to the Schroedinger equation. The wavefunction is constructed to be an eigenfunction of all symmetry operators which commute with the Hamiltonian operator $\hat{H}$. Hence the wavefunction has certain symmetries which are in accord with the postulates (in this case fermion antisymmetry) or with the physics of the problem (e.g. the spin operators $\hat{S}_z$ or $\hat{S}^2$). In particular, the wavefunction is frequently written in terms of space and spin orbitals, i.e. one-electron space functions, $\phi_i(\underline{r})$ and spin functions α and β.

The space orbitals $\phi_i(\underline{r})$ are usually expanded in terms of a number of appropriate spatial basis functions $\chi_k(\underline{r})$

$$(1) \quad \phi_i(\underline{r}) = \sum_k \chi_k(\underline{r})\; c_{ki}$$

which define a finite Hilbert space. Solution for Ψ implies determination of the matrix of linear coefficients $\underline{C}$ which define the best orbitals obtainable in terms of this basis. It is apparent that the quality of the basis is of critical importance for the <u>quality</u> of the wavefunction that can be obtained. Furthermore, reviewing the calculational procedure, one quickly realizes that the size of the basis is of critical importance for the <u>amount of effort</u> that must be expended. This investigation deals therefore with the basis, its form and selection, and ways of efficiently manipulating the data generated from it in connection with substantial atomic and molecular problems.

There are many kinds of *ab initio* approaches, each dictated by a particular approximation to the wavefunction in terms of orbitals. In the following we adopt the Hartree-Fock approximation, in which the wavefunction is an antisymmetrized product of orthonormal spin orbitals, u_i, defined as products of pure space and pure spin orbitals,

$$(2) \quad \Psi = \Psi(1,2,\ldots N) = \hat{A}\{u_1(1)u_2(2)\ldots u_N(N)\}$$

where $\hat{A}$ is the antisymmetrization operator. This product is formally equivalent to an N by N determinant and hence is also called a Slater determinant (6).

By virtue of the variational principle, one seeks the lowest energy possible for such a determinant, and this determines the Hartree-Fock orbitals. As is the case for the exact wavefunction, limitation to a finite Hilbert space by the expansion of Eq. 1, means that one obtains only an approximation to the Hartree-Fock approximation. Here too, the quality of the basis is essential for the quality of this approximation. Now, in all cases of ^1S closed shell states, the Hartree-Fock wavefunction is a very good approximation to the true wavefunction. It is therefore a safe assumption that a basis which is effective for obtaining a good representation of the Hartree-Fock wavefunction will also be desirable for the construction of more sophisticated wavefunctions.

The Hartree-Fock approach has the advantage that computationally simple techniques exist so that calculations can be repeated a sufficient number of times with the objective to test the performance of various bases.

THE LCAO-MO-SCF METHOD

The Matrix Formulation

The LCAO-MO-SCF (linear-combination-of-atomic-orbitals molecular-orbital self-consistent-field) method is a technique for solving the Hartree-Fock equations,

$$(3) \qquad \hat{F}\phi_i = e_i\phi_i \quad .$$

The Fock operator, $\hat{F}$, is a pseudo-one-electron operator which depends on the system space orbitals ϕ_i implicit in Eq. 2. If each orbital ϕ_i, is expanded in a set of suitable symmetry adapted basis functions X_{ls} according to

$$(4) \qquad \phi_{il} = \sum_s X_{ls}\, c_{sil} \;=\; |X\rangle\, \underline{c}_{il}$$

the problem becomes one of matrix algebra. The solution of the matrix Hartree-Fock equations has been described by Roothaan (7,8) and Roothaan and Bagus (9). If the density matrices are defined

$$\underline{D}_T(l) = \underline{D}_C(l) + \underline{D}_O(l)$$

$$(5) \qquad \underline{D}_C(l) = \sum_{i\in \text{closed}} N(il)\, \underline{c}_{il}\underline{c}^{+}_{il}$$

$$\underline{D}_O(l) = \sum_{i\in \text{open}} N(il)\, \underline{c}_{il}\underline{c}^{+}_{il}$$

in terms of column vectors $\underline{c}_{il}$ of the coefficient matrix $\underline{C}(l)$ and occupation numbers $N(il)$, corresponding to the i-th orbital of symmetry or irreducible representation l, then one may write the energy compactly as

$$(6) \qquad E = \frac{1}{2}\sum_{l}\{[2\underline{H}^{+}(l) + \underline{P}^{+}(l)]\,\underline{D}_{T}(l) - \underline{Q}^{+}(l)\,\underline{D}_{O}(l)\}$$

where the lower triangular matrices $\underline{H}(l)$, $\underline{D}_O(l)$, $\underline{D}_T(l)$, $\underline{P}(l)$, and $\underline{Q}(l)$ are considered supervectors, with the off-diagonal elements of the density matrices being doubled. The supervector $\underline{H}(l)$ represents a collection of one-electron integrals over the basis functions.

Application of the variation principle to the energy formula results in a set of coupled eigenvalue equations

$$(7) \qquad \underline{F}_{O}(l)\,\underline{c}_{il} = e_{i}\,\underline{S}(l)\,\underline{c}_{il}$$

$$(8) \qquad \underline{F}_{C}(l)\,\underline{c}_{jl} = e_{j}\,\underline{S}(l)\,\underline{c}_{jl}$$

for each symmetry l, which must be solved for the coefficient vectors $\underline{c}_{il}$ and $\underline{c}_{jl}$ defining orbitals of Eq. 4. A set of initial orbitals is chosen to start the process. These are orthogonalized with respect to the metric matrix $\underline{S}$ and are used to construct the density matrices of Eq. 5. The Fock matrices $\underline{F}_C$ and $\underline{F}_O$ may then be formed. By virtue of their definition below, each has components from both closed- and open-shells and from every symmetry. Now, each of these equations is treated as a general matrix eigenvalue problem

$$\underline{F}\,\underline{C} = \underline{S}\,\underline{C}\,\underline{e}, \tag{9}$$

where $\underline{e}$ is assumed diagonal. The problem is converted to an ordinary eigenvalue problem by finding a transformation matrix, $\underline{U}$, which brings $\underline{S}$ to the identity,

$$\underline{U}^{+}\underline{S}\,\underline{U} = \underline{I}\ .$$

The eigenvectors which solve Eq. 9 are assumed to be of the form $\underline{C}=\underline{U}\underline{V}$ so that Eq. 9 becomes

$$\underline{F}\,\underline{U}\,\underline{V} = \underline{S}\,\underline{U}\,\underline{V}\,\underline{e}\ .$$

Multiplication on the left by U^{+} gives

$$\underline{U}^{+}\underline{F}\,\underline{U}\,\underline{V} = \underline{U}^{+}\underline{S}\,\underline{U}\,\underline{V}\,\underline{e}\ ,$$

which is equivalent to

$$\underline{F}'\underline{V} = \underline{V}\,\underline{e}\ , \tag{10}$$

where $\underline{F}' = \underline{U}^{+}\underline{F}\,\underline{U}$. Eq. 10 is solved by diagonalizing the real, symmetric matrix $\underline{F}'$. The orthogonal matrix which effects this is $\underline{V}$. The process is done first for closed-shells and then open. In this way one gets two solution matrices $\underline{C}$(open) and $\underline{C}$(closed). Certain vectors from each are chosen according to their associated eigenvalues e_i to be used as occupied orbitals. Then new density matrices are constructed and the entire process is recycled until input orbitals equal output. If convergence of this iterative process is obtained, orbitals derived from Eqs. 7 and 8 will be mutually orthogonal. However, during early iterations this orthogonality must be forced.

If the problem is closed shell, $\underline{D}_o(1)$, $\underline{Q}(1)$, and $\underline{F}_o(1)$ are not defined so that the problem is simpler, requiring solution of only the closed-shell equations.

The following equations serve to complete the definition of all quantities used above;

$$\underline{F}_c(1) = \underline{H}(1) + \underline{P}(1) + \underline{R}_o(1)$$

$$\underline{F}_o(1) = \underline{H}(1) + \underline{P}(1) - \underline{Q}(1) + \underline{R}_c(1)$$

$$\underline{P}(1) = \sum_{1'} \underline{\mathcal{P}}(11')\ \underline{D}_T(1')$$

$$\underline{Q}(1) = \sum_{1'} \mathcal{Q}(11')\ \underline{D}_o(1')$$

$$\underline{R}_c(1) = [N_c(1)/(N_c(1)-N_o(1))] \sum_{i \in \text{closed}} [\underline{V}_i(1) + \underline{V}_i^{+}(1)]$$

$$\underline{R}_o(1) = [N_o(1)/(N_c(1)-N_o(1))] \sum_{i \in \text{open}} [\underline{V}_i(1) + \underline{V}_i^{+}(1)]$$

$$\underline{V}_i(l) = \underline{S}(l)\ \underline{c}_{il}\underline{c}^{+}{}_{il}\underline{Q}^{+}(l)$$

$$N_o(l) = \sum_{i \in \text{open}} N(il), \qquad N_c(l) = \sum_{i \in \text{closed}} N(il) .$$

The supermatrices $\underline{\mathcal{P}}(ll')$ and $\underline{\mathcal{Q}}(ll')$ contain the two-electron integrals arising from the electron-repulsion term of an atomic or molecular Hamiltonian and computed in terms of the basis functions.

Matrix Elements

One-electron integrals

The quantity $\underline{H}(l)$ mentioned above represents a supervector or lower triangular matrix of expectation values of the one-electron Hamiltonian terms computed over a symmetry adapted basis. The one-electron Hamiltonian operator is

$$\hat{H}_1 = \sum_i \hat{h}(i)$$

where

$$\hat{h}(i) = -\hat{\Delta}_i/2 - \sum_\alpha (Z_\alpha/r_{i\alpha}),$$

the i sum being over all electrons and α summing over all nuclei. The first term arises from the kinetic energy of the electrons with the operator

$$\hat{\Delta} = \hat{\nabla}^2 = (\partial/\partial x)^2 + (\partial/\partial y)^2 + (\partial/\partial z)^2 .$$

The second represents the Coulomb attraction of the nuclei for the electrons. If symmetry adapted basis functions χ_{lr} are taken to be real, the integrals are defined such that

$$(11)\qquad H(lrs) = \int dV_1 \chi_{lr}(1)\ h(1)\ \chi_{ls}(1)$$

$$= \langle \chi_{lr} | h | \chi_{ls} \rangle$$

where the second line is written in the bra-ket notation of Dirac (10). The overlap matrix $\underline{S}(l)$ is computed with respect to the symmetry adapted functions such that

$$(12)\qquad S(lrs) = \int dV_1 \chi_{lr}(1)\ \chi_{ls}(1)$$

$$= \langle \chi_{lr} | \chi_{ls} \rangle \ .$$

All one-electron integrals between symmetries l and l' are identically zero.

<u>Two-electron integrals</u>

The integral supermatrices $\underline{\mathcal{P}}(ll')$ and $\underline{\mathcal{Q}}(ll')$ are combinations of the more basic supermatrices $\underline{\mathcal{J}}(ll')$ and $\underline{\mathcal{K}}(ll')$. These in turn are formed from the basic electron repulsion integrals arising from the two-electron term of the molecular Hamiltonian operator

$$\hat{H}_2 = \sum_{i<j} r_{ij}^{-1}$$

where the sums are over the electrons. The basic integral is commonly written

(13) $$[rs|tu] = \langle rt|r_{12}^{-1}|su\rangle = \int dV_1 \int dV_2 \; X_r(1) \; X_t(2)\,(1/r_{12}) \; X_s(1) \; X_u(2)$$

with the general indices referring to basis functions, either symmetry adapted or not. The supermatrix derives its form from the three integral symmetry properties

(14) $$[rs|tu] = [tu|rs]$$
$$[rs|tu] = [rs|ut]$$
$$[rs|tu] = [sr|tu] \quad .$$

Unique integrals form a lower triangular supermatrix with rows and columns numbered by the (rs) pairs in the sequence (rs) = (11), (21), (22), (31), (32),...etc. corresponding to row-wise lower triangular supervector elements. Hence there are $M(M+1)/2$ unique integrals where $M=N(N+1)/2$ and N is the number of basis functions X_s.

Elements of the Coulomb and exchange supermatrices $\mathcal{J}(ll')$ and $\mathcal{K}(ll')$ are

(15) $$\mathcal{J}(lrs,l'tu) = [lr\ ls|l't\ l'u]$$

and

$$\mathcal{K}(lrs,l'tu) = \{[lr\ lt|l's\ l'u] + [lr\ lu|l's\ l't]\}/2\ . \tag{16}$$

In terms of these, elements of $\mathcal{P}(ll')$ and $\mathcal{Q}(ll')$ are

$$\mathcal{P}(lrs,l'tu) = \mathcal{J}(lrs,l'tu) - (1/2)\mathcal{K}(lrs,l'tu) \tag{17}$$

and

$$\mathcal{Q}(lrs,l'tu) = A(ll')\mathcal{J}(lrs,l'tu) - (B(ll')/2)\mathcal{K}(lrs,l'tu). \tag{18}$$

The quantities $A(ll')$ and $B(ll')$ are vector coupling constants peculiar to the degeneracy of a symmetry and are necessary in order to obtain an eigenfunction of correct spin state in open-shell systems. Constants used in this work are discussed in Appendix A. The symmetry classification (ll') of the constants is the reason for using symmetry adapted functions and integrals. It is convenient to insert them in the definition of $\mathcal{Q}(ll')$ if the basis is symmetry adapted. The closed-shell problem has no such requirement and is often carried out without explicit symmetry adaptation of integrals over the basis. A more detailed descriptions of the open-shell SCF procedure are given by Roothaan and Bagus (9) and Wahl et al. (11).

EVEN-TEMPERED ATOMIC ORBITAL BASES

The Role of the Basis

It seems clear that the selection of a basis rates high on the scale of important considerations. One must select a basis such that the function space of the system may be well represented. Naively one might suggest an infinite number of functions comprising a "complete set" capable of representing any function in any local function space. This is of course an impossible choice due to an inability to handle an infinite amount of data. The usual approach has been to select a finite set of functions, most frequently termed atomic orbitals (AO's), which are found separately for each atom of the molecular system, to combine them, and to use them as a basis for the calculation. The idea is that the electrostatic potential seen by the electrons near the atoms in the molecule is similar to that of the isolated atoms, so that the "atomic" functions provide a good description of that part of the wavefunction local to the atoms. To account for the modification of single atom potentials in interatomic regions, the set is normally augmented with extra functions the purpose of which is to better provide for this molecular polarization of the atoms. Various types of molecular basis have been tried. For example, Preuss (12) and Whitten (13,14) have used off-nucleus 1s Gaussians or "lobe functions" to simulate atomic orbitals, and others have used single-centered bases (15) for molecules with one heavy atom. These have not met the practical success in terms of consistently attaining the accuracy of the nuclear-centered analytic atomic function basis used here. The lobe function bases have not yet been extended to include d-type functions. On the other hand, the single-centered bases require very many terms and still do not describe atoms away from the heavy nucleus very well. This investigation has been confined to nuclear-centered basis types.

Within this limitation, several considerations may be made. Although any finite basis could be handled successfully in principle, there are practical limits to be considered. Integrals must be computed which consist of expectation values of various terms of the molecular Hamiltonian $\hat{H}$ over the basis functions. The occurrence of a two-electron term in $\hat{H}$ requires computation of a quantity of unique two-electron integrals of the order of $N^4/8$ where N is the number of basis functions. This number gets large quite fast as N increases, implying the need to handle very large numbers of these integrals, a formidable data management problem. Moreover, these two-electron integrals are very time consuming to compute even by the very best available techniques so that a large basis implies a substantial amount of time just to get the integrals. This is not only a problem of practicality but of expense considering the high cost of computer time.

Furthermore, the larger the basis, the larger the matrices which must be handled at one time. This fact first of all reflects the practicality with respect to the programming of matrix manipulations. Provision must be made to carry out intricate calculations as far as possible in the high-speed core rather than to make heavy use of either low-speed core or external storage. Consequently, the size of available high-speed core is a limitation. Secondly, the manipulation of large arrays increases the number of arithmetic operations, in turn affecting the degree of accuracy which may be maintained (considering truncation, roundoff, differencing, etc.). The larger the basis, the greater will be the accuracy required in for example the values of integrals in order that their subsequent handling will not diminish the accuracy of results below the desired level.

Definition of the Even-Tempered Basis

This investigation introduces a new concept in the selection of a basis to be used for the type of calculation described previously. Although the individual basis functions are not of a new analytic form, the fact that several basis functions are often needed prompted this author to consider them collectively. As a result, the "even-tempered" atomic basis is defined as a collection or group of _pure_ exponential or *pure* Gaussian functions multiplied by a real solid spherical harmonic. The latter consists of r^l multiplied by a normalized real spherical harmonic $S_l^m(\theta,\phi)$ given by,

$$S_l^m(\theta,\phi) = \mathcal{P}_l^{|m|}(\cos\theta)\,\Phi_m(\phi)$$

$$\Phi_m(\phi) = \begin{cases} \pi^{-1/2}\cos m\phi & m>0 \\ (2\pi)^{-1/2} & m=0 \\ \pi^{-1/2}\sin|m|\phi & m<0 \end{cases}$$

and $\mathcal{P}_l^{|m|}$ are associated Legendre functions (16) which are normalized. A set of even-tempered atomic orbitals is defined by

$$\chi(klm) = N_l(\zeta_k)\exp(-\zeta_k r^p)\,r^l S_l^m(\theta,\phi) \tag{19}$$

with

$$p = \begin{cases} 1 & \text{exponential} \\ 2 & \text{Gaussian} \end{cases}$$

and the radial normalization factor

$$N_l(\zeta_k) = \begin{cases} (2\zeta_k)^{l+3/2}\,[(2l+2)!]^{-1/2} & p=1 \\ (2\zeta_k)^{(2l+3)/4}\,\pi^{-1/4}\,[(2l+1)!!]^{-1/2} & p=2\,. \end{cases}$$

Consequently, *different even-tempered atomic orbitals for a given S_l^m do not differ in the power of r, but only in the values of the exponents ζ_k.* This is in contrast to Slater-type orbitals which, from the present point of view, form a "mixed" basis. In linear combinations of primitive functions X(klm),

$$(20)\quad G_{lm}(\underline{r}) = \sum_{k=1}^{M} c_k\, X(klm),$$

the solid harmonic may be factored, yielding,

$$(21)\quad G_{lm}(\underline{r}) = r^l S_l^{\,m}(\theta,\varphi)\cdot\sum_{k=1}^{M} c_k N_l(\zeta_k)\exp(-\zeta_k r\ ).$$

A second condition, which suggests the name "even-tempered" governs the choice of the exponential parameters $\{\ \zeta_k\colon k=1,2,\ldots,M\}$. These are taken to form a geometric sequence dependent upon two parameters, α and β, by the relation

$$(22)\qquad \zeta_k = \alpha\cdot\beta^k\ ,\qquad \alpha,\beta > 0,\qquad \beta \neq 1,\qquad k=1,2,\ldots M.$$

The reason for choosing this progression, was that, for expansions of the type of Eq. 20 used for atomic calculations, independent optimal determination of all zeta's did yield a set of values which gave an almost linear plot of $\log(\zeta_k)$ vs. k. The next step then was the assumption of such a straight line determined by two parameters a, the intercept, and b, the slope, which is equivalent to selecting the zeta's in a geometric progression and is the restriction given by Eq. 6, since α and β may be taken as exp(a) and exp(b) respectively. The selection of exponential parameters in a geometric sequence had been previously recommended by Reeves (17) for Gaussian primitive functions. In 1963 Reeves and Harrison (18) presented calculations on ammonia in which the s Gaussian primitives were chosen in this way and optimized in terms of an α and β. Since that time, the concept of an even-tempered basis has not been used, even for Gaussians.

Adequacy of the Even-Tempered Basis

A first question of interest is the completeness of the radial part of the new basis. It is pertinent to discuss the Laplace-Stieltjes transform

$$f(r) = \int_0^\infty \exp(-\zeta r)\ du(\zeta), \tag{23}$$

which is a generalization of the Laplace transform for which

$$u(\zeta) = \int_0^\zeta c(s)\ ds.$$

This transform correctly represents a large class of functions f(r). Representation of a single exponential is of course trivial, if $u(\zeta)$ is taken as the unit step function $u(\zeta-\zeta')$ such that

$$du(\zeta-\zeta') = \delta(\zeta-\zeta')\ d\zeta$$

and so

$$f(r) = \int_0^\infty \exp(-\zeta r) \quad \delta(\zeta-\zeta') \; d\zeta$$

$$= \exp(-\zeta' r)$$

where $\delta(\zeta-\zeta')$ is the delta function introduced by Dirac (10). Since exponential functions are known to be the best analytic functions representing atomic orbitals, it is natural to assume that the real atomic orbitals are also representable by such transforms. Moreover, the Laplace-Stieltjes transform generates a Dirichlet series (19,20)

$$(24) \qquad f(r) = \sum_{k=1}^{\infty} a_k \; \exp(-\zeta_k r), \qquad 0 \leq \zeta_1 < \zeta_2 < \zeta_3 \ldots, \qquad \lim_{k\to\infty} \zeta_k = \infty,$$

if

$$u(\zeta) = 0 \qquad -\infty < \zeta \leq \zeta_1$$

$$= s(n) \qquad \zeta_n < \zeta \leq \zeta_{n+1} \qquad n=1,2,\ldots\infty$$

with

$$s(n) = \sum_{k=1}^{n} a_k \qquad\qquad n=1,2,\ldots\infty \; .$$

Although infinite, this series clearly is of the form of the radial part of the linear combination of even-tempered exponential functions in Eq. 21. Thus, the constraint of Eq. 22 defines a special class of Dirichlet series. We make the conjecture that the exponent selection prescribed by Eq. 22, with k ranging to infinity, would result in a set of exponentials which form a complete basis, just as the Laplace transform does. In that case, one could interpret Eq. 22 as a practical grid for a numerical approximation to the Laplace transform. If this is so, then there is no loss of generality in the restriction to a single power of r. Similar arguments may be made for Gaussian series generated from Gaussian transforms.

From a practical point of view, it is more important whether or not this type of basis is adequate to expand the type of radial functions occurring in atomic SCF orbitals. It must be proved that impractical summation limits need not be used to attain the necessary accuracy. Furthermore, the question of appropriateness with respect to molecular calculations must be answered. Experience described in this work shows that the basis is not only very practical in many ways but is appropriate in terms of the molecular results which may be obtained.

Advantages and Disadvantages
of the Even-Tempered Basis

Before attempting to show that the present basis is sufficient to replace other earlier bases, it is of interest to review the possible advantages of using such a basis. Even if the new basis is not strictly competitive with others, a careful evaluation of all points for and against is necessary in order that adoption might be considered. It is to this end that the following lists are given.

Advantages

1. The new basis, instead of having one optimizable parameter per basis function, has two such parameters per group of atomic functions belonging to the same symmetry species of an atom or in some cases per atom. In either case, the net result is a marked decrease in the number of optimizable parameters. Presently there is little possibility of subjecting any basis to full optimization in polyatomic molecule calculations. The crucial fact is that optimization methods are based on quadratic fits and are iterative, with each fit requiring $(n+1)(n+2)/2$ points, where n is the number of free parameters per independent group. Change of basis functions or their determining parameters implies the recomputation of integrals requiring a large fraction of the computation time. Together, these facts render the use of full basis optimiza-

tion impractical. It may be that with a smaller number of largely independent parameters, optimization will become feasible.

2. Restriction of the basis to fewer analytic forms means that programs to compute integrals over the functions will be simpler than for alternative cases. This will alleviate some of the difficult programming and will most likely mean that less of the fast core will be needed for the code instructions and certain constant arrays.

3. Another reason for using the even-tempered basis is connected with the analysis required to formulate expressions for integral evaluation. The limitation to a solid harmonic multiplied by an exponential or Gaussian is the key here. The evaluation of two-electron integrals is often accomplished using some expansion of r_{12}^{-1} (21-26). For a general four-centered integral the problem is to express the four basis functions in coordinates of two centers. It is desirable then to have explicit formulae, preferably in closed form (finite series), for this expression. It has been shown that the solid spherical harmonic translates to parallel coordinate systems simply and in closed form (27-30). A special property allows the product of two pure Gaussian primitives located at separate points to be expressed as a single Gaussian on a point along the line joining the original Gaussians. Translating the solid harmonics to the same point produces a

bipolar problem which coupled with a bipolar expansion of r_{12}^{-1} may be solved in closed form. There is no convenient property for simple exponentials but the zeta-function expansions of Barnett and Coulson (31,32) and others (33-35) involve the expansion of one exponential at the site of the other. Coupled with the solid-harmonic translation, the integrals could in principle be carried out. This has in fact been used with the more general exponential for four-centered integrals but resulting programs (34) are very slow and therefore impractical Perhaps with the aforementioned restrictions and with more concentration on providing for fewer cases, a practical set of programs could be written. In summary then, it is this neat property of the solid harmonic which may be of practical aid in future integral analysis.

4. Since many basis functions are of the same symmetry subspecies (i.e. have the same quantum numbers l and m from the spherical harmonic), calculations may be set up so that large blocks of integrals of uniform type are computed at the same time. This is particularly useful if the molecular calculation is to be carried out in terms of "contracted" or linear combination of primitive basis functions (18). In this event, the integrals over the primitives need not be stored even temporarily since they may be used right away in forming contracted integrals. Efficient techniques for this process keep the storage area to a minimum. In this way a

large block of integrals is "condensed" into a smaller block. No other contribution to the smaller block is needed and these integrals may be written on a peripheral device for later use. This contraction procedure (Appendix C) is used here for all molecular calculations.

5. The even-tempered basis has a unique space covering feature as a result of the geometric sequence of exponents. The expressions for the overlap integral between two normalized Gaussians or two normalized exponentials X(klm) and X(k'lm) at the same point in space may be rearranged to reveal that the value of the overlap integral is a function of the <u>ratio</u> of the exponents ζ and ζ'. For an example, refer to Appendix A. Because of this, a set of even-tempered functions of the same symmetry type has a matrix of overlap integrals, the peculiar feature of which is that values along diagonal lines are constant. This feature suggests that the basis "covers" the Hilbert space evenly, or equivalently, that no part of the Hilbert space intercepted by the basis is covered better (i.e. may be represented better) than any other part except near the limits of the space. A feature such as this is not necessary but is valuable if one wishes to use the same basis over regions of space other than that for which the basis was originally designed by replacing the radial argument r by the "scaled" argument (tr). This introduction of such a scale parameter t is an important device

when atomic functions are used for molecular calculations.

6. The uncontracted basis cannot become linearly dependent if the spacing parameter beta is forced to stay greater than one. This has been easy to avoid even with free optimization of beta since $\beta=1$ would imply only one function with one exponent, a situation which is clearly not as good as a collection of functions with several different exponents. If beta would approach unity, the energy would increase as would the possibility of linear dependence.

7. Because of the small number of optimizable parameters upon which the basis depends, it may be possible to formulate a set of rules allowing one to quickly determine parameters for any atom. The utility of such a set of rules is proven by the wide and successful usage of Slater's empirically derived rules (36) for minimal basis sets. There are no similar rules for larger basis sets. In essence these rules would be a further parametrization of the optimizable parameters which are now found by other means. Such a parametrization would be useful where the parameters could not otherwise be optimally determined or as a first guess in their determination.

8. The proper mixing of the basis need not be prescribed since no mixing is used. This in effect is also a removal of parameters from the specification of the basis.

Disadvantages

1. The limitation of the basis for atom and molecule calculations as a product of a solid harmonic times a Gaussian with no additional power of r is not new. O-ohata et al. (37) showed that a uniform Gaussian s-basis of this type is sufficient to expand either 1s, 2s, or 3s Slater-type orbitals. In fact, the mean square deviations for the 2s and 3s orbitals are shown to be smaller than for the 1s orbital. This is probably due to the absence of a cusp. Similarly, Slater-type 2p, 3p, and 3d orbitals were fit very well with 2p and 3d Gaussians. Subsequently, it has been common practice to limit a Gaussian-type basis in this way although perhaps some mixing of basis forms could give better results.

2. The same type of restriction as above has apparently never been used or conceived of before in the case of exponential-type bases. Early *ab initio* calculations on molecules used "minimal" bases of Slater-type atomic orbitals where the orbital exponents were fixed by Slater's rules (36). The word minimal is used to imply that just one basis function per fully or partially occupied atomic orbital in the atomic ground state configuration is used as the molecule basis. The minimal basis returns quite a good energy for diatomic molecules (38,39). It seems to have developed that the mixed Slater-type minimal basis was augmented by adding other functions of the same mixed variety, for example, the

mixed double-zeta basis invented by Richardson (40).

3. For Gaussian calculations, the practice of using the same functional exponents ζ, for all symmetries of the basis of one atom was adopted. This is a further restriction to be sure and separate ζ's for the separate symmetries would have to be better as a consequence of the variational principle. It has been found, in determining Gaussian atomic bases, that the difference between least-square approximations to the same exponential atomic orbitals with and without this restriction is not overwhelmingly large, in most cases less than an order of magnitude.

4. Another disadvantage is that the primitives are not independently optimized which means that the best result per basis size is not attainable. This again is a consequence of the variational principle and certainly is true. One must weigh the small loss in quality against the enormous gain in feasibility of parameter optimization. An important question is how many more even-tempered basis functions are needed as compared to the standard mixed bases.

5. In order to apply constraints to the calculation to satisfy certain theoretical requirements, a loss in variational freedom is suffered. Because the number of free parameters is already small, this may have a deleterious effect on the results. Little work of this sort has been attempted here so the possibility remains untested. Constraints such

as the cusp constraint have been applied to mixed bases without affecting the energy measurably (41). However, more basis functions were needed to maintain the quality.

ATOM CALCULATIONS

Intention

The logical first test of the even-tempered basis concept is an application to atoms. Here a test of the "completeness" of the basis is easily possible since the symmetry classification of Hartree-Fock atomic orbitals is identical to the symmetry classification of the basis functions. Hence one does not need to be concerned that some other atomic functions of different symmetry might contribute to a given atomic orbital. For example, the helium ^1S state is described by a single spherically symmetric atomic orbital. This means that only basis functions of spherical form, the s functions where $l=0$, need be used to describe it. Because of this type of limitation, the possibility of approaching the Hartree-Fock limit may be tested. In molecules, this is not generally possible. A diatomic orbital of sigma symmetry for instance, may have a contribution from all atomic function symmetries $l=0,1,2,\ldots\infty$.

Furthermore, atom calculations do not require extensive computer time since the integrals may be computed quickly in simple closed form with exponential functions as a basis. The exponentials exhibit proper analytic behavior at the origin (42) and at long range (43) and fewer of these functions are needed in comparison to Gaussian functions (44).

Several compilations of atomic SCF results are available with which to compare the new approach (45-48). These all employ a mixed basis, i.e. not restricted to 1s, 2p, 3d, etc., so that the effect of the restriction may be assessed. It is fair to compare the results of the present work to these results since the approach taken is similar.

The aim of the atom calculations was that the best possible even-tempered atomic orbitals would be found for a given basis size. To fulfill this purpose, the parameters of the basis, α and β, were varied automatically to minimize the SCF energy. Separate parameters were taken for each symmetry s, p, d, and f. Moreover, the primitive basis functions of Eq. 19 (p=1) were used as the variational functions of the SCF procedure. This means that the atomic orbitals which result have the form of an even-tempered function, that being a normalized linear combination of appropriately defined primitives. According to the SCF technique, these even-tempered basis atomic orbitals are the best atomic orbitals expressible in terms of the basis. It is therefore fair to compare the results of these calculations to the existing atomic SCF results since the approach is similar. In the other calculations, the primitive functions are also the variational functions and the orbital exponents ζ are usually optimized to some extent. A group of efficient programs were written to carry out the proposed calculations. These are described in

Appendix A.

In order to arrive at a good initial guess for the parameters α and β, a program was written to find the best weighted (r^{-1}) least-squares approximation of an even-tempered basis to some given mixed exponential atomic orbital or orbitals. This technique was used to get initial values whenever an atomic SCF calculation for a specific atom was available. Heavy atoms have often not been computed beforehand with analytic basis functions although calculations by numerical procedures for all atoms have been made. The resultant numerical orbitals are described by tables of values which the orbitals attain at various values of r, the distance from the nucleus. Although they are often the best results available, numerical procedures are not easily used for molecular calculations. Therefore analytic functions in the form of exponentials or Gaussians are used here in order that ultimate extension to molecular calculations may be made. For the heavy atoms extrapolation from lighter atoms was used to get values of α and β prior to optimization. Specific starting values of α and β were found to be of little importance since the optimization procedure automatically tests values about those given. Very bad starting values were avoided however.

Investigation of Basis Size for Adequacy and Accuracy

Because of restrictions placed on the composition of the even-tempered function as described in its definition, it was thought that more primitives would be needed in the even-tempered function to equal the results obtainable with a freer basis containing mixed analytic forms within a symmetry. Thus a group of preliminary calculations were made on the ^1S ground states of helium, beryllium, and neon in order to find out just what the actual case is. Tables 1, 2, and 3 collect the results of these calculations. Several even-tempered basis results are given, followed by some results where basis mixing was allowed. All even-tempered calculations are optimum with respect to basis parameters α and β. The other results are also optimized at least in part with respect to individual exponential parameters.

The composition of the basis is given by telling the number of primitives of each standard analytic form which were used. The energy is the SCF energy, truncated to the number of figures shown. Truncation is used instead of round-off in order that a more credible value is available for comparison in for instance the checking of new programs. The quantity $|2-V/E|$ is a measure of the deviation of the virial coefficient V/E (potential energy divided by total energy) from its theoretical value of two. This is an indication of how well the virial theorem is satisfied and is a measure of the optimization of the wavefunction (49). For complete optimization, that is when the minimum energy with respect to the parameter space of the wavefunction which is being searched is found, the virial theorem is satisfied. The value 4.9(-8) means that the deviation is 4.9 in the eighth decimal place while 0.0(-10) means that it is exactly zero to the ten decimals printed in the program output. The column or columns headed "Cusp" contain values of the computed orbital cusp (42),

$$\partial\phi_{nlm}(\underline{r})/\partial r\Big|_{r=0}\Big/\phi_{nlm}(0) ,$$

which theoretically assumes the value $-Z/(l+1)$ for each atomic orbital $\phi_{nlm}(r)$, n being the atomic orbital number analogous to the principal quantum number n in the hydrogen atom wavefunctions.

All quantities in these tables and in other tables included in this work are in atomic units (50 or 51) unless otherwise specified.

Helium

The first group of calculations in Table 1 represents the even-tempered results with the comparison values following. The three term basis of Gilbert and Bagus (45) surpasses the three-term even-tempered energy but the difference is hardly significant. It is of interest that the four-term even-tempered energy is lower than the four-term energy of Clementi (46). This should not be true since the basis is composed of similar analytic functions (four 1s functions) with the even-tempered basis more restricted. It has to be that optimization of the unrestricted basis is incomplete or that the optimization leads to a false or relative minimum.

In all even-tempered results, the virial coefficient is close to the theoretical value while the other calculations are not as good. It is perhaps difficult to compare these though, since the calculations may have been made with different numbers of significant figures carried by separate machines. Of further interest is the value of the cusp. This property of the wavefunction at the nucleus is an even finer test of the basis than the energy or other properties calculated from the wavefunction. The even-tempered basis is capable of representing the proper behavior even though several basis functions are required.

Beryllium

The general features of Table 2 are the same as Table 1. Notable are the energies for the four-term calculations. It is seen that the energy for the even-tempered basis falls between the two energies from four-term mixed bases. This would suggest that the mixed basis could be best in certain cases if the mixing of the basis is appropriate. However no prescription exists for selection of the analytic form of the primitive basis functions and some trial and error procedure might be necessary. With an increase in the number of basis functions, the number of mixing arrangements becomes large and as a consequence, determination of the best mixed basis would be highly impractical. The even-tempered basis avoids this problem since the mixing question is not left open. Furthermore, the result obtained is not significantly worse, at least for the four-term wavefunction. The two five-term comparison functions attain a better energy than the five-term even-tempered function although at worst, the difference is only five ten-thousandths of a percent. Again, the virial theorem is easily satisfied and the cusp is represented reasonably well.

Neon

The neon energies are displayed in Table 3 according to the same format as above. It is somewhat difficult to compare the bases here since all comparison calculations used p primitives only of 2p analytic form. These are the same as the even-tempered functions and therefore, difference effects of the p parts of the wavefunctions are minimal and difficult to identify. However, general trends in for example, the 2p cusp suggest that the p part of the wavefunction is as adequately represented as the s part. Again it is seen that the even-tempered basis lags the more traditional mixed basis with respect to energy lowering but the difference between energies computed with bases of similar size is not really significant.

Summary

In summary, the results for helium, beryllium, and neon indicate that the even-tempered basis is an adequate basis for the representation of Hartree-Fock atomic orbitals. The standards of low energy, accurate cusp values, and satisfaction of the virial theorem are all met successfully. This suggests that the basis set is complete, at least to the same degree as the mixed bases used for comparison. A general fact that emerges is that more often than not, more even-tempered exponentials would be needed to attain the accuracy obtained with a good mixed basis. With optimization however, this must be a minor consideration since the total time of calculation is of sole import. For helium and beryllium, the number of optimizable parameters is reduced to just two, and for neon, just four. Bases good enough to attain the Hartree-Fock accuracy limit require large numbers of basis functions. Consequently, widely differing numbers of optimizable parameters are required for the two types of basis, implying an even-tempered advantage. For example, the neon eighteen primitive mixed basis of Table 3 requires optimization of ten parameters as opposed to four.

It is difficult to identify the effects of the individual even-tempered basis restrictions because those bases available for comparison are not designed to bring out the differences. The programs used here could not be used to make other mixed basis calculations because of the built-in restrictions.

It was deemed worthwhile nevertheless, to carry out an extensive group of calculations on several atoms with basis sizes governed by these preliminary results and by practical considerations. In this way some good even-tempered atomic bases would be made available and furthermore, this new basis might be proved useful in other ways.

Double-Zeta-Type SCF Calculations

Because of computational limitations, some limit to the size of a computational basis must be imposed. Although molecular calculations are not widely carried out with exponential-type basis functions, the "double-zeta" (DZ) exponential basis has been proposed as a basis of proper and adequate size for molecular work (40,52). In fact, atomic Gaussian bases which duplicate atomic double-zeta SCF energy results are often chosen to be used for molecular calculations. The double-zeta basis is therefore a kind of benchmark or standard of accuracy.

By definition, the double-zeta basis is a mixed basis, which is made up of two non-orthogonal Slater-type primitives of the same designation as the corresponding atomic orbital which is to be represented. For example, neon has a ground state configuration $1s^2 2s^2 2px^2 2py^2 2pz^2$ or $1s^2 2s^2 2p^6$. Consequently, the double-zeta basis for neon consists of two 1s type functions, two 2s type, and two each of 2px, 2py, and 2pz. Recent optimum double-zeta bases for helium through argon are given by Huzinaga and Arnau (53). The exponents of each of these primitive functions were carefully varied to attain best energy minima. These bases are found sufficient to obtain a large part of the Hartree-Fock atomic energy and contain enough functions so that each electron could be represented by one analytic basis function. This property means that the basis has enough variational freedom for use in configuration interaction theories. Minimal basis sets cannot be used for that purpose.

As a comparison we have found the even-tempered double-zeta (ETDZ) bases for the atoms lithium through argon. The even-tempered double-zeta basis is an even-tempered basis which is of the same size (same number of primitives) as the ordinary double-zeta basis but with the even-tempered restrictions. For example, neon requires four 1s primitives and two each of the 2px, 2py, and 2pz primitives. Because there is no basis mixing within a symmetry, a notation similar to that introduced for Gaussians by Neumann and Moskowitz (54) may be conveniently used. The symbol (ks,lp,md) is used to denote the basis of k s functions, l independent p functions, and m independent d functions. Each symmetry is degenerate of degree 2l+1 so that, for instance, each independent p function implies three primitives; px, py, and pz. The parentheses further mean that each function is a variational function in the theoretical procedure. The neon basis above is (4s,2p). Square brackets denote the number of contracted functions, a concept to be treated at length in the following sections on molecular calculations. The letters s, p, d, or f, or the commas may be left out in order to be more compact.

The energies from these calculations are collected in Table 4. Some basis parameters are presented in Table 9 along with corresponding coefficients describing the even-tempered SCF atomic orbitals. This table contains basis information for only the atoms boron through magnesium since the even-tempered double-zeta basis is identical to the even-tempered augmented double-zeta (ETADZ) basis to be described below. Basis information for the remaining atoms is given under the ETADZ classification.

In Table 4 we find that the even-tempered double zeta basis gives a lower energy for beryllium and boron. For all other atoms the regular double-zeta basis gives a lower energy although either way, the difference is smaller than two-hundredths of one-percent. Therefore, the even-tempered double-zeta basis is quite good in comparison, and in fact would probably retain the same standard of accuracy in a molecular calculation. This contention has however not been tested at this time. A simple test would be to use both of the optimum double-zeta bases for calculations on a group of first- and second-row diatomic molecules.

Augmented Basis SCF Calculations

In order to provide other fully optimized atomic bases which might be more suitable for future molecule calculations, especially for heavy atoms, two bases other than the double-zeta size were considered. First of all, we have taken what we call the even-tempered augmented double-zeta basis which is near double-zeta size. The difference is that whenever only two basis functions are used to represent a symmetry for the double-zeta case, the basis for that symmetry is augmented by one function. For example, neon, which requires two 2p functions in the double-zeta basis, would be given three in the augmented basis, i.e. (4s,3p) as opposed to (4s,2p). For argon, the basis is (6s,4p), so the augmented basis is identical to the double-zeta basis.

The reason for this augmentation is to achieve a "balance" (55) among the bases of all symmetries. It is reasonable to have each symmetry represented equally well so that for example, the addition of a single function to *any* symmetry will result upon optimization in an approximately equal energy lowering. In the case of double-zeta neon, only two basis functions can represent the 2p atomic orbital, whereas in argon, all four p basis functions share in the representation of the 2p and 3p atomic orbitals. The extra function of the augmented basis adds extra potential linear variation for the neon p orbital.

As a second basis we have chosen the even-tempered augmented triple-zeta (ETATZ) basis. This is a triple-zeta sized basis (i.e. three primitives per occupied or partially occupied orbital) of even-tempered variety which is augmented in the same way as the double-zeta basis above. Here neon would have a (6s,4p) basis while that for argon would be (9s,6p).

In order to evaluate the results obtained with the augmented bases it is convenient to divide them into the separate classifications of light atoms and heavy atoms. The division is chosen to be at atomic number Z=21, which is the first atom requiring d orbitals in its ground state configuration.

Light atoms

A complete set of results has been compiled for the light atoms in both of the augmented bases. The energies are presented in Table 5 along with accurate SCF values approaching Hartree-Fock (47,48) for comparison.

By a comparison of Table 5 with Table 4, one sees that for the atoms boron through neon, for which the double-zeta and augmented double-zeta bases are different, a substantial difference is observed. In fact, this difference is greater than that between the two augmented bases of Table 5. Thus, it would appear that the augmented double-zeta basis is a significant improvement over the ordinary double-zeta basis and that consequently it may be a good computational choice for molecules.

Of further interest is the accuracy characteristic of the triple-zeta energies. The energies obtained for silicon, phosphorus, sulfur, and potassium are lower than the previous accurate values while the others remain higher but close. The important point may be reiterated that just four parameters were varied to obtain these optimum energies whereas, for example, the accurate argon wavefunction, a cusp-constrained function, depends on fourteen non-linear variational parameters.

Heavy atoms

The heavy atoms, as defined here require d and/or f orbitals for the ground state configuration. It was not possible to try each atom in the transition or lanthanide series because the proper coupling coefficients are not available with which to form the correct ground states. However, results given include both open and closed d- and f-shells and should be sufficient to test the performance of the new basis, since prior results for light atoms show no dependence on the state.

For these heavy atoms, the basis used for the most part was the smaller augmented double-zeta basis, purely for economic reasons. In instances where the triple-zeta basis was tried, the energy comparison with accurate results is very good, the difference being a very small percentage of the total energy. The energies are displayed along with light atom energies in Tables 5, 10, and 11.

The calculations for the series rubidium through lanthanum represent the first tabulation of analytic basis SCF calculations for this group of atoms. Furthermore, these analytic bases are designed to have a balanced composition, with no symmetry emphasized. In the past, some SCF calculations were made on heavy atoms, especially the lanthanide series (56), in which the outer f-shells were emphasized. A basis which could be considered nearly minimal (viz. one basis function per pair of electrons) was used for s, p, and d electrons. Four or five f basis functions were then used for each f orbital. It may be argued that the symmetries are largely independent so this may be done. However they are not completely independent and just how much so is an important question if one is to justify reaching any practical conclusions on the basis of the results. This is especially true here since the core orbitals have a large shielding effect on outer orbitals. This kind of calculation most probably was done because of a lack of computing power and general methods for the selection of good bases.

Although present calculations obtained for heavy atoms past krypton cannot be compared to other analytic basis SCF calculations, it appears that there is no loss of computing ability with the extension to greater numbers of electrons or higher symmetry. The fifth period of the table involves a second occupied d-level. Moreover, we include two calculations involving f orbitals, those of gadolinium ion and radon. The linear coefficients for the f orbitals shown in Table 10 are quite similar to corresponding cases where a new symmetry was occupied for the first time, for example, the d shell of krypton or the p shell of neon. Also the optimal slope parameter β is consistent as expected.

A comparison of energies may be made with the numerical SCF results of Fischer (57) or Mann (58,59). Mann's calculations do not treat the orthogonality of open-shells properly so that in that sense they do not exactly correspond to the Hartree-Fock solutions. The calculations of Fischer apparently do treat this criterion correctly. Both sets of numerical calculation apparently were done with low precision arithmetic so that due to accumulation of machine error, the latter figures of the energy values might be considered dubious. Nevertheless, Fischer records an energy of -21866.79 Hartrees for radon while the present calculation yielded a value of -21866.62648 Hartrees. This is quite a good comparison. A similar result for Gd^{+3} was not found. Numerical results are said to be very close to exact Hartree-Fock since no problem of only partial representation of the Hilbert space of an atom exists. One in effect solves for the solution space directly. If these numerical results are indeed well done, then the even-tempered basis has also performed very well.

Local minima

Although no serious problems occurred while running the programs, it was found that local minima in the energy surfaces do occur. A scan of Tables 10 and 11 reveals that the slope or spacing parameter, β, is often approximately constant through a similar group of atoms within one type of basis (e.g. boron through neon). This holds for the augmented triple-zeta bases in Table 11 but it is not strictly true for the augmented double-zeta basis as seen in Table 10. If now the coefficients in Table 10 corresponding to the latter are examined, one finds a change of the primitive function which has the largest coefficient in the 1s and 2s atomic orbitals. In particular, the largest coefficient of the 2s orbital is always the first function, but in the sequence boron to neon, the largest coefficient of the 1s atomic orbital changes at carbon from the third primitive to the fourth. This coincides with the change in the slope parameter. It was possible to find a set of optimum bases where the parameter β was more constant throughout this group of atoms but bases other than those displayed produced a slightly higher energy. Such minima were true local minima since extensive optimization about the point did not reveal a false minimum or saddle point. In fact, the virial coefficient was close to two at these points.

Although these local minima can occur, it is sometimes possible to spot irregularities in sequences such as that described above so that the true minimum may be found. For example, if the β parameter switched back in the sequence discussed above, one would expect that something is amiss and look to resolve it.

It is hoped that none of the wavefunctions given represents a local minimum of the energy surface but no assurance can be given that all are true optima. For the most part, extensive trials were made, especially for the light atoms in the smaller bases. Often it was found that even though the basis parameters were quite different for separate minima, the corresponding energy values were equal to a large number of significant figures. Thus the results given here may be considered a good indication of the capability of the even-tempered basis.

We feel that apart from the problem of possible local minima, the even-tempered basis has been demonstrated to be quite useful for atomic calculations. It seems to be at least adequate, and may be used conveniently to attain high standards of accuracy. It is hoped furthermore, that the even-tempered basis approach contains improvements which will prove useful to cope with problems arising in atomic as well as molecular problems.

Properties

A compilation of properties computed in each basis for all atoms listed in this work is included in Table 12. The table is arranged by atomic number and within this classification by basis size, the smaller bases taken first. The atomic number and name of the atom or ion along with the spectroscopic state and orbital configuration preceeds the basis composition. The quantity $|2-V/E|$ described before is given along with |1-Norm| which is the deviation from the value one of the computed overlap, $\langle\Psi|\Psi\rangle$, of the total wavefunction Ψ. Values of the cusp summed over all orbitals of the same symmetry are given next. Finally expectation values of several operators, $\langle\phi_i|O|\phi_i\rangle$, are given for each atomic orbital ϕ_i and also summed over all occupied orbitals

$$\langle\Psi|O|\Psi\rangle = \sum_{i}^{occ.} N(i)\langle\phi_i|O|\phi_i\rangle$$

for the total wavefunction, with occupation numbers $N(i)$. The total is listed just below the operator heading with the orbital values following according to the conventional atomic orbital notation. The operators are in order: T, kinetic energy; V(1), one-electron potential energy; V(2), two-electron potential energy; V(T), total potential energy; E, total energy or T+V(T); e, orbital energy (the total represents [T+V(1)]+2•V(2)); -cusp, orbital values; r max, the value of r at which the orbital distribution attains a maximum; and r^{-3}, r^{-2}, r^{-1}, r, r^2, r^4, r^6, various powers of the operator r. The cusp and r max are not expectation values but orbital properties so that a total is not given. The expectation value of r^{-3} is not defined for s orbitals and therefore the total is not possible. The ordering of the orbitals in this table is according to a numerical sequencing of the orbital eigenvalues e. Table 12 is computer printed and as a consequence, all values printed here have been automatically rounded off, including the total energy.

Table 1. SCF ground state helium calculations

Number of Basis Functions 1s	2s	Total	Energy	|2-V/E|	-Cusp	Ref.
3	-	3	-2.861679036686	5.0(-10)	2.015	a
4	-	4	-2.861679875316	1.3(-7)	2.0013	a
5	-	5	-2.861679986833	4.0(-8)	2.0004	a
6	-	6	-2.861679987495	1.0(-10)	2.0011	a
7	-	7	-2.861679994968	4.9(-8)	2.00060	a
8	-	8	-2.861679995610	2.0(-10)	2.000029	a
12	-	12	-2.861679995615	3.7(-8)	1.999968	a
2	-	2	-2.8616725			b
1	2	3	-2.861680	7.0(-6)	2.012	c
4	-	4	-2.8616785	1.2(-6)		d
5	-	5	-2.8616799	2.3(-6)		d

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a. This work
b. Huzinaga and Arnau (53)
c. Bagus and Gilbert (45)
d. Clementi (46)

Table 2. SCF ground state beryllium calculations

Number of Basis Functions				Energy	|2-V/E|	-Cusp		Ref.
1s	2s	3s	Total			1s	2s	
4	-	-	4	-14.57282754	2.9(-7)	4.08	4.03	a
5	-	-	5	-14.57294014	1.7(-8)	3.95	4.11	a
6	-	-	6	-14.57301487	5.0(-10)	4.03	4.05	a
7	-	-	7	-14.57302122	7.2(-9)	3.993	3.96	a
8	-	-	8	-14.57302308	4.6(-9)	4.003	4.006	a
12	-	-	12	-14.57302316	2.0(-9)	3.9998	4.0001	a
2	2	-	4	-14.572371				b
2	1	1	4	-14.57299	1.3(-5)	4.02	3.95	c
2	3	-	5	-14.573014	1.2(-6)			d
2	2	1	5	-14.57302	0.0(-6)	4.02	4.03	c
2	4	-	6	-14.573020	1.5(-6)			d

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a. This work
b. Huzinaga and Arnau (53)
c. Bagus and Gilbert (45)
d. Clementi (46)

Table 3. SCF ground state neon calculations

Number of Basis Functions					Energy	|2-V/E|	-Cusp			Ref.
1s	2s	3s	2p	Total			1s	2s	2p	
4	-	-	2	10	-128.5342215	5.7(-8)	9.87	9.91	4.16	a
4	-	-	3	13	-128.5449241	3.1(-8)	9.87	9.90	4.62	a
5	-	-	3	14	-128.5465597	2.0(-10)	10.02	9.97	4.62	a
5	-	-	4	17	-128.5469298	2.5(-8)	10.02	9.97	4.76	a
6	-	-	4	18	-128.5469510	1.5(-8)	10.02	10.12	4.75	a
6	-	-	5	21	-128.5470677	4.0(-8)	10.02	10.12	5.10	a
8	-	-	6	26	-128.5470968	3.8(-8)	10.001	9.98	5.07	a
2	2	-	2	10	-128.53508					b
2	1	1	3	13	-128.54648	8.0(-6)	10.01	10.01	4.68	c
2	3	-	4	17	-128.54698	3.2(-6)				d
2	2	1	4	17	-128.54709	2.0(-6)	10.02	10.05	5.0003	c
2	4	-	4	18	-128.54701	4.9(-6)				d

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a. This work
b. Huzinaga and Arnau (53)
c. Bagus and Gilbert (45)
d. Clementi (46)

Table 4. Double-zeta vs. even-tempered double-zeta energies

Atomic State	Energy This work	 Reference (53)	Percent Diff.
Li(^{2}S)	-7.431888	-7.4327223	0.0112
Be(^{1}S)	-14.572827	-14.572371	0.0031
B(^{2}P)	-24.528240	-24.527921	0.0013
C(^{3}P)	-37.686548	-37.686751	0.0005
N(^{4}S)	-54.397139	-54.397950	0.0014
O(^{3}P)	-74.803506	-74.804316	0.0010
F(^{2}P)	-99.400464	-99.401302	0.0008
Ne(^{1}S)	-128.534221	-128.53508	0.0006
Na(^{2}S)	-161.848025	-161.85002	0.0012
Mg(^{1}S)	-199.604884	-199.60702	0.0010
Al(^{2}P)	-241.865719	-241.87320	0.0030
Si(^{3}P)	-288.844336	-288.85120	0.0024
P(^{4}S)	-340.709037	-340.71597	0.0020
S(^{3}P)	-397.491350	-397.50230	0.0209
Cl(^{2}P)	-459.458310	-459.47962	0.0046
Ar(^{1}S)	-526.795062	-526.81512	0.0038

Table 5. Augmented double- and triple-zeta energies

Atomic State	Energy		
	ADZ	ATZ	Reference (48)
He(^{1}S)	-2.861679	-2.861679	-2.8616799
Li(^{2}S)	-7.431888	-7.432720	-7.4327257
Be(^{1}S)	-14.572827	-14.573014	-14.573020
B(^{2}P)	-24.528484	-24.529049	-24.529052
C(^{3}P)	-37.687365	-37.688598	-37.688611
N(^{4}S)	-54.398981	-54.400895	-54.400911
O(^{3}P)	-74.807525	-74.809286	-74.809359
F(^{2}P)	-99.407396	-99.409204	-99.409284
Ne(^{1}S)	-128.544924	-128.546951	-128.54701
Na(^{2}S)	-161.855877	-161.858803	-161.85889
Mg(^{1}S)	-199.606331	-199.614546	-199.61458
Al(^{2}P)	-241.865719	-241.876625	-241.87665
Si(^{3}P)	-288.844336	-288.854277	-288.85426
P(^{4}S)	-340.709037	-340.718696	-340.71866
S(^{3}P)	-397.491350	-397.504766	-397.50475
Cl(^{2}P)	-459.458310	-459.481799	-459.48187
Ar(^{1}S)	-526.795052	-526.817019	-526.81734
K(^{2}S)	-599.147486	-599.164566	-599.16446
Ca(^{1}S)	-676.743435	-676.757145	-676.75803
Sc(^{2}D)	-759.717952		-759.73555
Cr(^{7}S)	-1042.333876		-1043.3539
Mn(^{6}S)	-1149.834817		-1149.8651
Cu(^{2}S)	-1638.880127		-1638.9614
Zn(^{1}S)	-1777.780153		-1777.8470

Table 5. (Continued)

Atomic State	Energy		
	ADZ	ATZ	Reference (48)
Ga(^{2}P)	-1923.158789	-1923.259911	-1923.2602
Ge(^{3}P)	-2075.252892		-2075.3590
As(^{4}S)	-2234.127989		-2234.2382
Se(^{3}P)	-2399.794470		-2399.8669
Br(^{2}P)	-2572.371868		-2572.4406
Kr(^{1}S)	-2751.989840		-2752.0543
Rb(^{2}S)	-2938.301898		
Sr(^{1}S)	-3131.497207		
Y(^{2}D)	-3331.580682		
Mo(^{7}S)	-3975.348771		
Tc(^{6}S)	-4203.747941		
Pd(^{1}S)	-4937.518502		
Ag(^{2}S)	-5197.389750		
Cd(^{1}S)	-5464.891360		
In(^{2}P)	-5739.955617		
Sn(^{3}P)	-6022.778861		
Sb(^{4}S)	-6313.332880		
Te(^{3}P)	-6611.644773		
I(^{2}P)	-6917.851512		
Xe(^{1}S)	-7232.015542	-7232.136903	
Cs(^{2}S)	-7553.835452		
Ba(^{1}S)	-7883.462981		
La(^{2}D)	-8220.974409		
Gd^{+3}(^{8}S)	-10819.244854		
Rn(^{1}S)	-21866.626489		

Table 6. Even-tempered helium orbitals

Num. of Primitives	α/β	Coefficients 1s	Num. of Primitives	α/β	Coefficients 1s
3	0.932625	0.754230	8	0.791863	0.002257
	1.517207	0.176473		1.326345	0.670548
		0.094288			0.195043
					0.077427
4	0.852996	0.770410			0.069819
	1.662827	0.212485			0.011532
		0.044500			-0.000622
		-0.002390			-0.000911
5	0.520556	0.003783	12	0.886077	0.002039
	1.654836	0.772507		1.250257	0.632834
		0.204780			0.188303
		0.046655			0.077297
		-0.002620			0.070527
					0.039531
6	0.520505	0.003942			0.019261
	1.655188	0.772942			-0.005271
		0.204117			0.001719
		0.046742			-0.001360
		-0.002718			0.000240
		0.000021			-0.000027
7	0.743184	0.003370			
	1.373390	0.699106			
		0.181136			
		0.092362			
		0.048028			
		0.002940			
		-0.001848			

Table 7. Even-tempered beryllium orbitals

Num. of Primitives	α/β	Coefficients 1s	2s
5	0.341735	-0.003323	1.423143
	2.181110	0.020668	-0.600065
		0.944531	-0.135170
		0.050992	-0.004535
		-0.001715	-0.000186
7	0.445690	0.000086	1.466503
	1.668493	-0.001087	-0.322507
		0.012748	-0.370989
		0.894730	-0.069240
		0.096131	-0.017014
		0.009841	-0.002451
		-0.001086	0.000432
8	0.514111	-0.000914	1.601002
	1.472859	0.005444	-0.433816
		-0.019970	-0.124325
		0.086934	-0.343648
		0.864124	0.025367
		0.034619	-0.037930
		0.045149	-0.002806
		-0.004028	0.009515
12	0.582434	-0.000584	1.789901
	1.318837	0.004106	-0.612197
		-0.015097	0.030074
		0.040205	-0.198415
		-0.096614	-0.261399
		0.568058	-0.040633
		0.512672	0.014270
		-0.071786	-0.034889
		0.071893	-0.001886
		-0.000247	-0.001052
		-0.000896	0.000503
		-0.000347	0.000015

Table 8. Even-tempered neon orbitals

Primitive s orbs.	α/β	Coefficients 1s	Coefficients 2s	Primitive p orbs.	α/β	Coefficients 2p
6	1.183392	0.001522	1.085652	5	0.945886	0.379104
	1.683379	-0.002025	0.317739		1.730264	0.471489
		0.041120	-0.626813			0.232068
		0.924005	-0.126793			0.014380
		0.043768	0.002019			0.001433
		-0.000197	-0.001120			
7	1.186983	0.001692	1.096454	5	0.945945	0.379168
	1.683024	-0.002824	0.298667		1.730272	0.471472
		0.044342	-0.615346			0.232028
		0.924064	-0.133471			0.014369
		0.040441	0.007127			0.001433
		0.000642	-0.003291			
		-0.000161	0.000475			
8	1.328402	-0.000079	1.016811	6	1.016690	0.274020
	1.487490	0.005844	0.357148		1.518533	0.376742
		-0.012690	-0.173826			0.289370
		0.095221	-0.485263			0.149715
		0.884190	-0.061623			0.005168
		0.025912	0.001422			0.003801
		0.011006	-0.004812			
		-0.001232	0.000744			

Table 9. Even-tempered double-zeta atomic orbitals

	Li(^{2}S)	Be(^{1}S)	B(^{2}P)	C(^{3}P)	N(^{4}S)	O(^{3}P)	F(^{2}P)	Ne(^{1}S)
α	0.307856	0.340407	0.473478	0.596363	0.831171	0.955814	1.073954	1.187882
β	1.819795	2.191497	2.130513	2.107092	1.718128	1.713781	1.713069	1.714098
1s	0.040383	-0.005416	-0.004106	-0.003359	0.023833	0.021349	0.019280	0.017584
	-0.160234	0.030455	0.029201	0.029763	-0.092634	-0.081961	-0.073120	-0.065909
	0.629373	0.945497	0.950047	0.953092	0.298659	0.267849	0.243306	0.223818
	0.507880	0.040503	0.034552	0.029537	0.779664	0.801869	0.819366	0.833149
2s	1.747934	1.422549	1.447173	1.451785	1.331797	1.270778	1.216481	1.169547
	-1.005712	-0.604531	-0.619446	-0.613568	-0.115896	-0.002848	0.091891	0.170392
	0.023828	-0.130205	-0.160126	-0.182008	-0.480427	-0.534955	-0.575754	-0.606555
	-0.078399	-0.004865	-0.001243	0.001841	-0.077345	-0.078874	-0.081021	-0.083446
α			0.455209	0.577616	0.690710	0.743435	0.817103	0.900784
β			2.203933	2.172201	2.165283	2.226565	2.260341	2.278920
2p			0.839385	0.801671	0.775851	0.742980	0.726153	0.715755
			0.216592	0.260567	0.290777	0.334277	0.356594	0.370114

Table 9. (Continued)

	Na (^2S)	Mg (^1S)
α	0.290947	0.379323
β	1.836890	1.784254
1s	0.005192	0.005290
	-0.019411	-0.020411
	0.043093	0.046080
	-0.076456	-0.082053
	0.182226	0.194774
	0.873338	0.863933
2s	0.043694	0.055187
	-0.187687	-0.239363
	0.782709	0.944856
	0.886052	0.775013
	-0.785336	-0.821832
	-0.103060	-0.090682
3s	1.849880	1.791271
	-1.212085	-0.971433
	0.108614	-0.208562
	-0.168976	-0.075757
	0.134383	0.151598
	0.012730	0.017434
α	1.196692	1.490216
β	2.136139	2.040478
2p	0.732854	0.744486
	0.338102	0.316733

Table 10. Even-tempered augmented double-zeta atomic orbitals

	B(^{2}P)	C(^{3}P)	N(^{4}S)	O(^{3}P)	F(^{2}P)	Ne(^{1}S)
α	0.473537	0.596677	0.831533	0.956576	1.075176	1.187882
β	2.130513	2.106704	1.717951	1.713445	1.712584	1.714098
	-0.004163	-0.003360	0.023842	0.021355	0.019289	0.017610
1s	0.029415	0.029770	-0.092683	-0.082012	-0.073182	-0.066011
	0.949949	0.953064	0.298839	0.268055	0.243536	0.224006
	0.034492	0.029560	0.779524	0.801706	0.819184	0.833035
	1.447285	1.452187	1.331992	1.271281	1.217363	1.167772
2s	-0.619675	-0.614147	-0.115889	-0.003089	0.091253	0.173780
	-0.160039	-0.181890	-0.480841	-0.535558	-0.576435	-0.608672
	-0.001245	0.001822	-0.077219	-0.078675	-0.080769	-0.083075
α	0.506643	0.628198	0.735915	0.759646	0.814197	0.890710
β	1.895047	1.876172	1.877756	1.943099	1.966034	1.911663
	0.755251	0.687456	0.638197	0.568813	0.521448	0.452051
2p	0.274521	0.340733	0.388061	0.458217	0.498248	0.524900
	0.030547	0.039495	0.046753	0.059188	0.073570	0.120834

Table 10. (Continued)

	Na(^2S)	Mg(^1S)	Al(^2P)	Si(^3P)	P(^4S)	S(^3P)	Cl(^2P)	Ar(^1S)
α	0.290910	0.379303	0.504009	0.547043	0.638558	0.739189	0.829412	0.924977
β	1.836890	1.784253	1.726074	1.903839	1.871659	1.841115	1.821166	1.802225
1s	0.005162	0.005277	0.005667	-0.001608	-0.001312	-0.000893	-0.000622	-0.000260
	-0.019299	-0.020357	-0.022709	0.006014	0.005015	0.003539	0.002532	0.001182
	0.042873	0.045977	0.052237	-0.013969	-0.012121	-0.009234	-0.007276	-0.004619
	-0.076147	-0.081919	-0.093048	0.057151	0.054256	0.049355	0.045786	0.040994
	0.181775	0.194579	0.217325	0.944044	0.944929	0.946737	0.948365	0.950625
	0.873611	0.864052	0.847797	0.015146	0.015724	0.016729	0.017209	0.017843
2s	0.043408	0.054991	0.065350	0.002533	-0.000843	-0.005723	-0.006021	-0.006498
	-0.185634	-0.237936	-0.288134	0.006915	0.021625	0.044535	0.046725	0.052602
	0.778505	0.941960	1.185580	1.662561	1.698594	1.725791	1.759736	1.788861
	0.890045	0.777793	0.550223	-0.894349	-0.960646	-1.024543	-1.073387	-1.120724
	-0.786947	-0.823033	-0.823494	-0.180903	-0.167682	-0.153533	-0.144777	-0.135235
	-0.102902	-0.090526	-0.076834	0.005518	0.004248	0.002805	0.002077	0.001208
3s	1.840723	1.785693	1.920029	1.890233	1.940176	2.010165	2.044823	2.089977
	-1.191602	-0.959045	-1.090592	-1.304205	-1.355841	-1.453003	-1.484125	-1.540341
	0.092869	-0.218280	-0.341121	-0.206467	-0.264487	-0.286746	-0.337346	-0.366725
	-0.164919	-0.073213	0.000693	0.239128	0.295459	0.340587	0.388375	0.428762
	0.134227	0.151571	0.170622	0.042501	0.035822	0.030396	0.023386	0.017262
	0.013055	0.017604	0.018545	-0.001327	-0.000255	0.000570	0.001551	0.002383
α	1.238510	1.578058	0.455807	0.541613	0.603840	0.662097	0.797545	0.820346
β	1.840941	1.764896	1.991736	1.955839	2.016551	2.028799	1.857083	1.993139
2p	0.540021	0.575075	0.007284	0.010654	-0.005755	-0.007839	0.027044	-0.006503
	0.466062	0.429179	0.008828	-0.005489	0.066672	0.076309	-0.071825	0.064570
	0.072052	0.061991	0.773604	0.789900	0.842321	0.856230	0.782553	0.871163
			0.270127	0.258736	0.144255	0.119140	0.305895	0.108307
3d			1.197201	1.166101	1.144724	1.113911	1.069998	1.089682
			-0.270025	-0.197767	-0.172111	-0.117159	0.009000	-0.059845
			-0.125751	-0.181131	-0.223382	-0.260169	-0.305873	-0.311454
			-0.056780	-0.056241	-0.031696	-0.024701	-0.070805	-0.020545

Table 10. (Continued)

	K(^{2}S)	Ca(^{1}S)	Sc(^{2}D)	Cr(^{7}S)	Mn(^{6}S)	Cu(^{2}S)	Zn(^{1}S)
α	0.193922	0.343262	0.263126	0.352324	0.396031	0.409456	0.459794
β	1.776909	1.782463	1.732148	1.697936	1.662137	1.705810	1.688416
	0.001510	-0.000122	0.001333	0.000877	0.001019	0.000868	0.000740
	-0.005877	0.000529	-0.005384	-0.003694	-0.004329	-0.003609	-0.003147
	0.013277	-0.001467	0.012504	0.008958	0.010497	0.008617	0.007686
1s	-0.023803	0.003224	-0.022889	-0.017225	-0.019978	-0.016232	-0.014847
	0.038226	-0.007957	0.037317	0.029662	0.033726	0.027341	0.025670
	-0.060646	0.045935	-0.060140	-0.051085	-0.056273	-0.046173	-0.044541
	0.141405	0.949088	0.142526	0.130212	0.136674	0.112723	0.111783
	0.901427	0.016114	0.899830	0.906835	0.903067	0.920337	0.920410
	0.014434	-0.002772	0.021732	0.025638	0.028621	0.014281	0.018589
	-0.055543	0.010291	-0.085961	-0.102785	-0.117095	-0.057106	-0.075363
	0.123336	-0.019607	0.193596	0.234065	0.268449	0.128113	0.170765
2s	-0.215179	0.051404	-0.339109	-0.409435	-0.470466	-0.216323	-0.291955
	0.405278	1.843742	0.626299	0.743353	0.860758	0.380755	0.516169
	1.550034	-1.187484	1.427626	1.394319	1.311645	1.745317	1.655284
	-1.159450	-0.123644	-1.205952	-1.268999	-1.275244	-1.387954	-1.396131
	-0.085620	0.000909	-0.067517	-0.052852	-0.045229	-0.052245	-0.043688
	-0.017668	0.096609	-0.016847	0.025497	0.007222	-0.055971	-0.044386
	0.059015	-0.413305	0.056707	-0.075448	-0.003769	0.207085	0.159487
	-0.070583	2.621276	-0.072400	0.024230	-0.198710	-0.358089	-0.231886
3s	2.355684	-1.760550	2.601548	-2.667596	-2.480177	2.866494	2.854218
	-2.031462	-0.483729	-2.490041	2.727879	2.780368	-2.448012	-2.651293
	-0.081624	0.543374	0.111532	-0.193055	-0.280755	-0.187467	-0.041954
	0.384082	0.001088	0.392877	-0.426529	-0.411272	0.578318	0.554905
	0.020907	0.004647	0.019001	-0.013029	-0.012428	-0.002049	-0.001607
	1.168058	2.312155	-0.987379	1.449794	1.939448	2.133012	1.961376
	0.325305	-2.024376	-0.784649	-0.079027	-1.086542	-1.703447	-1.237000
	-1.069121	0.029374	1.448903	-0.889710	-0.204049	0.603518	0.127024
4s	0.072696	0.298300	0.019375	-0.278211	-0.456106	-0.825651	-0.685636
	0.229964	0.168087	-0.468728	0.625212	0.662520	0.630139	0.676927
	0.067890	-0.153660	-0.007577	-0.047152	-0.089357	-0.041710	-0.047061
	-0.088391	0.005718	0.105073	-0.104334	-0.084806	-0.082656	-0.099969
	-0.001339	-0.001939	0.002223	-0.001861	-0.002670	-0.001418	-0.000569
α	1.018843	1.215501	1.335553	1.641460	1.725853	2.035471	2.185093
β	1.889991	1.815976	1.797167	1.686892	1.781532	1.795653	1.777885
	-0.003524	-0.001962	-0.000891	0.030727	0.000693	0.001314	0.001049
2p	0.053256	0.045521	0.042040	-0.102286	0.042390	0.044676	0.047170
	0.858100	0.846153	0.849390	0.747169	0.870057	0.897799	0.885729
	0.127654	0.143792	0.141478	0.354573	0.114971	0.092026	0.091320
	1.140557	1.187755	1.193261	1.025141	1.183573	1.147546	1.171331
3p	-0.110759	-0.156268	-0.153111	0.195680	-0.119911	-0.061098	-0.090996
	-0.334388	-0.353141	-0.371087	-0.502079	-0.419698	-0.455758	-0.455737
	-0.027322	-0.033332	-0.032300	-0.090356	-0.021931	-0.011773	-0.012069
α			0.658687	0.533402	0.978752	0.945582	1.150641
β			2.124709	2.208727	2.018390	2.040090	1.972380
			0.537951	0.388789	0.454829	0.343518	0.345979
3d			0.524132	0.558042	0.568905	0.568746	0.578565
			0.097099	0.274431	0.123918	0.268914	0.236307

Table 10. (Continued)

	Ga (^2P)	Ge (^3P)	As (^4S)	Se (^3P)	Br (^2P)	Kr (^1S)
α	0.538402	0.637392	0.753626	0.823619	0.897175	1.018984
β	1.662350	1.634359	1.711996	1.697318	1.683338	1.565084
	0.000594	0.000519	0.000419	0.000613	0.000810	0.000801
	-0.002626	-0.002399	-0.001605	-0.002400	-0.003227	-0.003906
	0.006685	0.006377	0.003302	0.005107	0.007007	0.010648
1s	-0.013503	-0.013429	-0.004864	-0.007929	-0.011172	-0.022162
	0.024374	0.025053	0.003821	0.008235	0.012889	0.039405
	-0.043923	-0.046008	0.021131	0.014803	0.008196	-0.066169
	0.113811	0.119842	0.967091	0.969810	0.972666	0.151044
	0.918237	0.913602	0.014241	0.015219	0.016211	0.893596
	0.026019	-0.033916	0.004126	0.000776	-0.002454	0.047925
	-0.107784	0.143936	-0.017620	-0.004164	0.009030	-0.217307
	0.248016	-0.336867	0.046351	0.014892	-0.016425	0.532882
2s	-0.430678	0.593340	-0.077425	-0.011650	0.055163	-0.972850
	0.771636	-1.087023	2.134996	2.109655	2.081600	1.954400
	1.464603	-1.209114	-1.453893	-1.486330	-1.516792	0.409936
	-1.387456	1.357751	-0.088028	-0.074376	-0.060995	-1.208611
	-0.031748	0.020350	0.001129	-0.000303	-0.001721	0.000952
	0.022474	-0.004357	0.120974	0.117151	0.112834	-0.069543
	-0.068252	0.051396	-0.520805	-0.510239	-0.496229	0.364056
	-0.047971	-0.452221	2.890218	3.004752	3.114914	-1.754039
3s	-2.716076	-2.408991	-1.849784	-2.082617	-2.317919	-1.036775
	2.925693	3.143605	-0.872210	-0.754357	-0.629177	3.298353
	-0.209249	-0.484533	0.869794	0.861242	0.848565	-1.114128
	-0.501000	-0.433224	-0.055865	-0.057001	-0.057165	-0.256261
	-0.000729	-0.004138	0.010376	0.010408	0.010308	-0.013268
	1.958264	2.105454	2.484167	2.499421	2.562312	2.668671
	-1.032649	-1.231747	-2.182328	-2.125493	-2.196173	-1.926050
	-0.213144	-0.380281	-0.187986	-0.432291	-0.538898	-0.868508
4s	-0.553456	-0.434572	0.474025	0.712864	0.879170	0.194731
	0.750437	0.856339	0.272673	0.193359	0.132183	0.987681
	-0.090157	-0.162035	-0.265268	-0.260240	-0.258552	-0.383412
	-0.107311	-0.103266	0.022686	0.019499	0.018168	-0.076837
	-0.000387	-0.001066	-0.003813	-0.003360	-0.003166	-0.003959

Table 10. (Continued)

	Ga(^{2}P)	Ge(^{3}P)	As(^{4}S)	Se(^{3}P)	Br(^{2}P)	Kr(^{1}S)
α	0.696547	0.708026	0.751527	0.760648	0.804871	0.854333
β	1.790710	1.798003	1.789553	1.682593	1.675264	1.667047
2p	0.001338	0.001585	0.001636	0.012598	0.012419	0.012314
	-0.003363	-0.004203	-0.004402	-0.044987	-0.044657	-0.044513
	0.003446	0.004949	0.005179	0.096888	0.096449	0.096434
	0.049649	0.046022	0.046117	-0.172268	-0.171786	-0.172025
	0.890622	0.895697	0.896177	0.519131	0.516286	0.516074
	0.083028	0.080155	0.078989	0.612056	0.614191	0.614139
3p	0.033406	0.041236	0.044169	0.021931	0.024379	0.024583
	-0.054644	-0.099708	-0.119834	-0.089491	-0.096116	-0.102101
	1.186480	1.207956	1.232700	0.554248	0.545453	0.543674
	-0.067981	-0.045200	-0.052915	0.951674	0.979383	1.000540
	-0.470229	-0.486533	-0.494815	-0.640964	-0.660154	-0.680477
	-0.008045	-0.006097	-0.005305	-0.202177	-0.203783	-0.204053
4p	1.590420	1.487097	1.436202	1.235484	1.146865	1.074870
	-0.932807	-0.711794	-0.591404	-0.176584	-0.006362	0.133899
	0.058034	-0.091049	-0.193453	-0.253685	-0.354746	-0.441498
	-0.102057	-0.057367	-0.026484	-0.248919	-0.251233	-0.253324
	0.135952	0.130336	0.131882	0.174378	0.187269	0.200053
	-0.004586	-0.002634	-0.001557	0.046768	0.051041	0.054034
α	1.362749	1.585101	1.809814	2.052312	2.288205	2.523336
β	1.920683	1.879020	1.845455	1.813346	1.784316	1.756748
3d	0.353956	0.371114	0.390883	0.418014	0.437820	0.454058
	0.585103	0.584422	0.579264	0.565091	0.552328	0.539606
	0.205666	0.176308	0.151289	0.129318	0.114781	0.104889

Table 10. (Continued)

	Rb(^{2}S)	Sr(^{1}S)	Y(^{2}D)	Mo(^{7}S)	Tc(^{6}S)	Pd(^{1}S)	Ag(^{2}S)	Cd(^{1}S)
α	0.307132	0.374861	0.386023	0.419244	0.441493	1.929641	0.467969	0.506288
β	1.616878	1.589542	1.588910	1.587330	1.582854	1.491100	1.587379	1.578295
	0.000198	0.000266	0.000210	0.000084	0.000064	0.001903	-0.000083	-0.000110
	-0.000913	-0.001258	-0.001002	-0.000431	-0.000343	-0.009630	0.000331	0.000455
	0.002388	0.003331	0.002697	0.001279	0.001069	0.026022	-0.000626	-0.000923
	-0.004854	-0.006760	-0.005596	-0.002986	-0.002623	-0.050784	0.000543	0.001047
1s	0.008807	0.012057	0.010276	0.006258	0.005752	0.080469	0.000777	0.000126
	-0.015322	-0.020320	-0.017901	-0.012397	-0.011797	-0.114106	-0.004792	-0.004167
	0.026031	0.033065	0.030072	0.023181	0.022559	0.204194	0.013507	0.013160
	-0.045743	-0.054901	-0.051471	-0.043400	-0.042821	0.864605	-0.031816	-0.032002
	0.114796	0.128786	0.123932	0.111894	0.111051		0.094167	0.095336
	0.917768	0.908831	0.911811	0.919356	0.919871		0.930560	0.929605
	-0.019320	0.023584	0.023404	0.022806	0.023318	0.049069	0.021556	0.023015
	0.084928	-0.106513	-0.105774	-0.103301	-0.106048	-0.241289	-0.097572	-0.105160
	-0.205726	0.263037	0.261342	0.255560	0.263220	0.626543	0.241348	0.261866
	0.372441	-0.481601	-0.478605	-0.468257	-0.483276	-1.194944	-0.442101	-0.481550
2s	-0.570413	0.741085	0.736245	0.719942	0.743569	2.869590	0.679083	0.740732
	0.796336	-1.036860	-1.029623	-1.006326	-1.039575	-0.643181	-0.948566	-1.034999
	-1.256819	1.673559	1.653550	1.595138	1.648014	-0.939224	1.470557	1.612085
	-1.148335	0.791321	0.820012	0.901034	0.862908	0.012551	1.052182	0.937367
	1.390255	-1.320011	-1.335223	-1.377688	-1.376135		-1.446251	-1.427066
	0.010592	-0.002451	-0.001045	0.002975	0.005132		0.008214	0.011495
	0.003616	-0.011715	-0.011256	-0.007446	-0.008871	0.134636	0.006079	-0.000290
	-0.012850	0.056819	0.054357	0.035998	0.042375	-0.716163	-0.027064	0.001764
	0.017919	-0.159553	-0.151222	-0.099553	-0.114796	3.698719	0.066091	-0.005798
	0.006096	0.359929	0.334625	0.211874	0.238129	-1.647614	-0.131723	0.004280
3s	-0.221076	-0.989408	-0.881307	-0.522164	-0.556294	-2.616428	0.211378	-0.036185
	-2.948795	-2.258424	-2.440256	-2.979628	-3.004148	1.612942	-3.898602	-3.730558
	3.707173	3.760757	3.887910	4.247592	4.349073	0.074360	4.765807	4.859235
	-0.688357	-0.974463	-1.000943	-1.072454	-1.139695	0.021097	-1.131967	-1.264978
	-0.439569	-0.352691	-0.358753	-0.376635	-0.365899		-0.419133	-0.383364
	-0.002019	-0.006841	-0.006291	-0.004472	-0.004903		0.000139	-0.002087
	-0.060759	-0.082695	-0.066618	0.014115	0.007199	3.474169	0.066245	0.064151
	0.305509	0.429899	0.347714	0.014024	-0.007442	-2.682641	-0.278024	-0.269682
	-1.321321	-1.828830	-1.443778	-0.438872	-0.224558	-2.574620	0.541496	0.538948
	-1.352999	-0.941078	-1.604310	-2.998929	-3.455601	2.579404	-4.108974	-4.337397
4s	2.728129	3.170587	3.633125	4.325090	4.756638	0.302524	4.256258	4.789715
	-0.143454	-0.742762	-0.803375	-0.572708	-0.705275	-0.503633	0.495048	0.104555
	-1.133686	-1.013719	-1.098202	-1.500140	-1.563149	-0.060831	-2.371953	-2.312149
	0.247337	0.304470	0.335028	0.477249	0.520763	-0.003591	0.753877	0.788848
	0.151309	0.140685	0.143958	0.135720	0.133741		0.109561	0.102366
	-0.000876	-0.000916	-0.000749	0.001640	0.002010		0.006595	0.006788

Table 10. (Continued)

	Rb(^{2}S)	Sr(^{1}S)	Y(^{2}D)	Mo(^{7}S)	Tc(^{6}S)	Pd(^{1}S)	Ag(^{2}S)	Cd(^{1}S)
	-3.194113	-3.154585	-3.032932	-3.180161	2.823796		-3.458394	-3.042873
	3.845138	3.476460	3.199840	3.782551	-2.806829		4.681154	3.500282
	-1.879896	-1.103242	-0.971842	-2.103449	1.070159		-3.404981	-2.107325
	1.371329	0.923190	1.023321	2.162100	-1.651990		3.057069	2.461434
5s	-1.173604	-1.277949	-1.389747	-2.013035	1.870772		-2.211301	-2.139089
	0.300569	0.428401	0.445252	0.632523	-0.517937		0.545159	0.467971
	0.141409	0.176174	0.195874	0.162109	-0.277849		0.222777	0.358795
	-0.021597	-0.053082	-0.061089	-0.052559	0.098894		-0.071454	-0.130842
	-0.039478	-0.042447	-0.042495	-0.045757	0.040822		-0.039306	-0.034751
	0.001274	0.001135	0.001046	0.001664	-0.000594		0.001342	0.000167
α	1.023908	1.191272	1.287009	1.474807	1.637720	1.670979	1.829600	1.987744
β	1.630316	1.601883	1.589930	1.573549	1.556146	1.562669	1.547345	1.533964
	0.012727	0.012892	0.012812	0.012307	0.012323	0.011511	0.011562	0.011652
	-0.047344	-0.049071	-0.049306	-0.048327	-0.049126	-0.046014	-0.046896	-0.047806
2p	0.103854	0.108697	0.109700	0.108537	0.110919	0.104365	0.106934	0.109305
	-0.183788	-0.190552	-0.191900	-0.191599	-0.193910	-0.187752	-0.191382	-0.194174
	0.575375	0.628200	0.642656	0.633285	0.671524	0.597800	0.627438	0.655220
	0.561147	0.511356	0.497114	0.505620	0.467714	0.538436	0.510363	0.483483
	0.032755	0.036247	0.039069	0.046722	0.047942	0.051773	0.055423	0.057403
	-0.134666	-0.149023	-0.160387	-0.192409	-0.198413	-0.210618	-0.226888	-0.235567
3p	0.745754	0.915844	0.971635	0.986747	1.115500	0.906893	1.028921	1.137067
	0.812537	0.628477	0.579033	0.625130	0.469951	0.789305	0.657770	0.531315
	-0.703852	-0.707642	-0.717057	-0.765643	-0.754537	-0.840072	-0.834359	-0.823992
	-0.175962	-0.152890	-0.146450	-0.147660	-0.131652	-0.157723	-0.144191	-0.132173
	1.191289	1.318392	1.328904	1.191639	1.307477	-0.964707	-1.085978	-1.200615
	0.026710	-0.119684	-0.098718	0.219019	0.081312	-0.658824	-0.517935	-0.377480
4p	-0.561326	-0.638219	-0.715952	-0.969871	-1.036272	1.202524	1.263331	1.313243
	-0.182257	-0.113642	-0.083428	-0.052841	0.030139	0.101794	0.019648	-0.059335
	0.216127	0.226979	0.235687	0.265410	0.262298	-0.322736	-0.316684	-0.308855
	0.052247	0.049409	0.049496	0.054007	0.051176	-0.058876	-0.055995	-0.053572
α	2.772643	3.023167	0.996917	1.052897	1.129936	1.170472	1.320666	1.420105
β	1.729781	1.705237	1.882927	1.876034	1.858816	1.853921	1.823712	1.934544
	0.471783	0.487714	-0.000727	0.017486	0.017649	0.030084	0.026950	-0.008796
3d	0.524489	0.510043	0.068351	-0.025520	-0.028064	-0.082243	-0.069431	0.092627
	0.096309	0.089549	0.735244	0.721726	0.724899	0.661313	0.694828	0.843816
			0.282185	0.361807	0.358007	0.457480	0.412088	0.132062
			1.057302	0.908072	0.891383	0.754083	0.771840	0.901271
4d			-0.055639	0.187460	0.216665	0.401425	0.391817	0.210577
			-0.179931	-0.232786	-0.251901	-0.249631	-0.291849	-0.358635
			-0.077331	-0.099087	-0.102826	-0.141108	-0.132908	-0.038568

Table 10. (Continued)

	In(^{2}P)	Sn(^{3}P)	Sb(^{4}S)	Te(^{3}P)	I(^{2}P)	Xe(^{1}S)
α	0.596136	0.693171	0.771089	0.847500	0.917865	0.984008
β	1.556172	1.536291	1.523249	1.512065	1.503076	1.495581
	-0.000068	0.000074	0.000216	0.000368	0.000501	0.000622
	0.000258	-0.000429	-0.001133	-0.001903	-0.002593	-0.003228
	-0.000396	0.001416	0.003294	0.005380	0.007274	0.009037
	-0.000056	-0.003582	-0.007230	-0.011300	-0.015019	-0.018498
1s	0.002151	0.007882	0.013701	0.020155	0.026048	0.031551
	-0.007575	-0.015826	-0.023896	-0.032707	-0.040678	-0.048065
	0.018356	0.029031	0.038943	0.049498	0.058888	0.067466
	-0.039157	-0.051659	-0.062529	-0.073730	-0.083459	-0.092161
	0.106474	0.122491	0.135084	0.147455	0.157793	0.166715
	0.922502	0.913059	0.905972	0.899170	0.893597	0.888879
	0.026317	0.028473	0.029466	0.029881	0.029955	0.029842
	-0.123114	-0.136181	-0.143038	-0.146969	-0.148921	-0.149714
	0.311891	0.350698	0.372443	0.386476	0.394812	0.399679
	-0.579632	-0.658556	-0.704245	-0.735469	-0.755352	-0.768178
2s	0.895990	1.023245	1.097700	1.150058	1.184349	1.207269
	-1.255094	-1.437648	-1.544638	-1.621451	-1.672589	-1.707452
	2.004557	2.366605	2.600432	2.794295	2.943494	3.062755
	0.585901	0.235855	-0.003038	-0.213747	-0.384144	-0.526471
	-1.345896	-1.254572	-1.188597	-1.127297	-1.076213	-1.032588
	0.016277	0.018668	0.019502	0.019641	0.019480	0.019197
	-0.021406	-0.038061	-0.047630	-0.054087	-0.058223	0.060991
	0.101307	0.184520	0.234776	0.270716	0.295167	-0.312616
	-0.263174	-0.489752	-0.631364	-0.737504	-0.812620	0.868240
	0.508205	0.975323	1.274858	1.509624	1.681239	-1.811969
3s	-1.001570	-1.999123	-2.686603	-3.284310	-3.760409	4.152427
	-2.855162	-1.807552	-1.025467	-0.292407	0.323393	-0.852195
	4.810302	4.562510	4.314061	4.039484	3.787771	-3.558940
	-1.541968	-1.725712	-1.812805	-1.864448	-1.892940	1.908798
	-0.284493	-0.203982	-0.158068	-0.122514	-0.096692	0.076846
	-0.009027	-0.014182	-0.016708	-0.018440	-0.019519	0.020225
	0.036445	0.002594	-0.022775	-0.046159	-0.066131	-0.083779
	-0.137821	0.032644	0.162102	0.283290	0.387021	0.478514
	0.058061	-0.604974	-1.114450	-1.611286	-2.037002	-2.408277
	-4.220711	-3.711910	-3.226817	-2.687349	-2.201048	-1.767555
4s	5.895779	6.652784	7.026228	7.258333	7.408493	7.520528
	-1.180564	-2.391529	-3.159223	-3.819499	-4.353647	-4.810199
	-1.842860	-1.305494	-0.943251	-0.604666	-0.320222	-0.071122
	0.774467	0.716529	0.674024	0.626075	0.583137	0.543604
	0.091834	0.090397	0.090798	0.093389	0.096579	0.100147
	0.005923	0.004140	0.002888	0.001563	0.000394	-0.000676
	-3.194492	-3.397819	-3.602381	-3.731879	-3.825485	-3.895039
	3.628940	3.853820	4.177341	4.287997	4.323199	4.309593
	-1.863862	-1.593495	-1.556783	-1.244099	-0.874900	-0.475082
	2.434131	2.250173	2.160127	1.826669	1.430913	1.002870
5s	-2.606173	-3.005207	-3.291894	-3.423168	-3.468115	-3.459587
	0.856009	1.302861	1.656259	1.943018	2.171137	2.360086
	0.287152	0.155822	0.026865	-0.082241	-0.175548	-0.258206
	-0.146707	-0.144563	-0.130946	-0.122600	-0.115666	-0.109469
	-0.036434	-0.040595	-0.045146	-0.048495	-0.051071	-0.053167
	0.000291	0.000836	0.001511	0.001987	0.002362	0.002674

Table 10. (Continued)

	In(^{2}P)	Sn(^{3}P)	Sb(^{4}S)	Te(^{3}P)	I(^{2}P)	Xe(^{1}S)
α	0.738113	0.637502	0.781632	0.811162	0.849520	0.892860
β	1.625032	1.589438	1.621584	1.617733	1.611646	1.604594
	-0.000569	0.005728	-0.000393	-0.000307	-0.000214	-0.000102
	0.002269	-0.022440	0.001622	0.001309	0.000970	0.000545
	-0.005567	0.050578	-0.004175	-0.003509	-0.002790	-0.001874
2p	0.011174	-0.088625	0.008871	0.007777	0.006593	0.005076
	-0.024691	0.136240	-0.021593	-0.020112	-0.018486	-0.016358
	0.113459	-0.204312	0.106996	0.104138	0.101287	0.097669
	0.860333	0.529581	0.865099	0.866720	0.867737	0.868794
	0.060751	0.610148	0.060164	0.060308	0.060967	0.062064
	0.021407	0.012804	0.023879	0.024504	0.024598	0.024551
	-0.079708	-0.050292	-0.089494	-0.092356	-0.093422	-0.093773
	0.175729	0.115266	0.197974	0.204871	0.208037	0.209639
3p	-0.297971	-0.212640	-0.343352	-0.357605	-0.364382	-0.368105
	1.698318	0.541075	1.736380	1.754461	1.772800	1.791185
	-0.512005	1.231647	-0.512630	-0.519731	-0.534196	-0.551221
	-0.473121	-0.912385	-0.486604	-0.490742	-0.492287	-0.493039
	-0.002281	-0.197968	-0.000574	-0.000132	-0.000145	-0.000406
	0.034626	-0.011699	-0.048208	-0.055903	-0.062542	-0.064563
	-0.093046	0.029071	0.181289	0.214492	0.240861	0.261859
	1.389693	0.230873	-1.409678	-1.420738	-1.445209	-1.477260
4p	0.021718	1.669219	-0.169828	-0.223055	-0.244604	-0.251144
	-1.279660	-1.333063	1.442662	1.515836	1.576734	1.633045
	0.464395	-0.410269	-0.517464	-0.546376	-0.577023	-0.608916
	0.143637	0.432307	-0.147414	-0.147884	-0.147133	-0.145897
	0.007094	0.072975	-0.007607	-0.008033	-0.008625	-0.009331
	2.197670	1.682106	1.904592	1.787340	1.699310	1.630805
	-2.084051	-0.970845	-1.357313	-1.073850	-0.852569	-0.672462
	0.806230	0.290734	0.144563	-0.106789	-0.320027	-0.504372
5p	-0.612565	-0.680870	-0.330214	-0.246509	-0.173659	-0.106701
	0.605440	0.474802	0.550648	0.560252	0.576017	0.590431
	-0.223798	0.043928	-0.201581	-0.206583	-0.216021	-0.226273
	-0.003787	-0.088626	-0.022784	-0.028601	-0.033054	-0.036200
	-0.006636	-0.018641	-0.004585	-0.004256	-0.004138	-0.004125
α	1.608219	1.754309	1.890998	2.031747	2.175617	2.322247
β	1.783317	1.772571	1.762978	1.744809	1.725615	1.707339
	0.019569	0.013827	0.008420	0.005292	0.002972	0.000890
3d	-0.036824	-0.009889	0.015257	0.028634	0.038239	0.046945
	0.749158	0.776423	0.791021	0.790946	0.787957	0.784467
	0.328438	0.277950	0.241628	0.229670	0.223736	0.219068
	0.815810	0.850590	0.877970	0.894557	0.909562	0.925450
4d	0.355216	0.315328	0.282577	0.266043	0.252146	0.236914
	-0.360600	-0.388986	-0.409901	-0.425764	-0.439449	-0.451452
	-0.112133	-0.096107	-0.084222	-0.081308	-0.080491	-0.079985

Table 10. (Continued)

	Cs(^2S)	Ba(^1S)	La(^2D)		Cs(^2S)	Ba(^1S)	La(^2D)
α	0.378072	0.411680	0.428286				
β	1.516492	1.508160	1.505417				
1s	0.000172	0.000256	0.000261	4s	0.005082	-0.003706	-0.004426
	-0.000879	-0.001309	-0.001341		-0.020470	0.023193	0.026483
	0.002449	0.003639	0.003738		0.032507	-0.085860	-0.092796
	-0.005069	-0.007461	-0.007676		0.002268	0.245396	0.248817
	0.008897	0.012851	0.013225		-0.395551	-0.893512	-0.835168
	-0.014232	-0.019957	-0.020519		-4.766528	-4.370596	-4.606281
	0.021713	0.029211	0.029966		8.630773	8.928735	9.313634
	-0.032338	-0.041327	-0.042236		-3.883651	-4.492032	-4.768607
	0.046927	0.056736	0.057694		-0.954258	-0.657879	-0.590481
	-0.068938	-0.078612	-0.079451		0.770311	0.729007	0.735966
	0.137666	0.147505	0.147870		0.081361	0.083538	0.082460
	0.905904	0.900711	0.900678		0.003731	0.002686	0.002610
2s	0.018223	0.018467	0.018551	5s	-0.075283	-0.095512	-0.082418
	-0.090595	-0.092801	-0.093556		0.438730	0.564352	0.490228
	0.242663	0.250665	0.253418		-2.717219	-2.818330	-2.403824
	-0.473984	-0.492433	-0.498831		0.205439	-0.226251	-1.139720
	0.765187	0.797450	0.808738		3.172317	4.252471	5.180043
	-1.090633	-1.137476	-1.153982		-0.151614	-0.992172	-1.334012
	1.427816	1.487555	1.508682		-3.053750	-2.982409	-3.132777
	-1.800675	-1.873591	-1.899504		1.620384	1.826732	1.995402
	2.805501	2.961057	3.007351		0.319809	0.256686	0.230450
	-0.118407	-0.281531	-0.323545		-0.297857	-0.309607	-0.320006
	-1.173071	-1.125875	-1.116969		-0.024998	-0.023863	-0.024387
	0.021750	0.021792	0.022454		-0.001970	-0.002105	-0.002095
3s	-0.027622	-0.030667	-0.031562	6s	-6.025698	-5.236979	-5.160674
	0.137525	0.154388	0.159438		11.477281	8.748098	8.543513
	-0.369873	-0.418969	-0.433800		-10.501892	-6.561709	-6.490014
	0.730804	0.833447	0.864284		8.178001	5.105928	5.369003
	-1.210484	-1.387699	-1.439449		-6.116963	-4.578641	-4.947416
	1.830849	2.111645	2.189480		3.108905	2.273148	2.455405
	-3.108248	-3.646581	-3.770534		-0.832219	-0.171046	-0.170952
	-0.905765	-0.304156	-0.200637		0.329304	-0.058125	-0.088627
	4.469795	4.250304	4.252867		-0.366560	-0.252474	-0.250858
	-1.941364	-1.981280	-2.018625		0.168703	0.147104	0.151768
	-0.139568	-0.112110	-0.101680		-0.018149	-0.008538	-0.008880
	-0.016617	-0.017947	-0.018498		0.003630	0.002555	0.002608

Table 10. (Continued)

	Cs(^{2}S)	Ba(^{1}S)	La(^{2}D)		Cs(^{2}S)	Ba(^{1}S)	La(^{2}D)
α	1.004893	1.116925	1.193349	α	2.477668	2.637982	1.000774
β	1.582588	1.563309	1.552705	β	1.689604	1.672721	1.665982
	-0.000282	-0.000378	-0.000360		-0.001454	-0.003755	-0.000496
	0.001256	0.001659	0.001601		0.057266	0.067744	0.002375
	-0.003482	-0.004421	-0.004312	3d	0.780712	0.776685	-0.010187
2p	0.007812	0.009388	0.009189		0.213370	0.207820	0.087442
	-0.020522	-0.022838	-0.022565				0.777806
	0.107035	0.112587	0.112539				0.190464
	0.860073	0.853319	0.851390				
	0.063664	0.065990	0.067588		0.946200	0.969100	0.027577
					0.214308	0.188231	-0.031515
	0.020256	0.016507	0.015042	4d	-0.461115	-0.468879	1.009931
	-0.079051	-0.065658	-0.060531		-0.079025	-0.078050	0.151631
	0.178747	0.149756	0.138706				-0.474833
3p	-0.304771	-0.243064	-0.219001				-0.071713
	1.808138	1.815171	1.825718				
	-0.637244	-0.708011	-0.744390				1.273093
	-0.466012	-0.443894	-0.435423				-0.325780
	-0.003587	-0.006548	-0.007876	5d			-0.253139
							-0.098867
	0.065586	0.063912	0.066382				0.160888
	-0.267869	-0.261995	-0.274523				0.017603
	1.672328	1.837347	1.930378				
4p	-0.047633	-0.324041	-0.447467				
	-1.557895	-1.476235	-1.462399				
	0.647319	0.674991	0.700839				
	0.135192	0.127729	0.124117				
	0.010775	0.011938	0.012736				
	1.694391	1.775499	1.791256				
	-0.696980	-0.764421	-0.731257				
	-0.713291	-0.884503	-1.038378				
5p	0.079291	0.263978	0.383766				
	0.575679	0.548838	0.539526				
	-0.246498	-0.262110	-0.274665				
	-0.039039	-0.041912	-0.043830				
	-0.004410	-0.004635	-0.004810				

Table 10. (Continued)

	Gd(^{8}S)				
α	1.366622				
β	1.525425				
	0.003240		-3.972376		1.770812
	-0.015694		4.251203		-0.644411
	0.040708		1.538433		-0.668959
	-0.076182		-3.385796	5p	-0.510139
1s	0.115873	5s	0.075855		0.991252
	-0.151944		1.637424		-0.134210
	0.176712		-0.707212		-0.152170
	-0.186066		0.034869		-0.020633
	1.058417		-0.022318		
	0.036982		0.002622	α	3.261845
				β	1.653774
	0.016423	α	1.410400		
	-0.079933	β	1.491535		0.004196
	0.209632			3d	0.038130
	-0.402592		0.005825		0.802800
2s	0.663780		-0.025630		0.198270
	-1.190996		0.062285		
	-1.491098	2p	-0.112941		0.913966
	1.810278		0.172581	4d	0.296103
	-0.078978		-0.248287		-0.541993
	0.014203		0.655874		-0.073977
			0.503867		
	-0.012322			α	1.874408
	0.065924		0.028027	β	1.903542
	-0.201449		-0.121363		
	0.462202		0.292063		0.392601
3s	-4.956003	3p	-0.535915	4f	0.595891
	6.286138		1.315230		0.181809
	-1.753547		0.640777		
	-0.442338		-0.989806		
	0.009959		-0.126864		
	-0.002504				
			-0.008992		
	0.197269		0.061776		
	-1.030268		-0.790264		
	5.763025	4p	-1.551073		
	-5.650291		2.362691		
4s	-1.519904		-0.232153		
	4.515749		-0.432518		
	-1.836269		-0.057441		
	0.104077				
	-0.063734				
	0.007729				

Table 10. (Continued)

Rn (^1S)

α	1.017676			α	0.841669			α	2.199251
β	1.449446			β	1.489038			β	1.554579
	0.000466		-0.024845		0.002845		-0.001602		0.009144
	-0.002576		0.145763		-0.012782		0.009725		-0.032063
	0.007579		-0.467440		0.031906		0.121620	3d	0.065764
	-0.016047		1.139391		-0.059613		2.218165		-0.087416
	0.027735		-3.160704	2p	0.094202	5p	-1.579721		0.767824
1s	-0.041866	4s	-2.929483		-0.134208		-1.502026		0.310770
	0.057502		11.879178		0.179594		1.588623		
	-0.073595		-8.795040		-0.243222		0.071344		0.027975
	0.088633		0.934302		0.520566		-0.334233		-0.100449
	-0.104406		0.789093		0.631058		-0.024610	4d	0.857088
	0.157524		0.019838						0.574123
	0.900588		0.004078		0.006520		1.572076		-0.681098
					-0.028889		-0.506724		-0.137825
	0.019295		-0.100137		0.070733		-0.067365		
	-0.105241		0.588960		-0.129113		-1.199985		0.921531
	0.303445		-2.961369	3p	0.198391	6p	0.965536		0.427918
	-0.624378		-2.341382		-0.283844		0.317594	5d	-0.729967
	1.038865		10.669775		0.575116		-0.469110		-0.203816
2s	-1.495459	5s	-6.595263		1.514425		-0.040657		0.281027
	1.946786		-2.606659		-1.275925		0.114338		0.054848
	-2.433675		3.579441		-0.165326		0.006793		
	4.049441		-0.298870					α	4.748574
	-1.345022		-0.450378		-0.020870			β	1.667104
	-0.860008		0.016792		0.090362				
	0.028973		-0.005116		-0.214984				0.414795
					0.379545			4f	0.570171
	0.046604		-5.375386	4p	-0.494401				0.120157
	-0.253836		7.841727		3.029392				
	0.732717		-3.911756		-2.495463				
	-1.519581		4.377012		-0.473784				
	2.582968		-7.624111		0.774931				
3s	-3.953163	6s	5.270034		0.054525				
	6.983192		-0.535025						
	-3.127942		-0.678666						
	-3.456980		-0.143392						
	2.588508		0.252462						
	-0.115965		-0.027153						
	0.029135		0.004506						

Table 11. Even-tempered augmented triple-zeta atomic orbitals

	Li(^{2}S)	Be(^{1}S)	B(^{2}P)	C(^{3}P)	N(^{4}S)	O(^{3}P)	F(^{2}P)	Ne(^{1}S)
α	0.351242	0.447163	0.581716	0.704515	0.822525	0.946188	1.066337	1.183685
β	1.604735	1.659528	1.659501	1.666496	1.673719	1.676262	1.679609	1.683251
	-0.002603	-0.001260	-0.000400	0.000221	0.000668	0.001026	0.001306	0.001517
	0.017558	0.005646	0.003377	0.001614	0.000311	-0.000632	-0.001403	-0.001997
1s	-0.053651	-0.011621	0.003385	0.015836	0.025324	0.031520	0.036751	0.041033
	0.834283	0.888665	0.904948	0.913218	0.917787	0.920815	0.922698	0.924008
	0.198973	0.124440	0.095751	0.076914	0.064100	0.055540	0.048989	0.043833
	0.021222	0.005473	0.002870	0.001443	0.000667	0.000266	-0.000009	-0.000200
	1.934306	1.457189	1.334494	1.251604	1.193151	1.147665	1.113605	1.086141
	-1.104538	-0.295732	-0.072032	0.061520	0.149710	0.224605	0.277007	0.317050
2s	-0.022867	-0.388255	-0.497893	-0.545656	-0.570568	-0.600146	-0.616571	-0.626564
	-0.083137	-0.064645	-0.075986	-0.091830	-0.105520	-0.112710	-0.120123	-0.126861
	-0.029565	-0.022989	-0.017079	-0.010847	-0.005894	-0.002973	-0.000278	0.002025
	-0.003024	-0.000747	-0.000610	-0.000721	-0.000872	-0.000929	-0.001025	-0.001121
α			0.509473	0.624700	0.731294	0.758132	0.848776	0.929874
β			1.802049	1.805955	1.813350	1.896120	1.736217	1.733414
			0.669543	0.607656	0.565058	0.525330	0.381974	0.360763
2p			0.355289	0.409494	0.443993	0.483657	0.492795	0.486189
			0.030349	0.046316	0.060523	0.076099	0.203134	0.231366
			0.008344	0.006817	0.005474	0.002142	0.017047	0.020451

Table 11. (Continued)

	Na(^{2}S)	Mg(^{1}S)	Al(^{2}P)	Si(^{3}P)	P(^{4}S)	S(^{3}P)	Cl(^{2}P)	Ar(^{1}S)
α	0.325177	0.409171	0.527348	0.630010	0.727210	0.820042	0.911962	1.003757
β	1.643118	1.610974	1.572014	1.549692	1.534194	1.523061	1.514069	1.506496
1s	-0.000090	-0.000081	0.000010	0.000005	-0.000048	-0.000151	-0.000247	-0.000328
	0.000421	0.000409	-0.000011	-0.000014	0.000213	0.000685	0.001127	0.001509
	-0.001215	-0.001236	-0.000256	-0.000308	-0.000961	-0.002248	-0.003480	-0.004571
	0.003677	0.003783	0.002155	0.002321	0.003576	0.005994	0.008322	0.010398
	-0.004762	-0.005085	-0.002645	-0.003184	-0.005495	-0.009658	-0.013694	-0.017339
	0.048284	0.052070	0.051613	0.055191	0.061189	0.069851	0.077997	0.085242
	0.918725	0.915683	0.912845	0.910458	0.907867	0.904637	0.901703	0.899156
	0.042671	0.041732	0.042995	0.041760	0.039462	0.036292	0.033323	0.030679
	0.000030	0.000219	0.000453	0.000615	0.000745	0.000869	0.000964	0.001031
2s	-0.001123	-0.004976	-0.003068	-0.004152	-0.006156	-0.008423	-0.010648	-0.012719
	0.010821	0.026888	0.020255	0.028224	0.040793	0.054744	0.068400	0.081187
	-0.048214	-0.097127	-0.077618	-0.098510	-0.131103	-0.168046	-0.203205	-0.235328
	1.265600	1.428293	1.585429	1.715391	1.828621	1.926844	2.012284	2.086895
	0.158835	0.018277	-0.199331	-0.340963	-0.448990	-0.532021	-0.600178	-0.657333
	-0.632270	-0.638238	-0.605834	-0.593061	-0.589250	-0.592858	-0.599646	-0.608349
	-0.119693	-0.112260	-0.110311	-0.106013	-0.099540	-0.090823	-0.081366	-0.071606
	0.001765	0.001270	0.002406	0.002611	0.002140	0.001063	-0.000330	-0.001915
	-0.001101	-0.001039	-0.001266	-0.001278	-0.001165	-0.000952	-0.000697	-0.000420
3s	2.008829	1.728457	1.666489	1.603998	1.562918	1.500894	-1.468466	-1.455493
	-1.270181	-0.584350	-0.264302	-0.019534	0.141431	0.324185	-0.427913	-0.481230
	0.045634	-0.495880	-0.910442	-1.165152	-1.306623	-1.437804	1.490799	1.498042
	-0.148866	-0.072906	0.007920	-0.007626	-0.081694	-0.163840	0.276721	0.401786
	-0.024873	-0.018102	0.006927	0.079330	0.176808	0.275729	-0.383826	-0.492435
	0.101444	0.130688	0.152125	0.145846	0.125689	0.103835	-0.076654	-0.048138
	0.016661	0.020498	0.023194	0.031041	0.040938	0.049974	-0.059429	-0.068406
	-0.000476	-0.000852	-0.001243	-0.003130	-0.005577	-0.007810	0.010124	0.012287
	0.000208	0.000307	0.000420	0.000698	0.001025	0.001306	-0.001587	-0.001841
α	0.702393	0.934504	0.405759	0.515606	0.613755	0.639211	0.689268	0.751677
β	1.884022	1.799327	1.727817	1.681310	1.657403	1.688668	1.698387	1.697587
2p	0.034229	0.039008	0.002372	0.002318	0.001886	0.002391	0.002762	0.001564
	0.617761	0.644457	-0.008599	-0.008072	-0.007500	-0.007621	-0.007320	-0.007440
	0.392288	0.352757	0.066053	0.065525	0.065192	0.067889	0.069170	0.067194
	0.036026	0.032324	0.665414	0.680044	0.699030	0.738971	0.762545	0.778620
			0.305688	0.285048	0.264310	0.229179	0.205392	0.190815
			0.028763	0.028353	0.025077	0.013775	0.009332	0.007287
3p			0.851748	0.798531	0.753145	0.639134	0.580502	0.545963
			0.291913	0.388353	0.464941	0.585501	0.646028	0.681742
			-0.182731	-0.227329	-0.255889	-0.233414	-0.218062	-0.206214
			-0.102031	-0.127815	-0.152356	-0.199921	-0.234151	-0.259852
			-0.059216	-0.064698	-0.065087	-0.053686	-0.046034	-0.040274
			-0.004472	-0.005347	-0.005364	-0.003905	-0.003541	-0.003555

Table 11. (Continued)

	K (^{2}S)	Ca (^{1}S)	Ga (^{2}P)		K (^{2}S)	Ca (^{1}S)	Ga (^{2}P)
α	0.344127	0.415657	0.626256				
β	1.431709	1.412682	1.422508				
	0.000692	0.000859	0.000294		0.024248	0.026060	0.007195
	-0.003925	-0.005036	-0.001687		-0.141268	-0.145778	-0.037191
	0.011767	0.015521	0.005101		0.428800	0.432117	0.089260
	-0.025186	-0.033957	-0.010955		-1.148394	-1.101725	-0.137111
	0.043546	0.059069	0.018888		-1.098396	-1.528933	-1.870855
1s	-0.065312	-0.090353	-0.028032	3s	0.185153	0.749602	-0.292703
	0.087392	0.121465	0.036338		1.930174	1.846766	2.150993
	-0.106302	-0.148003	-0.041832		-0.403768	-0.456729	0.512898
	0.124703	0.171786	0.044118		-0.215116	-0.252148	-0.959373
	-0.105490	-0.160685	-0.003447		-0.148320	-0.138708	-0.015756
	0.955232	0.968641	0.942562		-0.032653	-0.037291	-0.046376
	0.088442	0.105445	0.042369		-0.000088	0.000099	0.003076
	0.005446	0.006490	-0.004135		3.245425	2.744139	1.911767
	-0.029818	-0.036536	0.023664		-3.180614	-2.019746	-0.674825
	0.084759	0.106512	-0.071482		1.037371	0.505968	0.080229
	-0.167966	-0.215496	0.154181		-0.839436	-1.451081	-1.203780
	0.266072	0.345997	-0.268099		0.426321	1.003725	0.498019
2s	-0.338044	-0.448641	0.426957	4s	-0.453330	-0.728483	-0.516610
	0.462808	0.635336	-0.575922		0.722308	1.009223	0.786645
	1.850473	1.809734	2.848532		-0.254985	-0.384358	0.013041
	-0.988226	-1.086456	-1.384317		0.020028	0.031873	-0.214374
	-0.466848	-0.437525	-0.557700		-0.046367	-0.058283	-0.001435
	-0.097289	-0.101106	-0.035505		-0.002331	-0.003541	-0.011109
	-0.004776	-0.005360	-0.004422		-0.000470	-0.000558	0.000773

Table 11. (Continued)

	K(^{2}S)	Ca(^{1}S)	Ga(^{2}P)
α	0.996699	0.860080	0.484890
β	1.607603	1.701137	1.596937
2p	0.001040	0.000043	-0.000052
	-0.005290	-0.002769	0.000297
	0.064294	0.051364	-0.001106
	0.754980	0.806402	0.004071
	0.205056	0.173608	-0.009351
	0.015565	0.004221	0.092071
			0.822570
			0.113551
			0.002556
3p	0.634364	0.222882	-0.000309
	0.648581	1.080168	0.006413
	-0.287611	-0.290656	-0.027035
	-0.257837	-0.308059	0.456448
	-0.050662	-0.043142	0.924291
	-0.005765	-0.002594	-0.340715
			-0.382806
			-0.016599
			-0.003414
4p			1.056243
			-0.032286
			0.038001
			-0.215719
			-0.106264
			0.036132
			0.074251
			-0.000661
			0.001069
α			1.272385
β			1.801427
3d			0.232149
			0.522349
			0.356762
			0.039480

Table 11. (Continued)

Xe(^{1}S)

α	0.985547			α	0.806807		
β	1.362618			β	1.411697		
	-0.000244		-0.031416		0.000301		-0.912624
	0.001578		0.223955		-0.001552		-0.154501
	-0.005301		-0.766626		0.004347		-0.550929
	0.012472		2.504756		-0.008934		1.159031
	-0.023267		2.483870		0.015219		0.000687
	0.036909		-4.633794	2p	-0.024117	5p	0.150349
	-0.051783		-3.677212		0.036534		-0.681576
1s	0.065903	4s	5.950003		-0.059181		0.182969
	-0.078884		-1.391547		0.255573		0.058860
	0.091292		0.428162		0.736198		0.047685
	-0.106792		-0.679573		0.054345		-0.001429
	0.196972		0.120670		0.007087		0.000688
	0.861843		-0.038746				
	-0.000445		0.006193		0.006215	α	2.003283
	0.002072		-0.000612		-0.031637	β	1.549698
					0.086987		
	-0.000195		-3.130750		-0.175421		0.000035
	0.001261		2.360574		0.299870		-0.003509
	-0.003961		-2.002153	3p	-0.456712	3d	0.084378
	0.008412		6.563380		1.413939		0.700356
	-0.013307		-5.842315		0.465814		0.251216
	0.011262		3.185441		-0.833649		0.018680
	0.007887		-4.823678		-0.234090		
2s	-0.069082	5s	4.605616		-0.021982		0.322112
	0.525315		-1.896770		-0.001531		0.817320
	2.486635		0.804098			4d	-0.007650
	-2.268725		-0.514305		0.006861		-0.388754
	-0.105909		0.143409		-0.035284		-0.091938
	-0.050255		-0.043181		0.086805		-0.009658
	0.005575		0.008351		-0.332268		
	-0.000876		-0.000894		-1.456535		
				4p	0.143827		
	0.016813				1.665899		
	-0.109053				-0.340972		
	0.365076				-0.258708		
	-0.864145				-0.137973		
	1.675289				0.000612		
	-2.832154				-0.001789		
	6.834554						
3s	-3.708565						
	-2.751227						
	1.273534						
	0.584744						
	0.063158						
	0.001480						
	0.001947						
	-0.000187						

Table 12. Atom properties

2 Helium Atom Singlet S State 1s(2) Configuration (3s) Basis

|2-V/E| = 3.9D-10 |1-Norm| = 1.1D-15

Total S Cusp: -2.014980

	T	V(1)	V(2)	V(T)	E	e	-Cusp	r max
	2.861679	-6.749128	1.025770	-5.723358	-2.861679	-1.835909		
1s	1.430840	-3.374564	0.512885	-2.861679	-1.430840	-0.917955	2.014980	0.569172
	r^{-3}	r^{-2}	r^{-1}	r	r^2	r^4	r^6	
		11.99343	3.374564	1.854516	2.369346	7.764691	50.26258	
1s		5.996716	1.687282	0.9272581	1.184673	3.882345	25.13129	

2 Helium Atom Singlet S State 1s(2) Configuration (4s) Basis

|2-V/E| = 1.3D-07 |1-Norm| = 6.7D-16

Total S Cusp: -2.001257

	T	V(1)	V(2)	V(T)	E	e	-Cusp	r max
	2.861680	-6.749128	1.025769	-5.723359	-2.861680	-1.835911		
1s	1.430840	-3.374564	0.512885	-2.861680	-1.430840	-0.917955	2.001257	0.569151
	r^{-3}	r^{-2}	r^{-1}	r	r^2	r^4	r^6	
		11.99113	3.374564	1.854518	2.369399	7.766994	50.31303	
1s		5.995563	1.687282	0.9272592	1.184700	3.883497	25.15651	

2 Helium Atom Singlet S State 1s(2) Configuration (5s) Basis

|2-V/E| = 4.8D-08 |1-Norm| = 1.8D-15

Total S Cusp: -2.000351

	T	V(1)	V(2)	V(T)	E	e	-Cusp	r max
	2.861680	-6.749129	1.025769	-5.723360	-2.861680	-1.835911		
1s	1.430840	-3.374564	0.512884	-2.861680	-1.430840	-0.917956	2.000351	0.569149
	r^{-3}	r^{-2}	r^{-1}	r	r^2	r^4	r^6	
		11.99100	3.374564	1.854547	2.369655	7.775827	50.56506	
1s		5.995498	1.687282	0.9272735	1.184828	3.887914	25.28253	

2 Helium Atom Singlet S State 1s(2) Configuration (6s) Basis

|2-V/E| = 1.7D-08 |1-Norm| = 2.2D-15

Total S Cusp: -2.001078

	T	V(1)	V(2)	V(T)	E	e	-Cusp	r max
	2.861680	-6.749129	1.025769	-5.723360	-2.861680	-1.835911		
1s	1.430840	-3.374564	0.512884	-2.861680	-1.430840	-0.917956	2.001078	0.569140
	r^{-3}	r^{-2}	r^{-1}	r	r^2	r^4	r^6	
		11.99105	3.374564	1.854546	2.369653	7.775896	50.56977	
1s		5.995525	1.687282	0.9272732	1.184827	3.887948	25.28488	

2 Helium Atom Singlet S State 1s(2) Configuration (7s) Basis

|2-V/E| = 7.5D-08 |1-Norm| = 4.4D-16

Total S Cusp: -2.000596

	T	V(1)	V(2)	V(T)	E	e	-Cusp	r max
	2.861680	-6.749129	1.025769	-5.723360	-2.861680	-1.835911		
1s	1.430840	-3.374564	0.512884	-2.861680	-1.430840	-0.917956	2.000596	0.569139
	r^{-3}	r^{-2}	r^{-1}	r	r^2	r^4	r^6	
		11.99104	3.374564	1.854547	2.369657	7.775824	50.55414	
1s		5.995520	1.687282	0.9272735	1.184829	3.887912	25.27707	

2 Helium Atom Singlet S State 1s(2) Configuration (8s) Basis

|2-V/E| = 1.4D-08 |1-Norm| = 2.2D-16

Total S Cusp: -2.000029

	T	V(1)	V(2)	V(T)	E	e	-Cusp	r max
	2.861680	-6.749129	1.025769	-5.723360	-2.861680	-1.835911		
1s	1.430840	-3.374564	0.512884	-2.861680	-1.430840	-0.917956	2.000029	0.569145
	r^{-3}	r^{-2}	r^{-1}	r	r^2	r^4	r^6	
		11.99101	3.374564	1.854547	2.369657	7.775896	50.55694	
1s		5.995504	1.687282	0.9272734	1.184829	3.887948	25.27847	

Table 12. (Continued)

2 Helium Atom Singlet S State 1s(2) Configuration (12s) Basis

|2-V/E| = 3.7D-08 |1-Norm| = 9.2D-13
Total S Cusp: -1.999968

	T	V(1)	V(2)	V(T)	E	e	-Cusp	r max
	2.861680	-6.749129	1.025769	-5.723360	-2.861680	-1.835911		
1s	1.430840	-3.374564	0.512884	-2.861680	-1.430840	-0.917956	1.999968	0.569145

	r^{-3}	r^{-2}	r^{-1}	r	r^2	r^4	r^6
		11.99101	3.374564	1.854547	2.369657	7.775898	50.55682
1s		5.995503	1.687282	0.9272735	1.184829	3.887949	25.27841

3 Lithium Atom Doublet S State 1s(2)2s(1) Configuration (4s) Basis

|2-V/E| = 5.4D-08 |1-Norm| = 2.2D-16
Total S Cusp: -2.925391

	T	V(1)	V(2)	V(T)	E	e	-Cusp	r max
	7.431889	-17.148921	2.285144	-14.863778	-7.431889	-5.146745		
1s	3.609675	-8.052189	0.983641	-7.068548	-3.458873	-2.475231	2.923866	0.361917
2s	0.212539	-1.044544	0.317861	-0.726682	-0.514143	-0.196282	2.986008	3.085527

	r^{-3}	r^{-2}	r^{-1}	r	r^2	r^4	r^6
		30.10711	5.716307	4.981412	18.24392	542.4181	27438.38
1s		14.83276	2.684063	0.5740390	0.4502143	0.6366592	9.373911
2s		0.4415863	0.3481812	3.833334	17.34349	541.1448	27419.63

3 Lithium Atom Doublet S State 1s(2)2s(1) Configuration (6s) Basis

|2-V/E| = 1.9D-08 |1-Norm| = 0.0
Total S Cusp: -3.026972

	T	V(1)	V(2)	V(T)	E	e	-Cusp	r max
	7.432721	-17.146387	2.280945	-14.865442	-7.432721	-5.151776		
1s	3.611943	-8.055086	0.982708	-7.072378	-3.460435	-2.477727	3.026489	0.363808
2s	0.208836	-1.036215	0.315529	-0.720686	-0.511850	-0.196321	3.046704	3.102344

	r^{-3}	r^{-2}	r^{-1}	r	r^2	r^4	r^6
		30.22036	5.715462	5.020426	18.64596	570.2094	29525.39
1s		14.89233	2.685029	0.5731307	0.4468134	0.5322173	1.251309
2s		0.4357004	0.3454049	3.874165	17.75233	569.1450	29522.89

4 Beryllium Atom Singlet S State 1s(2)2s(2) Configuration (4s) Basis

|2-V/E| = 3.0D-07 |1-Norm| = 1.3D-15
Total S Cusp: -4.082137

	T	V(1)	V(2)	V(T)	E	e	-Cusp	r max
	14.572823	-33.636816	4.491166	-29.145651	-14.572828	-10.081662		
1s	6.784751	-14.726838	1.605086	-13.121752	-6.337001	-4.731916	4.083918	0.267840
2s	0.501661	-2.091570	0.640497	-1.451073	-0.949413	-0.308915	4.028147	2.064675

	r^{-3}	r^{-2}	r^{-1}	r	r^2	r^4	r^6
		57.68049	8.409204	6.115663	17.20395	265.6462	7104.469
1s		27.78412	3.681709	0.4148970	0.2328330	0.1433224	0.2058896
2s		1.056124	0.5228926	2.642935	8.369144	132.6798	3552.029

4 Beryllium Atom Singlet S State 1s(2)2s(2) Configuration (5s) Basis

|2-V/E| = 2.5D-08 |1-Norm| = 2.2D-15
Total S Cusp: -3.951671

	T	V(1)	V(2)	V(T)	E	e	-Cusp	r max
	14.572940	-33.636162	4.490282	-29.145880	-14.572940	-10.082658		
1s	6.785122	-14.727219	1.604887	-13.122332	-6.337211	-4.732324	3.946357	0.267119
2s	0.501348	-2.090862	0.640254	-1.450608	-0.949259	-0.309006	4.110219	2.064781

	r^{-3}	r^{-2}	r^{-1}	r	r^2	r^4	r^6
		57.60666	8.409040	6.118865	17.22709	266.5261	7142.737
1s		27.74689	3.681805	0.4149581	0.2328961	0.1425037	0.1813852
2s		1.056442	0.5227154	2.644474	8.380649	133.1205	3571.187

Table 12. (Continued)

4 Beryllium Atom Singlet S State 1s(2)2s(2) Configuration (6s) Basis

|2-V/E| = 3.9D-09 |1-Norm| = 3.1D-15
Total S Cusp: -4.029381

	T	V(1)	V(2)	V(T)	E	e	-Cusp	r max
	14.573015	-33.635161	4.489131	-29.146030	-14.573015	-10.083884		
1s	6.785389	-14.727517	1.604728	-13.122789	-6.337400	-4.732672	4.028746	0.267112
2s	0.501118	-2.090063	0.639837	-1.450226	-0.949108	-0.309270	4.048468	2.052478

	r^{-3}	r^{-2}	r^{-1}	r	r^{2}	r^{4}	r^{6}
		57.62992	8.408790	6.129706	17.33243	272.1175	7432.327
1s		27.75891	3.681879	0.4149965	0.2329608	0.1420663	0.1675701
2s		1.056044	0.5225158	2.649856	8.433256	135.9167	3715.996

4 Beryllium Atom Singlet S State 1s(2)2s(2) Configuration (7s) Basis

|2-V/E| = 2.7D-09 |1-Norm| = 1.1D-15
Total S Cusp: -3.991817

	T	V(1)	V(2)	V(T)	E	e	-Cusp	r max
	14.573021	-33.635179	4.489136	-29.146042	-14.573021	-10.083885		
1s	6.785385	-14.727508	1.604725	-13.122783	-6.337398	-4.732673	3.992821	0.267081
2s	0.501125	-2.090081	0.639843	-1.450238	-0.949112	-0.309269	3.961536	2.052365

	r^{-3}	r^{-2}	r^{-1}	r	r^{2}	r^{4}	r^{6}
		57.61672	8.408795	6.129449	17.32909	271.8251	7410.553
1s		27.75283	3.681877	0.4149944	0.2329552	0.1420581	0.1666988
2s		1.055531	0.5225203	2.649730	8.431592	135.7705	3705.110

4 Beryllium Atom Singlet S State 1s(2)2s(2) Configuration (8s) Basis

|2-V/E| = 3.7D-09 |1-Norm| = 6.7D-16
Total S Cusp: -4.003358

	T	V(1)	V(2)	V(T)	E	e	-Cusp	r max
	14.573023	-33.635190	4.489144	-29.146046	-14.573023	-10.083879		
1s	6.785384	-14.727507	1.604726	-13.122780	-6.337396	-4.732670	4.003260	0.267040
2s	0.501127	-2.090088	0.639846	-1.450243	-0.949115	-0.309270	4.006305	2.050472

	r^{-3}	r^{-2}	r^{-1}	r	r^{2}	r^{4}	r^{6}
		57.61869	8.408798	6.128857	17.31960	270.7910	7321.707
1s		27.75367	3.681877	0.4149941	0.2329548	0.1420613	0.1668065
2s		1.055674	0.5225221	2.649435	8.426843	135.2534	3660.687

4 Beryllium Atom Singlet S State 1s(2)2s(2) Configuration (12s) Basis

|2-V/E| = 4.4D-09 |1-Norm| = 1.9D-15
Total S Cusp: -3.999834

	T	V(1)	V(2)	V(T)	E	e	-Cusp	r max
	14.573023	-33.635191	4.489144	-29.146046	-14.573023	-10.083879		
1s	6.785384	-14.727507	1.604726	-13.122781	-6.337396	-4.732670	3.999825	0.267051
2s	0.501127	-2.090088	0.639846	-1.450243	-0.949115	-0.389270	4.000114	2.050592

	r^{-3}	r^{-2}	r^{-1}	r	r^{2}	r^{4}	r^{6}
		57.61801	8.408798	6.128816	17.31878	270.6595	7306.160
1s		27.75336	3.681877	0.4149941	0.2329547	0.1420594	0.1667011
2s		1.055648	0.5225221	2.649414	8.426436	135.1877	3652.914

5 Boron Atom Doublet P State 1s(2)2s(2)2p(1) Configuration (4s, 2p) Basis

|2-V/E| = 5.4D-07 |1-Norm| = 0.0
Total S Cusp: -5.073734 Total P Cusp: -1.788877

	T	V(1)	V(2)	V(T)	E	e	-Cusp	r max
	24.528227	-56.901364	7.844895	-49.056468	-24.528241	-16.683345		
1s	10.931726	-23.370658	2.372494	-20.998164	-10.066436	-7.693942	5.080380	0.211418
2s	0.959937	-3.567523	1.057021	-2.510502	-1.550566	-0.493544	4.907958	1.543332
2p	0.744898	-3.025002	0.985865	-2.039136	-1.294238	-0.308373	1.788877	1.582409

	r^{-3}	r^{-2}	r^{-1}	r	r^{2}	r^{4}	r^{6}
		93.72012	11.38027	6.762485	15.60899	158.4529	2862.890
1s		44.57464	4.674132	0.3258172	0.1433045	5.3829164D-02	4.2222384D-02
2s		2.022015	0.7135047	1.967759	4.639374	40.60129	597.6724
2p	0.7500906	0.5268124	0.6050003	2.195333	6.043637	77.14266	1667.461

Table 12. (Continued)

5 Boron Atom Doublet P State 1s(2)2s(2)2p(1) Configuration (4s, 3p) Basis

|2-V/E| = 6.4D-06 |1-Norm| = 2.2D-16
Total S Cusp: -5.073434 Total P Cusp: -2.017699

	T	V(1)	V(2)	V(T)	E	e	-Cusp	r max
	24.528642	-56.900835	7.843708	-49.057127	-24.528485	-16.684777		
1s	10.931650	-23.370576	2.372336	-20.998239	-10.066589	-7.694252	5.080064	0.211418
2s	0.960103	-3.567802	1.056929	-2.510873	-1.550770	-0.493842	4.908107	1.543256
2p	0.745135	-3.024079	0.985178	-2.038902	-1.293767	-0.308589	2.017699	1.588736

	r^{-3}	r^{-2}	r^{-1}	r	r^2	r^4	r^6
		93.72128	11.38017	6.789022	15.66995	161.6712	3026.200
1s		44.57398	4.674115	0.3258195	0.1433085	5.3839513D-02	4.2319145D-02
2s		2.022352	0.7135604	1.967606	4.638598	40.58605	597.3098
2p	0.7635405	0.5286142	0.6048159	2.202172	6.106136	80.39144	1831.496

5 Boron Atom Doublet P State 1s(2)2s(2)2p(1) Configuration (6s, 4p) Basis

|2-V/E| = 4.5D-08 |1-Norm| = 1.8D-16
Total S Cusp: -5.028306 Total P Cusp: -2.469785

	T	V(1)	V(2)	V(T)	E	e	-Cusp	r max
	24.529051	-56.897230	7.839130	-49.058100	-24.529050	-16.689920		
1s	10.932716	-23.371710	2.371831	-20.999879	-10.067163	-7.695332	5.027266	0.210997
2s	0.958949	-3.564389	1.055370	-2.509019	-1.550070	-0.494700	5.053762	1.526133
2p	0.745720	-3.025032	0.984728	-2.040304	-1.294585	-0.309857	2.469785	1.586061

	r^{-3}	r^{-2}	r^{-1}	r	r^2	r^4	r^6
		93.66887	11.37945	6.810623	15.84964	168.9558	3330.818
1s		44.54432	4.674342	0.3258677	0.1433639	5.3619827D-02	3.8831894D-02
2s		2.025185	0.7128777	1.977253	4.711459	42.94596	673.1221
2p	0.7749421	0.5298487	0.6050065	2.204381	6.139992	82.95667	1984.496

6 Carbon Atom Triplet P State 1s(2)2s(2)2p(2) Configuration (4s, 2p) Basis

|2-V/E| = 9.2D-07 |1-Norm| = 0.0
Total S Cusp: -6.071222 Total P Cusp: -2.274349

	T	V(1)	V(2)	V(T)	E	e	-Cusp	r max
	37.686514	-88.145619	12.772556	-75.373063	-37.686549	-24.913993		
1s	16.050233	-33.984781	3.305789	-30.678992	-14.628759	-11.322970	6.083464	0.174686
2s	1.540119	-5.385846	1.571215	-3.814631	-2.274512	-0.703297	5.795374	1.240202
2p	1.252906	-4.702183	1.509274	-3.192909	-1.940003	-0.430729	2.274349	1.201700

	r^{-3}	r^{-2}	r^{-1}	r	r^2	r^4	r^6
		138.8308	14.69094	7.109677	13.53897	92.47112	1122.493
1s		65.27954	5.664130	0.2684114	9.7163301D-02	2.4687937D-02	1.2730322D-02
2s		3.248397	0.8976410	1.580018	2.993874	16.91549	160.6728
2p	1.641699	0.8874430	0.7836971	1.706409	3.678448	29.29538	400.5611

6 Carbon Atom Triplet P State 1s(2)2s(2)2p(2) Configuration (4s, 3p) Basis

|2-V/E| = 6.2D-08 |1-Norm| = 0.0
Total S Cusp: -6.071152 Total P Cusp: -2.540326

	T	V(1)	V(2)	V(T)	E	e	-Cusp	r max
	37.687368	-88.142880	12.768146	-75.374733	-37.687366	-24.919219		
1s	16.049736	-33.984306	3.305289	-30.679017	-14.629231	-11.323943	6.083358	0.174688
2s	1.540714	-5.386832	1.570980	-3.815852	-2.275138	-0.704158	5.796262	1.240051
2p	1.253194	-4.700302	1.507804	-3.192498	-1.939313	-0.431509	2.540326	1.210093

	r^{-3}	r^{-2}	r^{-1}	r	r^2	r^4	r^6
		138.8356	14.69048	7.122237	13.63431	95.77773	1232.190
1s		65.27781	5.664051	0.2684156	9.7166455D-02	2.4699428D-02	1.2730362D-02
2s		3.249552	0.8978053	1.579710	2.992608	16.89923	160.4207
2p	1.670565	0.8904302	0.7833837	1.712993	3.727379	30.96495	455.6617

6 Carbon Atom Triplet P State 1s(2)2s(2)2p(2) Configuration (6s, 4p) Basis

|2-V/E| = 1.7D-07 |1-Norm| = 1.1D-16
Total S Cusp: -6.026968 Total P Cusp: -2.956471

	T	V(1)	V(2)	V(T)	E	e	-Cusp	r max
	37.688605	-88.136933	12.759731	-75.377203	-37.688598	-24.928868		
1s	16.051993	-33.986643	3.304574	-30.682069	-14.630076	-11.325502	6.025222	0.174383
2s	1.538631	-5.380768	1.568266	-3.812502	-2.273871	-0.705605	6.065351	1.223025
2p	1.253679	-4.701056	1.507025	-3.194031	-1.940352	-0.433327	2.956471	1.212576

	r^{-3}	r^{-2}	r^{-1}	r	r^2	r^4	r^6
		138.7791	14.68949	7.144196	13.78709	100.0826	1356.536
1s		65.24100	5.664441	0.2684434	9.7199701D-02	2.4634102D-02	1.2176827D-02
2s		3.256549	0.8967947	1.599455	3.053259	18.22154	188.9267
2p	1.690289	0.8920001	0.7835093	1.714199	3.743084	31.79513	489.3290

Table 12. (Continued)

7 Nitrogen Atom Quartet S State 1s(2)2s(2)2p(3) Configuration (4s, 2p) Basis

|2-V/E| = 2.3D-08 |1-Norm| = 6.9D-17
Total S Cusp: -6.877657 Total P Cusp: -2.752317

	T	V(1)	V(2)	V(T)	E	e	-Cusp	r max
	54.397141	-128.361098	19.566818	-108.794280	-54.397140	-34.830322		
1s	22.141149	-46.570850	4.402969	-42.167880	-20.026732	-15.623763	6.878964	0.148354
2s	2.243819	-7.550067	2.181450	-5.368617	-3.124798	-0.943348	6.850611	1.024972
2p	1.875736	-6.706422	2.132660	-4.573762	-2.698027	-0.565367	2.752317	0.972435

	r^{-3}	r^{-2}	r^{-1}	r	r^2	r^4	r^6
		192.6679	18.33730	7.325116	11.91391	59.10916	521.9469
1s		89.60379	6.652979	0.2283131	7.0397797D-02	1.3555142D-02	1.3073483D-02
2s		4.735389	1.078581	1.330343	2.138804	8.897468	63.76832
2p	3.014161	1.329840	0.9580603	1.402601	2.498501	13.76237	131.4614

7 Nitrogen Atom Quartet S State 1s(2)2s(2)2p(3) Configuration (4s, 3p) Basis

|2-V/E| = 3.6D-07 |1-Norm| = 0.0
Total S Cusp: -6.877538 Total P Cusp: -3.069696

	T	V(1)	V(2)	V(T)	E	e	-Cusp	r max
	54.399001	-128.354253	19.556270	-108.797983	-54.398981	-34.842711		
1s	22.140290	-46.569946	4.401944	-42.168002	-20.027712	-15.625769	6.878882	0.148357
2s	2.244934	-7.551842	2.180943	-5.370898	-3.125964	-0.945021	6.849708	1.024800
2p	1.876184	-6.703559	2.130165	-4.573394	-2.697210	-0.567044	3.069696	0.981672

	r^{-3}	r^{-2}	r^{-1}	r	r^2	r^4	r^6
		192.6790	18.33632	7.342938	12.02892	61.97858	590.1746
1s		89.60046	6.652849	0.2283176	7.0400429D-02	1.3555105D-02	1.3058291D-02
2s		4.737294	1.078835	1.330032	2.137748	8.887851	63.65895
2p	3.068702	1.334480	0.9576513	1.408746	2.537540	14.72526	154.2768

7 Nitrogen Atom Quartet S State 1s(2)2s(2)2p(3) Configuration (6s, 4p) Basis

|2-V/E| = 3.2D-08 |1-Norm| = 9.7D-17
Total S Cusp: -7.025662 Total P Cusp: -3.436500

	T	V(1)	V(2)	V(T)	E	e	-Cusp	r max
	54.400897	-128.351432	19.549640	-108.801793	-54.400896	-34.851256		
1s	22.143163	-46.572650	4.400232	-42.172419	-20.029255	-15.629024	7.023037	0.148606
2s	2.242675	-7.547200	2.179626	-5.367575	-3.124900	-0.945274	7.079598	1.022675
2p	1.876407	-6.703910	2.129975	-4.573935	-2.697528	-0.567553	3.436500	0.985131

	r^{-3}	r^{-2}	r^{-1}	r	r^2	r^4	r^6
		193.2164	18.33592	7.349479	12.07655	63.37354	627.0363
1s		89.84875	6.653236	0.2282979	7.0265808D-02	1.2877208D-02	4.6403231D-03
2s		4.755178	1.078171	1.332356	2.150191	9.110311	67.59884
2p	3.096545	1.336182	0.9577015	1.409391	2.585212	15.04239	163.9431

8 Oxygen Atom Triplet P State 1s(2)2s(2)2p(4) Configuration (4s, 2p) Basis

|2-V/E| = 8.5D-08 |1-Norm| = 0.0
Total S Cusp: -7.876184 Total P Cusp: -3.216561

	T	V(1)	V(2)	V(T)	E	e	-Cusp	r max
	74.803513	-178.094937	28.487918	-149.607019	-74.803506	-46.315589		
1s	29.211825	-61.136289	5.631669	-55.504620	-26.292795	-20.661126	7.876847	0.129286
2s	3.108121	-10.123007	2.887068	-7.235938	-4.127817	-1.240749	7.863258	0.877582
2p	2.540905	-8.894086	2.862611	-6.031476	-3.490570	-0.627960	3.216561	0.819586

	r^{-3}	r^{-2}	r^{-1}	r	r^2	r^4	r^6
		256.5828	22.26187	7.576212	10.96340	43.65565	314.9102
1s		118.1036	7.642036	0.1985882	5.3223717D-02	7.6790083D-03	4.9755616D-03
2s		6.568890	1.265376	1.140957	1.575900	4.864186	26.06945
2p	4.833886	1.809443	1.111761	1.224280	1.926288	8.477979	65.69034

8 Oxygen Atom Triplet P State 1s(2)2s(2)2p(4) Configuration (4s, 3p) Basis

|2-V/E| = 2.3D-07 |1-Norm| = 0.0
Total S Cusp: -7.875927 Total P Cusp: -3.655664

	T	V(1)	V(2)	V(T)	E	e	-Cusp	r max
	74.807543	-178.077804	28.462736	-149.615068	-74.807525	-46.344789		
1s	29.210230	-61.134625	5.629494	-55.505131	-26.294901	-20.665407	7.876656	0.129289
2s	3.110423	-10.126628	2.886096	-7.240532	-4.130109	-1.244012	7.861701	0.877369
2p	2.541559	-8.888825	2.857889	-6.030936	-3.489376	-0.631487	3.656664	0.833505

	r^{-3}	r^{-2}	r^{-1}	r	r^2	r^4	r^6
		256.6094	22.25973	7.605164	11.13561	47.27898	387.1456
1s		118.0971	7.641828	0.1985931	5.3226078D-02	7.6795592D-03	4.9635999D-03
2s		6.572726	1.265829	1.140533	1.574643	4.855488	25.99404
2p	4.945938	1.817414	1.111103	1.231728	1.969968	9.388161	93.78690

Table 12. (Continued)

8 Oxygen Atom Triplet P State 1s(2)2s(2)2p(4) Configuration (6s, 4p) Basis

|2-V/E| = 3.1D-08 |1-Norm| = 0.0

Total S Cusp: -8.024434 Total P Cusp: -3.858964

	T	V(1)	V(2)	V(T)	E	e	-Cusp	r max
	74.809289	-178.075735	28.457159	-149.618576	-74.809287	-46.352128		
1s	29.213141	-61.137298	5.627829	-55.509470	-26.296329	-20.668500	8.021117	0.129458
2s	3.108134	-10.122077	2.884918	-7.237159	-4.129025	-1.244107	8.088723	0.876297
2p	2.541685	-8.889246	2.857916	-6.031330	-3.489645	-0.631729	3.858964	0.835674

	r^{-3}	r^{-2}	r^{-1}	r	r^2	r^4	r^6
		257.2394	22.25947	7.608392	11.15811	47.89124	401.8153
1s		118.3892	7.642162	0.1985897	5.3146131D-02	7.3665677D-03	2.0217410D-03
2s		6.593398	1.265260	1.142006	1.581583	4.951478	27.30140
2p	4.966836	1.818551	1.111156	1.231800	1.972162	9.493387	86.80211

9 Fluorine Atom Doublet P State 1s(2)2s(2)2p(5) Configuration (4s, 2p) Basis

|2-V/E| = 6.1D-08 |1-Norm| = 0.0

Total S Cusp: -8.875667 Total P Cusp: -3.686905

	T	V(1)	V(2)	V(T)	E	e	-Cusp	r max
	99.400471	-238.703573	39.902638	-198.800935	-99.400465	-59.497827		
1s	37.254477	-77.673059	7.023046	-70.650013	-33.395536	-26.372490	8.875306	0.114563
2s	4.096893	-13.046382	3.691264	-9.355118	-5.258225	-1.566960	8.882412	0.768438
2p	3.339546	-11.452938	3.694803	-7.758135	-4.418589	-0.723785	3.686905	0.707603

	r^{-3}	r^{-2}	r^{-1}	r	r^2	r^4	r^6
		330.2860	26.52262	7.736725	10.01082	32.03673	187.0033
1s		150.5148	8.630340	0.1757380	4.1661359D-02	4.6784499D-03	2.1805296D-03
2s		8.672250	1.449598	1.000584	1.213836	2.904465	12.15493
2p	7.334980	2.382390	1.272549	1.076816	1.499964	5.243689	32.53781

9 Fluorine Atom Doublet P State 1s(2)2s(2)2p(5) Configuration (4s, 3p) Basis

|2-V/E| = 7.2D-07 |1-Norm| = 0.0

Total S Cusp: -8.875273 Total P Cusp: -4.217840

	T	V(1)	V(2)	V(T)	E	e	-Cusp	r max
	99.407468	-238.674052	39.859188	-198.814865	-99.407396	-59.548209		
1s	37.252002	-77.670490	7.019566	-70.650924	-33.398922	-26.379356	8.875004	0.114568
2s	4.100526	-13.052059	3.689885	-9.362174	-5.261648	-1.571762	8.880302	0.768221
2p	3.340483	-11.445791	3.688057	-7.757734	-4.417251	-0.729194	4.217840	0.723820

	r^{-3}	r^{-2}	r^{-1}	r	r^2	r^4	r^6
		330.3367	26.51934	7.772418	10.20625	35.48869	244.2187
1s		150.5045	8.630054	0.1757430	4.1663363D-02	4.6780465D-03	2.1736120D-03
2s		8.678214	1.450229	1.000115	1.212601	2.897689	12.10822
2p	7.526867	2.394259	1.271755	1.084141	1.539544	5.936791	43.99959

9 Fluorine Atom Doublet P State 1s(2)2s(2)2p(5) Configuration (6s, 4p) Basis

|2-V/E| = 3.4D-08 |1-Norm| = 1.8D-16

Total S Cusp: -9.023295 Total P Cusp: -4.241562

	T	V(1)	V(2)	V(T)	E	e	-Cusp	r max
	99.409208	-238.667630	39.849218	-198.818412	-99.409204	-59.559987		
1s	37.254865	-77.673059	7.017820	-70.655239	-33.400374	-26.382553	9.019095	0.114700
2s	4.098514	-13.047925	3.688455	-9.359470	-5.260956	-1.572501	9.101509	0.767700
2p	3.340490	-11.445132	3.687333	-7.757799	-4.417309	-0.729976	4.241562	0.721435

	r^{-3}	r^{-2}	r^{-1}	r	r^2	r^4	r^6
		331.0506	26.51863	7.777788	10.23614	36.18641	261.0193
1s		150.8403	8.630340	0.1757479	4.1612716D-02	4.5175887D-03	9.7756642D-04
2s		8.700078	1.449769	1.001089	1.216666	2.942098	12.58807
2p	7.520728	2.393965	1.271681	1.084923	1.543917	6.059635	47.16824

10 Neon Atom Singlet S State 1s(2)2s(2)2p(6) Configuration (4s, 2p) Basis

|2-V/E| = 6.1D-08 |1-Norm| = 2.2D-16

Total S Cusp: -9.875971 Total P Cusp: -4.158744

	T	V(1)	V(2)	V(T)	E	e	-Cusp	r max
	128.534229	-311.191109	54.122658	-257.068451	-128.534222	-74.911563		
1s	46.269254	-96.181397	9.576570	-87.604827	-41.335573	-32.759002	9.874298	0.102853
2s	5.210515	-16.321763	4.594395	-11.727368	-6.516853	-1.922458	9.906305	0.684059
2p	4.262449	-14.364131	4.630121	-9.734010	-5.471562	-0.841440	4.158744	0.622675

	r^{-3}	r^{-2}	r^{-1}	r	r^2	r^4	r^6
		414.0282	31.11911	7.844745	9.144046	23.78079	113.1103
1s		186.8383	9.618140	0.1575178	1.3502430D-02	3.0138231D-03	1.0596831D-03
2s		11.04654	1.632176	0.8919715	0.9656722	1.843770	5.230640
2p	10.60865	3.043076	1.436413	0.9576277	1.190949	3.346203	16.77448

Table 12. (Continued)

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 10     Neon Atom           Singlet S State        1s(2)2s(2)2p(6) Configuration       ( 4s, 3p) Basis

                         |2-V/E| = 3.0D-08                    |1-Norm| = 8.9D-16
                     Total S Cusp:  -9.875525           Total P Cusp:   -4.620815

              T            V(1)          V(2)          V(T)           E             e           -Cusp        r max
          128.544926   -311.141847    54.051995   -257.089852   -128.544924   -74.492929

 1s        46.265773    -96.177778     8.571645    -87.606132    -41.340360   -32.768715     9.874017     0.102856
 2s         5.215610    -16.329393     4.592160    -11.737232     -6.521622    -1.929461     9.902839     0.683790
 2p         4.263694    -14.354584     4.620731     -9.733854     -5.470160    -0.849430     4.620815     0.637273

             r^-3          r^-2          r^-1          r            r^2           r^4          r^6
                        414.1042      31.11418      7.886849      9.354106      26.90934     157.2475

 1s                     186.8246      9.617778     0.1576238    3.3504859D-02 3.0143859D-03 1.0613401D-03
 2s                     11.05476      1.632939     0.8914855     0.9648399      1.845744     6.216905
 2p        10.86220     3.057572      1.435458     0.9647717     1.226236       3.868637     24.13526

 10     Neon Atom           Singlet S State        1s(2)2s(2)2p(6) Configuration       ( 5s, 3p) Basis

                         |2-V/E| = 8.3D-09                    |1-Norm| = 1.6D-15
                     Total S Cusp:  -10.019158          Total P Cusp:   -4.622214

              T            V(1)          V(2)          V(T)           E             e           -Cusp        r max
          128.546561   -311.139019    54.045899   -257.093121   -128.546560   -74.500661

 1s        46.268611    -96.180304     8.570054    -87.610250    -41.341639   -32.771585    10.021991     0.102964
 2s         5.213441    -16.325327     4.591118    -11.734209     -6.520769    -1.929651     9.967609     0.683769
 2p         4.263743    -14.354626     4.620592     -9.734034     -5.470291    -0.849698     4.622214     0.637293

             r^-3          r^-2          r^-1          r            r^2           r^4          r^6
                        414.8901      31.11390      7.888188      9.359183      26.95830     157.7070

 1s                     187.2072      9.618030     0.1576312    3.3470287D-02 2.9243120D-03 5.1490624D-04
 2s                     11.06492      1.632533     0.8921185     0.9672702      1.868438     6.423556
 2p        10.86306     3.057641      1.435463     0.9647814     1.226284       3.869263     24.14314

 10     Neon Atom           Singlet S State        1s(2)2s(2)2p(6) Configuration       ( 5s, 4p) Basis

                         |2-V/E| = 2.4D-07                    |1-Norm| = 1.8D-15
                     Total S Cusp:  -10.019187          Total P Cusp:   -4.758186

              T            V(1)          V(2)          V(T)           E             e           -Cusp        r max
          128.546899   -311.133177    54.039349   -257.093829   -128.546930   -74.507581

 1s        46.268715    -96.180412     8.569722    -87.610690    -41.341975   -32.772254    10.022027     0.102964
 2s         5.213804    -16.325866     4.590845    -11.735021     -6.521217    -1.930373     9.967528     0.683752
 2p         4.263644    -14.353437     4.619703     -9.733734     -5.470091    -0.850388     4.758186     0.635038

             r^-3          r^-2          r^-1          r            r^2           r^4          r^6
                        414.8942      31.11332      7.891476      9.374312      27.21867     163.1597

 1s                     187.2077      9.618041     0.1576310    3.3470199D-02 2.9242844D-03 5.1481620D-04
 2s                     11.06559      1.632587     0.8920914     0.9672108      1.868213     6.422492
 2p        10.87634     3.057941      1.435344     0.9653386     1.228825       3.912732     25.05229

 10     Neon Atom           Singlet S State        1s(2)2s(2)2p(6) Configuration       ( 6s, 4p) Basis

                         |2-V/E| = 1.8D-08                    |1-Norm| = 1.8D-15
                     Total S Cusp:  -10.022245          Total P Cusp:   -4.758178

              T            V(1)          V(2)          V(T)           E             e           -Cusp        r max
          128.546953   -311.133172    54.039268   -257.093905   -128.546951   -74.507683

 1s        46.268626    -96.180319     8.569729    -87.610590    -41.341964   -32.772235    10.017054     0.102958
 2s         5.213842    -16.325770     4.590768    -11.735002     -6.521160    -1.930392    10.116102     0.683601
 2p         4.263669    -14.353499     4.619712     -9.733787     -5.470117    -0.850405     4.758178     0.635038

             r^-3          r^-2          r^-1          r            r^2           r^4          r^6
                        414.9040      31.11332      7.891426      9.373889      27.21129     163.0664

 1s                     187.2029      9.618032     0.1576312    3.3470035D-02 2.9238240D-03 5.1217515D-04
 2s                     11.07519      1.632577     0.8920988     0.9671224      1.865915     6.395334
 2p        10.87638     3.057956      1.435350     0.9653276     1.228784       3.912268     25.04578

 10     Neon Atom           Singlet S State        1s(2)2s(2)2p(6) Configuration       ( 6s, 5p) Basis

                         |2-V/E| = 3.8D-08                    |1-Norm| = 2.0D-15
                     Total S Cusp:  -10.022289          Total P Cusp:   -5.102837

              T            V(1)          V(2)          V(T)           E             e           -Cusp        r max
          128.547063   -311.133201    54.039071   -257.094131   -128.547068   -74.507997

 1s        46.268868    -96.180575     8.569631    -87.610943    -41.342076   -32.772444    10.017097     0.102958
 2s         5.213770    -16.325661     4.590760    -11.734901     -6.521131    -1.930371    10.116181     0.683593
 2p         4.263631    -14.353455     4.619715     -9.733740     -5.470109    -0.850394     5.102837     0.634126

             r^-3          r^-2          r^-1          r            r^2           r^4          r^6
                        414.9104      31.11332      7.890971      9.370007      27.09784     160.5854

 1s                     187.2037      9.618057     0.1576305    3.3469740D-02 2.9237684D-03 5.1219343D-04
 2s                     11.07499      1.632566     0.8921100     0.9671597      1.866190     6.397477
 2p        10.90699     3.058849      1.435346     0.9652483     1.228125       3.893268     24.63158
```

Table 12. (Continued)

10 Neon Atom Singlet S State 1s(2)2s(2)2p(6) Configuration (8s, 6p) Basis

|2-V/E| = 3.7D-08 |1-Norm| = 1.1D-15
Total S Cusp: -10.000639 Total P Cusp: -5.071045

	T	V(1)	V(2)	V(T)	E	e	-Cusp	r max
	128.547102	-311.133193	54.038995	-257.094198	-128.547097	-74.508102		
1s	46.268832	-96.180536	8.569632	-87.610904	-41.342072	-32.772440	10.001778	0.102960
2s	5.213763	-16.325537	4.590693	-11.734845	-6.521081	-1.930389	9.979973	0.682948
2p	4.263652	-14.353508	4.619724	-9.733783	-5.470132	-0.850407	5.071045	0.633984

	r^{-3}	r^{-2}	r^{-1}	r	r^2	r^4	r^6
		414.8904	31.11332	7.891090	9.371473	27.17098	162.9213
1s		187.1977	9.618054	0.1576305	3.3469633D-02	2.9233003D-03	5.0824314D-04
2s		11.07099	1.632554	0.8921064	0.9670310	1.863751	6.374413
2p	10.90657	3.058855	1.435351	0.9652694	1.228412	3.906272	25.02858

11 Na Sodium Atom Doublet S State Ne(10)3s(1) Configuration (6s, 2p) Basis

|2-V/E| = 3.4D-06 |1-Norm| = 2.2D-16
Total S Cusp: -10.864433 Total P Cusp: -4.748217

	T	V(1)	V(2)	V(T)	E	e	-Cusp	r max
	161.848578	-389.779604	66.083000	-323.696604	-161.848026	-95.765026		
1s	56.271758	-116.678349	9.969925	-106.709424	-50.436666	-40.466742	10.859188	0.093329
2s	6.841511	-20.535435	5.451619	-15.083816	-8.242306	-2.790687	10.951904	0.607033
2p	5.892241	-18.669965	5.633115	-13.036850	-7.144608	-1.511493	4.748217	0.542641
3s	0.268592	-3.332245	1.441220	-1.891025	-1.622432	-0.181212	10.867003	3.386084

	r^{-3}	r^{-2}	r^{-1}	r	r^2	r^4	r^6
		508.4143	35.43451	10.78417	26.62588	725.5168	40363.44
1s		227.0500	10.60712	0.1428382	2.7537202D-02	4.3221791D-03	0.1910096
2s		14.43891	1.866858	0.7802357	0.7360041	1.177055	14.99565
2p	16.67923	4.173207	1.697270	0.7950046	0.8078898	1.475900	4.755842
3s		0.3971652	0.3029313	4.167994	20.25146	714.2986	40304.53

11 Na Sodium Atom Doublet S State Ne(10)3s(1) Configuration (6s, 3p) Basis

|2-V/E| = 1.7D-07 |1-Norm| = 1.1D-16
Total S Cusp: -10.863704 Total P Cusp: -5.229613

	T	V(1)	V(2)	V(T)	E	e	-Cusp	r max
	161.855904	-389.752694	66.040913	-323.711781	-161.855877	-95.814964		
1s	56.269397	-116.675938	9.966708	-106.709230	-50.439834	-40.473126	10.858547	0.093332
2s	6.845126	-20.540606	5.450439	-15.090167	-8.245041	-2.794602	10.949415	0.606877
2p	5.892416	-18.662445	5.626885	-13.035561	-7.143145	-1.516260	5.229613	0.550317
3s	0.272305	-3.344934	1.445311	-1.899623	-1.627258	-0.181947	10.877803	3.374450

	r^{-3}	r^{-2}	r^{-1}	r	r^2	r^4	r^6
		508.4848	35.43206	10.79407	26.62157	721.6806	40064.06
1s		227.0377	10.60690	0.1428395	2.7537015D-02	4.2964615D-03	0.1889821
2s		14.44420	1.867328	0.7800909	0.7358063	1.176144	14.87818
2p	16.95992	4.186273	1.696586	0.7983085	0.8209822	1.598510	5.824981
3s		0.4032928	0.3040849	4.158359	20.16899	709.7287	39998.97

11 Na Sodium Atom Doublet S State Ne(10)3s(1) Configuration (9s, 4p) Basis

|2-V/E| = 1.5D-09 |1-Norm| = 4.4D-16
Total S Cusp: -11.023714 Total P Cusp: -5.335814

	T	V(1)	V(2)	V(T)	E	e	-Cusp	r max
	161.858803	-389.735087	66.017481	-323.717606	-161.858803	-95.841322		
1s	56.275147	-116.681119	9.963793	-106.717326	-50.442179	-40.478386	11.019105	0.093395
2s	6.842603	-20.540721	5.450575	-15.090145	-8.247542	-2.796967	11.098653	0.608157
2p	5.892669	-18.662691	5.625969	-13.036722	-7.144053	-1.518085	5.335814	0.549783
3s	0.267288	-3.315262	1.432932	-1.882330	-1.615042	-0.182110	11.121875	3.393012

	r^{-3}	r^{-2}	r^{-1}	r	r^2	r^4	r^6
		509.5188	35.43046	10.84477	27.18390	766.7016	43978.33
1s		227.5417	10.60737	0.1428585	2.7480809D-02	1.9684474D-03	3.0958285D-04
2s		14.45684	1.867338	0.7790703	0.7315237	1.028874	2.493025
2p	16.98391	4.187200	1.696608	0.7984679	0.8221578	1.626442	6.369628
3s		0.3984917	0.3013875	4.210100	20.73295	754.8813	43935.13

Table 12. (Continued)

12 Mg Magnesium Atom Singlet S State Ne(10)3s(2) Configuration (6s, 2p) Basis

|2-V/E| = 1.7D-07 |1-Norm| = 8.9D-16
Total S Cusp: -11.870415 Total P Cusp: -5.308386

	T	V(1)	V(2)	V(T)	E	e	-Cusp	r max
	199.604919	-479.074012	79.864209	-399.209803	-199.604885	-119.740676		
1s	67.268884	-139.170214	11.439632	-127.730581	-60.461697	-49.022065	11.868109	0.085395
2s	8.743921	-25.288758	6.390840	-18.897918	-10.153997	-3.763157	11.902707	0.544787
2p	7.751856	-23.427460	6.698887	-16.728573	-8.976716	-2.277829	5.308386	0.479657
3s	0.534085	-4.795655	2.004971	-2.790684	-2.256599	-0.251628	11.973865	2.603688

	r^{-3}	r^{-2}	r^{-1}	r	r^2	r^4	r^6
		613.6989	39.92283	12.21999	29.27968	535.4044	18449.94
1s		271.3527	11.59752	0.1305798	2.2986566D-02	2.1825819D-03	4.3146350D-03
2s		18.34370	2.107396	0.6915158	0.5747958	0.6894749	5.431199
2p	24.55561	5.456039	1.952288	0.6829220	0.5903631	0.7672681	1.744307
3s		0.7849288	0.3996379	3.239132	12.27097	264.7087	9214.263

12 Mg Magnesium Atom Singlet S State Ne(10)3s(2) Configuration (6s, 3p) Basis

|2-V/E| = 2.5D-08 |1-Norm| = 8.9D-16
Total S Cusp: -11.870023 Total P Cusp: -5.725956

	T	V(1)	V(2)	V(T)	E	e	-Cusp	r max
	199.611354	-479.057162	79.834458	-399.222704	-199.611349	-119.776891		
1s	67.267492	-139.168793	11.437245	-127.731548	-60.464056	-49.026811	11.867799	0.085396
2s	8.746653	-25.292505	6.390031	-18.902474	-10.155819	-3.765787	11.900825	0.544695
2p	7.751261	-23.420562	6.694041	-16.726522	-8.975261	-2.281221	5.725956	0.483992
3s	0.537749	-4.805596	2.007831	-2.797764	-2.260017	-0.252185	11.977453	2.598971

	r^{-3}	r^{-2}	r^{-1}	r	r^2	r^4	r^6
		613.7736	39.92143	12.22272	29.25961	533.6114	18364.23
1s		271.3457	11.59740	0.1305805	2.2986588D-02	2.1787603D-03	4.2950798D-02
2s		18.34760	2.107709	0.6914469	0.5747211	0.6892943	5.410186
2p	24.84436	5.467609	1.951714	0.6847995	0.5966252	0.8089734	2.001523
3s		0.7906824	0.4004663	3.234934	12.24222	263.6873	9170.656

12 Mg Magnesium Atom Singlet S State Ne(10)3s(2) Configuration (9s, 4p) Basis

|2-V/E| = 1.4D-08 |1-Norm| = 1.6D-15
Total S Cusp: -12.024235 Total P Cusp: -5.823350

	T	V(1)	V(2)	V(T)	E	e	-Cusp	r max
	199.614549	-479.045675	79.816579	-399.229096	-199.614547	-119.797968		
1s	67.274493	-139.175283	11.434611	-127.740672	-60.466179	-49.031568	12.020221	0.085454
2s	8.743416	-25.293802	6.391341	-18.902461	-10.159045	-3.767704	12.083444	0.546605
2p	7.751269	-23.420357	6.693433	-16.726924	-8.975654	-2.282221	5.823350	0.484227
3s	0.535557	-4.792681	2.002038	-2.790643	-2.255086	-0.253048	12.120110	2.588710

	r^{-3}	r^{-2}	r^{-1}	r	r^2	r^4	r^6
		614.8759	39.92047	12.25807	29.62202	557.3229	20001.20
1s		271.8564	11.59794	0.1305946	2.2956106D-02	1.3712857D-03	1.6743340D-04
2s		18.38604	2.107817	0.6903396	0.5710982	0.6114108	1.119243
2p	24.88358	5.468948	1.951696	0.6849901	0.5976918	0.8241269	2.180171
3s		0.7886473	0.3993901	3.253131	12.42388	275.5763	9992.942

13 Aluminum Atom Doublet P State Ne(10)3s(2)3p(1) Configuration (6s, 4p) Basis

|2-V/E| = 1.2D-06 |1-Norm| = 1.7D-16
Total S Cusp: -12.880181 Total P Cusp: -5.967803

	T	V(1)	V(2)	V(T)	E	e	-Cusp	r max
	241.866006	-578.676002	94.944277	-483.731726	-241.865720	-146.921443		
1s	79.256515	-163.652759	12.956492	-150.696267	-71.439752	-58.483260	12.881026	0.078699
2s	10.888507	-30.535866	7.377539	-23.158327	-12.269820	-4.897281	12.863084	0.494426
2p	9.844927	-28.644699	7.799514	-20.845185	-11.000258	-3.200743	5.961022	0.430385
3s	0.923190	-6.560446	2.628761	-3.931685	-3.008495	-0.379734	12.966136	2.119387
3p	0.660019	-5.309665	2.221607	-3.088058	-2.428039	-0.206432	6.140237	2.590241

	r^{-3}	r^{-2}	r^{-1}	r	r^2	r^4	r^6
		729.2571	44.51354	13.39602	30.57517	422.9971	10438.47
1s		319.6535	12.58867	0.1202515	1.9476381D-02	1.2602477D-03	9.5090367D-03
2s		22.74295	2.348913	0.6208680	0.4610946	0.4195232	1.701163
2p	34.71642	6.905496	2.203438	0.6009811	0.4552307	0.4630836	1.074274
3s		1.339788	0.5046497	2.599711	7.861769	106.1643	2279.469
3p	1.256798	0.3516277	0.4084357	3.108469	11.15911	207.0484	5869.661

Table 12. (Continued)

13 Aluminum Atom Doublet P State Ne(10)3s(2)3p(1) Configuration (9s, 6p) Basis

|2-V/E| = 3.1D-08 |1-Norm| = 6.4D-16
Total S Cusp: -13.024610 Total P Cusp: -6.331564

	T	V(1)	V(2)	V(T)	E	ε	-Cusp	r max
	241.876633	-578.498493	94.745234	-483.753259	-241.876626	-147.131391		
1s	79.264147	-163.660040	12.947438	-150.712602	-71.448455	-58.501017	13.020480	0.078755
2s	10.884504	-30.537118	7.370904	-23.166214	-12.281710	-4.910806	13.081059	0.496223
2p	9.856110	-28.666595	7.796020	-20.870575	-11.014465	-3.218445	6.332328	0.432684
3s	0.936142	-6.588718	2.629503	-3.959216	-3.023074	-0.393571	13.110699	2.099341
3p	0.570388	-4.927172	2.073425	-2.853746	-2.283358	-0.209932	6.307795	2.682285

	r^{-3}	r^{-2}	r^{-1}	r	r^{2}	r^{4}	r^{6}
		730.4027	44.49968	13.72112	33.53146	587.7327	20632.54
1s		320.1396	12.58923	0.1202586	1.9458840D-02	9.8365515D-04	9.7776372D-05
2s		22.80173	2.349009	0.6200267	0.4589042	0.3880183	0.5452388
2p	34.89545	6.914968	2.205123	0.6005404	0.4553750	0.4638484	0.9277647
3s		1.360006	0.5068245	2.599198	7.891539	109.1331	2454.423
3p	1.085576	0.3102157	0.3790132	3.438909	14.05941	365.9054	15717.04

14 Silicon Atom Triplet P State Ne(10)3s(2)3p(2) Configuration (6s, 4p) Basis

|2-V/E| = 3.7D-05 |1-Norm| = 1.4D-16
Total S Cusp: -14.023738 Total P Cusp: -6.522623

	T	V(1)	V(2)	V(T)	E	ε	-Cusp	r max
	288.853280	-689.665202	111.967586	-577.697616	-288.844337	-176.876751		
1s	92.247688	-190.138984	14.548260	-175.590725	-83.343037	-68.794777	14.048654	0.073055
2s	13.249725	-36.249210	8.433095	-27.816115	-14.566389	-6.133294	13.687902	0.456302
2p	12.184385	-34.362347	8.972404	-25.389942	-13.205558	-4.233153	6.519317	0.389387
3s	1.383045	-8.456623	3.275065	-5.181557	-3.798512	-0.523446	13.712242	1.809746
3p	0.993026	-6.900744	2.810160	-4.090584	-3.097558	-0.287398	6.590906	2.168859

	r^{-3}	r^{-2}	r^{-1}	r	r^{2}	r^{4}	r^{6}
		856.2189	49.26180	14.19048	30.03826	321.5661	5996.590
1s		372.4382	13.56136	0.1114296	1.6703245D-02	7.4191666D-04	6.3000829D-04
2s		27.62406	2.589229	0.5628772	0.3768372	0.2580852	0.2936926
2p	47.09810	8.512448	2.454453	0.5359199	0.3596072	0.2848013	0.5570291
3s		1.986339	0.6040445	2.192486	5.571044	52.46117	778.8074
3p	2.145427	0.5235366	0.4929103	2.620686	7.975123	107.2086	2217.522

14 Silicon Atom Triplet P State Ne(10)3s(2)3p(2) Configuration (9s, 6p) Basis

|2-V/E| = 4.3D-08 |1-Norm| = 7.2D-16
Total S Cusp: -14.024903 Total P Cusp: -6.838460

	T	V(1)	V(2)	V(T)	E	ε	-Cusp	r max
	288.854290	-689.413790	111.705222	-577.708568	-288.854278	-177.149056		
1s	92.244674	-190.135917	14.539421	-175.596496	-83.351822	-68.612401	14.020883	0.073029
2s	13.262032	-36.265602	8.423477	-27.842125	-14.580093	-6.156616	14.074356	0.454205
2p	12.197942	-34.389532	8.967724	-25.421807	-13.223866	-4.256141	6.838538	0.390974
3s	1.385795	-8.445669	3.259965	-5.185704	-3.799909	-0.539944	14.134960	1.799791
3p	0.940819	-6.691111	2.726575	-3.964537	-3.023718	-0.297143	6.836760	2.169502

	r^{-3}	r^{-2}	r^{-1}	r	r^{2}	r^{4}	r^{6}
		856.2939	49.24384	14.44222	32.28344	411.0197	9909.060
1s		372.3937	13.58114	0.1114308	1.6700923D-02	7.2345547D-04	6.1392436D-05
2s		27.69547	2.590400	0.5629430	0.3772620	0.2591384	0.2935487
2p	47.21579	8.519355	2.456395	0.5354066	0.3596912	0.2830200	0.4196690
3s		1.948678	0.6032621	2.207002	5.676555	55.87638	891.1602
3p	2.051648	0.5010398	0.4779365	2.753514	8.992129	148.5245	4061.817

15 Phosphorus Atom Quartet S State Ne(10)3s(2)3p(3) Configuration (6s, 4p) Basis

|2-V/E| = 4.8D-09 |1-Norm| = 1.9D-16
Total S Cusp: -15.031754 Total P Cusp: -7.418585

	T	V(1)	V(2)	V(T)	E	ε	-Cusp	r max
	340.709054	-812.436092	131.018000	-681.418091	-340.709038	-209.691037		
1s	106.217160	-218.604013	16.214218	-202.389795	-96.172635	-79.958417	15.050979	0.068302
2s	15.869178	-42.471328	9.555804	-32.915524	-17.046346	-7.490542	14.773925	0.419893
2p	14.762983	-40.569069	10.212821	-30.356248	-15.593265	-5.380444	7.420894	0.359278
3s	1.878789	-10.402858	3.921065	-6.481793	-4.603004	-0.681938	14.962464	1.600714
3p	1.400300	-8.688426	3.452966	-5.235460	-3.835160	-0.382194	7.377912	1.862307

	r^{-3}	r^{-2}	r^{-1}	r	r^{2}	r^{4}	r^{6}
		992.6780	54.16241	14.76800	28.83492	243.4261	3506.784
1s		428.6697	14.57360	0.1038028	1.4488751D-02	5.5016711D-04	1.4146706D-04
2s		33.01061	2.831422	0.5155529	0.3156778	0.1798733	0.1683359
2p	62.46562	10.28912	2.704605	0.4834103	0.2913499	0.1825845	0.2209902
3s		2.694711	0.6935239	1.928996	4.310738	31.23905	355.0287
3p	3.386650	0.7310563	0.5792284	2.256944	5.935003	59.83056	931.6877

Table 12. (Continued)

15 Phosphorus Atom Quartet S State Ne(10)3s(2)3p(3) Configuration (9s, 6p) Basis

|2-V/E| = 2.8D-08 |1-Norm| = 4.7D-16
Total S Cusp: -15.025183 Total P Cusp: -7.355186

	T	V(1)	V(2)	V(T)	E	ε	-Cusp	r max
	340.718706	-812.220577	130.783174	-681.437403	-340.718697	-209.935522		
1s	106.216330	-218.603129	16.208585	-202.394544	-96.178213	-79.969628	15.021421	0.068078
2s	15.872784	-42.475508	9.545803	-32.929704	-17.056921	-7.511117	15.065879	0.418694
2p	14.777952	-40.594224	10.207639	-30.386585	-15.608633	-5.400994	7.354270	0.356586
3s	1.890428	-10.421425	3.917269	-6.504156	-4.613728	-0.696459	15.161415	1.586836
3p	1.363970	-8.551703	3.398008	-5.153695	-3.789725	-0.391717	7.371360	1.843921

	r^{-3}	r^{-2}	r^{-1}	r	r^2	r^4	r^6
		992.6338	54.14804	14.97380	30.28339	290.6397	5135.406
1s		428.6195	14.57354	0.1038048	1.4488361D-02	5.4365538D-04	3.9920737D-05
2s		33.06095	2.831701	0.5156625	0.3159242	0.1801708	0.1688733
2p	62.08818	10.28302	2.706282	0.4833996	0.2918019	0.1830307	0.2096196
3s		2.713847	0.6947617	1.932560	4.346843	32.52840	393.0325
3p	3.309090	0.7156770	0.5701136	2.323116	6.392689	74.70775	1449.248

16 Sulfur Atom Triplet P State Ne(10)3s(2)3p(4) Configuration (6s, 4p) Basis

|2-V/E| = 1.5D-05 |1-Norm| = 3.1D-16
Total S Cusp: -16.043080 Total P Cusp: -8.028432

	T	V(1)	V(2)	V(T)	E	ε	-Cusp	r max
	397.497247	-947.138460	152.149863	-794.988597	-397.491350	-245.341487		
1s	121.178120	-249.060702	17.945215	-231.115487	-109.937366	-91.992151	16.056493	0.063778
2s	18.725206	-49.178820	10.735147	-38.443673	-19.718467	-8.983320	15.860484	0.388841
2p	17.569863	-47.242438	11.505842	-35.736596	-18.166733	-6.660891	8.040873	0.330628
3s	2.459675	-12.557871	4.617226	-7.940644	-5.480969	-0.863743	16.112154	1.434844
3p	1.838016	-10.522261	4.129908	-6.392353	-4.554337	-0.424429	7.830062	1.648938

	r^{-3}	r^{-2}	r^{-1}	r	r^2	r^4	r^6
		1139.638	59.19615	15.27839	27.81692	194.8681	2315.039
1s		488.8872	15.56629	9.7148817D-02	1.2685731D-02	4.1785161D-04	4.6824689D-05
2s		38.87934	3.073676	0.4756676	0.2684444	0.1294624	0.1024200
2p	80.22668	12.20776	2.952652	0.4410498	0.2418474	0.1252288	0.1306682
3s		3.519638	0.7648669	1.717474	3.412985	19.42398	172.1253
3p	4.894278	0.9546963	0.6576413	2.012877	4.744402	38.75224	492.4499

16 Sulfur Atom Triplet P State Ne(10)3s(2)3p(4) Configuration (9s, 6p) Basis

|2-V/E| = 1.3D-08 |1-Norm| = 4.4D-16
Total S Cusp: -16.025568 Total P Cusp: -7.891790

	T	V(1)	V(2)	V(T)	E	ε	-Cusp	r max
	397.504772	-946.895811	151.886274	-795.009538	-397.504766	-245.618493		
1s	121.180474	-249.063048	17.939174	-231.123874	-109.943400	-92.004226	16.022246	0.063754
2s	18.719514	-49.170873	10.723613	-38.447260	-19.727747	-9.004134	16.056033	0.388285
2p	17.588756	-47.271210	11.500040	-35.771170	-18.182414	-6.682373	7.884593	0.327737
3s	2.471739	-12.578032	4.613443	-7.964589	-5.492799	-0.879356	16.180206	1.421111
3p	1.807171	-10.411162	4.083393	-6.327769	-4.520598	-0.437205	8.001266	1.619732

	r^{-3}	r^{-2}	r^{-1}	r	r^2	r^4	r^6
		1139.500	59.16099	15.47466	29.15374	234.4578	3525.857
1s		488.8215	15.56644	9.7150833D-02	1.2686473D-02	4.1626645D-04	2.6940874D-05
2s		38.90303	3.073180	0.4757766	0.2685337	0.1293160	0.1021937
2p	79.71800	12.20184	2.954451	0.4410406	0.2420896	0.1247812	0.1196442
3s		3.535898	0.7861270	1.720545	3.442352	20.29039	192.6958
3p	4.843623	0.9420325	0.6506976	2.060369	5.063514	48.21721	784.8857

17 Cl Chlorine Atom Doublet P State Ne(10)3s(2)3p(5) Configuration (6s, 4p) Basis

|2-V/E| = 5.9D-08 |1-Norm| = 2.2D-16
Total S Cusp: -17.051202 Total P Cusp: -7.969611

	T	V(1)	V(2)	V(T)	E	ε	-Cusp	r max
	459.458338	-1094.670985	175.754336	-918.916649	-459.458311	-283.703975		
1s	137.128168	-281.506481	19.756769	-261.749713	-124.621545	-104.864776	17.061359	0.059970
2s	21.809033	-56.360507	11.983947	-44.376560	-22.567557	-10.593610	16.901477	0.362284
2p	20.601825	-54.368987	12.860345	-41.508642	-20.906918	-8.046472	7.975220	0.301321
3s	3.082322	-14.820011	5.344440	-9.475571	-6.393248	-1.048808	17.269074	1.305064
3p	2.361681	-12.616612	4.884391	-7.732222	-5.370541	-0.486150	7.890744	1.459291

	r^{-3}	r^{-2}	r^{-1}	r	r^2	r^4	r^6
		1297.015	64.39241	15.59193	26.22674	151.0589	1470.815
1s		553.0698	16.55920	9.1295673D-02	1.1199528D-02	3.2447789D-04	2.3210475D-05
2s		45.20757	3.315324	0.4416149	0.2311415	9.5487779D-02	6.4386343D-02
2p	100.0214	14.26171	3.198176	0.4066259	0.2053457	9.4152045D-02	0.1728079
3s		4.406613	0.8717653	1.556608	2.803272	13.06267	94.46842
3p	6.767910	1.215398	0.7421537	1.794627	3.760688	24.33540	256.1425

Table 12. (Continued)

17 Cl Chlorine Atom Doublet P State Ne(10)3s(2)3p(5) Configuration (9s, 6p) Basis

|2-V/E| = 2.2D-08 |1-Norm| = 6.4D-16
Total S Cusp: -17.025736 Total P Cusp: -8.407281

	T	V(1)	V(2)	V(T)	E	ε	-Cusp	r max
	459.481809	-1094.358119	175.394510	-918.963609	-459.481799	-284.087289		
1s	137.136165	-281.514657	19.747277	-261.767380	-124.631215	-104.883939	17.022919	0.059947
2s	21.796218	-56.344230	11.970486	-44.373744	-22.577527	-10.607040	17.045711	0.361993
2p	20.632495	-54.425926	12.860811	-41.565115	-20.932620	-8.071809	8.392289	0.303273
3s	3.108727	-14.873317	5.346084	-9.527233	-6.418506	-1.072422	17.198605	1.290413
3p	2.320924	-12.467631	4.820390	-7.647241	-5.326316	-0.505927	8.609551	1.445810

	r^{-3}	r^{-2}	r^{-1}	r	r^2	r^4	r^6
		1296.953	64.37401	15.81656	27.60339	183.8916	2295.749
1s		552.9963	16.55969	9.1295556D-02	1.1200051D-02	3.2402374D-04	1.8672868D-05
2s		45.21027	3.314366	0.4417199	0.2311974	9.5374994D-02	6.4544189D-02
2p	100.3288	14.27680	3.201525	0.4057149	0.2043261	8.8265958D-02	7.2246622D-02
3s		4.436038	0.8749010	1.555426	2.811850	13.48343	103.9302
3p	6.779612	1.201482	0.7333900	1.841077	4.053788	31.24075	417.4653

18 Argon Atom Singlet S State Ne(10)3s(2)3p(6) Configuration (6s, 4p) Basis

|2-V/E| = 2.6D-07 |1-Norm| = 1.8D-15
Total S Cusp: -18.059978 Total P Cusp: -9.072040

	T	V(1)	V(2)	V(T)	E	ε	-Cusp	r max
	526.795197	-1255.336564	201.746305	-1053.590259	-526.795062	-325.048757		
1s	154.075376	-315.949802	21.638592	-294.311209	-140.235834	-118.597241	18.068470	0.056590
2s	25.115479	-64.012129	13.297782	-50.714347	-25.598868	-12.301086	17.947435	0.339140
2p	23.906761	-62.056027	14.299952	-47.756075	-23.849294	-9.549342	9.101151	0.284339
3s	3.781833	-17.273924	6.116870	-11.157054	-7.375221	-1.258351	18.383319	1.197016
3p	2.901523	-14.754782	5.640017	-9.114765	-6.213242	-0.573225	8.673567	1.330655

	r^{-3}	r^{-2}	r^{-1}	r	r^2	r^4	r^6
		1465.340	69.74092	15.89295	24.95780	121.1281	982.2783
1s		621.2432	17.55277	8.6102265D-02	9.9584716D-03	2.5590122D-04	1.3186154D-05
2s		51.98545	3.556229	0.4122139	0.2012333	7.2111647D-02	4.2058598D-02
2p	124.9925	16.52729	3.447557	0.3753963	0.1742064	6.3394738D-02	4.3646714D-02
3s		5.399718	0.9596624	1.421750	2.337404	9.041646	54.05251
3p	8.999443	1.486603	0.8197101	1.633406	3.135895	17.08662	145.6379

18 Argon Atom Singlet S State Ne(10)3s(2)3p(6) Configuration (9s, 6p) Basis

|2-V/E| = 1.5D-08 |1-Norm| = 2.0D-15
Total S Cusp: -18.025687 Total P Cusp: -8.917114

	T	V(1)	V(2)	V(T)	E	ε	-Cusp	r max
	526.817028	-1255.071022	201.436974	-1053.634048	-526.817020	-325.380046		
1s	154.083517	-315.958046	21.632488	-294.325558	-140.242041	-118.609553	18.023428	0.056568
2s	25.102045	-63.994895	13.285738	-50.709156	-25.607112	-12.321373	18.035259	0.339038
2p	23.937266	-62.099199	14.295614	-47.803585	-23.866320	-9.570706	8.894105	0.282175
3s	3.802612	-17.315905	6.118402	-11.197504	-7.394892	-1.276490	18.214024	1.183748
3p	2.869514	-14.656356	5.598339	-9.058017	-6.188502	-0.590163	9.203995	1.306747

	r^{-3}	r^{-2}	r^{-1}	r	r^2	r^4	r^6
		1465.074	69.72617	16.06267	25.98869	144.0840	1491.566
1s		621.1442	17.55322	8.6103706D-02	9.9597063D-03	2.5592678D-04	1.3197406D-05
2s		51.98094	3.555272	0.4122867	0.2012310	7.1969587D-02	4.2232589D-02
2p	124.2993	16.52428	3.449956	0.3753310	0.1743402	6.3361754D-02	4.1101867D-02
3s		5.416362	0.9619947	1.421962	2.349268	9.382530	60.09784
3p	8.994831	1.474265	0.8142420	1.661664	3.303622	20.79905	228.5065

19 K Potassium Atom Doublet S State Ar(18)4s(1) Configuration (8s, 4p) Basis

|2-V/E| = 1.5D-07 |1-Norm| = 3.7D-16
Total S Cusp: -18.861670 Total P Cusp: -9.394533

	T	V(1)	V(2)	V(T)	E	ε	-Cusp	r max
	599.147398	-1423.023512	224.728627	-1198.294884	-599.147486	-374.418859		
1s	172.000026	-352.371938	23.422968	-328.948971	-156.948945	-133.525977	18.857434	0.053538
2s	28.703337	-72.200410	14.506669	-57.693742	-28.990405	-14.483736	18.917861	0.317802
2p	27.447801	-70.211665	15.625277	-54.586388	-27.138587	-11.513311	9.421151	0.264829
3s	4.795166	-20.384210	6.923467	-13.460742	-8.665577	-1.742109	18.831746	1.091686
3p	3.869057	-17.908555	6.545547	-11.363008	-7.493951	-0.948403	9.092230	1.179154
4s	0.249189	-4.389073	1.997477	-2.391597	-2.142407	-0.144930	18.400386	4.221807

	r^{-3}	r^{-2}	r^{-1}	r	r^2	r^4	r^6
		1642.119	74.89597	19.59614	54.59116	2411.787	271608.1
1s		692.2692	18.54589	8.1452881D-02	8.9210516D-03	1.1610335D-03	0.1970928
2s		59.23132	3.800022	0.3865665	0.1775398	0.1434715	18.16242
2p	152.1247	18.92639	3.695351	0.3494961	0.1507307	4.6955473D-02	2.6056755D-02
3s		6.777432	1.072853	1.277864	1.883080	5.953920	57.41210
3p	12.91777	1.954643	0.9425555	1.422749	2.366988	9.527785	59.20747
4s		0.2770037	0.2310039	5.470902	35.34577	2342.141	271101.2

Table 12. (Continued)

19 Potassium Atom Doublet S State Ar(18)4s(1) Configuration (12s, 6p) Basis

|2-V/E| = 1.5D-09 |1-Norm| = 7.5D-16
Total S Cusp: -19.005836 Total P Cusp: -9.419008

	T	V(1)	V(2)	V(T)	E	e	-Cusp	r max
	599.164566	-1422.963291	224.634158	-1198.329133	-599.164567	-374.530409		
1s	172.028834	-352.399732	23.419009	-328.980723	-156.951890	-133.532881	19.007893	0.053543
2s	28.663569	-72.156261	14.501443	-57.654819	-28.991250	-14.489808	18.986372	0.318827
2p	27.470104	-70.243382	15.627067	-54.616316	-27.146212	-11.519145	9.404983	0.263866
3s	4.814097	-20.422256	6.929775	-13.492481	-8.678385	-1.748610	18.955879	1.082359
3p	3.844419	-17.841901	6.521618	-11.320283	-7.475865	-0.954247	9.567913	1.164861
4s	0.264439	-4.495093	2.041598	-2.453495	-2.189056	-0.147457	18.990606	4.342923

	r^{-3}	r^{-2}	r^{-1}	r	r^{2}	r^{4}	r^{6}
		1644.179	74.89280	19.44982	51.21887	1706.546	128758.2
1s		693.2549	18.54735	8.1466519D-02	8.9134911D-03	2.0840315D-04	6.5846087D-04
2s		59.25327	3.797698	0.3863912	0.1765980	5.5428552D-02	7.0861324D-02
2p	151.7354	18.92578	3.697020	0.3494274	0.1508014	4.7060072D-02	2.5790760D-02
3s		6.815766	1.074856	1.277067	1.883531	5.849312	28.89977
3p	12.97095	1.946853	0.9390474	1.436681	2.439839	10.73114	78.45415
4s		0.2951501	0.2365839	5.243322	31.53695	1630.067	128229.4

20 Calcium Atom Singlet S State Ar(18)4s(2) Configuration (8s, 4p) Basis

|2-V/E| = 3.2D-06 |1-Norm| = 1.6D-15
Total S Cusp: -20.058110 Total P Cusp: -9.770592

	T	V(1)	V(2)	V(T)	E	e	-Cusp	r max
	676.745597	-1603.449527	249.960495	-1353.489032	-676.743435	-426.782940		
1s	190.964375	-390.831778	25.258368	-365.573410	-174.609035	-149.350668	20.059035	0.050850
2s	32.477135	-80.822914	15.768362	-65.054553	-32.577418	-16.809056	19.963541	0.300790
2p	31.233046	-78.861836	17.006748	-61.855088	-30.622042	-13.615294	9.795464	0.248032
3s	5.920201	-23.687301	7.770768	-15.916533	-9.996332	-2.225564	20.685430	1.007590
3p	4.937520	-21.226203	7.482475	-13.743728	-8.806209	-1.323734	9.525445	1.063786
4s	0.499391	-6.118655	2.715083	-3.403572	-2.904181	-0.189097	21.173675	3.432077

	r^{-3}	r^{-2}	r^{-1}	r	r^{2}	r^{4}	r^{6}
		1834.692	80.17248	20.92369	53.24249	1182.162	52280.65
1s		769.5065	19.54159	7.7300069D-02	8.0226649D-03	1.6627349D-04	4.5568642D-05
2s		67.03826	4.041146	0.3635003	0.1562012	4.3366228D-02	4.1131850D-02
2p	182.9927	21.48758	3.943092	0.3269165	0.1316932	3.5615776D-02	1.6917545D-02
3s		8.390152	1.184365	1.163773	1.556420	4.143376	38.45585
3p	17.63857	2.467560	1.061310	1.266561	1.869690	5.853062	27.98163
4s		0.5456185	0.3059327	4.076839	18.89645	569.2280	26017.83

20 Calcium Atom Singlet S State Ar(18)4s(2) Configuration (12s, 6p) Basis

|2-V/E| = 2.9D-09 |1-Norm| = 2.0D-15
Total S Cusp: -20.004697 Total P Cusp: -9.892207

	T	V(1)	V(2)	V(T)	E	e	-Cusp	r max
	676.757143	-1603.203436	249.689148	-1353.514288	-676.757145	-427.067997		
1s	190.970878	-390.838377	25.252024	-365.586353	-174.615475	-149.363451	20.006679	0.050829
2s	32.472551	-80.817365	15.761178	-65.056187	-32.583536	-16.822358	19.987064	0.300799
2p	31.245500	-78.879380	17.002489	-61.876892	-30.631392	-13.628903	9.866255	0.247691
3s	5.956542	-23.774973	7.786706	-15.988267	-10.031725	-2.245019	19.956239	0.996868
3p	4.917906	-21.177420	7.459652	-13.717768	-8.799862	-1.340210	10.132201	1.056101
4s	0.488283	-6.000601	2.658244	-3.342358	-2.854074	-0.195830	19.983525	3.472454

	r^{-3}	r^{-2}	r^{-1}	r	r^{2}	r^{4}	r^{6}
		1834.403	80.16017	21.24388	56.53172	1424.831	72163.01
1s		769.3793	19.54192	7.7300663D-02	8.0231921D-03	1.6775211D-04	2.7704533D-04
2s		67.03438	4.040868	0.3635034	0.1561733	4.3114709D-02	3.5827453D-02
2p	182.8650	21.48875	3.[illegible]3969	0.3268734	0.1317160	3.5671116D-02	1.6884110D-02
3s		8.395973	1.188749	1.159437	1.546094	3.853961	14.80655
3p	17.76096	2.463060	1.058871	1.275403	1.914740	6.548427	38.42472
4s		0.5365927	0.3000301	4.214870	20.41620	688.7660	35951.34

Table 12. (Continued)

21 Scandium Atom Doublet D State Ar(18)3d(1)4s(2) Configuration (8s, 4p, 3d) Basis

|2-V/E| = 2.6D-06 |1-Norm| = 5.1D-16

Total S Cusp: -20.857402 Total P Cusp: -10.272454 Total D Cusp: -5.306532

	T	V(1)	V(2)	V(T)	E	e	-Cusp	r max
	759.719897	-1799.890619	280.452769	-1519.437849	-759.717952	-479.265183		
1s	210.883798	-431.249679	27.236122	-404.013557	-193.129759	-165.893637	20.860621	0.048376
2s	36.573014	-90.021351	17.185011	-72.836340	-36.263327	-19.078316	20.825511	0.283468
2p	35.257052	-87.996840	18.536180	-69.460660	-34.203608	-15.667428	10.302110	0.233661
3s	6.955990	-26.892793	8.686318	-18.206476	-11.250486	-2.564169	20.827413	0.936178
3p	5.864446	-24.247247	8.405696	-15.841552	-9.977106	-1.571411	9.996762	0.983234
3d	3.070933	-16.773086	6.680494	-10.092592	-7.021659	-0.341165	5.306532	1.135380
4s	0.547188	-6.662680	2.953059	-3.709621	-3.162432	-0.209373	20.561045	3.188911

	r^{-3}	r^{-2}	r^{-1}	r	r^2	r^4	r^6
		2031.695	85.70908	21.58488	55.02059	1402.313	83036.62
1s		848.4337	20.53570	7.3522371D-02	7.2607229D-03	3.4144462D-04	2.5443605D-02
2s		75.18829	4.286731	0.3434638	0.1401039	8.9704988D-02	6.862830
2p	218.2738	24.21907	4.190326	0.3071233	0.1160741	2.7549940D-02	1.1460331D-02
3s		9.775644	1.280609	1.079590	1.339012	2.911522	13.93964
3p	22.26633	2.916774	1.154631	1.167379	1.588391	4.216427	17.05545
3d	1.417980	0.8845160	0.7987184	1.670181	3.579294	29.71851	437.6016
4s		0.5999457	0.3172705	4.037266	19.12088	670.5636	[illegible]

24 Cr Chromium Atom Heptuplet S State Ar(18)3d(5)4s(1) Configuration (8s, 4p, 3d) Basis

|2-V/E| = 1.3D-04 |1-Norm| = 3.1D-16

Total S Cusp: -23.846223 Total P Cusp: -11.386543 Total D Cusp: -5.372573

	T	V(1)	V(2)	V(T)	E	e	-Cusp	r max
	1042.200231	-2477.183821	392.649714	-2084.534107	-1042.333876	-649.684162		
1s	276.721267	-564.580581	33.613758	-530.966823	-254.245556	-220.631798	23.855166	0.042261
2s	50.157527	-120.408048	21.884877	-98.523171	-48.365644	-26.480767	23.763208	0.244156
2p	48.764256	-118.317995	23.572929	-94.745066	-45.980810	-22.407881	11.407520	0.197802
3s	10.265393	-37.110257	11.683171	-25.427086	-15.161693	-3.478522	23.733232	0.784702
3p	8.897261	-34.010940	11.442246	-22.568694	-13.671433	-2.229186	11.213731	0.801833
4s	0.788475	-9.021788	3.987062	-5.034726	-4.246251	-0.259190	23.598269	2.703284
3d	4.230855	-21.998130	8.841598	-13.156532	-8.925677	-0.084080	5.372573	0.875784

	r^{-3}	r^{-2}	r^{-1}	r	r^2	r^4	r^6
		2692.943	103.2160	21.08757	39.69751	521.5379	17334.67
1s		1112.611	23.52419	6.4136037D-02	5.5195990D-03	1.0374737D-04	1.9163362D-03
2s		102.7659	5.017002	0.2941976	0.1025979	4.0968607D-02	1.699993
2p	349.0249	33.35744	4.929916	0.2602934	8.3216350D-02	1.4359949D-02	6.2704936D-03
3s		14.38553	1.546261	0.9023238	0.9368879	1.441733	5.300880
3p	39.45412	4.379534	1.417122	0.9600201	1.080563	1.996269	5.759512
4s		0.8729656	0.3759078	3.426731	13.75825	339.5470	14003.82
3d	2.399488	1.224611	0.9165888	1.563529	3.373315	33.39230	656.4505

25 Mn Manganese Atom Hextuplet S State Ar(18)3d(5)4s(2) Configuration (8s, 4p, 3d) Basis

|2-V/E| = 5.2D-06 |1-Norm| = 2.9D-16

Total S Cusp: -24.851969 Total P Cusp: -12.387922 Total D Cusp: -6.809069

	T	V(1)	V(2)	V(T)	E	e	-Cusp	r max
	1149.840774	-2735.392604	435.717012	-2299.675592	-1149.834818	-714.117806		
1s	300.690919	-613.048283	35.917895	-577.130388	-276.439469	-240.521574	24.864128	0.040547
2s	55.112596	-131.454047	23.621476	-107.832571	-52.719975	-29.098499	24.730534	0.233393
2p	53.710549	-129.369271	25.427186	-103.942085	-50.231536	-24.804350	12.443990	0.189973
3s	11.335881	-40.593789	12.726325	-27.867464	-16.531583	-3.805257	24.759092	0.746862
3p	9.910490	-37.386345	12.504208	-24.882137	-14.971646	-2.467438	11.923364	0.766712
3d	6.477806	-29.194272	11.046674	-18.147597	-11.675791	-0.629117	6.809069	0.785875
4s	0.738358	-9.347655	4.181940	-5.165715	-4.427356	-0.245416	24.770624	2.735041

	r^{-3}	r^{-2}	r^{-1}	r	r^2	r^4	r^6
		2935.815	109.4157	21.75565	42.98042	559.6554	22943.22
1s		1208.890	24.52193	6.1517490D-02	5.0770389D-03	8.7021337D-05	1.2899041D-03
2s		112.8108	5.258162	0.2809156	9.3515919D-02	3.2186895D-02	1.048830
2p	404.5828	36.74304	5.174771	0.2475816	7.5165558D-02	1.1442964D-02	3.0597276D-03
3s		15.89049	1.623752	0.8604677	0.8523304	1.175345	2.596410
3p	46.37952	4.879824	1.495454	0.9080023	0.5626566	1.551620	3.815395
3d	4.139456	1.850276	1.167771	1.124870	1.612762	6.068127	42.06938
4s		0.8224293	0.3739062	3.396000	13.39391	308.7606	11351.33

Table 12. (Continued)

29 Cu Copper Atom Doublet S State Ar(18)3d(10)4s(1) Configuration (8s, 4p, 3d) Basis

|2-V/E| = 3.2D-05 |1-Norm| = 3.7D-16
Total S Cusp: -28.845242 Total P Cusp: -14.523154 Total D Cusp: -7.380582

	T	V(1)	V(2)	V(T)	E	e	-Cusp	r max
	1638.828038	-3929.582035	651.873869	-3277.708166	-1638.880128	-987.006258		
1s	406.498381	-826.849685	45.795419	-781.054266	-374.555884	-328.760465	28.855091	0.034897
2s	77.386193	-180.618298	31.223997	-149.394301	-72.008108	-40.784112	28.811461	0.198608
2p	75.933332	-178.485789	33.484671	-145.001118	-69.067786	-35.583115	14.620179	0.160147
3s	16.362138	-56.365832	17.517309	-38.848523	-22.486385	-4.969076	28.335242	0.629255
3p	14.650832	-52.608429	17.336998	-35.271431	-20.620599	-3.283601	13.750842	0.633161
3d	9.416209	-40.438163	15.283501	-25.154662	-15.738453	-0.454952	7.380582	0.613264
4s	0.667546	-10.967471	5.035396	-5.932075	-5.264529	-0.229132	28.711186	2.708303

	r^{-3}	r^{-2}	r^{-1}	r	r^2	r^4	r^6
		4010.136	135.5028	20.86858	31.08151	331.2857	10126.20
1s		1633.208	28.51206	5.2871449D-02	3.7475632D-03	4.9958974D-05	7.6482960D-04
2s		158.1413	6.228217	0.2376165	6.6687280D-02	1.1634136D-02	0.2138300
2p	674.0800	51.80923	6.154682	0.2075905	5.2734597D-02	5.6052223D-03	1.0515511D-03
3s		22.86378	1.943649	0.7236100	0.6047464	0.6573753	4.361818
3p	81.30670	7.182696	1.814084	0.7530005	0.6641529	0.7455596	1.285138
3d	7.407473	2.699573	1.394419	0.9757738	1.261087	4.258261	28.91314
4s		0.7620723	0.3781887	3.319098	12.81896	282.8580	9820.198

30 Zn Zinc Atom Singlet S State Ar(18)3d(10)4s(2) Configuration (8s, 4p, 3d) Basis

|2-V/E| = 7.3D-07 |1-Norm| = 1.3D-15
Total S Cusp: -29.840743 Total P Cusp: -15.005522 Total D Cusp: -7.964649

	T	V(1)	V(2)	V(T)	E	e	-Cusp	r max
	1777.781456	-4262.488097	706.926488	-3555.561609	-1777.780153	-1070.853666		
1s	435.436477	-885.286297	48.285468	-837.000828	-401.564351	-353.278883	29.854941	0.033723
2s	83.529370	-194.102265	33.118382	-160.983883	-77.454513	-44.336131	29.755241	0.191366
2p	82.075166	-191.973619	35.499130	-156.474488	-74.399323	-38.900192	15.100229	0.154031
3s	18.000183	-61.109701	18.750788	-42.358913	-24.358730	-5.607942	29.396545	0.602359
3p	16.225721	-57.267441	18.615725	-38.651716	-22.425996	-3.810271	14.277231	0.604547
3d	11.206623	-45.973960	17.005031	-28.968929	-17.762307	-0.757275	7.964649	0.578057
4s	0.988925	-13.152804	5.938883	-7.213920	-6.224995	-0.286111	29.566787	2.319211

	r^{-3}	r^{-2}	r^{-1}	r	r^2	r^4	r^6
		4307.457	142.0829	21.90471	34.46551	363.1574	9257.971
1s		1749.255	29.50954	5.1076689D-02	3.4967342D-03	3.7364013D-05	2.7634844D-04
2s		170.5289	6.470076	0.2288782	6.1893763D-02	1.0658119D-02	0.1815011
2p	755.6069	55.96243	6.399121	0.1995597	4.8718219D-02	4.7789946D-03	8.2512028D-04
3s		25.14047	2.036990	0.6910245	0.5505609	0.5152293	1.798298
3p	93.63238	7.933745	1.908915	0.7152592	0.5983550	0.6011601	0.9227161
3d	9.371680	3.200479	1.532465	0.8677248	0.9755015	2.384128	11.47684
4s		1.113416	0.4384268	2.898295	9.798074	167.3143	4566.851

31 Gallium Atom Doublet P State Ar(18)3d(10)4s(2)4p(1) Configuration (8s, 6p, 3d) Basis

|2-V/E| = 2.9D-07 |1-Norm| = 4.7D-16
Total S Cusp: -30.838202 Total P Cusp: -15.512165 Total D Cusp: -8.534074

	T	V(1)	V(2)	V(T)	E	e	-Cusp	r max
	1923.159351	-4609.929631	763.611492	-3846.318140	-1923.158789	-1159.547297		
1s	465.376472	-945.724774	50.797657	-894.927116	-429.550645	-378.752987	30.857671	0.032624
2s	89.891136	-208.051325	35.028857	-173.022468	-83.131332	-48.102476	30.681135	0.184682
2p	88.452157	-205.946139	37.531811	-168.414328	-79.962170	-42.430359	15.643225	0.148442
3s	19.780966	-66.139890	20.019152	-46.120738	-26.339771	-6.320619	30.527714	0.576570
3p	17.838526	-61.977449	19.866407	-42.111042	-24.272516	-4.406110	14.627223	0.578335
3d	13.121513	-51.679221	18.716876	-32.962345	-19.840832	-1.123956	8.534074	0.543662
4s	1.410158	-15.634041	6.920155	-8.713886	-7.303728	-0.383573	30.575350	2.043272
4p	1.282556	-14.495839	6.521780	-7.974059	-6.691403	-0.169623	12.577706	2.258240

	r^{-3}	r^{-2}	r^{-1}	r	r^2	r^4	r^6
		4615.539	148.7074	22.63959	35.04047	296.0049	5367.904
1s		1869.352	30.50725	4.9400014D-02	3.2703353D-03	2.9232596D-05	6.8124400D-05
2s		183.3388	6.711333	0.2207802	5.7615115D-02	9.6656769D-03	0.1380431
2p	843.7378	60.27617	6.643424	0.1921233	4.5143350D-02	4.1335641D-03	1.3555675D-03
3s		27.62608	2.133545	0.6605362	0.5024527	0.4106859	0.6322315
3p	106.8172	8.707907	1.999273	0.6854078	0.5519309	0.5438376	1.290495
3d	11.61397	3.733341	1.667072	0.7842662	0.7839374	1.461103	5.246643
4s		1.568341	0.5043239	2.535109	7.462589	95.66381	1953.470
4p	4.605428	0.5295487	0.4676077	2.600087	7.566797	85.93771	1399.205

Table 12. (Continued)

31 Gallium Atom Doublet P State Ar(18) 3d(10) 4s(2) 4p(1) Configuration (12s, 9p, 4d) Basis

|2-V/E| = 8.8D-09 |1-Norm| = 1.0D-15
Total S Cusp: -31.011532 Total P Cusp: -15.478789 Total D Cusp: -9.618867

	T	V(1)	V(2)	V(T)	E	e	-Cusp	r max
	1923.259894	-4608.214406	761.694601	-3846.519805	-1923.259911	-1161.565310		
1s	465.454933	-945.801504	50.764831	-895.036672	-429.581740	-378.816909	31.011860	0.032622
2s	89.806530	-207.970577	34.998598	-172.971979	-83.165448	-48.166850	31.020491	0.185281
2p	88.516154	-206.023408	37.507438	-168.515970	-79.999816	-42.492377	15.419652	0.148005
3s	19.811756	-66.189639	19.992406	-46.197234	-26.385477	-6.393072	30.930846	0.573203
3p	17.872358	-62.080845	19.863894	-42.216951	-24.344593	-4.480699	15.858684	0.573885
3d	13.100111	-51.610357	18.659230	-32.951127	-19.851016	-1.191786	9.618867	0.539280
4s	1.500056	-15.977620	7.027073	-8.950547	-7.450491	-0.423418	30.928395	1.998749
4p	0.781154	-11.606636	5.308492	-6.298144	-5.516989	-0.208497	16.377728	2.667877

	r^{-3}	r^{-2}	r^{-1}	r	r^2	r^4	r^6
		4620.458	148.6521	23.35959	40.52678	520.4434	15833.89
1s		1871.200	30.50973	4.9407745D-02	3.2708234D-03	2.7343020D-05	3.4216600D-06
2s		183.7540	6.708728	0.2206332	5.7352644D-02	5.7098992D-03	1.4979742D-03
2p	841.6717	60.27602	6.645916	0.1920862	4.5149669D-02	4.1045338D-03	6.5685300D-04
3s		27.75816	2.135150	0.6604676	0.5026458	0.4071123	0.5022711
3p	108.2402	8.732772	2.002608	0.6840698	0.5506713	0.5295440	0.8348544
3d	11.64535	3.729706	1.664850	0.7879965	0.7965059	1.565849	6.269046
4s		1.669477	0.5154071	2.489596	7.209955	90.31731	1831.680
4p	2.928782	0.3455349	0.3744076	3.382482	13.44034	320.1228	12101.82

32 Germanium Atom Triplet P State Ar(18) 3d(10) 4s(2) 4p(2) Configuration (8s, 6p, 3d) Basis

|2-V/E| = 1.9D-07 |1-Norm| = 4.4D-16
Total S Cusp: -31.841506 Total P Cusp: -16.045836 Total D Cusp: -9.087922

	T	V(1)	V(2)	V(T)	E	e	-Cusp	r max
	2075.253267	-4972.463907	821.957728	-4150.506179	-2075.252893	-1253.295165		
1s	496.319860	-1008.166501	53.335883	-954.830618	-458.510758	-405.174875	31.864702	0.031594
2s	96.474095	-222.471224	36.959602	-185.511622	-89.037527	-52.077924	31.625564	0.178445
2p	95.055393	-220.391955	39.584757	-180.807197	-85.751804	-46.167047	16.194896	0.143269
3s	21.691675	-71.429340	21.313049	-50.116291	-28.424616	-7.111567	31.678075	0.552551
3p	19.686764	-67.179905	21.208131	-45.971774	-26.285010	-5.076879	15.037788	0.553730
3d	15.104474	-57.453752	20.394962	-37.058790	-21.954316	-1.559354	9.087922	0.512229
4s	1.895019	-18.218283	7.909125	-10.309158	-8.414139	-0.505014	31.692432	1.848041
4p	1.497155	-15.962268	7.107728	-8.854540	-7.357385	-0.249657	13.793105	2.124681

	r^{-3}	r^{-2}	r^{-1}	r	r^2	r^4	r^6
		4935.177	155.3895	23.45031	36.24701	272.6996	4018.070
1s		1993.536	31.50520	4.7830547D-02	3.0653797D-03	2.4648047D-05	1.8552520D-05
2s		196.6360	6.952226	0.2132193	5.3730553D-02	8.1069871D-03	8.4548142D-02
2p	938.6977	64.74869	6.887249	0.1852268	4.1941521D-02	3.5765826D-03	1.3862509D-03
3s		30.29428	2.232167	0.6322092	0.4598929	0.3388629	0.3781392
3p	122.1507	9.583728	2.099372	0.6527825	0.4997597	0.4481747	1.161848
3d	14.08631	4.283204	1.795430	0.7191022	0.6509390	0.9651535	2.691355
4s		2.088233	0.5693213	2.253902	5.860166	57.47645	883.1138
4p	5.786543	0.6203882	0.4988209	2.468453	6.866852	72.34534	1108.512

33 As Arsenic Atom Quartet S State Ar(18) 3d(10) 4s(2) 4p(3) Configuration (8s, 6p, 3d) Basis

|2-V/E| = 7.5D-06 |1-Norm| = 4.4D-16
Total S Cusp: -33.090210 Total P Cusp: -16.540729 Total D Cusp: -9.608061

	T	V(1)	V(2)	V(T)	E	e	-Cusp	r max
	2234.144774	-5351.466305	883.193542	-4468.272763	-2234.127990	-1350.934447		
1s	528.302270	-1072.645469	55.915793	-1016.729677	-488.427406	-432.511614	33.081410	0.030636
2s	103.222152	-237.318708	38.932958	-198.385750	-95.163598	-56.230641	32.942742	0.173276
2p	101.913690	-235.345984	41.680040	-193.665944	-91.752253	-50.072213	16.697737	0.138384
3s	23.641201	-76.774195	22.602238	-54.171957	-30.530756	-7.928519	34.481850	0.534509
3p	21.678134	-72.680183	22.610037	-50.070146	-28.391962	-5.781925	15.503502	0.530682
3d	17.176562	-63.362406	22.080735	-41.281671	-24.105110	-2.024375	9.608061	0.483491
4s	2.517701	-21.283764	9.068981	-12.214783	-9.697082	-0.628101	34.970686	1.679831
4p	1.820421	-17.880326	7.868599	-10.011727	-8.191306	-0.322707	14.720147	1.966482

	r^{-3}	r^{-2}	r^{-1}	r	r^2	r^4	r^6
		5271.647	162.1656	24.03072	36.23038	237.8253	2932.028
1s		2123.725	32.50441	4.6363104D-02	2.8792335D-03	2.1435895D-05	5.1130367D-06
2s		210.9663	7.191476	0.2059752	4.9966001D-02	4.3420344D-03	1.0250415D-03
2p	1040.207	69.38514	7.131696	0.1787963	3.9065838D-02	3.0975289D-03	1.0721716D-03
3s		33.24419	2.326491	0.6079387	0.4248933	0.3026213	0.6469314
3p	139.2760	10.52364	2.202430	0.6221584	0.4531636	0.3655831	0.8735797
3d	16.81881	4.856033	1.920073	0.6659724	0.5530090	0.6733317	1.508935
4s		2.755687	0.6449625	1.976750	4.439418	31.09627	326.9538
4p	7.486580	0.7505057	0.5418280	2.297073	5.970866	55.35779	752.1624

Table 12. (Continued)

34 Selenium Atom Triplet P State Ar(18)3d(10)4s(2)4p(4) Configuration (8s, 6p, 3d) Basis

|2-V/E| = 5.3D-06 |1-Norm| = 5.3D-16

Total S Cusp: -34.101477 Total P Cusp: -16.115989 Total D Cusp: -10.095927

	T	V(1)	V(2)	V(T)	E	e	-Cusp	r max
	2399.781802	-5744.349683	944.773411	-4799.576272	-2399.794471	-1455.021060		
1s	561.229087	-1139.070621	58.510245	-1080.560376	-519.331289	-460.821044	34.087427	0.029727
2s	110.316223	-252.757448	40.904746	-211.852703	-101.536480	-60.631734	34.019353	0.167737
2p	109.057847	-250.841662	43.780535	-207.061127	-98.003280	-54.222745	16.088103	0.132640
3s	25.778568	-82.539326	23.938026	-58.601300	-32.822732	-8.884707	35.408507	0.514674
3p	23.843792	-78.583646	24.058816	-54.524830	-30.681038	-6.622222	16.283541	0.505646
3d	19.312643	-69.374239	23.724530	-45.649709	-26.337066	-2.612536	10.095927	0.457873
4s	3.113566	-23.938481	10.006065	-13.932415	-10.818849	-0.812784	35.525949	1.558283
4p	2.092662	-19.360923	8.443460	-10.917463	-8.824801	-0.381341	16.261649	1.864234

	r^{-3}	r^{-2}	r^{-1}	r	r^{2}	r^{4}	r^{6}
		5613.051	168.9515	25.08175	39.02913	270.9303	3555.644
1s		2255.870	33.50208	4.4977522D-02	2.7094182D-03	1.9145538D-05	6.2789429D-06
2s		225.4070	7.434043	0.1993420	4.6796652D-02	3.7834157D-03	4.9243232D-04
2p	1135.940	74.03579	7.377696	0.1728677	3.6643515D-02	4.3499630D-03	3.7826689D-02
3s		36.19050	2.427627	0.5831493	0.3904775	0.2506487	0.4178966
3p	158.7526	11.53305	2.311284	0.5924390	0.4108895	0.2893522	0.4136633
3d	19.78967	5.445359	2.040419	0.6218229	0.4782565	0.4884403	0.8975558
4s		3.391776	0.7040730	1.828013	3.798630	22.73316	203.8434
4p	9.278179	0.8661295	0.5694389	2.240180	5.771036	54.57713	783.8590

35 Bromine Atom Doublet P State Ar(18)3d(10)4s(2)4p(5) Configuration (8s, 6p, 3d) Basis

|2-V/E| = 4.1D-06 |1-Norm| = 3.1D-16

Total S Cusp: -35.111234 Total P Cusp: -16.620335 Total D Cusp: -10.520769

	T	V(1)	V(2)	V(T)	E	e	-Cusp	r max
	2572.361427	-6155.320454	1010.587159	-5144.733295	-2572.371869	-1561.784710		
1s	595.150342	-1207.490242	61.160812	-1146.329430	-551.179088	-490.018276	35.092484	0.028870
2s	117.647739	-268.683902	42.934490	-225.749412	-108.101703	-65.167213	35.089325	0.162545
2p	116.400933	-266.781698	45.934148	-220.847550	-104.446647	-58.512499	16.591201	0.128452
3s	28.035687	-88.546859	25.339963	-63.206896	-35.171209	-9.831246	36.321569	0.496078
3p	26.072086	-84.567557	25.525505	-59.042053	-32.969967	-7.444462	16.787386	0.485993
3d	21.563101	-75.593907	25.421114	-50.172793	-28.609692	-3.188578	10.520769	0.434600
4s	3.696669	-26.536597	10.934732	-15.601865	-11.905196	-0.970464	36.294923	1.462324
4p	2.566333	-21.754131	9.375622	-12.378508	-9.812175	-0.436553	16.800817	1.711967

	r^{-3}	r^{-2}	r^{-1}	r	r^{2}	r^{4}	r^{6}
		5966.555	175.8663	25.60869	38.84096	243.1521	2837.863
1s		2391.987	34.49972	4.3672246D-02	2.5541791D-03	1.7145643D-05	6.5183215D-06
2s		240.3221	7.676683	0.1931167	4.3917112D-02	3.3340980D-03	4.6039635D-04
2p	1251.017	78.99024	7.622334	0.1672397	3.4273009D-02	3.6207250D-03	2.6337716D-02
3s		39.29559	2.529910	0.5601253	0.3598871	0.2096484	0.2798345
3p	179.3562	12.57857	2.416216	0.5667917	0.3756505	0.2409429	0.3264742
3d	23.06984	6.064745	2.159826	0.5837029	0.4187238	0.3656097	0.5647981
4s		4.010799	0.7581885	1.707330	3.311691	17.19113	133.0639
4p	11.96234	1.052587	0.6215466	2.071797	4.951617	40.64408	512.6819

36 Krypton Atom Singlet S State Ar(18)3d(10)4s(2)4p(6) Configuration (8s, 6p, 3d) Basis

|2-V/E| = 4.9D-08 |1-Norm| = 1.1D-15

Total S Cusp: -35.871318 Total P Cusp: -17.127311 Total D Cusp: -10.905569

	T	V(1)	V(2)	V(T)	E	e	-Cusp	r max
	2751.989705	-6583.273757	1079.294211	-5503.979546	-2751.989841	-1672.695630		
1s	630.059206	-1277.898942	63.856284	-1214.042658	-583.983452	-520.127168	35.896646	0.028049
2s	125.197293	-285.061106	44.995849	-240.065257	-114.867964	-69.872114	35.591191	0.157514
2p	123.989407	-283.218087	48.126172	-235.091915	-111.102509	-62.976337	17.097850	0.124521
3s	30.499081	-94.953121	26.814367	-68.138753	-37.639673	-10.825305	35.997292	0.474985
3p	28.437768	-90.823180	27.039109	-63.784071	-35.346303	-8.307195	17.289320	0.467649
3d	23.901073	-81.977076	27.136750	-54.840326	-30.939253	-3.802502	10.905569	0.413816
4s	4.265358	-29.010629	11.804773	-17.205856	-12.940498	-1.135725	35.981787	1.386601
4p	3.062341	-24.234632	10.332080	-13.902552	-10.840212	-0.508132	17.324608	1.585128

	r^{-3}	r^{-2}	r^{-1}	r	r^{2}	r^{4}	r^{6}
		6325.922	182.8687	26.04892	38.32276	215.1377	2220.567
1s		2530.292	35.49719	4.2437801D-02	2.4119878D-03	1.4994234D-05	2.5448623D-06
2s		254.9010	7.918364	0.1873816	4.1404022D-02	3.6664257D-03	9.5430543D-03
2p	1373.778	84.11003	7.867169	0.1619606	3.2122204D-02	3.0320564D-03	1.8240084D-02
3s		42.50410	2.637587	0.5379437	0.3320105	0.1738961	0.1486396
3p	201.8965	13.68465	2.522866	0.5428357	0.3440575	0.2000359	0.2380125
3d	26.64155	6.707319	2.277141	0.5506901	0.3707214	0.2810035	0.3716588
4s		4.609365	0.8058508	1.619383	2.985747	14.04131	98.62253
4p	14.85370	1.244731	0.6731842	1.923157	4.272553	30.44525	336.2919

Table 12. (Continued)

37 Rubidium Atom Doublet S State Kr(36)5s(1) Configuration (10s, 6p, 3d) Basis

|2-V/E| = 2.7D-08 |1-Norm| = 6.8D-16

Total S Cusp: -36.842977 Total P Cusp: -17.702223 Total D Cusp: -11.278893

	T	V(1)	V(2)	V(T)	E	ε	-Cusp	r max
	2938.301818	-7018.504513	1141.900797	-5876.603717	-2938.301898	-1796.401102		
1s	665.939069	-1350.277831	66.456431	-1283.821400	-617.882331	-551.425899	36.870510	0.027288
2s	133.059679	-302.023139	46.968260	-255.054979	-121.995200	-75.026940	36.595286	0.152839
2p	131.822513	-300.149278	50.221802	-249.927476	-118.104963	-67.883161	17.688251	0.120887
3s	32.976283	-101.408714	29.157570	-73.251144	-40.274861	-12.117291	36.688941	0.460326
3p	30.901088	-97.278545	28.452867	-68.825678	-37.924590	-9.471723	17.770659	0.450257
3d	26.363510	-88.598244	28.758209	-59.840036	-33.476525	-4.718317	11.278893	0.395002
4s	5.162567	-32.398903	12.862786	-19.536117	-14.373549	-1.510763	36.573943	1.291043
4p	3.956807	-27.932256	11.588485	-16.343771	-12.386964	-0.798478	17.860359	1.449234
5s	0.309065	-8.144418	3.849689	-4.294728	-3.985664	-0.135974	36.134463	4.744102

	r^{-3}	r^{-2}	r^{-1}	r	r^2	r^4	r^6
		6700.778	189.6893	29.58581	65.73524	1940.075	140621.3
1s		2673.734	36.49400	4.1271847D-02	2.2810922D-03	1.4985310D-05	2.1132519D-04
2s		270.7345	8.162788	0.1818727	3.9163125D-02	2.0153467D-02	2.108257
2p	1506.446	89.42294	8.112143	0.1569953	3.0142644D-02	2.2777746D-03	6.7663341D-03
3s		45.82125	2.740776	0.5180992	0.3076300	0.1487669	0.1939542
3p	225.9216	14.83031	2.629150	0.5210451	0.3166211	0.1679523	0.1718192
3d	30.56920	7.382878	2.394547	0.5211529	0.3303909	0.2191110	0.2501626
4s		5.537150	0.8756460	1.500693	2.563320	10.41842	79.57948
4p	20.04602	1.583013	0.7549259	1.719664	3.391623	18.58161	153.9641
5s		0.2785287	0.2201194	5.504187	34.17622	1804.198	139530.2

38 Strontium Atom Singlet S State Kr(36)5s(2) Configuration (10s, 6p, 3d) Basis

|2-V/E| = 2.7D-07 |1-Norm| = 6.7D-16

Total S Cusp: -37.856226 Total P Cusp: -18.270574 Total D Cusp: -11.640973

	T	V(1)	V(2)	V(T)	E	ε	-Cusp	r max
	3131.498055	-7470.077830	1207.082566	-6262.995263	-3131.497208	-1924.414641		
1s	702.874055	-1424.711065	69.088013	-1355.623052	-652.748997	-583.660984	37.884290	0.026563
2s	141.075040	-319.382008	48.968483	-270.413524	-129.338484	-80.370000	37.580505	0.148635
2p	139.903022	-317.579159	52.349888	-265.229271	-125.326249	-72.976361	18.267876	0.117456
3s	35.600161	-108.136479	29.537615	-78.598865	-42.998704	-13.461089	37.849693	0.444504
3p	33.472932	-103.958480	29.900026	-74.058454	-40.585521	-10.685495	18.273616	0.434527
3d	28.931818	-95.422803	30.404535	-65.018269	-36.086451	-5.681916	11.640973	0.377965
4s	6.167774	-36.007343	13.977545	-22.029798	-15.862023	-1.884478	37.611770	1.215796
4p	4.901927	-31.604107	12.807646	-18.796462	-13.894535	-1.086889	18.391509	1.343254
5s	0.539265	-10.262766	4.774275	-5.488491	-4.949226	-0.174951	37.355211	3.916535

	r^{-3}	r^{-2}	r^{-1}	r	r^2	r^4	r^6
		7089.155	196.5810	31.60875	73.76282	1801.518	91797.24
1s		2822.038	37.49240	4.0170815D-02	2.1607886D-03	1.3149832D-05	1.1187503D-04
2s		286.9867	8.404790	0.1766583	3.6908668D-02	1.2872706D-02	0.9187178
2p	1646.994	94.89518	8.357346	0.1523211	2.8347773D-02	1.8423562D-03	2.8723160D-03
3s		49.46916	2.845697	0.4997220	0.2861028	0.1297777	0.2932085
3p	252.12[illegible]4	16.02993	2.735749	0.5008061	0.2921365	0.1415029	0.1216356
3d	34.84346	8.086582	2.511126	0.4948542	0.2966204	0.1738257	0.1733564
4s		6.585318	0.9475617	1.392184	2.196455	7.468908	45.48278
4p	25.83474	1.937031	0.8316870	1.566532	2.600674	12.37075	80.94248
5s		0.4790403	0.2700728	4.562390	23.51321	854.7361	45607.86

39 Yttrium Atom Doublet D State Kr(36)4d(1)5s(2) Configuration (10s, 6p, 4d) Basis

|2-V/E| = 8.7D-08 |1-Norm| = 3.7D-16

Total S Cusp: -38.853042 Total P Cusp: -18.792647 Total D Cusp: -11.226519

	T	V(1)	V(2)	V(T)	E	ε	-Cusp	r max
	3331.580973	-7943.273709	1280.112053	-6663.161656	-3331.580683	-2051.468630		
1s	740.789201	-1501.124944	71.824499	-1429.300445	-688.511244	-616.686744	38.882021	0.025876
2s	149.363808	-337.266909	51.075261	-286.191648	-136.827840	-85.752579	38.569718	0.144579
2p	148.222540	-335.497999	54.583945	-280.914054	-132.691514	-78.107569	18.793252	0.114174
3s	38.322000	-115.073266	31.025095	-84.048172	-45.726171	-14.701076	38.844024	0.430418
3p	36.168612	-110.883890	31.459608	-79.424282	-43.255671	-11.796063	18.775942	0.419805
3d	31.574604	-102.391112	32.136991	-70.254121	-38.679517	-6.542527	11.212759	0.362122
4s	7.032040	-39.214444	15.033968	-24.180476	-17.148397	-2.114429	38.634333	1.156786
4p	5.682873	-34.720508	13.892147	-20.828361	-15.145488	-1.253340	18.909647	1.266151
4d	3.181457	-25.290066	10.942550	-14.347516	-11.166059	-0.223509	11.422475	1.666517
5s	0.597574	-11.049505	5.133874	-5.915631	-5.318057	-0.184183	38.393007	3.718601

	r^{-3}	r^{-2}	r^{-1}	r	r^2	r^4	r^6
		7486.915	203.6737	31.97852	71.06464	1547.892	72750.99
1s		2973.995	38.49038	3.9125627D-02	2.0496173D-03	1.1373978D-05	5.7508879D-05
2s		303.7366	8.647869	0.1717354	3.4871557D-02	1.1285549D-02	0.7579914
2p	1794.594	100.5105	8.602513	0.1479212	2.6719550D-02	1.5891093D-03	1.8085284D-03
3s		53.20027	2.950597	0.4825221	0.2665950	0.1121926	0.2298401
3p	280.4799	17.28556	2.843177	0.4819873	0.2703476	0.1205111	9.3971169D-02
3d	39.36729	8.808899	2.625413	0.4714920	0.2682117	0.1415778	0.1342032
4s		7.491479	1.005499	1.317195	1.964843	5.934043	30.61385
4p	31.01708	2.230411	0.8902694	1.469139	2.461482	9.507728	54.18575
4d	2.394567	0.7579129	0.6484632	1.927639	4.226438	27.79321	263.2688
5s		0.5317771	0.2833206	4.360259	21.53404	724.3946	36048.74

Table 12. (Continued)

42 Molybdenum Atom Heptuplet S State Kr(36)4d(5)5s(1) Configuration (10s, 6p, 4d) Basis

|2-V/E| = 7.4D-08 |1-Norm| = 4.3D-16
Total S Cusp: -41.845040 Total P Cusp: -20.292499 Total D Cusp: -11.953260

	T	V(1)	V(2)	V(T)	E	e	-Cusp	r max
	3975.349065	-9476.117307	1525.419472	-7950.697836	-3975.348771	-2449.929299		
1s	860.535180	-1742.367420	80.370853	-1661.996567	-801.461388	-721.090535	41.876688	0.024015
2s	175.688055	-393.882721	57.726773	-336.155948	-160.467883	-102.741110	41.537317	0.133631
2p	174.649108	-392.225673	61.620031	-330.605642	-155.956534	-94.336503	20.294901	0.105285
3s	47.067595	-137.120414	35.790045	-101.330370	-54.262775	-18.472730	41.821513	0.393087
3p	44.845547	-132.897555	36.438947	-96.458608	-51.613061	-15.174114	20.262367	0.380927
3d	40.160374	-124.571464	37.621174	-86.950290	-46.789916	-9.168742	11.946839	0.320092
4s	9.680411	-48.915576	18.295594	-30.619982	-20.939571	-2.643977	41.829733	1.018971
4p	8.037914	-43.959210	17.153125	-26.806085	-18.768171	-1.615046	20.423397	1.092859
4d	4.385985	-31.698464	13.515833	-18.182631	-13.796646	-0.280813	12.038250	1.402233
5s	0.677477	-12.843458	5.989429	-6.854029	-6.176552	-0.187124	41.203386	3.440586

	r^{-3}	r^{-2}	r^{-1}	r	r^{2}	r^{4}	r^{6}
		8746.300	225.6218	31.20179	53.01123	669.5959	24149.22
1s		3453.883	41.48494	3.6292217D-02	1.7630584D-03	7.9706929D-06	5.2420176D-06
2s		356.9041	9.378160	0.1584695	2.9671137D-02	7.7386681D-03	0.4372656
2p	2288.105	118.3165	9.338706	0.1361162	2.2599634D-02	1.0976427D-03	7.5155359D-04
3s		65.17211	3.264772	0.4374959	0.2188631	7.4304812D-02	7.9282479D-02
3p	377.4622	21.31465	3.164228	0.4334710	0.2182830	7.7848893D-02	4.9496093D-02
3d	55.37170	11.15378	2.965987	0.4142402	0.2054579	8.2697618D-02	9.2692816D-02
4s		10.28281	1.164657	1.148717	1.494203	3.402828	11.65861
4p	48.20444	3.113016	1.046648	1.262898	1.821801	5.225615	22.26175
4d	3.733759	1.040937	0.7547253	1.693553	3.319632	18.18421	149.0720
5s		0.6075518	0.3057966	4.034764	18.49339	539.0507	23244.72

43 Technetium Atom Hextuplet S State Kr(36)4d(5)5s(2) Configuration (10s, 6p, 4d) Basis

|2-V/E| = 2.2D-06 |1-Norm| = 3.3D-16
Total S Cusp: -42.845283 Total P Cusp: -20.843312 Total D Cusp: -12.332300

	T	V(1)	V(2)	V(T)	E	e	-Cusp	r max
	4203.738576	-10009.583676	1602.097159	-8407.486517	-4203.747941	-2601.650782		
1s	902.445371	-1826.776339	83.134384	-1743.641956	-841.196585	-758.062201	42.877580	0.023452
2s	184.951776	-413.745463	59.849547	-353.895916	-168.944140	-109.094594	42.527417	0.130350
2p	183.953801	-412.132257	63.872520	-348.259738	-164.305937	-100.433417	20.852648	0.102656
3s	50.220004	-144.940918	37.287681	-107.653237	-57.433233	-20.145551	42.842559	0.381874
3p	47.956583	-140.661881	38.006370	-102.675510	-54.718927	-16.712557	20.775396	0.369663
3d	43.252690	-132.426229	39.359710	-93.066518	-49.813828	-10.454118	12.325468	0.309223
4s	10.907974	-52.891848	19.430766	-33.461082	-22.559108	[illegible]	42.860610	0.975937
4p	9.228308	-48.008595	18.381326	-29.627268	-20.398960	-2.017634	20.972357	1.038210
5s	0.878908	-14.528134	6.713950	-7.814184	-6.935276	-0.221326	42.563392	3.089534
4d	5.116691	-34.923918	14.821220	-20.102698	-14.986007	-0.164787	12.413908	1.306232

	r^{-3}	r^{-2}	r^{-1}	r	r^{2}	r^{4}	r^{6}
		9190.144	232.7810	33.10947	61.61075	875.8915	29761.79
1s		3621.880	42.48317	3.5437003D-02	1.6808167D-03	7.2083551D-06	2.1493551D-06
2s		375.6163	9.621988	0.1544814	2.8186502D-02	6.5521157D-03	0.3329369
2p	2472.571	124.6010	9.584477	0.1325808	2.1430171D-02	9.6193331D-04	4.2048904D-04
3s		69.49207	3.370719	0.4242050	0.2057032	6.5639594D-02	7.5162560D-02
3p	414.4963	22.75947	3.271672	0.4193084	0.2041007	6.7599145D-02	3.7751700D-02
3d	61.59513	11.99851	3.079680	0.3980335	0.1892811	6.9400419D-02	6.7645704D-02
4s		11.55387	1.230043	1.091165	1.346023	2.732053	8.038571
4p	57.09189	3.550071	1.116479	1.186975	1.605164	3.997710	14.56253
5s		0.7854987	0.3378636	3.690472	15.54349	387.8500	14577.97
4d	4.569869	1.207876	0.8121841	1.580886	2.896720	13.89826	100.1355

46 Palladium Atom Singlet S State Kr(36)4d(10)5s(0) Configuration (8s, 6p, 4d) Basis

|2-V/E| = 6.7D-08 |1-Norm| = 1.1D-15
Total S Cusp: -45.920017 Total P Cusp: -22.263162 Total D Cusp: -12.949547

	T	V(1)	V(2)	V(T)	E	e	-Cusp	r max
	4937.518831	-11778.695258	1903.657925	-9875.037334	-4937.518502	-3033.860577		
1s	1034.279286	-2092.105949	92.345182	-1999.760767	-965.481481	-873.136299	45.940370	0.021908
2s	214.097206	-476.186378	67.158215	-409.030163	-194.938958	-127.780743	45.665502	0.121610
2p	213.312152	-474.796556	71.570641	-403.225915	-189.913762	-118.343121	22.265241	0.095358
3s	60.127073	-169.455571	42.653061	-126.802511	-66.675438	-24.022377	46.208747	0.351878
3p	57.820971	-165.189046	43.590576	-121.598470	-63.777499	-20.186924	22.239675	0.338980
3d	53.024322	-157.020733	45.414689	-111.606044	-58.576722	-13.162033	12.934657	0.278034
4s	13.657098	-62.961585	22.966329	-39.995255	-26.344158	-3.377828	45.989952	0.883664
4p	11.619052	-57.326248	21.789876	-35.536372	-23.921320	-2.131444	22.350550	0.932319
4d	6.643923	-42.319386	17.755890	-24.563496	-17.919572	-0.163682	13.107792	1.133503

	r^{-3}	r^{-2}	r^{-1}	r	r^{2}	r^{4}	r^{6}
		10586.69	256.0586	30.30270	36.68374	117.5331	680.8592
1s		4151.395	45.48056	3.3098373D-02	1.4659166D-03	5.5036289D-06	2.7938977D-07
2s		434.9696	10.35192	0.1435882	2.4243323D-02	1.0397991D-03	2.3209700D-04
2p	3076.296	144.3368	10.32166	0.1230041	1.8433516D-02	7.1394563D-04	3.1556838D-04
3s		83.16084	3.683817	0.3893041	0.1731195	4.5879719D-02	1.8333353D-02
3p	537.5307	27.31679	3.591066	0.3824437	0.1697083	4.6753006D-02	2.3771256D-02
3d	82.15737	14.64983	3.413494	0.3577562	0.1528165	4.8812584D-02	8.0850124D-02
4s		14.45402	1.368730	0.9856997	1.098103	1.807016	4.225651
4p	77.63423	4.441588	1.246723	1.071424	1.313594	2.730791	8.526189
4d	6.601469	1.562165	0.9199866	1.416053	2.355128	9.666755	62.02606

Table 12. (Continued)

47 Silver Atom Doublet S State Kr(36)4d(10)5s(1) Configuration (10s, 6p, 4d) Basis

|2-V/E| = 6.5D-08 |1-Norm| = 4.6D-16

Total S Cusp: -46.830944 Total P Cusp: -22.799722 Total D Cusp: -13.512573

	T	V(1)	V(2)	V(T)	E	ε	-Cusp	r max
	5197.390089	-12389.767452	1994.987613	-10394.779839	-5197.389750	-3202.402138		
1s	1080.090617	-2184.417744	95.311542	-2089.106202	-1009.015585	-913.704044	46.867269	0.021443
2s	224.427569	-498.117836	69.471100	-428.646736	-204.219166	-134.748066	46.485662	0.118640
2p	223.583247	-496.669304	74.015992	-422.653311	-199.070064	-125.054072	22.809065	0.093188
3s	63.634531	-178.067867	44.322323	-133.745544	-70.111013	-25.788689	46.728801	0.343513
3p	61.300185	-173.765059	45.324861	-128.440199	-67.140014	-21.815153	22.739779	0.330044
3d	56.531312	-165.710539	47.319400	-118.391139	-61.859827	-14.540427	13.500420	0.270810
4s	14.810641	-66.804220	24.069952	-42.734268	-27.923627	-3.853675	47.202386	0.855749
4p	12.804464	-61.371863	23.014187	-38.357676	-25.553212	-2.539025	22.884238	0.897095
4d	7.930369	-47.148053	19.400528	-27.747525	-19.817155	-0.416627	13.627473	1.054830
5s	0.719183	-15.528838	7.308252	-8.220586	-7.501403	-0.193151	46.235548	3.197225

	r^{-3}	r^{-2}	r^{-1}	r	r^2	r^4	r^6
		11070.29	263.6121	32.23486	47.30994	460.9189	13841.06
1s		4333.581	46.47697	3.2382482D-02	1.4031591D-03	5.0606210D-06	3.4912408D-06
2s		455.2454	10.59825	0.1403559	2.3253183D-02	4.5109343D-03	0.2021049
2p	3300.051	151.2656	10.56743	0.1201100	1.7569375D-02	6.3719762D-04	1.9331583D-04
3s		87.78290	3.788678	0.3787390	0.1637898	4.1180803D-02	3.0938784D-02
3p	583.6610	28.92696	3.697129	0.3715559	0.1601115	4.1418172D-02	1.8895871D-02
3d	90.38329	15.61298	3.525756	0.3455951	0.1420954	3.9840563D-02	4.1270674D-02
4s		15.69315	1.421366	0.9530421	1.028940	1.639418	5.714109
4p	87.85513	4.876830	1.305784	1.023561	1.196289	2.237261	6.191643
4d	8.226564	1.848255	1.003150	1.298473	1.972072	6.661739	34.82580
5s		0.6528436	0.3304008	3.693769	15.48967	376.8570	13443.24

48 Cadmium Atom Singlet S State Kr(36)4d(10)5s(2) Configuration (10s, 6p, 4d) Basis

|2-V/E| = 9.9D-08 |1-Norm| = 2.9D-15

Total S Cusp: -47.833861 Total P Cusp: -23.334410 Total D Cusp: -16.076621

	T	V(1)	V(2)	V(T)	E	ε	-Cusp	r max
	5464.891904	-13019.060468	2089.277204	-10929.783264	-5464.891360	-3375.614156		
1s	1126.997372	-2278.823261	98.302879	-2180.520382	-1053.523011	-955.220131	47.870353	0.020993
2s	234.927862	-520.471706	71.809639	-448.662067	-213.734206	-141.924567	47.473769	0.116051
2p	234.126496	-519.068334	76.485781	-442.582553	-208.456056	-131.970275	23.349225	0.091110
3s	67.254744	-186.899421	46.022832	-140.876590	-73.621846	-27.599014	47.802507	0.334784
3p	64.868771	-182.539183	47.091845	-135.447338	-70.578567	-23.486722	23.246233	0.321572
3d	60.065330	-174.548844	49.261454	-125.287390	-65.222060	-15.960606	16.114823	0.270853
4s	16.136627	-71.044994	25.278293	-45.766701	-29.630074	-4.351781	48.207539	0.827727
4p	14.086794	-65.605778	24.278253	-41.327525	-27.240731	-2.962478	23.425054	0.864131
4d	9.297920	-51.940735	20.980774	-30.959961	-21.662032	-0.681257	15.722783	0.997759
5s	1.066868	-18.203069	8.446177	-9.756892	-8.690024	-0.243847	47.694292	2.745393

	r^{-3}	r^{-2}	r^{-1}	r	r^2	r^4	r^6
		11571.09	271.2304	33.61069	52.61010	545.7437	14530.37
1s		4521.618	47.47548	3.1699843D-02	1.3445425D-03	4.6626191D-06	3.6635039D-06
2s		476.4361	10.84316	0.1372020	2.2210932D-02	3.7052057D-03	0.1415142
2p	3534.673	158.3721	10.81392	0.1173382	1.6761672D-02	5.7304807D-04	1.2645648D-04
3s		92.75444	3.893738	0.3688582	0.1553439	3.6747423D-02	1.2416239D-02
3p	632.1693	30.57774	3.802900	0.3612870	0.1513265	3.6845322D-02	1.5202274D-02
3d	100.0125	16.61109	3.636434	0.3337283	0.1318573	3.2122128D-02	1.4015693D-02
4s		17.07037	1.480104	0.9167312	0.9505559	1.379901	3.988421
4p	99.16920	5.344356	1.366787	0.9791269	1.092682	1.846613	4.559609
4d	10.14873	2.153498	1.082099	1.206839	1.695967	4.788403	20.26816
5s		0.9599650	0.3792306	3.274759	12.25417	241.6968	7145.909

Table 12. (Continued)

49 Indium Atom Doublet P State Kr(36) 4d(10) 5s(2) 5p(1) Configuration (10s, 8p, 4d) Basis

|2-V/E| = 3.8D-06 |1-Norm| = 4.4D-16

Total S Cusp: -48.849443 Total P Cusp: -24.306223 Total D Cusp: -14.626701

	T	V(1)	V(2)	V(T)	E	e	-Cusp	r max
	5739.933618	-13665.609555	2185.720318	-11479.889236	-5739.955618	-3554.235299		
1s	1174.932908	-2375.257574	101.313377	-2273.944197	-1099.011288	-997.697911	48.883135	0.020561
2s	245.579431	-543.221557	74.172903	-469.048654	-223.469223	-149.296319	48.485554	0.113620
2p	244.891621	-541.937446	78.983567	-462.953878	-218.062257	-139.078690	24.424922	0.089340
3s	71.017967	-195.993940	47.731198	-148.262742	-77.244776	-29.513578	48.998271	0.326289
3p	68.510248	-191.474752	48.852146	-142.622606	-74.112358	-25.260212	23.641705	0.315031
3d	63.829587	-183.697133	51.194973	-132.502160	-68.672573	-17.477600	14.624565	0.257432
4s	17.534970	-75.433874	26.522591	-48.911283	-31.376313	-4.853722	49.132662	0.800206
4p	15.408345	-69.855782	25.528761	-44.327021	-28.918676	-3.389914	24.526527	0.831516
4d	10.634039	-56.739482	22.575130	-34.164352	-23.530313	-0.955183	14.643613	0.936332
5s	1.507860	-21.206450	9.685433	-11.521018	-10.013158	-0.327725	48.698334	2.438349
5p	1.289799	-19.408734	8.981438	-10.427296	-9.137496	-0.156058	27.024406	2.705074

	r^{-3}	r^{-2}	r^{-1}	r	r^{2}	r^{4}	r^{6}
		12083.77	278.8900	34.56254	54.14581	475.6452	9245.647
1s		4713.974	48.47464	3.1045498D-02	1.2895183D-03	4.2327092D-06	5.9331293D-07
2s		498.0452	11.08615	0.1341954	2.1227848D-02	2.5098145D-03	6.6360499D-02
2p	3790.203	165.7114	11.05995	0.1146920	1.6005412D-02	5.0777447D-04	1.1630329D-04
3s		97.97703	3.999876	0.3594449	0.1475451	3.4206230D-02	5.3820111D-02
3p	684.7567	32.29710	3.907648	0.3515611	0.1432752	3.7369489D-02	0.1439160
3d	108.1702	17.61303	3.748921	0.3238332	0.1241729	2.8708124D-02	1.5094479D-02
4s		18.51370	1.539467	0.8830671	0.8811240	1.163882	2.335166
4p	111.9611	5.833721	1.425628	0.9425680	1.014429	1.615220	4.194784
4d	11.91688	2.444624	1.157949	1.126262	1.475398	3.630485	13.56570
5s		1.339556	0.4327847	2.885091	9.462659	141.3669	3134.108
5p	6.646047	0.4408247	0.3960966	3.022978	10.08015	143.9997	2810.679

50 Tin Atom Triplet P State Kr(36) 4d(10) 5s(2) 5p(2) Configuration (10s, 8p, 4d) Basis

|2-V/E| = 7.2D-08 |1-Norm| = 7.9D-16

Total S Cusp: -49.867669 Total P Cusp: -24.218148 Total D Cusp: -15.249763

	T	V(1)	V(2)	V(T)	E	e	-Cusp	r max
	6022.778426	-14327.839681	2282.282393	-12045.557288	-6022.778862	-3740.496469		
1s	1223.865745	-2473.689077	104.334900	-2369.354177	-1145.488433	-1041.153533	49.898378	0.020146
2s	256.508491	-566.503294	76.537919	-489.965375	-233.456884	-156.918964	49.517393	0.111287
2p	255.877110	-565.273202	81.483179	-483.790023	-227.912912	-146.429733	24.188399	0.087118
3s	74.850908	-205.257684	49.435680	-155.822004	-80.971096	-31.535416	50.122542	0.318445
3p	72.411962	-200.871912	50.656768	-150.215143	-77.803182	-27.146413	24.343140	0.305721
3d	67.611012	-192.976398	53.132506	-139.843892	-72.232880	-19.100374	15.256885	0.251450
4s	19.018287	-79.987779	27.762881	-52.224898	-33.206611	-5.443731	50.019948	0.774190
4p	16.844427	-74.412514	26.832248	-47.580266	-30.735839	-3.903591	24.298196	0.805965
4d	12.078667	-61.627893	24.119634	-37.508258	-25.429591	-1.309957	15.197156	0.889664
5s	2.035281	-24.336401	10.923363	-13.413037	-11.377757	-0.454393	49.626786	2.208178
5p	1.261608	-19.451269	8.969166	-10.492103	-9.220494	-0.251328	24.550235	2.726084

	r^{-3}	r^{-2}	r^{-1}	r	r^{2}	r^{4}	r^{6}
		12606.52	286.5568	36.09347	60.34118	610.0074	13123.59
1s		4910.380	49.47378	3.0417737D-02	1.2378137D-03	3.8887613D-06	1.8265140D-07
2s		520.2467	11.33007	0.1313074	2.0304187D-02	1.6967081D-03	2.9843933D-02
2p	4026.101	172.9427	11.30546	0.1121857	1.5334349D-02	1.0279680D-03	2.2435486D-02
3s		103.2673	4.105154	0.3505505	0.1403475	3.1597509D-02	6.1371957D-02
3p	739.1425	34.06812	4.017438	0.3421207	0.1356947	3.2029548D-02	0.1209539
3d	117.7784	18.64754	3.859528	0.3140392	0.1165693	2.4882881D-02	1.0127520D-02
4s		20.03953	1.599756	0.8515141	0.8185689	0.9949393	1.708773
4p	124.0978	6.341313	1.488250	0.9035704	0.9306572	1.345043	2.996629
4d	14.02699	2.761220	1.232558	1.058833	1.300931	2.787076	8.968993
5s		1.789038	0.4867280	2.580432	7.534605	87.87416	1501.391
5p	6.663196	0.4395036	0.3890254	3.164523	11.32297	197.9072	5004.290

Table 12. (Continued)

51 Antimony Atom Quartet S State Kr(36)4d(10)5s(2)5p(3) Configuration (10s, 8p, 4d) Basis

|2-V/E| = 1.5D-08 |1-Norm| = 7.8D-16

Total S Cusp: -50.880008 Total P Cusp: -25.305444 Total D Cusp: -15.788276

	T	V(1)	V(2)	V(T)	E	e	-Cusp	r max
	6313.332786	-15011.601264	2384.935598	-12626.665666	-6313.332880	-3928.397282		
1s	1273.778666	-2574.100728	107.405528	-2466.695200	-1192.916534	-1085.511006	50.908750	0.019748
2s	267.713938	-590.313827	78.956966	-511.356861	-243.642923	-164.685957	50.544193	0.109027
2p	267.163788	-589.167365	84.033813	-505.133551	-237.969763	-153.935950	25.440632	0.085569
3s	78.777253	-214.727903	51.201464	-163.526439	-84.749186	-33.547722	51.176536	0.311100
3p	76.204562	-210.145737	52.463621	-157.682116	-81.477554	-29.013933	24.566565	0.299821
3d	71.530032	-202.518131	55.137402	-147.380728	-75.850697	-20.713294	15.805170	0.245285
4s	20.561721	-84.658605	29.062910	-55.595696	-35.033974	-5.971065	50.953466	0.750228
4p	18.380255	-79.124405	28.194642	-50.929764	-32.549508	-4.354867	25.589483	0.775514
4d	13.549797	-66.505862	25.676524	-40.829338	-27.279542	-1.603018	15.670740	0.849101
5s	2.466214	-26.879718	11.938083	-14.941636	-12.475421	-0.537339	50.543643	2.064445
5p	1.815762	-23.124910	10.504660	-12.620250	-10.804488	-0.299829	26.768877	2.386306

	r^{-3}	r^{-2}	r^{-1}	r	r^{2}	r^{4}	r^{6}
		13142.54	294.3451	36.47246	57.89871	449.7276	6768.879
1s		5110.606	50.47256	2.9814706D-02	1.1891468D-03	3.6135157D-06	8.0464912D-07
2s		542.9598	11.57478	0.1285379	1.9444338D-02	1.2836766D-03	1.6206340D-02
2p	4312.545	180.7017	11.55230	0.1097507	1.4649054D-02	4.2304615D-04	5.0060444D-05
3s		108.6490	4.210351	0.3420471	0.1336039	2.8644035D-02	4.9160179D-02
3p	795.0930	35.84485	4.120505	0.3335975	0.1289884	3.0994849D-02	0.1249221
3d	127.8500	19.71390	3.970944	0.3047979	0.1096794	2.1842081D-02	7.5645787D-03
4s		21.63188	1.659973	0.8223158	0.7628539	0.8593016	1.359040
4p	140.0238	6.909270	1.551459	0.8687605	0.8593683	1.142285	2.607945
4d	16.26275	3.082478	1.304037	1.001840	1.162833	2.206269	6.236178
5s		2.153824	0.5270533	2.390495	6.447054	63.48289	906.3937
5p	10.06143	0.6142000	0.4534296	2.702336	8.142419	97.22000	1624.803

52 Tellurium Atom Triplet P State Kr(36)4d(10)5s(2)5p(4) Configuration (10s, 8p, 4d) Basis

|2-V/E| = 2.9D-08 |1-Norm| = 6.9D-16

Total S Cusp: -51.891125 Total P Cusp: -25.806013 Total D Cusp: -16.143942

	T	V(1)	V(2)	V(T)	E	e	-Cusp	r max
	6611.644587	-15711.457670	2488.168315	-13223.289354	-6611.644774	-4123.476458		
1s	1324.691940	-2676.512817	110.486326	-2566.026490	-1241.334550	-1130.848224	51.918063	0.019366
2s	279.157774	-614.611934	81.381701	-533.230233	-254.072459	-172.690757	51.571773	0.106852
2p	278.668775	-613.526709	86.592286	-526.934423	-248.265648	-161.673362	25.944438	0.083798
3s	82.810130	-224.417206	52.964811	-171.452395	-88.642265	-35.677454	52.209533	0.304118
3p	80.214485	-219.815449	54.299245	-165.516204	-85.301715	-31.002469	25.049984	0.292722
3d	75.545256	-212.258816	57.137348	-155.121468	-79.576212	-22.438864	16.166561	0.238861
4s	22.181366	-89.477710	30.364666	-59.113044	-36.931678	-6.567012	51.891275	0.727767
4p	19.964387	-83.944373	29.553220	-54.391153	-34.426772	-4.873552	26.130693	0.750271
4d	15.078519	-71.472230	27.215579	-44.256651	-29.178132	-1.962553	15.995734	0.812699
5s	2.973895	-29.609483	12.989704	-16.619779	-13.645885	-0.656180	51.511471	1.933947
5p	2.172687	-25.292431	11.399031	-13.893400	-11.720713	-0.321682	26.985486	2.235432

	r^{-3}	r^{-2}	r^{-1}	r	r^{2}	r^{4}	r^{6}
		13688.80	302.1434	37.29529	59.02781	433.3072	5992.606
1s		5314.814	51.47140	2.9234999D-02	1.1432865D-03	3.3695423D-06	1.3008290D-06
2s		566.1515	11.81946	0.1258855	1.8640568D-02	1.0088189D-03	9.0983186D-03
2p	4590.843	188.4430	11.79859	0.1074352	1.4034347D-02	3.8746113D-04	3.2091378D-05
3s		114.1664	4.315716	0.3339354	0.1273181	2.5828456D-02	3.5686338D-02
3p	854.6373	37.69196	4.227220	0.3252583	0.1225994	2.7935390D-02	0.1052201
3d	138.2603	20.80096	4.081900	0.2961755	0.1034817	1.9364027D-02	6.0874648D-03
4s		23.30267	1.720725	0.7949389	0.7124766	0.7462680	1.100132
4p	155.6189	7.480862	1.614315	0.8364045	0.7959937	0.9784043	2.164350
4d	18.65520	3.414602	1.374466	0.9514221	1.047469	1.777260	4.465295
5s		2.583273	0.5694131	2.222716	5.562829	46.79775	566.5121
5p	12.49257	0.7295124	0.4863929	2.547825	7.269430	78.53971	1199.740

Table 12. (Continued)

53 Iodine Atom Doublet P State Kr(36)4d(10)5s(2)5p(5) Configuration (10s, 8p, 4d) Basis

|2-V/E| = 3.6D-08 |1-Norm| = 4.0D-16

Total S Cusp: -52.899852 Total P Cusp: -26.307352 Total D Cusp: -16.458023

	T	V(1)	V(2)	V(T)	E	e	-Cusp	r max
	6917.851263	-16430.103570	2594.400795	-13835.702776	-6917.851513	-4323.450718		
1s	1376.600020	-2780.919768	113.596693	-2667.323076	-1290.723055	-1177.126363	52.925342	0.018998
2s	290.849160	-639.407632	83.833589	-555.574043	-264.724883	-180.891294	52.595298	0.104754
2p	290.420049	-638.382724	89.178495	-549.204229	-258.784180	-169.605685	26.443990	0.082097
3s	86.951242	-234.328392	54.754613	-179.573780	-92.622538	-37.867925	53.228060	0.297443
3p	84.338245	-229.715771	56.163005	-173.552766	-89.214521	-33.051516	25.557078	0.285917
3d	79.664850	-222.209948	59.161160	-163.048789	-83.383939	-24.222779	16.484883	0.232657
4s	23.862476	-94.419264	31.690533	-62.728732	-38.866255	-7.175722	52.842231	0.706752
4p	21.608659	-88.881561	30.934073	-57.947488	-36.338829	-5.404756	26.677232	0.726754
4d	16.659710	-76.523556	28.764596	-47.758961	-31.099251	-2.334655	16.291549	0.779833
5s	3.490236	-32.281996	14.006575	-18.275421	-14.785186	-0.778611	52.496448	1.826348
5p	2.579537	-27.634816	12.345159	-15.289657	-12.710120	-0.364960	27.301252	2.095317

	r^{-3}	r^{-2}	r^{-1}	r	r^2	r^4	r^6
		14246.42	310.0020	37.97983	59.40816	406.2469	5121.461
1s		5522.962	52.47018	2.8677322D-02	1.1000235D-03	3.1395143D-06	1.4579989D-06
2s		589.8246	12.06429	0.1233409	1.7887645D-02	8.2968549D-04	5.4791033D-03
2p	4880.839	196.3482	12.04496	0.1052146	1.3457302D-02	3.5562606D-04	2.0790013D-05
3s		119.8228	4.421290	0.3261845	0.1214521	2.3313693D-02	2.5816485D-02
3p	917.3207	39.59033	4.334260	0.3172946	0.1166390	2.4909968D-02	8.0803600D-02
3d	149.1866	21.91538	4.192641	0.2880599	9.7821083D-02	1.7251822D-02	5.0248842D-03
4s		25.03740	1.781496	0.7693916	0.6670842	0.6518082	0.8986870
4p	172.2536	8.073042	1.677011	0.8065244	0.7397307	0.8437124	1.788838
4d	21.21455	3.756878	1.443841	0.9063849	0.9496068	1.451074	3.265269
5s		3.019102	0.6090943	2.086423	4.894833	35.96624	378.0292
5p	15.32007	0.8590596	0.5214116	2.398629	6.462041	62.61307	863.9243

54 Xenon Atom Singlet S State Kr(36)4d(10)5s(2)5p(6) Configuration (10s, 8p, 4d) Basis

|2-V/E| = 5.4D-08 |1-Norm| = 2.9D-15

Total S Cusp: -53.907013 Total P Cusp: -26.809882 Total D Cusp: -16.766265

	T	V(1)	V(2)	V(T)	E	e	-Cusp	r max
	7232.015934	-17167.726327	2703.694851	-14464.031476	-7232.015543	-4528.320692		
1s	1429.504220	-2887.322875	116.736633	-2770.596242	-1341.082022	-1224.345389	53.931333	0.018644
2s	302.787101	-664.699996	86.312609	-578.357387	-275.600286	-189.287678	53.615373	0.102733
2p	302.417596	-663.735380	91.792356	-571.942995	-269.525399	-177.733013	26.942441	0.080464
3s	91.200409	-244.460802	56.570944	-187.889858	-96.689450	-40.118506	54.239118	0.291048
3p	88.574570	-239.843621	58.054377	-181.789245	-93.214674	-35.160298	26.075308	0.279402
3d	83.888669	-232.372370	61.209474	-171.162896	-87.274227	-26.064753	16.796779	0.226758
4s	25.603767	-99.481508	33.040219	-66.441289	-40.837522	-7.797303	53.801353	0.686999
4p	23.346811	-94.004286	32.354406	-61.649879	-38.303068	-5.948662	27.224614	0.704625
4d	18.294866	-81.666777	30.326269	-51.340508	-33.045642	-2.719373	16.586563	0.749968
5s	4.017756	-34.930001	15.003984	-19.926017	-15.908261	-0.904276	53.489167	1.734857
5p	2.986704	-30.007461	13.300271	-16.707190	-13.720487	-0.420215	27.684092	1.970878

	r^{-3}	r^{-2}	r^{-1}	r	r^2	r^4	r^6
		14815.46	317.9209	38.55407	59.26617	374.6761	4288.672
1s		5735.072	53.46894	2.8140471D-02	1.0591672D-03	2.9237331D-06	1.4405342D-06
2s		613.9807	12.30926	0.1208971	1.7160579D-02	7.0416139D-04	3.4773101D-03
2p	5182.852	204.4177	12.29140	0.1030830	1.2914879D-02	3.2709323D-04	1.4710095D-05
3s		125.6209	4.527052	0.3187748	0.1159748	2.1101801D-02	1.8998171D-02
3p	983.1498	41.53918	4.441549	0.3096922	0.1110861	2.2201533D-02	6.0341744D-02
3d	160.6755	23.05781	4.303192	0.2803963	9.2625161D-02	1.5428212D-02	4.2016786D-03
4s		26.83420	1.842250	0.7455014	0.6260427	0.5722670	0.7394241
4p	190.2233	8.696958	1.740820	0.7791067	0.6878184	0.7232783	1.388394
4d	23.95735	4.109759	1.512348	0.8658209	0.8656181	1.198231	2.429318
5s		3.463575	0.6468519	1.971864	4.367658	28.46969	264.1665
5p	18.18821	0.9866219	0.5556937	2.262708	5.759499	49.98952	620.9646

Table 12. (Continued)

54 **Xenon Atom** Singlet S State Kr(36) 4d(10) 5s(2) 5p(6) Configuration (15s, 12p, 6d) **Basis**

|2-V/E| = 1.9D-08 |1-Norm| = 6.7D-16

Total S Cusp: -54.023967 Total P Cusp: -26.991783 Total D Cusp: -17.666220

	T	V(1)	V(2)	V(T)	E	e	-Cusp	r max
	7232.137042	-17165.235534	2700.961589	-14464.273946	-7232.136904	-4531.175315		
1s	1429.523327	-2887.341449	116.710535	-2770.630913	-1341.107587	-1224.397051	54.022672	0.018646
2s	302.811554	-664.735717	86.292373	-578.443344	-275.631790	-189.339417	54.037031	0.102750
2p	302.432166	-663.751459	91.768783	-571.962676	-269.550509	-177.781726	27.000756	0.080441
3s	91.202531	-244.472102	56.547309	-187.924793	-96.722262	-40.174953	54.011162	0.291274
3p	88.671649	-240.002070	58.054752	-181.947317	-93.275668	-35.220916	26.934383	0.278367
3d	83.926152	-232.433768	61.194743	-171.239024	-87.312872	-26.118129	17.603052	0.226693
4s	25.610114	-99.497511	33.015968	-66.481543	-40.871430	-7.855462	54.047022	0.687211
4p	23.345257	-94.041002	32.344110	-61.696892	-38.351635	-6.007525	27.062529	0.705090
4d	18.220537	-81.483440	30.242914	-51.240526	-33.019988	-2.777074	18.007484	0.748209
5s	4.055584	-34.980662	14.990633	-19.990029	-15.934445	-0.943813	54.177234	1.712948
5p	2.928249	-29.540233	13.077584	-16.462648	-13.534399	-0.456815	27.113556	1.940238

	r^{-3}	r^{-2}	r^{-1}	r	r^2	r^4	r^6
		14819.99	317.8747	39.05485	62.60167	468.1836	6951.993
1s		5736.284	53.46929	2.8141027D-02	1.0591620D-03	2.8421744D-06	8.0250815D-08
2s		614.9363	12.30992	0.1208726	1.7159530D-02	5.0022632D-04	2.2634830D-05
2p	5182.465	204.4189	12.29169	0.1030820	1.2915085D-02	3.2722555D-04	2.1652060D-05
3s		125.5044	4.527261	0.3186975	0.1158712	2.0300228D-02	5.3215347D-03
3p	989.6887	41.61152	4.444483	0.3094287	0.1108205	1.9484242D-02	8.3235281D-03
3d	160.8113	23.06614	4.304329	0.2803358	9.2632849D-02	1.5464221D-02	4.1897971D-03
4s		26.85896	1.842547	0.7452695	0.6255767	0.5706985	0.7185680
4p	189.5944	8.690340	1.741500	0.7770238	0.6855305	0.7074986	1.044943
4d	24.05210	4.100333	1.508953	0.8700037	0.8792026	1.286055	2.952122
5s		3.505438	0.6477900	1.980961	4.438842	30.42177	309.2911
5p	17.81369	0.9700469	0.5470413	2.337728	6.271783	64.79633	1049.347

55 **Cesium Atom** Doublet S State Xe(54)6s(1) Configuration (12s, 8p, 4d) **Basis**

|2-V/E| = 3.8D-08 |1-Norm| = 1.6D-15

Total S Cusp: -54.887153 Total P Cusp: -27.302629 Total D Cusp: -17.078395

	T	V(1)	V(2)	V(T)	E	e	-Cusp	r max
	7553.835737	-17912.289798	2804.618608	-15107.671189	-7553.835452	-4749.216844		
1s	1483.384797	-2995.702799	119.795317	-2875.907482	-1392.522685	-1272.727369	54.915839	0.018303
2s	314.987977	-690.501085	88.706819	-601.794267	-286.806290	-198.099471	54.545954	0.100743
2p	314.669275	-689.593377	94.323517	-595.269860	-280.600585	-186.277068	27.396740	0.078878
3s	95.577092	-254.839914	58.305575	-196.534339	-100.957248	-42.651673	55.191742	0.284792
3p	92.945995	-250.239165	59.870352	-190.368813	-97.422818	-37.552465	26.744038	0.273014
3d	88.218546	-242.749745	63.172435	-179.577309	-91.358763	-28.186328	17.111993	0.221157
4s	27.412210	-104.681302	34.308355	-70.372947	-42.960737	-8.652382	55.006846	0.669281
4p	25.115643	-99.194153	33.677159	-65.516994	-40.401351	-6.724192	27.783363	0.684731
4d	20.005774	-86.953584	31.806241	-55.147343	-35.141568	-3.335327	16.889939	0.722598
5s	4.804732	-38.326497	16.162525	-22.163973	-17.359240	-1.196716	55.094586	1.624876
5p	3.753859	-33.632956	14.614110	-19.018847	-15.264988	-0.650878	28.028101	1.822045
6s	0.350291	-11.195407	5.363830	-5.831577	-5.481286	-0.117457	56.894145	5.238542

	r^{-3}	r^{-2}	r^{-1}	r	r^2	r^4	r^6
		15394.74	325.6780	42.22756	88.35216	2190.687	138279.2
1s		5950.637	54.46732	2.7622842D-02	1.0205208D-03	2.9776149D-06	3.6842482D-05
2s		638.3913	12.55457	0.1185629	1.6562885D-02	4.4343330D-03	0.4257765
2p	5495.909	212.6461	12.53806	0.1010350	1.2404658D-02	3.0166546D-04	1.5507698D-05
3s		131.5656	4.633453	0.3116729	0.1109254	2.7606326D-02	0.9806526
3p	1053.442	43.55251	4.549803	0.3023411	0.1058018	1.8722227D-02	2.2617597D-02
3d	172.7365	24.22855	4.413632	0.2731405	8.7840141D-02	1.3044505D-02	3.5442089D-03
4s		28.72550	1.903296	0.7228326	0.5882168	0.5032501	0.6329075
4p	209.0621	9.331543	1.803530	0.7519475	0.6416747	0.6223063	1.005405
4d	26.90491	4.477807	1.580974	0.8285070	0.7917077	0.9956295	1.822733
5s		4.132173	0.6968454	1.844615	3.825795	21.93090	185.4061
5p	23.53771	1.222089	0.6115083	2.072124	4.822281	34.66409	353.2185
6s		0.2611857	0.2035529	5.795790	36.97867	1923.827	135760.6

Table 12. (Continued)

56 Barium Atom Singlet S State Xe(54)6s(2) Configuration (12s, 8p, 4d) Basis

|2-V/E| = 6.9D-08 |1-Norm| = 1.3D-15

Total S Cusp: -55.895976 Total P Cusp: -27.798069 Total D Cusp: -17.391112

	T	V(1)	V(2)	V(T)	E	e	-Cusp	r max
	7883.462430	-18675.051731	2908.126314	-15766.925417	-7883.462981	-4975.336667		
1s	1538.290234	-3106.107152	122.875986	-2983.231166	-1444.940932	-1322.064946	55.923269	0.017974
2s	327.419137	-716.788002	91.123758	-625.664245	-298.245108	-207.121350	55.567217	0.098875
2p	327.165322	-715.945847	96.876371	-619.069476	-291.904154	-195.027783	27.863551	0.077358
3s	100.049945	-265.422977	60.059315	-205.363661	-105.313717	-45.254401	56.217406	0.278897
3p	97.418990	-260.840539	61.704478	-199.136061	-101.717072	-40.012594	27.372671	0.266930
3d	92.657372	-253.345884	65.156110	-188.189774	-95.532402	-30.376292	17.427034	0.215824
4s	29.295115	-110.023630	35.600011	-74.423619	-45.128505	-9.528493	55.958184	0.651348
4p	26.948702	-104.511740	35.021522	-69.490218	-42.541516	-7.519994	28.299090	0.665747
4d	21.781234	-92.359119	33.303234	-59.055885	-37.274651	-3.971418	17.198639	0.697373
5s	5.678035	-41.915343	17.374870	-24.540473	-18.862438	-1.487568	56.098856	1.541730
5p	4.553618	-37.189023	15.877497	-21.311526	-16.757909	-0.680412	28.393979	1.704955
6s	0.545826	-13.282301	6.292898	-6.989403	-6.443577	-0.150680	56.982551	4.535627

	r^{-3}	r^{-2}	r^{-1}	r	r^{2}	r^{4}	r^{6}
		15987.37	333.4831	44.78245	102.6897	2585.524	138996.3
1s		6170.790	55.46620	2.7124404D-02	9.8397612D-04	2.9574742D-06	4.7394140D-05
2s		663.5446	12.79979	0.1162995	1.5925063D-02	3.1589453D-03	0.2538587
2p	5821.785	221.0406	12.78475	9.9066056D-02	1.1923733D-02	2.7854534D-04	1.3974710D-05
3s		137.6709	4.739696	0.3048803	0.1061266	2.4426035D-02	0.7019920
3p	1126.706	45.61125	4.657867	0.2953694	0.1009430	1.6481780D-02	1.0057371D-02
3d	185.3985	25.42858	4.524034	0.2662558	8.3418953D-02	1.2460254D-02	3.0110529D-03
4s		30.66437	1.964708	0.7015686	0.5539333	0.4445590	0.4945289
4p	228.9787	9.987177	1.866281	0.7275283	0.6001738	0.5395308	0.7563918
4d	30.06581	4.858679	1.649270	0.7943471	0.7269542	0.8339489	1.384283
5s		4.860340	0.7484883	1.724076	3.329719	16.27375	115.7739
5p	29.31835	1.465302	0.6640897	1.920830	4.138241	25.27607	216.7136
6s		0.4047664	0.2371839	5.085877	28.73246	1194.287	68721.54

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57 Lanthanum Atom Doublet D State Xe(54)5d(1)6s(2) Configuration (12s, 8p, 6d) Basis

|2-V/E| = 1.1D-07 |1-Norm| = 1.2D-15

Total S Cusp: -56.897470 Total P Cusp: -28.297596 Total D Cusp: -17.795249

	T	V(1)	V(2)	V(T)	E	e	-Cusp	r max
	8220.975312	-19462.631474	3020.681732	-16441.949742	-8220.974410	-5200.292678		
1s	1594.189127	-3218.505135	126.038943	-3092.466192	-1498.277056	-1372.238113	56.924625	0.017657
2s	340.099329	-743.573069	93.622058	-649.951011	-309.851682	-216.229623	56.567445	0.097063
2p	339.905279	-742.792255	99.510940	-643.281315	-303.376036	-203.865096	28.351313	0.075902
3s	104.628368	-276.223861	61.895183	-214.328678	-109.700309	-47.805126	57.231994	0.273215
3p	101.984020	-271.636130	63.616270	-208.019859	-106.035829	-42.419559	27.923293	0.261195
3d	97.205342	-264.158799	67.219446	-196.939353	-99.734011	-32.514565	17.896542	0.210886
4s	31.230447	-115.474876	36.971120	-78.503755	-47.273309	-10.302188	56.957150	0.634623
4p	28.851951	-109.962337	36.448316	-73.514021	-44.662070	-8.213754	28.814905	0.647462
4d	23.593311	-97.798457	34.848984	-62.949474	-39.356162	-4.507178	17.581140	0.673934
5s	6.407569	-44.978092	18.455030	-26.523062	-20.115472	-1.660442	57.090721	1.476500
5p	5.212134	-40.172847	16.975637	-23.197210	-17.985076	-1.009439	28.836460	1.620532
5d	2.937145	-29.784294	13.303522	-16.480772	-13.543627	-0.240105	17.171658	2.107526
6s	0.610776	-14.191571	6.711129	-7.480441	-6.869666	-0.158536	57.964145	4.319678

	r^{-3}	r^{-2}	r^{-1}	r	r^{2}	r^{4}	r^{6}
		16590.38	341.4497	45.30923	99.92461	2223.998	108489.6
1s		6394.785	56.46500	2.6643457D-02	9.4934722D-04	2.7223485D-06	3.8509583D-05
2s		689.1294	13.04514	0.1141235	1.5330561D-02	2.7009091D-03	0.1997536
2p	6160.959	229.6025	13.03144	9.7171762D-02	1.1469967D-02	2.5749443D-04	1.1513976D-05
3s		143.9731	4.846033	0.2983744	0.1016328	2.2152058D-02	0.5801360
3p	1202.532	47.70911	4.765546	0.2887487	9.6450553D-02	1.4898223D-02	6.7197423D-03
3d	198.8135	26.66169	4.634365	0.2597153	7.9319555D-02	1.1240939D-02	2.6112441D-03
4s		32.66159	2.025875	0.6815864	0.5226587	0.3946503	0.4139858
4p	250.1359	10.66658	1.929164	0.7047462	0.5628732	0.4722933	0.6073191
4d	33.43280	5.248170	1.715762	0.7647816	0.6752372	0.7407060	1.430748
5s		5.471101	0.7890893	1.641718	3.017357	13.29548	84.17081
5p	34.36513	1.665560	0.7047868	1.818236	3.707427	20.22736	154.3163
5d	2.847959	0.5897884	0.5225315	2.370234	6.275181	57.48013	727.3465
6s		0.4531288	0.2489749	4.857858	26.25934	1003.655	53323.82

Table 12. (Continued)

64 Gadolinium Ion (+3) Octuplet S State Xe(54)6s(0)4f(7) Configuration (10s, 8p, 4d, 3f) Basis

|2-V/E| = 3.5D-05 |1-Norm| = 1.0D-15

Total S Cusp: -64.192829 Total P Cusp: -31.370896 Total D Cusp: -20.333262 Total F Cusp: -11.941710

	T	V(1)	V(2)	V(T)	E	e	-Cusp	r max
	10818.862062	-25623.976782	3985.869866	-21638.106916	-10819.244854	-6833.374989		
1s	2013.506745	-4061.315548	149.790249	-3911.525299	-1898.018555	-1748.228306	64.175927	0.015723
2s	436.296705	-945.560134	112.866751	-832.693383	-396.396679	-283.529928	64.436200	0.085902
2p	436.393525	-945.072929	119.687281	-825.385648	-388.992123	-269.304843	31.387856	0.066953
3s	139.591058	-357.871755	76.643346	-281.228410	-141.637352	-64.994007	64.147144	0.239173
3p	136.912252	-353.276616	78.878256	-274.398361	-137.486108	-58.607853	31.275811	0.226690
3d	131.997049	-345.825569	83.480322	-262.345247	-130.348198	-46.967876	20.400677	0.181507
4s	42.997779	-151.549043	47.069936	-104.479108	-61.481328	-14.411393	62.765890	0.548087
4p	40.207861	-145.433886	46.693295	-98.740591	-58.532730	-11.839435	31.455710	0.552814
4d	34.024605	-131.807844	45.283153	-86.524691	-52.500086	-7.216933	20.008591	0.562115
5s	8.396077	-57.873683	23.300621	-34.573062	-26.176985	-2.876364	62.958286	1.283941
5p	6.872947	-51.854133	21.455460	-30.398673	-23.525726	-2.070266	31.487359	1.400329
4f	22.107042	-103.639563	39.801080	-63.838483	-41.731441	-1.930361	11.941710	0.572956

	r^{-3}	r^{-2}	r^{-1}	r	r^2	r^4	r^6
		21121.63	400.3746	33.94083	35.81981	99.56165	515.4729
1s		8078.213	63.45806	2.3701081D-02	7.5108427D-04	2.2266587D-06	6.3585997D-06
2s		884.7760	14.77438	0.1008285	1.1932830D-02	2.6063195D-04	1.6962206D-04
2p	8907.527	294.2919	14.76676	8.5639601D-02	8.8999930D-03	1.6944002D-04	1.6896640D-04
3s		191.3564	5.591746	0.2595316	7.6787545D-02	8.8529198D-03	1.5033052D-03
3p	1821.547	63.65530	5.519947	0.2497218	7.2156664D-02	8.4968990D-03	5.2044934D-03
3d	311.6792	36.11120	5.403525	0.2219158	5.7706296D-02	5.8832548D-03	9.7393118D-04
4s		44.83288	2.367954	0.5867731	0.3876568	0.2186396	0.1859852
4p	392.9116	14.74117	2.272404	0.6008767	0.4097162	0.2498510	0.2135234
4d	56.01774	7.514419	2.059498	0.6386783	0.4710427	0.3520874	0.3829200
5s		7.165784	0.9042763	1.429642	2.286619	7.625407	35.47774
5p	51.08755	2.191189	0.8102208	1.582756	2.815595	11.77814	69.46503
4f	8.954592	3.344071	1.619368	0.7742811	0.7380877	1.150808	3.171367

86 Radon Atom Singlet S State Xe(54)4f(14)5d(10)6s(2)6p(6) Config. (12s, 10p, 6d, 3f) Basis

|2-V/E| = 4.4D-08 |1-Norm| = 1.2D-15

Total S Cusp: -85.934328 Total P Cusp: -42.300270 Total D Cusp: -27.299712 Total F Cusp: -18.904578

	T	V(1)	V(2)	V(T)	E	e	-Cusp	r max
	21866.627446	-51979.840664	8246.586729	-43733.253935	-21866.626489	-13620.039761		
1s	3650.316405	-7348.115260	233.765125	-7114.350135	-3464.033730	-3230.268605	85.954552	0.011679
2s	816.992202	-1738.485914	182.311482	-1556.174433	-739.182141	-556.870659	85.614759	0.063283
2p	818.521941	-1739.469482	192.157638	-1547.311844	-728.789903	-536.632265	42.289574	0.048998
3s	280.921401	-681.077360	130.882715	-550.194644	-269.273243	-138.390528	86.474009	0.171642
3p	276.264311	-676.521202	134.807436	-541.713766	-263.449405	-128.641968	42.392215	0.161209
3d	273.978791	-670.128336	142.740497	-527.387838	-253.409048	-110.668550	27.316855	0.126050
4s	97.379798	-304.104520	86.418041	-217.686479	-120.306681	-33.888640	86.045663	0.377679
4p	93.705022	-296.713938	86.776014	-209.937924	-116.232902	-29.456888	42.118118	0.376699
4d	86.350937	-282.270664	87.311023	-194.959641	-108.608653	-21.297630	27.229259	0.365182
4f	73.357416	-257.781515	87.173503	-170.608012	-97.250598	-10.077095	18.904578	0.318004
5s	26.657935	-132.734467	49.601698	-83.132769	-56.474833	-6.873135	86.340491	0.804014
5p	23.862535	-124.506819	47.725275	-76.781544	-52.918959	-5.193685	42.240826	0.837935
5d	17.805332	-105.805718	42.851899	-62.953819	-45.148437	-2.296538	27.355766	0.933889
6s	4.422310	-50.509278	22.614667	-27.894612	-23.472301	-0.857635	86.975567	1.908538
6p	3.128053	-42.588338	19.522975	-23.065363	-19.937311	-0.414335	42.055759	2.165037

	r^{-3}	r^{-2}	r^{-1}	r	r^2	r^4	r^6
		39021.77	604.4168	53.43232	79.69693	587.1252	8488.617
1s		14630.91	65.44320	1.7591768D-02	4.1348254D-04	4.5757442D-07	5.0215742D-07
2s		1649.565	20.21495	7.3802157D-02	6.3854738D-03	1.1523511D-04	8.8284237D-04
2p	22680.45	550.4802	20.22639	6.2351197D-02	4.7061273D-03	7.0518743D-05	8.4430568D-04
3s		383.3463	7.919504	0.1846296	3.8856450D-02	2.5164176D-03	5.3346585D-03
3p	5064.098	128.1438	7.866526	0.1756236	3.5658269D-02	2.1199775D-03	4.6614250D-03
3d	911.3519	74.50338	7.792190	0.1529047	2.7259783D-02	1.3264165D-03	2.8144675D-04
4s		101.0031	3.536099	0.3983469	0.1784923	4.5472007D-02	1.6658100D-02
4p	1254.777	33.68033	3.450162	0.3998719	0.1811371	4.9320114D-02	6.4577807D-02
4d	204.7419	18.64457	3.282217	0.4005858	0.1844623	5.2682498D-02	2.2852923D-02
4f	49.26306	10.91193	2.997459	0.3982733	0.1865329	6.2945596D-02	3.4545456D-02
5s		22.48467	1.543424	0.8679231	0.8283858	0.9684189	1.532637
5p	248.5696	7.270370	1.447754	0.9112325	0.9305557	1.250720	2.317918
5d	31.30099	3.375901	1.230299	1.052435	1.253813	2.372411	6.386622
6s		3.206199	0.5873172	2.135709	5.086897	37.49135	381.9974
6p	25.71874	0.8803495	0.4952132	2.526460	7.206486	79.52510	1273.767

BASES FOR MOLECULE CALCULATIONS

General Considerations

Although exponential-type primitive functions are best for expanding atomic orbital components of molecular wavefunctions, the calculation of three- and four-centered integrals is a major bottleneck to their use. An alternative has been widely applied and accepted, namely the Gaussian type primitive functions defined by Eq. 19, with p=2. This function has been gaining popularity ever since it was introduced in 1950 by Boys (60). Reviews enumerating the molecules which have been treated using Gaussians have been written by Allen and Karo (61), Allen (62), and Clark and Stewart (63).

All integrals which form matrix elements of the molecular Hamiltonian operator are readily evaluated in closed form, the multi-centered integrals in particular being expressed in terms of the well-known incomplete gamma function. A defect of the Gaussian primitive is that it does not have the proper short- or long-range behavior required to satisfy the demonstrable boundary conditions of molecular or atomic wavefunctions (42,43). As a consequence, large numbers of Gaussian primitives centered at each atom nucleus with widely ranging exponential parameters must be used in order to simulate the proper behavior, especially the short-range one.

The use of Gaussians therefore implies relatively large bases for good calculations on polyatomic molecules. Now, the number of two-electron integrals generated by an n function basis is $[n(n+1)/2]\cdot[\{n(n+1)/2\}+1]/2$. SCF matrix elements formed from these and other integrals require at least $n(n+1)/2$ words of core. These figures rapidly approach certain practical limits. For example, in a (9s,5p) basis for diatomic nitrogen there are forty-eight primitive Gaussians ($n=48$). This implies of the order of $7\cdot 10^5$ integrals and symmetric matrices which require 1176 words. In order to reduce this number so that even larger molecules may be considered, the idea of independent variation of a basis of Gaussian primitives must be abandoned and instead certain linear combinations of Gaussian primitives taken as basis. These "contracted" or "combined" Gaussians play a role similar to that played by single exponentials. Integrals over Gaussian primitives need not be stored since only those over combined functions are ever used. This saves data handling time. Moreover, in the new basis the matrices are smaller and require less core storage during SCF processing.

Contracted Gaussian function bases representing atomic orbitals were suggested in 1963 by Reeves and Harrison (18). Subsequently, Taketa et al. (64) in 1966 discussed procedures for efficiently calculating integrals for combined functions. The functions have variously been called combined

Gaussian-type orbitals (CGTO's), contracted Gaussian functions, and combined Gaussian functions (CGF's). Since the individual Gaussian primitives are not separate variational functions, the coefficients in the linear combination which define the combined function $G_{lm}(\underline{r})$ are required prior to the molecular calculation. Various authors differ in the method of pre-forming the contracted basis functions. References (37, 44, 65-85) contain various Gaussian atomic orbitals and recommended contractions for molecular calculations. The following deals with a new method for generating the contracted or combined Gaussian functions.

Even-Tempered Gaussian Representations of SCF Atomic Orbitals

A logical procedure to construct combined Gaussian functions is first to seek such functions which represent good approximations of accurate SCF atomic orbitals. These also form a good zeroth order approximation for a molecular basis where those atoms so represented are involved. Accurate atomic SCF orbitals such as those described earlier in this work are available at this time for nearly every atom up to krypton and for many beyond. They are generally given in terms of a basis of exponential functions. In 1965, Reeves and Fletcher (86) described Gaussian approximations to single exponentials as linear combinations of Gaussians found by an optimized least-squares fitting. Subsequently O-ohata et al. (37) presented various length expansions of this type showing that "basic" Gaussians (i.e. composed of a solid harmonic and a pure Gaussian without additional powers of r) are sufficient to represent more general types of exponential-type functions. Shavitt (87) generalized the Gaussian fitting expressions to include arbitrary smooth functions of r while also including an arbitrary weighting function W(r).

In this work, even-tempered Gaussian primitives are used, and the weighted least-squares deviation

$$(25) \qquad D_{lm}(\alpha,\beta) = \int dV\, [\phi_{nlm}(\underline{r}) - G_{lm}(\underline{r})]^2\, W(r)$$

is minimized with respect to the orbital exponent parameters α and β of Eq. 22 and the coefficients in the even-tempered expansions $G_{lm}(r)$ of Eq 20. The accurate SCF atomic orbital is denoted by $\phi_{nlm}(r)$. Since dV is the ordinary three-dimensional volume element, the angular parts of $\phi_{nlm}(\underline{r})$ and $G_{lm}(\underline{r})$ integrate to unity leaving the radial integral with volume element r^2dr. The weighting function W(r) is discussed below.

Rather than using specific Gaussian primitives for fitting <u>each</u> atomic orbital, the <u>same</u> set of Gaussian primitives is used to fit <u>all</u> atomic SCF orbitals of the same symmetry in an atom, a symmetry being defined by a value of the quantum number l. In order to obtain optimal values for α and β, which serve equally well for all SCF atomic orbitals of one symmetry, the sum of deviations for those orbitals,

$$(26) \quad D_l(\alpha,\beta) = \sum_n w(n)N(n)D_{nl}(\alpha,\beta) \quad ,$$

is minimized. Here the N(n) are the SCF orbital occupation numbers and the w(n) are additional adjustable weighting factors. For the expansions included in this work, the atomic orbital weights were taken to decrease from core level to valence level by orders of magnitude. For example, the s orbitals of sodium were weighted by (wN)=2.0, 0.2, and 0.01 in the sequence 1s, 2s, and 3s. This is a matter of judgement and experience, but is felt to be logically consistent since first of all, the inner orbitals are more important to the energy. Energy quantities for atoms regularly vary in orders of magnitude in the same way the weights have been chosen. For examples, see Table 12. Secondly, since core orbitals describing inner shells are essentially constant in different molecular environments, it is anticipated that little adjustment of the atomic core orbitals is needed for molecules. Therefore it is consistent to represent these more invariant orbitals as well as possible and the more deformable valence atomic orbitals less well. The addition of correction terms may then be confined to only those corrections needed for the valence shells.

We return to the question of the weighting function $W(r)$ in Eq. 25. First, the possibilities r^{-2}, r^{-1}, and 1 were investigated. For several typical atoms, the corresponding Gaussian representations were calculated for all SCF atomic orbitals. Then the total atomic energies were calculated. It was found that the representations obtained using $W(r)=r^{-1}$ gave energies closest to the actual SCF energies. This is reasonable, because of the major role played by r^{-1} in the large nuclear attraction energy term of the atomic Hamiltonian. This weighting function was generally adopted.

Because of various quantities involved in the analytic expressions for integrals, it was thought that a great deal of time might be saved during integral computation if the exponents for Gaussian primitives of <u>all</u> <u>symmetries</u> of an atom were drawn from the same even-tempered set. To obtain the optimal basis set, one (α,β) pair was determined by minimizing a total atomic least-squares deviation. This total deviation was again taken as a weighted sum of individual values similar to Eq. 26

$$(27) \qquad D(\alpha,\beta) = \sum_{nl} w(n) N(n,l) D_{nl}(\alpha,\beta) \quad .$$

Again, the $N(n,l)$ are occupation numbers and $w(n)$ adds additional weight factors. As indicated in the equation, the additional factors $w(n)$ are assumed to depend only upon the principal quantum number n. These are taken to be 1, 0.1, 0.01, etc. for n=1,2,3,... For example, combined weights and occupation numbers (wN) for atomic orbitals 1s, 2s, and 2p of the nitrogen atom were taken to be 2.0, 0.2, and 0.3 respectively. This weighting produced fittings which appear satisfactory and logically consistent with the considerations applied in the case where the symmetries were left unmixed. This limitation to one pair, (α,β), for all symmetries is of course a substantial restriction on the primitive basis as compared to allowing separate pairs for different symmetries. The effect of the restriction was measured by comparing the optimal least-squares deviations obtained for the individual orbitals by the two methods. It was found that the unified (α,β) approach leads to worse least-squares deviations but the deterioration is not substantial.

Considering the 1s, 2s, and 3s orbitals of argon, the 2s orbital is more expanded radially than the 1s orbital, likewise the 3s is more expanded than the 2s. The optimal Gaussian s-basis will contain primitives required to represent all three atomic orbitals. Some primitives with large exponents are important for the 1s, others with smaller exponents for the 2s, and still smaller for the 3s. However, to some degree all Gaussians contribute to all the SCF atomic orbitals. This is mainly a consequence of the orthogonality requirement. The SCF orbital orthogonality is similar to that of orbitals obtained by Schmidt orthogonalizing Slater-type 1s, 2s, and 3s orbitals. That is, outer SCF atomic orbitals have considerable contributions of a similar character from inner SCF atomic orbitals and the nodal behavior is also mimicked. In view of this analogy, it is to be expected that one might express the orthogonal atomic SCF orbitals in terms of an equal number of non-orthogonal atomic SCF orbitals, which like the Slater-type atomic orbitals, would have substantial values over a smaller range of the radial variable. The resulting distribution of charge would be considerably more localized radially. For this reason, each non-orthogonal orbital would require a substantial contribution from a limited number of the Gaussian primitive set only and such "de-orthogonalized" SCF atomic orbitals would therefore offer certain advantages. It must be noted, however, that in contrast to specific orthogonalization procedures, the process of deorthogonalization is not unique in any sense. Nevertheless, a method was devised to form non-orthogonal SCF atomic orbitals which have just the desired qualities. It is described in Appendix B.

In this manner, it became feasible to restrict the number of Gaussian primitives contributing to each non-orthogonal SCF atomic orbital to less than the total number of primitives. This shortening of the expansions saves valuable time in summations defining contracted Gaussian integrals in terms of primitives. In the present work, all SCF atomic orbitals are non-orthogonal SCF atomic orbitals in Gaussian expansion. Examples are displayed in Tables 13-18, 20, and 22. The columns labelled with the unprimed ordinary atomic orbital designations, 1s, 2s, 2p, etc. are the Gaussian representations of non-orthogonal atomic orbitals. Note that the zetas for the p Gaussians are a subset of the s Gaussian zetas. Representations of SCF atomic orbitals restricted to include only a part of the Gaussian primitive functions as just discussed are found only in Tables 17, 18, 20, and 22.

Atomic Orbital Bases for Molecular Calculations

Certainly SCF atomic orbitals are the most important atomic orbitals for molecular calculations. They may be termed a minimal basis set of SCF atomic orbitals or a zeroth order basis. In particular, one finds that localized core or inner shell functions occupied by core electrons in a molecule are very nearly the same as compared to the atom inner shells. However, the physical environment of an atom in a molecule is substantially different from that of an isolated atom and the valence shells, which extend over the entire molecule, have substantial distortions arising from the extra-atomic molecular forces. In order to take these effects into account, additional contracted basis functions are provided. The distortions can be divided into two categories: scaling and polarization.

Scaling and pseudoscaling

Scaling of a basis function implies the inclusion of a scale parameter t (t>0) which multiplies the radial coordinate r wherever it appears. Each orbital is also multiplied by $t^{3/2}$ to keep it normalized to unity. This parameter has the effect of "contracting" (t>1) or "dilating" (t<1) the original function (t=1) while retaining its shape. Dilation creates a more diffuse charge while contraction causes the charge to concentrate about the nucleus. Infinite contraction ($t \longrightarrow \infty$) would simulate a point charge at the nucleus, while infinite dilation ($t \longrightarrow 0$) would approach a distribution uniformly spread over all space. The scale parameters of the contracted atomic orbitals represent valuable additional parameters for the molecular variational process and the best molecular energy is obtained by minimizing the energy with respect to the scale parameters (49). This is a procedure which implies recalculating the energy for many different t values. Explicit scaling such as this involves the repetition of almost all steps in the molecular calculation because the primitive basis actually changes with t. This is clearly to be avoided if possible. An alternative which avoids such non-linear parameter optimization consists in adding to the SCF minimal basis set additional atomic orbitals, judiciously chosen and of such nature that, in the enlarged linear space, reasonably good approximations to the scaled SCF orbitals may be found. If done effectively, this use of the enlarged basis set in a molecular calculation obviates the need for introducing explicit scale parameters. The determination of the contribution of each basis function to the molecular wavefunction is then reduced to that of finding coefficients for linear expansions.

The procedure for selecting additional effective variational functions (88) is as follows. First, a scaling range (t_i, t_f) is established for an SCF atomic orbital. For twenty different values of the scale parameter t distributed over the scaling range, Gaussian representations of the scaled SCF atomic orbitals are found in terms of the same Gaussian primitives determined for the unscaled (t=1) SCF atomic orbital. Finally, a set of orthogonal basis functions is determined in the space spanned by the resulting twenty expansions and its members are ranked in order of importance. The important ones are selected as additional contracted Gaussian functions. Good judgement and accumulated experience defines which atomic orbitals are to be used to form the extra functions. Since this procedure derives from the explicit scaling of SCF atomic orbitals, the functions created by it ought to be useful for the simulation of scaling through linear variation. Since the additional functions are found independently for each SCF atomic orbital, substantial overlap between those arising from separate SCF atomic orbitals may exist. Checks for such linear dependencies must be made and dependent functions discarded. This function so determined will be referred to as a "pseudo-scaled" basis.

The determination of the transformation is carried out as follows. Extending Eq. 20 one may write the twenty scaled Gaussian linear combinations

$$(28) \qquad G_{jlm}(\underline{r}) = G_{lm}(t_j\underline{r}) = \sum_{k=1}^{M} X(klm)\ c_{jk}$$

where $j=1,2,\ldots 20$, with $M \leq 20$, and with the t_j's equally distributed over the chosen scaling range. The Gaussian primitives $X(klm)$ depend on the same exponential parameters α and β which were determined for the original unscaled SCF atomic orbital. The new set of contracted Gaussian functions $G_{ilm}'(\underline{r})$ are formed according to the relations

$$(29) \qquad G_{ilm}'(\underline{r}) = \sum_{j} G_{jlm}(\underline{r})\ T_{ji}$$

where

$$(30) \qquad \underline{T} = \underline{U}\ \underline{S}_D^{-1/2} \quad .$$

The matrix $\underline{U}$ is that orthogonal matrix ($\underline{U}^{+}=\underline{U}^{-1}$) which diagonalizes $\underline{S}$, the real symmetric matrix of overlap integrals between the scaled functions $G_{jlm}(\underline{r})$. The diagonal matrix is $\underline{S}_D$. This transformation is called canonical orthonormalization (89) and has the important feature of allowing easy discrimination between the new functions with respect to importance. Each new function is associated with one of the eigenvalues of $\underline{S}$. Because of linear dependence, (20-N) of the eigenvalues will be exactly zero. The N functions G_{ilm}' corresponding to non-zero eigenvalues span the entire space and are mutually orthogonal. Moreover they may be ordered according to the magnitude of the eigenvalues, the largest being the most important, etc., with respect to expanding the scaled SCF atomic orbital in the given scaling range. In the present work, the first two or three of these transformed basis orbitals have been used as extra basis functions. It may be observed that the first, most important function is very nearly the same as the original unscaled (t=1) Gaussian contraction. Somewhat better results were obtained by replacing it with the original unscaled SCF atomic orbital although this introduced a slight non-orthogonality between this SCF atomic orbital and the second and third of the G' functions. A newer version of this method, not used here, first projects the unscaled SCF atomic orbitals out of the space of all scaled SCF atomic orbitals. The canonical orthonormalization is then used to obtain the extra functions G' from the remaining space which is orthogonal to the original unscaled SCF atomic orbital. The columns in Tables 13-18, 20, and 22, headed with primed atomic orbital designations (e.g. 2s', 2p'') are those obtained by the above procedure.

An extensive set of programs was developed to automatically form scaled atomic orbital contracted Gaussian basis functions as described (90). The input consists of a set of accurate atomic orbitals for some atom expressed as linear combinations of exponential functions, weight parameters $w(n)N(n,l)$ for the least-squares step, the numbers of Gaussian primitives to be used to expand each symmetry along with designated subsets for each non-orthogonal atomic orbital if desired, scaling ranges for each individual atomic orbital, and the number of scaled functions to be produced for each atomic orbital. Output consists of data defining the contracted Gaussian functions which may be used for molecular calculations.

Polarization

Polarization functions are those atomic orbitals used in a molecular calculation which belong to a symmetry not occupied in the SCF approximation to the ground states of constituent atoms. Examples are p functions in hydrogen atom and d functions in sulfur. In the atomic SCF wavefunctions they are excluded by symmetry constraints. However, the molecular symmetry orbitals are mixtures of atomic orbitals with much less restriction as to the symmetry of included atomic functions and hence, polarization functions play an important role in molecular orbitals. Early calculations showed that the incorporation of a pz function into the basis for a hydrogen molecule has a significant effect on the result (91). Mulliken distinguished between two classes of polarization effect (55): valence polarization, representing a redistribution of electrons among the valence orbitals, and Coulomb polarization, being a deformation of a valence orbital due to the field of neighboring nuclei. While atomic SCF orbitals are a good zeroth order expansion basis for a molecule, the addition of appropriate polarization functions is necessary to produce more realistic charge distributions. The selection of these functions is not trivial and often much work in terms of expensive calculations must be expended. Each function which is added must be optimal for a molecular environment in order that the number of such functions is kept small. This is because of the fact that functions of higher symmetry usually require more calculation time than those of lower symmetry.

The radial extent of useful polarization functions must be approximately that of the outermost valence atomic orbitals (55). Roos and Siegbahn (75) applied this criterion to recommend single d-Gaussian polarization functions for all atoms from boron through fluorine and aluminum through chlorine on the basis of their optimal results for oxygen and sulfur. They also recommended single and double p-Gaussians for polarization of hydrogen.

In the work described here which involves the atoms hydrogen, lithium, and sodium, only p-type polarization functions are included. It was not possible to incorporate d functions because of program restrictions. It can however be assumed that they are less important than the p functions. For these atoms, the highest occupied orbital in the neutral atom ^2S ground state is an ns orbital, n=1,2,3 respectively. In order to obtain p functions with an appropriate radial extent, the ^2P states of lithium and sodium, formed by moving the lone electron from the ns to the np orbital, were computed using the atomic SCF programs described in Appendix A. In this way an SCF p-atomic orbital was found which accurately describes the lone np electron and which is concentrated near the nucleus to about the same extent as a single ns electron. The radii at which these lithium 2s and 2p orbital distributions attain their respective maxima are 3.10 a.u. and 3.82 a.u.; for sodium they are 3.39 a.u. and 4.90 a.u.

For hydrogen a different tack was necessary. The 2p orbital of the ^2P state has a radial distribution maximum at

4.0 a.u., far beyond that of the 1s function, which is 1.0 a.u. It is desirable to determine "atomic orbitals" in the form of a 1s and a 2p Slater-type orbital for use in the fitting process. In order to do this, first of all, the exponent of a 1s exponential-type orbital was optimized with respect to the performance of its contracted even-tempered Gaussian pseudo-scaled (6s)/[3s] basis in an SCF calculation on the hydrogen diatomic molecule (r=1.4a.u.). The optimal energy was obtained for an exponent of 1.1. Secondly, a single 2p exponential was expanded in a Gaussian pseudo-scaled (4p)/[3p] p basis where the Gaussian exponents of the p primitives are the same as those of the s Gaussians obtained above, in accord with an earlier restriction. By a series of hydrogen molecule calculations with different fitted bases obtained from Slater-type p-orbitals with different exponents, the single p-exponent was fixed optimally at 1.30. Through trial of various weights, (wN), for these fittings it was found that unweighted p-orbitals produced the best energies. Hence molecule adapted single exponential atomic orbitals were determined for hydrogen to be used in generating even-tempered Gaussian pseudo-scaled bases of <u>any</u> desired expansion length. The distribution of the hydrogen s atomic orbital so found attains a radial maximum at 0.91 a.u. while the p orbital distribution has a maximum at 1.54 a.u.

Choice of Two Bases

With the methods described, two contracted even-tempered pseudo-scaled Gaussian bases were formed representing the SCF atomic orbitals and polarization atomic orbitals for each of the three atoms. Weights, w(n)N(n,l), of Eq. 27 for polarization orbitals were taken to be zero on the basis of some earlier exploratory calculations on the hydrogen molecule so that the expansions of SCF atomic orbitals which are important to the energy would not be biased by the less important polarization atomic orbitals. With the help of the procedure for adding functions to describe orbital scaling, this minimal, polarized basis was augmented with several contracted functions. The resulting pseudo-scaled bases, referred to as A(smaller) and B(larger), which are displayed in Tables 13-18 were then used for all molecular calculations described in the following section.

Although we have been forced to use least-squares approximations to SCF atomic orbitals, it is generally known that comparable Gaussian expansions, which are optimal for the atom in terms of the energy, are best as a zeroth order molecular basis. An improvement to the method described here then would be to determine even-tempered Gaussian SCF atomic orbitals directly as was done with exponentials in the preceding section using the energy criterion. These could be converted to non-orthogonal atomic orbitals and furthermore, a scaling procedure much like that used here could be constructed. Alternatively, the deorthogonalized virtual orbitals of an atomic SCF calculation might be used as added basis functions. It is hoped that these possibilities will be investigated in future work.

Before going on to the molecular calculations, we now display some results which serve to give some idea about the quality of the bases used here.

Comparison of Segmented Contracted Bases with Pseudo-Scaled Contracted Bases

Contracted Gaussian basis sets for molecular calculations are derived from a primary set of atomic orbitals. This is done because it has become apparent that the space spanned by the atomic orbitals as such forms a subspace of Hilbert space which is extremely important for the expansion of molecular orbitals. Many investigators in this field use SCF atomic orbitals directly. Here use is made of weighted least-squares approximations to SCF atomic orbitals as described. The present method of deriving a contracted pseudo-scaled basis from the primary atomic orbitals is substantially different from that used by others. Since new, it is therefore of interest to compare it with the conventional technique.

In the present method, the SCF atomic orbitals are used for some of the contracted basis functions. Additional linearly independent functions are formed such that the entire set spans a space designed to contain the space spanned by the scaled primary SCF atomic orbitals. In contrast, in other methods, the primary SCF atomic orbitals are not part of the molecular basis. Instead, the primary atomic orbitals are cut into segments, each expanded in terms of a subset of the primitive expansion basis. From these are selected those segments to be used as contracted functions. An important criterion used is that no one Gaussian primitive will contribute to more than one contracted basis function. The coefficients in these atomic orbital segments are ordinarily the self-consistent field coefficients defining the SCF atomic orbitals. In the common case in which several atomic orbitals of the same symmetry depend on the same group of Gaussian primitives, those specific linear coefficients are taken which correspond to the orbital to which each Gaussian primitive is the principal contributor. For example, the Gaussian primitives with large exponents are more important to inner shell atomic orbitals while those with small exponents are important for the outer or valence shells. This contraction scheme will be referred to as the segmented-basis scheme.

Recently Dunning has proposed segmented bases of this type for the first-row atoms (81) where the segmentation scheme is optimal. These contractions were optimized in the framework of a molecular calculation in order to remove any bias in favor of atoms. Several choices are given, depending on the number of contracted basis functions desired. The Gaussian primitives used are the energy optimized (9s,5p) results of Huzinaga (44).

A direct comparison is difficult since it is not possible using the present programs to form a pseudo-scaled basis with the same Gaussian primitives. Thus the comparison made here is to form a pseudo-scaled even-tempered basis as prescribed above, and compare it with a segmented even-tempered basis made using the same (9s,5p) Gaussian primitive set. The segmented basis contracted functions parallel those of Dunning (81) since the same numbers of Gaussian primitives, (9s,5p), were used and the zeta values are similar.

The segmented-basis and scaled-basis contractions are presented in Tables 19-22 for oxygen and nitrogen. For the segmented bases, each column of coefficients headed by the notation [ns] or [mp] represents a <u>group</u> of contracted functions. The horizontal lines separate <u>different</u> contracted functions, one from another (note that the s functions are rearranged from their normal increasing zeta order so that the contracted functions could be displayed in the simple fashion used). In the case of the scaled bases, <u>each column</u> adjacent to the column of zetas represents <u>one</u> contracted function. The 1s, 2s, and 2p contracted functions are the best weighted least-squares approximations to the SCF atomic orbitals used for fitting. The 2s', 2s'', 2p', and 2p'' are the extra contracted functions added to include "pseudo-scaling" in the basis. No 1s' or 1s'' functions are displayed since these were found to be relatively ineffective with respect to improvement of molecular energies. This is in accord with Dunning's observation that segments representing diffuse distributions are more important to the molecular energy. Since no primed functions of the 1s variety were used it is easy to see how a collection of scaled-contracted functions is selected. The 1s, 2s, and 2p SCF type functions serve as a core which is the zeroth-order or unscaled approximation. To these are added primed functions either 2s or 2p as desired. Presumably, if 1s primed functions were included, they would follow the 2s'' function in effectiveness with respect to molecular calculations. Calculations on H_2O and N_2 with Dunning's geometries were carried out. For H_2O, the same segmented-basis contracted functions were used for hydrogen in both cases since only the effect of the contracted oxygen bases is of interest.

The results of calculations with these bases on H_2O are presented in Table 23. We see that the pseudo-scaled basis far surpasses the segmented-basis in terms of the energy obtainable with the smallest number of contracted functions. The [2s,2p] pseudo-scaled basis gives a lower energy than the

[4s,3p] segmented basis. The difference is *five* contracted basis functions. Also it may be noted that the virial coefficient V/E attains a better value for the pseudo-scaled basis. This is a partial confirmation of the goal that the pseudo-scaled basis incorporates a large share of the variability obtainable by scaling. Moreover, this large reduction of the basis size saves substantial computation time.

Table 24 displays the corresponding results for the N_2 calculations. Here the advantage of the scaled-basis scheme is less distinct but an energy advantage over the segmented-basis is still held. There is also a better virial coefficient as before.

The two examples given do not prove conclusively that the pseudo-scaled technique is better than the segmented-basis technique in all cases, however, the comparison presented here is consistent within itself and does display a pseudo-scaled basis advantage. An interesting comparison would be one in which Dunning's results (81) are compared directly to pseudo-scaled basis results where the pseudo-scaled basis employs the same (9s,5p) Gaussian primitives as those used by Dunning. It is anticipated that the proposed comparison will show the same trend of results as those in Tables 23 and 24.

Table 13. Even-tempered Gaussian A basis for hydrogen

Alpha = 0.0427223860 Beta = 3.9731435139

k	Zeta(s)	1s	1s'	1s''
1	0.169742	0.534455	-1.208282	-0.826963
2	0.674410	0.468828	0.980996	1.774329
3	2.679528	0.101798	0.229149	-1.360457
4	10.646148	0.033332	0.108512	-0.136441

k	Zeta(p)	2p	2p'
1	0.169742	0.596790	-1.000601
2	0.674410	0.495517	0.899730
3	2.679528	0.070379	0.234315

Table 14. Even-tempered Gaussian A basis for lithium

Alpha = 0.0134244004 Beta = 4.4087312064

k	Zeta (s)	1s	1s'	2s	2s'	2s''
1	0.059185	0.003252	-0.130685	-1.061541	0.976542	-0.322977
2	0.260929	-0.066512	0.700168	0.069603	-1.767186	1.069250
3	1.150365	-0.591262	0.423309	0.069026	0.553693	-1.956915
4	5.071651	-0.401180	-0.723107	0.006087	-0.089143	0.843025
5	22.359547	-0.083839	-0.221324	0.000385	0.036194	-0.196413
6	98.577233	-0.022567	-0.065388	0.000021	-0.007027	0.043458

k	Zeta (p)	2p	2p'
1	0.059185	0.914106	-0.763537
2	0.260929	0.133451	1.205215
3	1.150365	0.041092	-0.070168
4	5.071651	0.002641	0.056667

Table 15. Even-tempered Gaussian A basis for sodium

Alpha = 0.0271184334 Beta = 3.9423341969

k	Zeta (s)	1s	2s	2s'	3s	3s'	3s''
1	0.106910	-0.007788	-0.033856	0.054357	1.360960	-0.804941	-0.262917
2	0.421475	0.019317	0.361320	-1.134960	-0.664814	2.042962	0.997811
3	1.661594	-0.032587	0.754129	0.618581	0.149688	-1.036179	-2.186997
4	6.550559	0.224629	-0.011300	0.705214	-0.065941	0.289267	1.211562
5	25.824492	0.601177	-0.091333	-0.219804	0.024256	-0.106019	-0.372887
6	101.808777	0.276783	-0.002165	-0.007127	-0.008173	0.037920	0.127342
7	401.364224	0.053918	-0.001910	-0.007504	0.002575	-0.011837	-0.041100
8	1582.311905	0.016922	0.000284	0.001206	-0.000547	0.002519	0.008750

k	Zeta (p)	2p	2p'	3p	3p'
1	0.106910	0.008281	0.078311	1.155731	-0.533538
2	0.421475	-0.284352	0.779946	-0.342481	1.448923
3	1.661594	-0.596840	-0.087016	0.101145	-0.470394
4	6.550559	-0.301361	-0.538045	-0.033729	0.134937
5	25.824492	-0.071911	-0.218352	0.007116	-0.034088

Table 16. Even-tempered Gaussian B basis for hydrogen

Alpha = 0.0418240224 Beta = 3.1025201259

k	Zeta (s)	1s	1s'	1s''
1	0.129760	0.344044	-1.203521	-1.419455
2	0.402583	0.504461	0.570174	2.530538
3	1.249021	0.208773	0.428332	-1.410156
4	3.875112	0.066852	0.199827	-0.072639
5	12.022612	0.012219	0.027673	-0.184594
6	37.300396	0.007000	0.021674	-0.023197

k	Zeta (p)	2p	2p'
1	0.129760	0.351883	-1.054385
2	0.402583	0.603455	0.523789
3	1.249021	0.166022	0.447151
4	3.875112	0.042314	0.112437

Table 17. Even-tempered Gaussian B basis for lithium

Alpha = 0.0115700412 Beta = 3.4255209394

k	Zeta (s)	1s	1s'	2s	2s'	2s''
1	0.039633	0.0	0.0	-0.800126	1.380438	-0.809067
2	0.135765	0.010834	0.003525	-0.326396	-1.795111	2.087963
3	0.465066	-0.210444	0.907008	0.138628	0.217677	-2.480206
4	1.593094	-0.537969	-0.007375	0.028699	0.031214	0.751112
5	5.457177	-0.299765	-0.587888	0.006591	0.031603	-0.053095
6	18.693674	-0.096477	-0.235659	0.0	0.0	0.0
7	64.035572	-0.019614	-0.060476	0.0	0.0	0.0
8	219.355193	-0.007962	-0.022461	0.0	0.0	0.0

k	Zeta (p)	2p	2p'
1	0.039633	0.755860	-1.051079
2	0.135765	0.289905	1.203019
3	0.465066	0.077801	0.016285
4	1.593094	0.012141	0.093219
5	5.457177	0.005053	0.000343

Table 18. Even-tempered Gaussian B basis for sodium

Alpha = 0.0163978687 Beta = 3.3577611334

k	Zeta (s)	1s	2s	2s'	3s	3s'	3s''
1	0.055060	0.0	0.0	0.0	1.194917	-1.277291	0.583843
2	0.184879	0.0	0.001993	-0.221654	-0.258506	2.306001	-1.824016
3	0.620779	0.0	0.515018	-0.992937	-0.021215	-0.872782	2.766856
4	2.084427	-0.007211	0.601007	0.898107	-0.049076	0.184419	-1.275815
5	6.999006	0.199525	-0.049888	0.522637	0.011826	-0.092733	0.306452
6	23.500992	0.549964	-0.078733	-0.174691	-0.001896	0.020937	-0.073667
7	78.910717	0.296943	-0.011472	-0.038524	0.0	0.0	0.0
8	264.963339	0.087799	0.0	0.0	0.0	0.0	0.0
9	889.683602	0.018048	0.0	0.0	0.0	0.0	0.0
10	2987.345019	0.007414	0.0	0.0	0.0	0.0	0.0

k	Zeta (p)	2p	2p'	3p	3p'
1	0.055060	0.0	0.0	1.105064	-0.837234
2	0.184879	-0.036207	0.311914	-0.195974	1.608357
3	0.620779	-0.375665	0.644501	0.079142	-0.440708
4	2.084427	-0.509383	-0.234273	-0.032909	0.135953
5	6.999006	-0.257626	-0.491214	0.006020	-0.037185
6	23.500992	-0.060573	-0.175109	0.0	0.0
7	78.910717	-0.012261	-0.041587	0.0	0.0

Table 19. Even-tempered segmented bases for oxygen

k	Zeta (s)	[3s]	[4s]	[5s]
1	0.237088	0.389215	1.0	1.0
2	0.764797	0.651556	1.0	1.0
4	7.958322	1.0	1.0	1.0
3	2.467084	0.069826	0.069826	0.069826
5	25.671964	0.413528	0.413528	0.413528
6	82.812644	0.141225	0.141225	0.141225
7	267.137104	0.041909	0.041909	0.041909
8	861.731117	0.007347	0.007347	0.007347
9	2779.773039	0.003797	0.003797	0.003797

k	Zeta (p)	[2p]	[3p]
1	0.237088	1.0	1.0
2	0.764797	0.473480	1.0
3	2.467084	0.303268	0.303268
4	7.958322	0.079705	0.079705
5	25.671964	0.022109	0.022109

Table 20. Even-tempered pseudo-scaled bases for oxygen

k	Zeta (s)	1s	2s	2s'	2s''
1	0.237088	0.0	0.389215	-1.145496	1.325788
2	0.764797	0.0	0.651556	0.601045	-2.378377
3	2.467084	0.069826	0.075350	0.767300	1.569574
4	7.958322	0.476983	-0.108228	-0.105985	0.244298
5	25.671964	0.413528	-0.018300	-0.074484	-0.165110
6	82.812644	0.141225	-0.003141	-0.008068	-0.027911
7	267.137104	0.041909	0.0	0.0	0.0
8	861.731117	0.007347	0.0	0.0	0.0
9	2779.773039	0.003797	0.0	0.0	0.0

k	Zeta (p)	2p	2p'	2p''
1	0.237088	0.369977	-0.921457	0.924088
2	0.764797	0.473480	0.274249	-1.375734
3	2.467084	0.303268	0.442420	0.481172
4	7.958322	0.079705	0.248480	0.407096
5	25.671964	0.022109	0.064976	0.212321

Table 21. Even-tempered segmented bases for nitrogen

k	Zeta (s)	[3s]	[4s]	[5s]
1	0.188809	0.438292	1.0	1.0
2	0.605375	0.623792	1.0	1.0
4	6.223404	1.0	1.0	1.0
3	1.941004	0.078531	0.078531	0.078531
5	19.953986	0.402541	0.402541	0.402541
6	63.978097	0.138554	0.138554	0.138554
7	205.131796	0.041123	0.041123	0.041123
8	657.710300	0.007311	0.007311	0.007311
9	2108.804429	0.003801	0.003801	0.003801

k	Zeta (p)	[2p]	[3p]
1	0.188809	1.0	1.0
2	0.605375	0.489950	1.0
3	1.941004	0.281715	0.281715
4	6.223404	0.070625	0.070625
5	19.953986	0.020051	0.020051

Table 22. Even-tempered pseudo-scaled bases for nitrogen

k	Zeta (s)	1s	2s	2s'	2s''
1	0.188809	0.0	0.438292	-1.204585	1.302996
2	0.605375	0.0	0.623792	0.764094	-2.447176
3	1.941004	0.078531	0.043756	0.677153	1.748323
4	6.223404	0.483364	-0.102515	-0.116432	0.120923
5	19.953986	0.402541	-0.016065	-0.067527	-0.138741
6	63.978097	0.138554	-0.002964	-0.007436	-0.029749
7	205.131796	0.041123	0.0	0.0	0.0
8	657.710300	0.007311	0.0	0.0	0.0
9	2108.804429	0.003801	0.0	0.0	0.0

k	Zeta (p)	2p	2p'	2p''
1	0.188809	0.374662	-0.952647	0.933998
2	0.605375	0.489950	0.335456	-1.474053
3	1.941004	0.281715	0.445845	0.650616
4	6.223404	0.070625	0.215303	0.344239
5	19.953986	0.020051	0.057069	0.183967

Table 23. Molecular comparison of contraction schemes: H_2O

Contraction	Segmented Basis		Scaled Basis	
	Energy	V/E	Energy	V/E
[2s,2p|2s]			-75.986463	2.00298
[3s,2p|2s]	-75.981672	1.99726	-75.987852	2.00043
[4s,2p|2s]	-75.984105	1.99802	-75.990762	2.00053
[4s,3p|2s]	-75.986285	1.99735	-75.995725	2.00016
[5s,3p|2s]	-75.990754	1.99764		
(9s,5p|4s)	-75.999510		-75.999510	

Table 24. Molecular comparison of contraction schemes: N_2

Contraction	Segmented Basis		Scaled Basis	
	Energy	V/E	Energy	V/E
[2s,2p]			-108.783000	2.00220
[3s,2p]	-108.784867	1.99659	-108.833053	2.00339
[4s,2p]	-108.861102	1.99720	-108.861188	2.00023
[4s,3p]	-108.866344	1.99752	-108.871894	1.99901
[5s,3p]	-108.870924	1.99777		
(9s,5p)	-108.877096		-108.877096	

MOLECULE CALCULATIONS

Triatomic Alkali Ions

The molecule H_3^+ has been known to mass spectroscopists since Thomson reported it in 1912 (92). It is of theoretical interest because it is the simplest prototype molecule for a three-center two-electron bond and possesses a high stability. It is as stable with respect to dissociation into H_2 and H^+ as H_2 itself is with respect to dissociation into neutral hydrogen atoms. A careful theoretical treatment of the dissociation of H_3^+ and H_2 was given by Schwartz and Schaad (93) in 1967.

Alkali-metal atoms are similar to hydrogen and, although their valence electron is shielded from the nucleus by an inner core of electrons, it is natural to inquire about the possible stability of the triatomic alkali ions. This inquiry is the object of the present calculations. Considered are the homonuclear triatomics H_3^+, Li_3^+, and Na_3^+ and the heteronuclear triatomics composed of at most two kinds of atom, i.e. LiH_2^+, Li_2H^+, NaH_2^+, $NaLi_2^+$, Na_2H^+, and Na_2Li^+. Also treated here are the atomic ions Li^+ and Na^+ and the neutral diatomics H_2, LiH, Li_2, NaH, NaLi, and Na_2. Some of these have been calculated previously. A tabulation of SCF calculations along with some more approximate results is presented in Table 25 with those obtained here. These results will be discussed later.

Because of the kind of atoms involved in the molecular calculations described here, the ground state configurations are rather straightforwardly assigned. All inner shell molecular orbitals resemble either the atomic inner shell orbitals or some symmetric linear combinations of them which are also easily identified. In diatomics, two electrons remain for the valence shell. They occupy a bonding orbital in order for the molecule to be stable. Although this could be an E1u (or πu) symmetry orbital, the A1g (or σg) bonding orbital is generally lower and provides better bonding, with the electrons distributed along the molecular bond axis. With very accurate open-shell SCF calculations on NaLi, Bertoncini et al. (94) found the $^1\Sigma^+$ state to be the most stable out of a set of possible states including the $^3\Pi$ and therefore predicted it to be the ground state. Analogously, in the positive triatomic ions there are also two electrons left for the valence shell. For these, the valence or highest occupied orbital is again most naturally one belonging to the totally symmetric irreducible representation for the molecular point group in question. Since the ions are electron deficient, with two electrons forming a three-center bond, the electrons most naturally would want to be in the plane of the atoms. Other bonding configurations would be analogous to the Π states of a diatomic, and would have a node in the atomic plane. Some experimentation with the alternate configurations was tried but all the molecules were finally predicted to have a ground state characterized by a totally symmetric valence orbital.

Equilibrium Nuclear Configurations

In order to establish the stability of the ions, it is necessary to first determine their ground state equilibrium structure. Using the smaller A bases, the geometry parameters were systematically varied and an energy computed for each new geometry to determine a minimum. Further variations were carried out using the larger B bases. These minima are predicted to be the ground state nuclear configurations. Table 26 contains all of the geometries so established with both A and B bases. All geometry parameters are in reference to Figure 1.

<u>Homonuclear triatomic ions</u>

H_3^+ has been found previously to have the conformation of an equilateral triangle (93). The same is true for Li_3^+ but from rather approximate calculations (95,96). We first of all optimized the geometry of Li_3^+ under an equilateral constraint. Secondly, small deviations from the equilibrium equilateral structure were made in order to determine whether some distorted equilateral triangle has a lower energy. In this way, Li_3^+ was shown to be equilateral in our calcula-

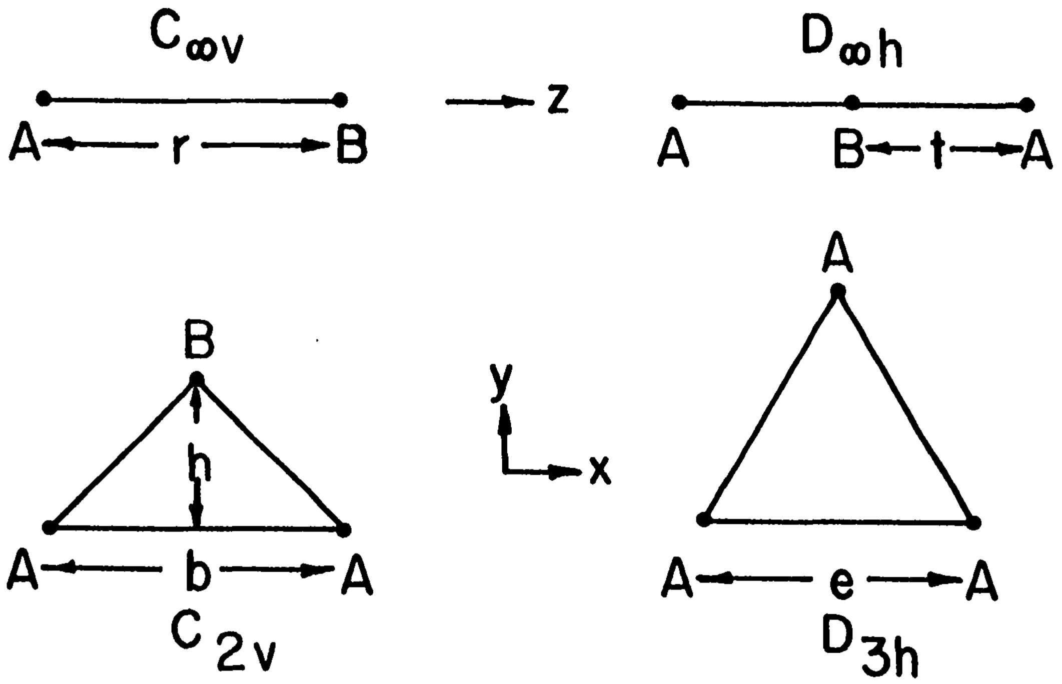

Figure 1. Parameters for molecule geometries

tions. For Na_3^+, only the equilateral geometry was optimized because of the large amount of time needed per geometry to compute the energy (see Table 77 in Appendix C). The equilibrium geometry of H_3^+ was also determined in order that consistent results for all homonuclear triatomics would be available with the bases described here. Edge lengths for the three homopolar triatomic ions are given in Table 26. For H_3^+ and Li_3^+ these values are within 1% of the best optimal values previously reported (see Table 25).

Dihydrogen-metal ions

The ions LiH_2^+ and NaH_2^+ were also subjected to extensive geometry optimization in the A bases. LiH_2^+ had been treated previously (see Table 25) in considerable detail and was found to have an isosceles conformation consisting of a hydrogen molecule located at some distance from the Li atom. Electrons are distributed in such a way that the Li atom is essentially a positive ion. Lester's calculation (97) is of comparable accuracy to ours and since all nuclear configurations were carefully considered by him, we restricted our geometry searches for both of the ions to the isosceles geometry characterized by base and height parameters b and h. A geometry optimum was successfully found in the present work, essentially duplicating that of Lester for LiH_2^+. A rationale of the geometries may be made in terms of the very slight binding experienced with respect to the separated species. The stabilities are to be discussed later in more detail.

Monohydrogen-metal ions

The ions Li_2H^+ and Na_2H^+ also fall into a separate category with respect to geometry. Again Li_2H^+ was computed previously (see Table 25), also with less accurate bases, and its shape was determined to be linear symmetric. We established the equilibrium linear symmetric geometry and then tried deviations from it in both bases but only higher energies were obtained. For Na_2H^+ a similar variation was attempted using the A basis for both symmetric linear and symmetric bent systems. The linear again was found the lowest in energy.

Lithium-sodium ions

The final two triatomic species, $NaLi_2^+$ and Na_2Li^+, have not been treated previously in either the experimental or theoretical literature. Therefore extensive geometry optimization had to be done. For $NaLi_2^+$, in view of a possible similarity to the MH_2^+ ions, an elongated isosceles triangular geometry was taken to be the initial guess. However, the bond distances were found to be less extreme as compared to MH_2^+ ions. A possible π-type valence orbital ground state configuration was tried but was found to be of higher energy.

On the other hand, the similarity of Na_2Li^+ to the previous M_2H^+ ions suggested the possibility of an optimum linear symmetric conformation. In the A basis a stable linear symmetric configuration with t=5.74 a.u. was found. However, lower energies were obtained for an isosceles or bent geometry.

Another possible ion ($NaLiH^+$) composed of all the atoms, although not computed, is predicted to be linear with the hydrogen atom in the middle on the basis of the present results.

Diatomic molecules and atomic ions

In order that predictions as to the stabilities of the above triatomic ions may be made, it is necessary to have data pertaining to dissociation products of the ions computed with the same bases. Consequently, all possible neutral homo- and heteronuclear diatomic molecules and positive atomic ions consisting of the atoms hydrogen, lithium and sodium were calculated in both bases. Diatomic bond lengths were optimized. A tabulation of experimental and previous theoretical geometries in Table 25 shows that those obtained here are, at worst, the same to within a few percent.

Comparison of bond lengths

It is instructive to compare the six possible interatomic distances in the various molecules. The following is a list of all optimum bond lengths in Angstroms, computed with the larger basis (B):

	H-H	Li-H	Na-H	Li-Li	Na-Li	Na-Na
H_2	0.734					
H_3^+	0.869					
Li_2				2.778		
Li_3^+				3.043		
Na_2						3.108
Na_3^+						3.557
NaLi					2.962	
Na_2Li^+					3.307	3.601
$NaLi_2^+$				3.029	3.338	
LiH		1.619				
Li_2H^+		1.674		3.348		
NaH			1.907			
Na_2H^+			2.002			4.004
LiH_2^+	0.743	2.103				
NaH_2^+	0.741		2.517			

These are arranged so that the bond length increases in going from left to right in each row and from top to bottom in each column.

The following observations can be made. Although the bond lengths increase from H_2 to Li_2 to Na_2, those of Na_2 and Li_2 are very close to each other. The heteronuclear diatomics have bond lengths intermediate to the corresponding homonuclear diatomics. Consequently, NaLi is very similar to Na_2 and Li_2.

The homonuclear triatomics have slightly longer bond lengths than the corresponding diatomics. This is presumably so because the diatomics are neutral, whereas the triatomics are positive ions and, hence, embody larger interatomic electrostatic repulsions. Because of the closeness of the Na_2, Li_2, and NaLi bond lengths, the heteronuclear triatomics made from Na and Li are nearly equilateral, in order to approximately maintain these interatomic distances.

If the triatomics Li_2H^+ and Na_2H^+ would preserve the diatomic bondlengths, they would be nearly, but not entirely, linear, i.e. very slightly bent. In fact, they are linear and both the M-H and the M-M bonds are stretched. The reason for this may be as follows. Hydrogen is about twice as electronegative as Li and Na. In agreement with this, the population analysis of the bonding orbital, to be discussed later, yields a charge of about 1.5 on the hydrogen and 0.25 on each of the metal atoms. The additional electrostatic repulsion between the metal atoms may well account for the linearity and the concomitant lengthening of the M-M bonds.

In LiH_2^+ and NaH_2^+, the electronegativity difference has an even stronger effect, since two hydrogens are pitted against one metal atom. Consequently, the bond orbital population on Li and Na is only 0.04 and 0.004 respectively. It is therefore not surprising that the metal-hydrogen distances are considerably elongated beyond those found in LiH and NaH. The unusual shape of these molecule ions, if indeed they are stable, corresponds to the fact that they really are just weak complexes between a hydrogen molecule and a metal ion.

Finally, there is a more subtle, but quite consistent regularity among all homonuclear and heteronuclear triatomics. Namely, the A-B bond lengths <u>decrease</u> in going from ABH^+ to $ABLi^+$ to $ABNa^+$. This, again, may be attributed to the decreasing electronegativity in going from H to Li to Na, which leads to a corresponding increase in the fraction of the bonding electrons available for the AB bond and, hence, to stronger AB bonding. This too is borne out by the population analyses of the bond orbitals.

Energies

An extensive set of total molecular energies expressed in atomic units (Hartrees) is displayed in Table 25 in order to compare the best results obtained here with other SCF results wherever available in the literature. Energies and geometries computed with basis B are tabulated. Of primary interest is the performance of the new pseudo-scaled even-tempered atomic orbital basis. It is therefore relevant to discuss the quality of the results in terms of the <u>relative magnitudes</u> of the energy obtained with the present basis. Very accurate treatments have been made previously for the atoms and diatomic molecules in terms of sets of many Slater-type functions. The present diatomic calculations with Gaussians do not attempt to compete with them, but the accurate values rather serve as benchmarks for our results. A certain consistency may be observed. For Li^+ our result lacks about 0.0035 a.u. while for Na^+ the discrepancy is 0.075 a.u. Likewise, the linear combination of Slater-type orbital results on diatomic molecules are estimated as being close to Hartree-Fock accuracy. Our result on LiH falls 0.0061 a.u. short. For Li_2, NaH, NaLi, and Na_2 the discrepancies are 0.0078, 0.078, 0.081, and 0.154 a.u. respectively. Such deviations seem substantial by chemical standards, however, they are approximately constant with respect to the included atoms, the values for H, Li, and Na respectively being about 0.0026, 0.0035, and 0.0749 a.u. This consistency in the defect of present energies from accurate Hartree-Fock energies is important since for chemical quantities one is generally interested in energy differences between related molecular systems. In lieu of energy differences between systems computed to Hartree-Fock accuracy it is sufficient to take energies which deviate from the Hartree-Fock by known amounts. It is expected that this constant-atomic-defect-property carries over to the triatomic ions where the comparison with more accurate calculations cannot be made. We believe that this constancy in atomic deviations comes about because our bases are designed to describe in detail the changes in going from the atoms to the molecules, in particular in the valence electrons. Because of this, the atomic basis inadequacies remain the same when the atom is incorporated in different molecules.

The SCF energies obtained for H_3^+ and LiH_2^+ are somewhat short of the best values in the literature; 0.0004 and 0.0038 a.u. respectively. For all others the values are the best and often the only ones yet obtained. For all molecules, the results are listed in Table 26 for both bases.

Wavefunctions

The wavefunctions for all molecular species are given for both bases A and B in Tables 27-60. Each column headed by a symmetry designation and an orbital energy corresponds to one molecular orbital. The orbital designation corresponds to the irreducible representation of the molecular point group to which it belongs. Rows in each column are labelled by the atomic orbital designations for the pseudo-scaled even-tempered Gaussian atomic orbital basis functions corresponding to those of Tables 13-18.

In order to interpret the orbitals correctly, they must be referred to external reference axes as shown in Figure 1. The linear systems are oriented along the z-axis while the triangular systems lie in the xy-plane. Moreover, the numbering of the atoms in a triatomic is such that the two equal atoms lying symmetric to the y-axis come first, the other atom coming last. This is the case for both hetero- and homonuclear triatomic ions. The linear triatomics are numbered similarly, the atom at the molecular midpoint being listed last. Of the two symmetrically placed atoms, the one placed at a more negative value of the x-coordinate is taken first. Calculation of integrals is with respect to a coordinate system of uniform handedness centered at each nucleus and displaced parallel to a master reference frame with no rotation. Therefore, the orientation of all p atomic orbitals contained in the basis is such that all positive lobes point in the same direction.

At the head of each wavefunction table is a list of energy quantities along with the value of V/E and the computed norm of the wavefunction. The quantity V/E is an indication of the satisfaction of the molecular virial theorem

$$2T + V + \underline{x}\bullet(\partial E/\partial \underline{x}) = \Delta(\underline{t}) ,$$

due to Wassermann (49). If the geometry is an optimum, the derivatives of the energy with respect to the internal coordinate variations ($\partial E/\partial x_i$) is zero, causing the third term to be zero. The quantity $\Delta(\underline{t})$ represents deviations resulting from incomplete variation of orbital scale factors $\underline{t}$ which are not explicitly included here. If V/E is perfectly equal to 2.0, then the parameters $\underline{x}$ and $\underline{t}$ must be assumed to be fully optimum. Values obtained here are in line with that to be expected as a consequence of comparison with other literature values. The norm is given as an indicator of calculational accuracy. If a basis is used which has linear dependence or near linear dependence, the matrices of expectation values are ill-conditioned. We have noticed that in our computer program, such ill-conditioning leads to a deviation of the norm of the final wavefunction from the correct value of unity. Thus a good value of the norm indicates no problem with linear dependence.

It can be observed that in certain cases some inner shell levels switch in going from the A basis to the B basis. This occurs for NaH_2^+, NaLi, Na_2Li^+, and Na_3^+. The levels in question (see Tables 47 - 50, and 57 - 60) are nearly degenerate, corresponding to the degenerate orbitals in the isolated atom. In the molecular environment they become slightly non-degenerate and the consequent splitting of the orbital energies is different in the separate calculations. The absolute ordering of these orbital energies appears to be a consequence of the basis and little physical significance is attributed to it. Furthermore, orbital energy differences in cases where switching occurs are of negligible magnitude (a maximum of 0.0003 a.u. or 0.2 kcal/mole).

Population Analyses

In 1955, Mulliken recommended a method of partitioning the electronic charge populations of LCAO-MO wavefunctions into net atom, overlap, and gross atom components (98-101). The basic definitions involved are:

$$\mathrm{NAP}(i,A) = \sum_{kl} c_{ik}{}^{A} c_{il}{}^{A} S_{kl}$$

$$\mathrm{OP}(i,AB) = \sum_{kl} c_{ik}{}^{A} c_{il}{}^{B} S_{kl}$$

and

$$\mathrm{GAP}(i,A) = \mathrm{NAP}(i,A) + (1/2) \sum_{B \neq A} \mathrm{OP}(i,AB) \ .$$

The quantity NAP(i,A) is the net atom population due to orbital i at atom A. The OP(i,AB) is the overlap population of orbital i for the bond between atoms A and B. The GAP(i,A) is the gross atom population of orbital i at atom A, one-half of the AB overlap population being added to the net atom population for every other atom in the molecule. The sums on k and l are over basis functions located on the atoms in question and the c's are molecular orbital coefficients. The quantity S_{kl} is the overlap integral between the respective basis functions denoted by k and l. These definitions are constructed such that a sum over all atoms results in

$$\sum_{A} \mathrm{GAP}(i,A) = N(i)$$

where N(i) is the orbital occupation number. For the closed-shell Hartree-Fock wavefunctions used here, two electrons occupy each orbital such that N(i)=2.0. Summing instead over all orbitals i gives the total NAP, the total OP, or the total GAP for each atom or bond. The GAP and the OP are the atom and bond populations ordinarily referred to. Further summing the total GAP over all atoms gives the total number of electrons for the molecule.

While this description may not be ideal, (the factor of one-half in the definition of the overlap population being somewhat arbitrary), it is sufficient to give a general picture of the distribution of electrons in lieu of detailed density maps, expectation values of charge distribution properties, etc. For the molecules calculated here, there is always just one valence orbital. Furthermore, the core orbital distributions are such that the core orbital net atom population is essentially equal to the core orbital gross atom population, with the overlap population due to core orbitals essentially negligible. In order to display the Mulliken population analyses for the molecules calculated here, it was felt adequate to sum these quantities over all core orbitals and present them for the core and valence orbitals separately along with totals. Tables 61-75 contain these population analyses for both basis A and B for all molecules including diatomics in order of increasing molecular weight.

Of prime interest are the valence electron distributions for the triatomic ions. It is convenient to break the entire group of molecules down into the classes described before. Populations in terms of the B bases are discussed unless otherwise noted.

Homonuclear triatomic ions

The homonuclear triatomic ions of H, Li, and Na are fairly uniform. The net atom populations are close to 0.30 while the overlap populations are close to 0.36. Na_3^+ deviates the most from this trend. However, comparison of the respective homonuclear diatomics reveals a similar trend with the sodium quantities again the farthest off. If the diatomic valence orbital overlap populations are compared to those of the triatomics, a smooth trend is observed. In the sequence where $X = H, Li, Na$, the ratio $OP(X_2)/OP(X_3^+)$ equals 2.32, 2.15, and 2.00. This relative comparison is further indication that our basis is adequate with respect to property differences rather than absolute values.

Dihydrogen-metal ions

In both LiH_2^+ and NaH_2^+ the two valence electrons reside primarily on the two H atoms and have "diatomic" charge populations very close to that of the isolated H_2 molecule. Very little of the electrons stray to the heavier atom.

Monohydrogen-metal ions

These linear symmetric "protonated homonuclear diatomics" are most similar in gross atom population. The valence orbital is essentially resident at the proton site contributing approximately 3/4 of the electrons. Though the valence orbital overlap populations are reasonably different, a comparison with those of LiH and NaH reveals an identical trend as in the case of homonuclear triatomics. For X = Li and Na, the ratio of valence overlap populations, Op(XH)/OP(X_2H^+), equals 2.03 and 2.37 respectively.

Sodium-lithium ions

Besides the obvious homonuclear triatomics, the species $NaLi_2^+$ and Na_2Li^+ correspond most closely to a three-center bonding situation. The bias for electron attraction is uniformly in favor of the Li atoms as in NaLi but not overly so as noted for hydrogen. The valence electrons seem to be distributed reasonably evenly around the whole triangular framework.

Dissociation Energy

A question of particular interest in treating an unknown molecule by *ab initio* methods is the predicted stability with respect to dissociation. In the case of known molecules, the calculated dissociation energies are good tests for our atomic orbital basis sets, since the energy changes are essentially due to valence orbitals and the design of the atomic orbital basis was meant to account for such valence shell deformations.

Furthermore, the presently considered triatomic ions are particularly interesting because, for them, adequate values of the dissociation energies can be expected in the Hartree-Fock approximation. For many chemical reactions, e.g. the dissociations of many diatomics, the Hartree-Fock approximation can predict only poor reaction energies, because the neglected correlation energy changes character in the course of the reaction. Therefore, it does not cancel out in the difference between the energy of the products and that of the reactants. This is so in particular, if the number of paired electrons in the products is different from that in the reactants. The situation is more favorable if reactants and products have an equal number of paired electrons. Thus, for example, the energy difference between HF and $(H^+ + F^-)$ can be calculated more accurately than that between HF and (H + F) by the Hartree-Fock approximation. However, since in fact, the dissociation proceeds to (H + F), the Hartree-Fock approximation cannot yield a useful internuclear distance dependence for the ground state energy of HF under dissociation. Only if all doubly filled orbitals of the reactants deform continuously into doubly occupied orbitals of the products, can the Hartree-Fock dissociation curve be useful in the sense that it differs only by an approximate constant from the actual energy curve. An example is the reaction He_2 —> 2He. Another example is the dissociation of the triatomic ions considered here into a neutral diatomic and an atomic ion: $ABC^+ \longrightarrow AB + C^+$. In this process the doubly filled three-center valence orbital goes continuously into the doubly-occupied diatomic valence orbital. As an illustration of the ability of the Hartree-Fock approximation to describe this process, Table 76 and Figure 2 show the results of calculations made for Li_3^+ in several very elongated isosceles conformations. The triangle base length is held fixed at the Li_2 equilibrium distance. The gross atomic populations given in Table 76 show clearly how the symmetric triatomic bond orbital deforms into a diatomic bond orbital while the energy approaches that of Li_2 plus Li^+.

In the foregoing reasoning, the correlation energy has been approximated as the sum of intra-orbital pair correlation energies. The implication is that the inter-orbital correlation can be neglected. This again is a favorable feature of the particular systems considered here. In general, molecular correlation energies are not the sum of intra-orbital pair correlation energies. However, separated pair calculations of Miller and Ruedenberg (102) have shown that in all four-electron atom systems (Li^- to Ne^{+6}), 92% of the correlation energy is recovered as the sum of the pair corre-

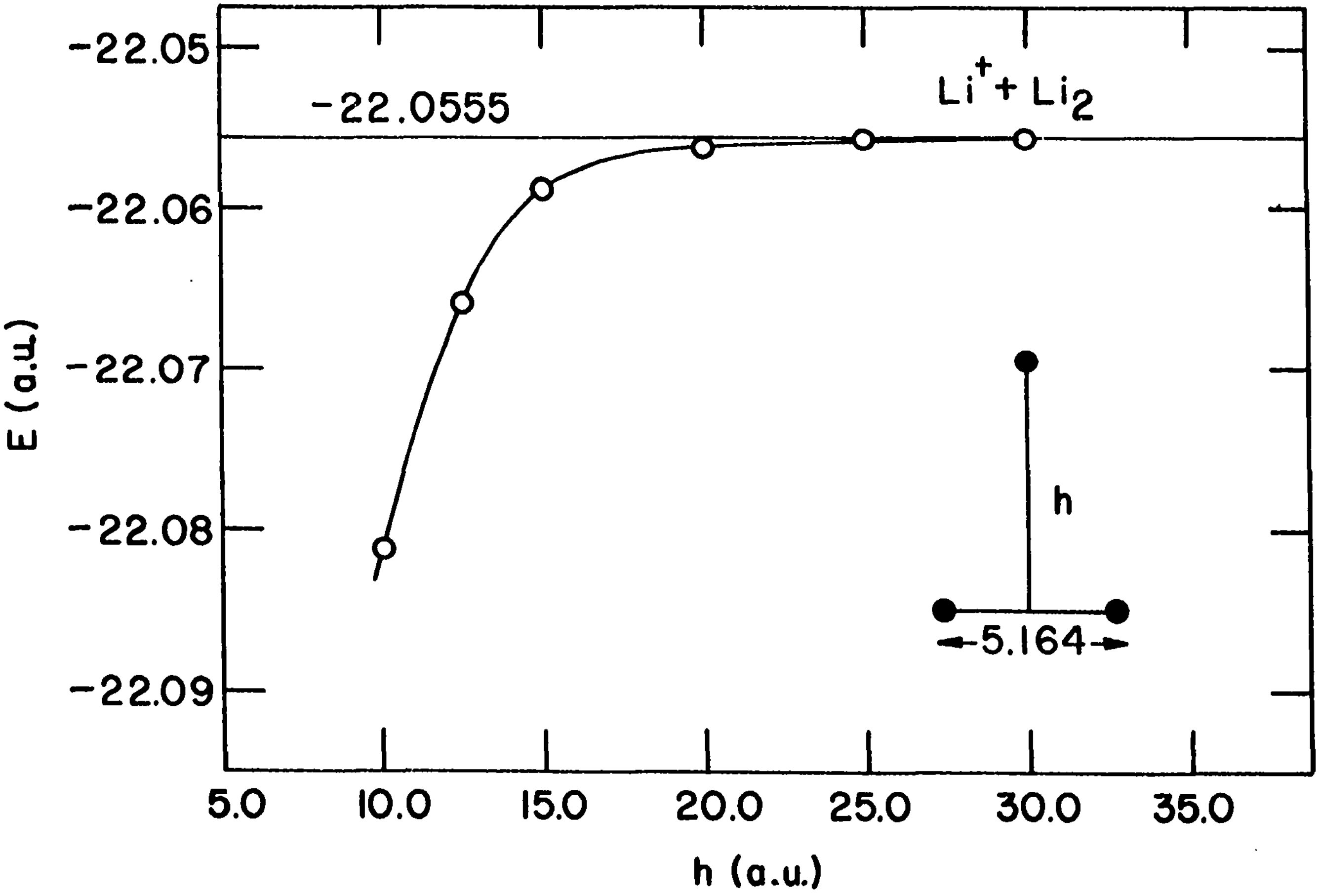

Figure 2. Dissociation energy curve for Li_3^+

lation energies of the inner orbital (about 0.042 a.u.) and that of the outer orbital (about 0.045 a.u.) for Be. Similar results have been obtained for LiH by Mehler et al. (103). It is to be expected that this additivity of inner and outer shell correlation energies remains valid for systems like Li_2 and Li_3^+ which consist of disjointed inner shells and only one valence orbital (104). These systems are probably optimal for description by a separated pair wavefunction. Similar expectations hold for Na_2, Na_3^+, etc.

The question arises, whether the triatomic ion ABC^+ dissociates into ($AB + C^+$) or into ($AB^+ + C$). The Hartree-Fock approximation can describe the former well but would be poor at describing the latter. This question is equivalent to the question which of the two sets of dissociation products has a lower energy. It is well known experimentally and theoretically (93), that $H_2 + H^+$ is more stable than $H + H_2^+$. Furthermore, accurate, near Hartree-Fock, self consistent-field calculations are available for the alternate products in some cases so that one may compare them. If the dissociation of Li_2H^+ is considered, the possible dissociation paths are to $Li_2 + H^+$, $Li_2^+ + H$, $LiH + Li^+$, or $LiH^+ + Li$. Respective total energies of the products are -14.87179, -15.20971, -15.22372, and -15.16216 Hartrees where individual diatomic energies are from the compendium of Krauss (105) and the atom energies are from the list of Clementi (46). Clearly, the products LiH + Li+ are favored. On the other hand, $NaLi_2^+$ has the possible products NaLi + Li+, NaLi+ + Li, Li_2 + Na+, or Li_2^+ + Na with respective product energies of -176.52985, -176.57132, -176.54855, and -176.56860 Hartrees. Energies for NaLi and NaLi+ are from Bertoncini et al. (94). Now, although it appears that the two lowest energy paths correspond to formation of the diatomic ions, there is a correlation energy difference between these products and those from paths which lead to neutral diatomics plus atomic ions. The energies of species which have paired valence electrons lack about -0.042 Hartrees of intra-pair correlation energy while this defect is absent in the case where products each have a single, unpaired valence electron. Therefore, if this quantity is added to the energies of the proper species, the total product energies, in the same sequence, become -176.57185, -176.57132, -176.59055, and -176.56860 Hartrees. Therefore, the paths leading to neutral diatomics, which are correctly described qualitatively by Hartree-Fock theory, are in fact predicted to be the lower energy dissociation paths.

We proceed to the quantitative consideration of the results for the various triatomic ions. The uncorrected dissociation energy,

$$D = \sum_{P} E(P) - \sum_{R} E(R) ,$$

is the sum of the energies of the dissociation products less the energy of the reactants, i.e. the undissociated molecules. Values computed for D are presented in Table 77 for all triatomic species treated here. Certain corrections may be applied to these values if needed.

Correlation correction

The accurate Hartree-Fock wavefunction accounts for approximately 99.5% of the absolute electronic energy of a molecule. The other 0.5% is called the correlation energy according to common usage. This energy is not trivial in a chemical sense since it usually is greater than typical bond energies. However, in the molecules considered here, 90% of the defect due to correlation energy can be accounted for in equal parts by the intrapair correlation contributions of each electron pair. Since the pairing of electrons is being preserved between the reactants and the products of the dissociation reactions considered here, a large cancellation of the correlation defect will occur if the dissociation energy is computed using Hartree-Fock or approximate Hartree-Fock energies. A test of this hypothesis may be made by comparing accurate Hartree-Fock and accurate correlated results. Csizmadia et al. (106) obtained the necessary values for H_3^+ and H_2. The electronic energy for H^+ is zero since there are no electrons. The dissociation energy, D, is found to be

0.1676 and 0.1658 Hartrees for correlated and uncorrelated wavefunctions respectively. The difference between these is 0.0018 Hartrees or 1.1 kcal/mole. This is small in comparison to ordinary bond energies which run between 40 and 100 kcal/mole. Therefore, it is assumed that a correlation correction is unnecessary due to an *essentially complete cancellation* of the correlation effects between products and reactants. The concomitant dissociation energy found with the best wavefunction computed here is 0.1657 which is very close to the accurate result (see Table 26). Even with the poorer wavefunction in the A basis, the dissociation energy is 0.1656 Hartree.

Zero point energy correction

An *ab initio* calculation for a molecule represents an isolated system in a ground electronic state. The energy computed is the value corresponding to the lowest point on the potential energy curve if the geometry is optimum. In actuality, the uncertainty principle dictates that the system cannot be represented as being at this point but that the lowest energy of a molecule is the above energy *plus* the sum of zero point energies for each molecular vibrational mode. In the reactions, some of this energy is cancelled by taking the difference, but in general the cancellation is not nearly as complete as that actually found in the case of the correlation energy. The product diatomic molecule has only one degree of freedom or one vibrational mode, while the triatomic species has four or three depending on whether the conformation is linear or non-linear. For quantification, we may refer to the accurate results of Schwartz and Schaad (93) who computed some zero point energies. They found 6.29 and 12.70 kcal/mole for H_2 and H_3^+ respectively, with a consequent difference for the dissociation reaction of 6.41 kcal/mole. This is a reasonably large fraction of the energy when one considers the uncorrected dissociation energy which is about 100 kcal/mole for H_3^+. Corresponding quantities from less accurate calculations on Li_3^+ (95) and for Li_2 from experiment (107) place the respective zero point energies at 0.60 and 0.50 kcal/mole. The absolute values of the zero point energies and their differences are, in this case, very small and clearly negligible. The large change from the case of the homonuclear hydrogen molecules is due to the large change in component atom weights. The frequency of vibration, ν_o, is proportional to the inverse of the square root of the reduced mass, μ, so that for the larger atomic weights, the zero point energy, $h\nu_o/2$, with $\nu_o=(2\pi)^{-1}(k/\mu)^{1/2}$, values are highly diminished since the force constants k change only little. For this reason we choose to consider the zero point energy effect on the dissociation energy as negligible except possibly where the hydrogen atom is involved and dominant.

Summary

The corrections which may be applied to the dissociation energy as computed directly from absolute ground state energies are largely cancelled by the differencing involved in the definition of dissociation energy or are negligible with respect to the total uncorrected dissociation energy. Therefore, the stability of the triatomic ions will be discussed in relation to the uncorrected results, shown in Table 77, keeping in mind that for marginal cases, the corrections may yet be invoked to govern the conclusions when the necessary data and conditions are given. The largest non-cancelling correction discussed, that of zero point energy, cannot be computed since not enough of each potential energy surface was obtained in order to be able to ascertain or estimate the force constants for the various vibrational modes.

Other corrections to be considered for certain experimental situations are due to population of higher quantum vibrational and electronic states. These are usually not highly populated unless there are unusually low lying states or some kind of high energy situation is involved. There is also the rotational and translational kinetic energy, usually taken proportional to RT/2 per degree of freedom. Finally, there is a pressure-volume term PV for a gas-phase. Depending on the situation, this might be estimated by considering the gas ideal so that PV=RT.

Homonuclear triatomic ions

According to the discussion above, we find all the homonuclear triatomic ions to be predicted stable. The best wavefunctions (basis B) for hydrogen, lithium, and sodium produce respective dissociation energies of 103.7, 41.8, and 37.8 kcal/mole. There exists a large disparity between the dissociation energies of sodium as computed from the A and B bases. The A basis yields 62.5 kcal/mole. This is in contrast to the equal A and B values for the hydrogen case. This is presumably related to the adequacy of the various bases involved. It would appear that the A basis is already quite good for hydrogen, but less good for sodium. It is in some ways reassuring that a large difference _is_ found since it shows that the wavefunctions are different and that one is substantially better than the other. Parenthetically, we may remark that Pitzer (108) has reported empirical bond energies, extrapolated to 0°K for homopolar bonds of the same atoms which are 103.2, 26, and 17.8 kcal/mole respectively. Our results are quantitatively in line with these values.

Dihydrogen-metal ions

The reaction path has two alternate routes, leading either to the hydrogen molecule plus metal ion or the hydride plus a proton. The equilibrium geometries of the species (Table 26) highly suggest the former of the two possibilities, being nearly that to begin with. The gross atom populations (Tables 64 and 69) reflect a situation close to that of the dissociated species. Moreover, the former is also energetically the most favorable. Dissociation energies found for LiH_2^+ and NaH_2^+ are low, being respectively 5.2 and 2.9 kcal/mole. It would seem that since these values are of such small magnitude, the effect of certain corrections might prove overwhelming and throw the reaction into reverse. The conclusion here would be that the ions are probably difficult to form even if marginally stable. A closer accounting of all energy terms would be necessary to make a final prediction. Certain experimental evidence in support of this will be discussed.

Monohydrogen-metal ions

It is well known theoretically and experimentally that $LiH + Li^+$ is more stable than $Li_2 + H^+$. Dissociation energies resulting in metal hydride plus metal ion are 57.2 and 51.4 kcal/mole for Li_2H^+ and Na_2H^+ respectively. Pitzer (108) recorded bond energies of Li-H and Na-H of 58 and 47 kcal/mole. These again show that our results are reasonable. We predict these ions to be stable due to the large magnitude of the dissociation energy. The zero point energy correction discussed above would be small since the metal atoms dominate and imply a large reduced mass.

Sodium-lithium ions

The two species $NaLi_2^+$ and Na_2Li^+ both have alternate reaction paths which are not dramatically different energywise. Those paths which are energetically favored are where a positive sodium ion separates from the triatomic species rather than the lithium ion. Although the respective dissociation energies of 31.2 and 33.6 kcal/mole for this case are of great enough magnitude that the species are predicted to be stable, the effect of various corrections and/or experimental conditions may change the preferred low energy dissociation path.

Experimental Discussion

Outside of H_3^+, there appears to be no experimental literature concerning the triatomic ions as such. However, some of these are known in mass spectra. Both Li_3^+ and Na_3^+ have been observed in spark spectra (109) where molecule lifetimes are about 1-15 microsec. Using the symmetric (A1') vibrational frequency estimate of 192 cm^{-1} or the doubly degenerate (E') vibration frequency estimate of 104 cm^{-1} as given by Pfeiffer and Ellison (95), one finds that after formation, the molecule undergoes of the order of 10^6 to 10^7 vibration cycles before it is collected for identification. Therefore, the lifetime is of such duration that one may safely say that there was indeed a stable ion. The opinion has also been given (109) that the ions $NaLi_2^+$ and Na_2Li^+ could be identified in the same situation if experiments were set up to do so. An interesting correlation may be drawn from mass spectrometric results. It is established (109) that metal-monohydrides are often detected while the metal-dihydrides are very rare. While this information is not from observations of alkali metal spectra, the correlation with present results is clear. It would seem reasonable from our arguments concerning the geometry that in any situation where two hydrogen atoms are involved in a three-center bond, their attraction for each other would be very great. Therefore, subsequent bonding of the H_2 molecule with any other atoms would be minimal. In other words, the energy of the two electrons in H_2 is so low compared to the available valence level of other species, that there is only little interaction.

Besides the mass spectroscopic evidence, one might wonder whether there are other situations in which the ions could play an important part. There is certain evidence that the ions could be present in the highly conductive molten alkali-metal alkali-halide solutions. Reviews by Corbett (110) and Bredig (111) cite measurements which show that although specific conductance increases with metal concentration, the equivalent conductance initially decreases. Some have ascribed this to the possible formation of metal diatomics and the resulting trapping of otherwise free conduction electrons. The homonuclear triatomic species, M_3^+, treated here would also appear to be in accord with this argument, the diatomic forming bonds with the free metal ions of the salt. Spin resonance measurements on the lithium-lithium iodide solution suggest that electrons are paired. In addition, it is found (112) that molten Na-NaCl solutions are largely diamagnetic and become only slightly paramagnetic as metal concentration increases. Such properties relating to the electron pairing are also consistent with M_3^+ as a possible participating species. Though there seems to be no evidence <u>for</u> presence of the triatomic ions in particular, they would not appear to be excluded by any evidence.

Alkali-metal liquid ammonia solutions are another situation in which the triatomic ions might exist. However, less is known about the nature of the concentrated solutions than about the molten salts. In high concentration, the metal solutions are excellent conductors and, in contrast to the dilute solutions, have no unpaired electrons (113,114). Here too, the evidence does not exclude the possibility of participation of the triatomic ions.

Table 25. Comparison with literature SCF results

Geometry Params.	Energy	Basis[a]	Year	Reference
		H_2		
r=1.402	-	Exp.	-	Herzberg (107)
r=1.4	-1.13342	LCGTO(ON)	1967	Schwartz & Schaad (115)
r=1.4	-1.1335	LCGTO	1970	Csizmadia et al. (106)
r=1.387	-1.133128	LCGTO	1971	This work
		H_3^+		
e=1.6405	-1.29993	LCGTO(ON)	1967	Schwartz & Schaad (93)
e=1.66	-1.2993	LCGTO	1970	Csizmadia et al. (106)
e=1.643	-1.298797	LCGTO	1971	This work
		Li^+		
-	-7.22140	LCGTO(ON)	1970	Janoschek (116)
-	-7.23641	LCSTO	1965	Clementi (46)
-	-7.232922	LCGTO	1971	This work
		LiH		
r=3.015	-	Exp.	-	Herzberg (107)
r=3.2260	-6.5727	FSGO	1967	Frost (117)
r=3.02	-7.985970	LCGTO	1966	Csizmadia (118)
r=3.015	-7.98731	LCSTO	1967	Cade & Huo (119)
r=3.059	-7.981232	LCGTO	1971	This work

---

[a] Abbreviations are as follows:

Exp.	Experimental (Conversion: 0.52917 a.u./A°)
DIM	Diatomics in molecules model-non SCF (120)
FSGO	Floating spherical Gaussian orbital model-non SCF (117)
LCSTO	Linear combination of Slater-type orbitals
LCGTO	Linear combination of Gaussian-type orbitals
ON	Off-nuclear Gaussians used

Table 25. (Continued)

Geometry Params.	Energy	Basis[a]	Year	Reference
		LiH_2^+		
b=1.4 h=4.95	A.T.[b]	DIM	1967	Wu & Ellison (121)
b=1.507 h=3.352	-6.920	FSGO	1970	Ray (96)
b=1.4 h=3.765	-8.37826	LCGTO	1970	Lester (97)
b=1.405 h=3.912	-8.374427	LCGTO	1971	This work
		Li_2		
r=5.051	-	Exp.	-	Herzberg (107)
r=5.155	-14.83163	LCGTO(ON)	1970	Janoschek (116)
r=5.37	-14.87179	LCSTO	1967	Cade & Wahl (105)
r=5.250	-14.863972	LCGTO	1971	This work
		Li_2H^+		
t=3.4	A.T.	DIM	1967	Wu & Ellison (121)
t=3.078	-12.618	FSGO	1970	Ray (96)
t=3.14	-15.289	LCGTO(ON)	1967	Diercksen & Preuss (122)
t=3.1635	-15.305500	LCGTO	1971	This work
		Li_3^+		
e=6.18	A.T.	DIM	1965	Pfeiffer & Ellison (95)
e=5.887	-18.292	FSGO	1970	Ray (96)
e=5.769	-22.12376	LCGTO(ON)	1970	Janoschek (116)
e=5.751	-22.163685	LCGTO	1971	This work

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[b] Approximate theory - No absolute energy value is obtained for a valid comparison

Table 25. (Continued)

Geometry Params.	Energy	Basis[a]	Year	Reference
		Na^+		
-	-161.67676	LCSTO	1965	Clementi (46)
-	-161.601805	LCGTO	1971	This work
		NaH		
r=3.567	-	Exp.	-	Herzberg (107)
r=3.566	-162.3928	LCSTO	1967	Cade & Huo (123)
r=3.603	-162.314134	LCGTO	1971	This work
		NaLi		
r=5.5	-169.29344	LCSTO	1970	Bertoncini et al. (94)
r=5.598	-169.212455	LCGTO	1971	This work
		Na_2		
r=5.819	-	Exp.	-	Herzberg (107)
r=5.8178	-323.7116	LCSTO	1967	LMSS (105)
r=5.874	-323.557963	LCGTO	1971	This work

Table 26. Optimum molecular geometries and energies

Molecule	Point Group	BASIS A		BASIS B	
		Geometry	Energy	Geometry	Energy
H_2	$D_{\infty h}$	r=1.391	-1.130829	r=1.387	-1.133128
H_3^+	D_{3h}	e=1.650	-1.296411	e=1.643	-1.298797
Li^+	O_3	-	-7.221335	-	-7.232922
LiH	$C_{\infty v}$	r=3.034	-7.968505	r=3.059	-7.981232
LiH_2^+	C_{2v}	b=1.415 h=3.879	-8.361201	b=1.405 h=3.912	-8.374427
Li_2	$D_{\infty h}$	r=5.164	-14.834200	r=5.250	-14.863972
Li_2H^+	$D_{\infty h}$	t=3.165	-15.283033	t=3.1635	-15.305500
Li_3^+	D_{3h}	e=5.812	-22.127484	e=5.751	-22.163685

Table 26. (Continued)

Molecule	Point Group	BASIS A		BASIS B	
		Geometry	Energy	Geometry	Energy
Na^+	O_3	-	-161.391975	-	-161.601805
NaH	$C_{\infty v}$	r=3.518	-162.088936	r=3.603	-162.314134
NaH_2^+	C_{2v}	b=1.400 h=4.700	-162.528050	b=1.400 h=4.705	-162.739526
NaLi	$C_{\infty v}$	r=5.228	-168.970398	r=5.598	-169.212455
$NaLi_2^+$	C_{2v}	b=5.650 h=5.485	-176.279469	b=5.725 h=5.622	-176.515658
Na_2	$D_{\infty h}$	r=5.412	-323.056571	r=5.874	-323.557963
Na_2H^+	$D_{\infty h}$	t=3.699	-323.573029	t=3.783	-323.997984
Na_2Li^+	C_{2v}	b=6.525 h=4.886	-330.424927	b=6.805 h=5.242	-330.867980
Na_3^+	D_{3h}	e=6.133	-484.548381	e=6.722	-485.220160

Table 27. Basis A wavefunction and energy terms for H_2

```
Molecular Energy =          -1.1308295313
Kinetic Energy =             1.1303431375
Potential Energy =          -2.2611726688
Virial Ratio =               1.9995698788

Elec-Elec Repulsion =          0.6608994966
Elec-Nucl Attraction =        -3.6409794264
Nucl-Nucl Repulsion =          0.7189072610
Wavefunction Norm =            1.0000000000



   Coefficient Vectors and Eigenvalues


          Orbital     1A1g
           Basis   -0.594419

       H   1s       0.535536
           1s'      0.002943
           1s''    -0.002414
           2px      0.0
           2px'     0.0
           2py      0.0
           2py'     0.0
           2pz      0.026489
           2pz'     0.008429
       H   1s       0.535536
           1s'      0.002943
           1s''    -0.002414
           2px      0.0
           2px'     0.0
           2py      0.0
           2py'     0.0
           2pz     -0.026489
           2pz'    -0.008429
```

Table 28. Basis B wavefunction and energy terms for H_2

Molecular Energy = -1.1331280499
Kinetic Energy = 1.1326324704
Potential Energy = -2.2657605203
Virial Ratio = 1.9995626448

Elec-Elec Repulsion = 0.6609395375
Elec-Nucl Attraction = -3.6476805913
Nucl-Nucl Repulsion = 0.7209805335
Wavefunction Norm = 1.0000000000

Coefficient Vectors and Eigenvalues

	Orbital	1A1g
	Basis	-0.596585
H	1s	0.535813
	1s'	0.001602
	1s''	-0.005896
	2px	0.0
	2px'	0.0
	2py	0.0
	2py'	0.0
	2pz	0.024979
	2pz'	0.011380
H	1s	0.535813
	1s'	0.001602
	1s''	-0.005896
	2px	0.0
	2px'	0.0
	2py	0.0
	2py'	0.0
	2pz	-0.024979
	2pz'	-0.011380

Table 29. Basis A wavefunction and energy terms for H_3^+

Molecular Energy = -1.2964116485
Kinetic Energy = 1.2856631466
Potential Energy = -2.5820747951
Virial Ratio = 1.9917090363

Elec-Elec Repulsion = 0.7001979399
Elec-Nucl Attraction = -5.1004545531
Nucl-Nucl Repulsion = 1.8181818182
Wavefunction Norm = 1.0000000000

Coefficient Vectors and Eigenvalues

	Orbital	1A1'
	Basis	-1.207198
H	1s	0.376118
	1s'	0.060327
	1s''	0.004536
	2px	-0.044112
	2px'	-0.004142
	2py	0.025468
	2py'	0.002392
	2pz	0.0
	2pz'	0.0
H	1s	0.376118
	1s'	0.060327
	1s''	0.004536
	2px	0.044112
	2px'	0.004142
	2py	0.025468
	2py'	0.002392
	2pz	0.0
	2pz'	0.0
H	1s	0.376118
	1s'	0.060327
	1s''	0.004536
	2px	0.0
	2px'	0.0
	2py	-0.050936
	2py'	-0.004783
	2pz	0.0
	2pz'	0.0

Table 30. Basis B wavefunction and energy terms for H_3^+

Molecular Energy = -1.2987971168
Kinetic Energy = 1.2953939885
Potential Energy = -2.5941911053
Virial Ratio = 1.9973797845

Elec-Elec Repulsion = 0.7024864521
Elec-Nucl Attraction = -5.1226057376
Nucl-Nucl Repulsion = 1.8259281802
Wavefunction Norm = 1.0000000000

Coefficient Vectors and Eigenvalues

	Orbital	1A1'
	Basis	-1.211119
H	1s	0.381434
	1s'	0.058052
	1s''	0.002863
	2px	0.032814
	2px'	0.014786
	2py	0.018945
	2py'	0.008537
	2pz	0.0
	2pz'	0.0
H	1s	0.381434
	1s'	0.058052
	1s''	0.002863
	2px	-0.032814
	2px'	-0.014786
	2py	0.018945
	2py'	0.008537
	2pz	0.0
	2pz'	0.0
H	1s	0.381434
	1s'	0.058052
	1s''	0.002863
	2px	0.0
	2px'	0.0
	2py	-0.037890
	2py'	-0.017074
	2pz	0.0
	2pz'	0.0

Table 31. Basis A wavefunction and energy terms for Li^+

Molecular Energy = -7.2213356810
Kinetic Energy = 7.1882479951
Potential Energy = -14.4095836762
Virial Ratio = 1.9954180657

Elec-Elec Repulsion = 1.6432000918
Elec-Nucl Attraction = -16.0527837679
Nucl-Nucl Repulsion = 0.0
Wavefunction Norm = 1.0000000000

Coefficient Vectors and Eigenvalues

	Orbital	1s
	Basis	-2.789068
Li	1s	0.992428
	1s'	-0.036679
	2s	0.002569
	2s'	0.005074
	2s''	0.007335

Table 32. Basis B wavefunction and energy terms for Li^+

Molecular Energy = -7.2329222582
Kinetic Energy = 7.2263051198
Potential Energy = -14.4592273780
Virial Ratio = 1.9990851363

Elec-Elec Repulsion = 1.6503269876
Elec-Nucl Attraction = -16.1095543656
Nucl-Nucl Repulsion = 0.0
Wavefunction Norm = 1.0000000000

Coefficient Vectors and Eigenvalues

	Orbital	1s
	Basis	-2.791298
Li	1s	0.998267
	1s'	-0.038969
	2s	0.002522
	2s'	-0.001592
	2s''	0.002328

Table 33. Basis A wavefunction and energy terms for LiH

Molecular Energy = -7.9685051214
Kinetic Energy = 7.9446666529
Potential Energy = -15.9131717743
Virial Ratio = 1.9970084140

Elec-Elec Repulsion = 3.4778463903
Elec-Nucl Attraction = -20.3798118364
Nucl-Nucl Repulsion = 0.9887936717
Wavefunction Norm = 1.0000000000

Coefficient Vectors and Eigenvalues

	Orbital	1A1	2A1
	Basis	-2.441669	-0.298057
Li	1s	0.990937	-0.130114
	1s'	-0.036723	0.012100
	2s	0.002834	0.347585
	2s'	0.006378	0.002468
	2s''	0.007637	-0.003465
	2px	0.0	0.0
	2px'	0.0	0.0
	2py	0.0	0.0
	2py'	0.0	0.0
	2pz	-0.004677	0.220743
	2pz'	-0.007075	0.051894
H	1s	-0.005124	-0.670123
	1s'	0.000754	0.079784
	1s''	-0.000235	0.005495
	2px	0.0	0.0
	2px'	0.0	0.0
	2py	0.0	0.0
	2py'	0.0	0.0
	2pz	-0.002177	-0.019215
	2pz'	-0.000904	-0.002201

Table 34. Basis B wavefunction and energy terms for LiH

Molecular Energy = -7.9812329381
Kinetic Energy = 7.9690643039
Potential Energy = -15.9502972419
Virial Ratio = 1.9984753441

Elec-Elec Repulsion = 3.4614059763
Elec-Nucl Attraction = -20.3924158694
Nucl-Nucl Repulsion = 0.9807126512
Wavefunction Norm = 1.0000000000

Coefficient Vectors and Eigenvalues

	Orbital Basis	1A1	2A1
		-2.450591	-0.299679
Li	1s	-0.995268	-0.131772
	1s'	0.038415	0.013917
	2s	0.008195	0.320950
	2s'	0.005297	0.008293
	2s''	-0.003598	-0.003625
	2px	0.0	0.0
	2px'	0.0	0.0
	2py	0.0	0.0
	2py'	0.0	0.0
	2pz	-0.011668	-0.198249
	2pz'	-0.010222	-0.062991
H	1s	0.016104	-0.689617
	1s'	-0.008059	0.105624
	1s''	-0.001933	0.014297
	2px	0.0	0.0
	2px'	0.0	0.0
	2py	0.0	0.0
	2py'	0.0	0.0
	2pz	-0.007529	0.022835
	2pz'	0.005407	0.002006

Table 35. Basis A wavefunction and energy terms for LiH_2^+

Molecular Energy = -8.3612012085
Kinetic Energy = 8.3152658786
Potential Energy = -16.6764670871
Virial Ratio = 1.9945061327

Elec-Elec Repulsion = 3.3569906032
Elec-Nucl Attraction = -22.2618580007
Nucl-Nucl Repulsion = 2.2284003104
Wavefunction Norm = 1.0000000000

Coefficient Vectors and Eigenvalues

Orbital Basis		1A1	2A1
		-2.767027	-0.849278
H	1s	-0.000948	-0.522794
	1s'	0.000090	-0.007031
	1s''	0.000179	0.001406
	2px	0.000319	-0.040793
	2px'	-0.000263	-0.001821
	2py	0.000569	-0.028187
	2py'	-0.000017	0.007769
	2pz	0.0	0.0
	2pz'	0.0	0.0
H	1s	-0.000948	-0.522794
	1s'	0.000090	-0.007031
	1s''	0.000179	0.001406
	2px	-0.000319	0.040793
	2px'	0.000263	0.001821
	2py	0.000569	-0.028187
	2py'	-0.000017	0.007769
	2pz	0.0	0.0
	2pz'	0.0	0.0
Li	1s	0.992202	-0.047476
	1s'	-0.036665	0.005618
	2s	0.002968	0.023037
	2s'	0.005626	0.007170
	2s''	0.007339	-0.001099
	2px	0.0	0.0
	2px'	0.0	0.0
	2py	-0.000329	0.020212
	2py'	-0.000090	0.022311
	2pz	0.0	0.0
	2pz'	0.0	0.0

Table 36. Basis B wavefunction and energy terms for LiH_2^+

Molecular Energy = -8.3744274235
Kinetic Energy = 8.3621883814
Potential Energy = -16.7366158049
Virial Ratio = 1.9985385219

Elec-Elec Repulsion = 3.3561632554
Elec-Nucl Attraction = -22.3141180156
Nucl-Nucl Repulsion = 2.2213389553
Wavefunction Norm = 1.0000000000

Coefficient Vectors and Eigenvalues

	Orbital	1A1	2A1
	Basis	-2.770741	-0.849061
H	1s	-0.001784	0.523300
	1s'	0.000365	0.007379
	1s''	0.000024	-0.003608
	2px	-0.000311	0.034882
	2px'	0.000156	0.007037
	2py	-0.001443	0.023703
	2py'	0.000637	-0.005548
	2pz	0.0	0.0
	2pz'	0.0	0.0
H	1s	-0.001784	0.523300
	1s'	0.000365	0.007379
	1s''	0.000024	-0.003608
	2px	0.000311	-0.034882
	2px'	-0.000156	-0.007037
	2py	-0.001443	0.023703
	2py'	0.000637	-0.005548
	2pz	0.0	0.0
	2pz'	0.0	0.0
Li	1s	0.997855	0.046055
	1s'	-0.038871	-0.005889
	2s	0.000810	-0.020888
	2s'	-0.002160	-0.015477
	2s''	0.002802	0.001533
	2px	0.0	0.0
	2px'	0.0	0.0
	2py	-0.001931	-0.021765
	2py'	-0.001879	-0.028893
	2pz	0.0	0.0
	2pz'	0.0	0.0

Table 37. Basis A wavefunction and energy terms for Li_2

Molecular Energy = -14.8342009936
Kinetic Energy = 14.8324641739
Potential Energy = -29.6666651676
Virial Ratio = 1.9998829179

Elec-Elec Repulsion = 6.5175716687
Elec-Nucl Attraction = -37.9270718479
Nucl-Nucl Repulsion = 1.7428350116
Wavefunction Norm = 1.0000000000

Coefficient Vectors and Eigenvalues

	Orbital	1A1g	1A2u	2A1g
	Basis	-2.430178	-2.429932	-0.169622
Li	1s	0.701209	-0.700920	-0.131031
	1s'	-0.026096	0.025894	0.009110
	2s	0.002997	0.003217	0.557299
	2s'	0.004331	-0.004978	-0.019885
	2s''	0.005364	-0.005249	-0.005455
	2px	0.0	0.0	0.0
	2px'	0.0	0.0	0.0
	2py	0.0	0.0	0.0
	2py'	0.0	0.0	0.0
	2pz	0.001048	-0.005201	-0.087466
	2pz'	0.002074	-0.001119	-0.027565
Li	1s	0.701209	0.700920	-0.131031
	1s'	-0.026096	-0.025894	0.009109
	2s	0.002997	-0.003217	0.557299
	2s'	0.004331	0.004978	-0.019885
	2s''	0.005364	0.005249	-0.005455
	2px	0.0	0.0	0.0
	2px'	0.0	0.0	0.0
	2py	0.0	0.0	0.0
	2py'	0.0	0.0	0.0
	2pz	-0.001048	-0.005201	0.087466
	2pz'	-0.002074	-0.001119	0.027565

Table 38. Basis B wavefunction and energy terms for Li_2

Molecular Energy = -14.8639724534
Kinetic Energy = 14.8581295966
Potential Energy = -29.7221020500
Virial Ratio = 1.9996069115

Elec-Elec Repulsion = 6.4163280795
Elec-Nucl Attraction = -37.8527158438
Nucl-Nucl Repulsion = 1.7142857143
Wavefunction Norm = 1.0000000000

Coefficient Vectors and Eigenvalues

	Orbital	1A1g	1A2u	2A1g
	Basis	-2.451490	-2.451291	-0.178185
Li	1s	0.705324	0.706152	-0.126912
	1s'	-0.027690	-0.027974	0.010004
	2s	0.002180	0.011196	0.541081
	2s'	-0.000238	-0.003818	-0.032930
	2s''	0.001740	0.002988	-0.002360
	2px	0.0	0.0	0.0
	2px'	0.0	0.0	0.0
	2py	0.0	0.0	0.0
	2py'	0.0	0.0	0.0
	2pz	0.000009	-0.003111	-0.099404
	2pz'	0.001038	0.004889	-0.035338
Li	1s	0.705324	-0.706152	-0.126912
	1s'	-0.027690	0.027974	0.010004
	2s	0.002180	-0.011196	0.541081
	2s'	-0.000238	0.003818	-0.032930
	2s''	0.001740	-0.002988	-0.002360
	2px	0.0	0.0	0.0
	2px'	0.0	0.0	0.0
	2py	0.0	0.0	0.0
	2py'	0.0	0.0	0.0
	2pz	-0.000009	-0.003111	0.099404
	2pz'	-0.001038	0.004889	0.035338

Table 39. Basis A wavefunction and energy terms for Li_2H^+

Molecular Energy = -15.2830335297
Kinetic Energy = 15.2026670240
Potential Energy = -30.4857005538
Virial Ratio = 1.9947414559

Elec-Elec Repulsion = 6.9002508775
Elec-Nucl Attraction = -40.7034869763
Nucl-Nucl Repulsion = 3.3175355450
Wavefunction Norm = 1.0000000000

Coefficient Vectors and Eigenvalues

	Orbital Basis	1A1g -2.646612	1A2u -2.646480	2A1g -0.557067
Li	1s	0.701031	-0.700920	0.102502
	1s'	-0.025932	0.025841	-0.011796
	2s	0.002996	0.001296	-0.128438
	2s'	0.004474	-0.004019	-0.008117
	2s''	0.005275	-0.005262	0.002566
	2px	0.0	0.0	0.0
	2px'	0.0	0.0	0.0
	2py	0.0	0.0	0.0
	2py'	0.0	0.0	0.0
	2pz	0.001087	-0.004717	0.097686
	2pz'	0.002296	-0.002970	0.046199
Li	1s	0.701031	0.700920	0.102502
	1s'	-0.025932	-0.025841	-0.011796
	2s	0.002996	-0.001296	-0.128438
	2s'	0.004474	0.004019	-0.008117
	2s''	0.005275	0.005262	0.002566
	2px	0.0	0.0	0.0
	2px'	0.0	0.0	0.0
	2py	0.0	0.0	0.0
	2py'	0.0	0.0	0.0
	2pz	-0.001087	-0.004717	-0.097686
	2pz'	-0.002296	-0.002970	-0.046199
H	1s	-0.003445	0.0	0.754874
	1s'	-0.000271	0.0	-0.107262
	1s''	-0.000251	0.0	-0.006519
	2px	0.0	0.0	0.0
	2px'	0.0	0.0	0.0
	2py	0.0	0.0	0.0
	2py'	0.0	0.0	0.0
	2pz	0.0	-0.003507	0.0
	2pz'	0.0	0.000438	0.0

Table 40. Basis B wavefunction and energy terms for Li_2H^+

Molecular Energy = -15.3055002391
Kinetic Energy = 15.2798066906
Potential Energy = -30.5853069297
Virial Ratio = 1.9983212866

Elec-Elec Repulsion = 6.9094097303
Elec-Nucl Attraction = -40.8138252422
Nucl-Nucl Repulsion = 3.3191085823
Wavefunction Norm = 1.0000000000

Coefficient Vectors and Eigenvalues

	Orbital	1A1g	1A2u	2A1g
	Basis	-2.650342	-2.650196	-0.557062
Li	1s	-0.704190	-0.705149	0.102553
	1s'	0.027170	0.027512	-0.012403
	2s	0.005062	-0.004338	-0.134973
	2s'	0.003124	0.004047	-0.028873
	2s''	-0.002653	-0.002603	0.005123
	2px	0.0	0.0	0.0
	2px'	0.0	0.0	0.0
	2py	0.0	0.0	0.0
	2py'	0.0	0.0	0.0
	2pz	-0.006457	0.000019	0.105906
	2pz'	-0.005598	-0.005341	0.068135
Li	1s	-0.704190	0.705149	0.102553
	1s'	0.027170	-0.027512	-0.012403
	2s	0.005062	0.004338	-0.134973
	2s'	0.003124	-0.004047	-0.028873
	2s''	-0.002653	0.002603	0.005123
	2px	0.0	0.0	0.0
	2px'	0.0	0.0	0.0
	2py	0.0	0.0	0.0
	2py'	0.0	0.0	0.0
	2pz	0.006457	0.000019	-0.105906
	2pz'	0.005598	-0.005341	-0.068135
H	1s	0.019253	0.0	0.721837
	1s'	-0.009630	0.0	-0.097211
	1s''	-0.002391	0.0	-0.006964
	2px	0.0	0.0	0.0
	2px'	0.0	0.0	0.0
	2py	0.0	0.0	0.0
	2py'	0.0	0.0	0.0
	2pz	0.0	-0.004973	0.0
	2pz'	0.0	0.003448	0.0

Table 41. Basis A wavefunction and energy terms for Li$_3^+$

Molecular Energy = -22.1274843420
Kinetic Energy = 22.0192776781
Potential Energy = -44.1467620201
Virial Ratio = 1.9951098524

Elec-Elec Repulsion = 10.2990972481
Elec-Nucl Attraction = -59.0914201767
Nucl-Nucl Repulsion = 4.6455609085
Wavefunction Norm = 1.0000000000

Coefficient Vectors and Eigenvalues

	Orbital	1A1'	1E'	1E'	2A1'
	Basis	-2.625838	-2.625735	-2.625735	-0.359666
Li	1s	0.572593	0.698065	0.409850	-0.110459
	1s'	-0.021246	-0.025757	-0.015123	0.009653
	2s	0.002770	-0.002232	-0.001310	0.358423
	2s'	0.003726	0.004945	0.002903	-0.003548
	2s''	0.004334	0.005234	0.003073	-0.003958
	2px	-0.000673	-0.004239	-0.001414	0.126110
	2px'	-0.001104	-0.001007	-0.000726	0.027374
	2py	0.000388	0.001363	0.002662	-0.072810
	2py'	0.000637	0.000717	0.000188	-0.015805
	2pz	0.0	0.0	0.0	0.0
	2pz'	0.0	0.0	0.0	0.0
Li	1s	0.572593	-0.703973	0.399617	-0.110459
	1s'	-0.021246	0.025975	-0.014745	0.009653
	2s	0.002770	0.002251	-0.001278	0.358423
	2s'	0.003726	-0.004987	0.002831	-0.003548
	2s''	0.004334	-0.005278	0.002996	-0.003958
	2px	0.000673	-0.004259	0.001351	-0.126110
	2px'	0.001104	-0.001017	0.000711	-0.027374
	2py	0.000388	-0.001402	0.002642	-0.072810
	2py'	0.000637	-0.000720	0.000177	-0.015805
	2pz	0.0	0.0	0.0	0.0
	2pz'	0.0	0.0	0.0	0.0
Li	1s	0.572593	0.005908	-0.809467	-0.110459
	1s'	-0.021246	-0.000218	0.029868	0.009653
	2s	0.002770	-0.000019	0.002588	0.358423
	2s'	0.003726	0.000042	-0.005734	-0.003548
	2s''	0.004334	0.000044	-0.006069	-0.003958
	2px	0.0	-0.001854	-0.000014	0.0
	2px'	0.0	0.000232	0.000002	0.0
	2py	-0.000777	-0.000037	0.005047	0.145619
	2py'	-0.001275	-0.000010	0.001427	0.031609
	2pz	0.0	0.0	0.0	0.0
	2pz'	0.0	0.0	0.0	0.0

Table 42. Basis B wavefunction and energy terms for Li_3^+

Molecular Energy = -22.1636852931
Kinetic Energy = 22.1415516840
Potential Energy = -44.3052369771
Virial Ratio = 1.9990013570

Elec-Elec Repulsion = 10.3696124386
Elec-Nucl Attraction = -59.3696850964
Nucl-Nucl Repulsion = 4.6948356808
Wavefunction Norm = 1.0000000000

Coefficient Vectors and Eigenvalues

	Orbital	1A1'	1E'	1E'	2A1'
	Basis	-2.627572	-2.627454	-2.627454	-0.361974
Li	1s	0.575855	0.002698	-0.815287	-0.112149
	1s'	-0.022563	-0.000107	0.032187	0.010819
	2s	0.001550	0.000044	-0.013238	0.349466
	2s'	-0.000314	-0.000014	0.004178	0.021688
	2s''	0.001209	0.000011	-0.003453	-0.008883
	2px	-0.000266	-0.000953	0.003409	-0.131400
	2px'	0.000760	0.000756	-0.004218	-0.045748
	2py	-0.000153	0.001625	0.001976	-0.075864
	2py'	0.000439	-0.001278	-0.002441	-0.026413
	2pz	0.0	0.0	0.0	0.0
	2pz'	0.0	0.0	0.0	0.0
Li	1s	0.575855	-0.707408	0.405307	-0.112149
	1s'	-0.022563	0.027928	-0.016001	0.010819
	2s	0.001550	-0.011487	0.006581	0.349466
	2s'	-0.000314	0.003625	-0.002077	0.021688
	2s''	0.001209	-0.002996	0.001717	-0.008883
	2px	0.000266	-0.002493	0.002513	0.131400
	2px'	-0.000760	0.003292	-0.002742	0.045748
	2py	-0.000153	0.002520	0.000436	-0.075864
	2py'	0.000439	-0.002753	0.000095	-0.026413
	2pz	0.0	0.0	0.0	0.0
	2pz'	0.0	0.0	0.0	0.0
Li	1s	0.575855	0.704710	0.409980	-0.112149
	1s'	-0.022563	-0.027822	-0.016186	0.010819
	2s	0.001550	0.011443	0.006657	0.349466
	2s'	-0.000314	-0.003611	-0.002101	0.021688
	2s''	0.001209	0.002985	0.001736	-0.008883
	2px	0.0	-0.000947	0.001628	0.0
	2px'	0.0	0.000747	-0.001284	0.0
	2py	0.000307	0.003406	0.001981	0.151727
	2py'	-0.000877	-0.004212	-0.002450	0.052825
	2pz	0.0	0.0	0.0	0.0
	2pz'	0.0	0.0	0.0	0.0

Table 43. Basis A wavefunction and energy terms for Na^+

Molecular Energy =	-161.3919755053	Elec-Elec Repulsion =	62.9117542176
Kinetic Energy =	161.0124558890	Elec-Nucl Attraction =	-385.3161856120
Potential Energy =	-322.4044313943	Nucl-Nucl Repulsion =	0.0
Virial Ratio =	1.9976484604	Wavefunction Norm =	1.0000000000

Coefficient Vectors and Eigenvalues

	Orbital	1s	2s	2py	2px	2pz
	Basis	-40.751529	-3.083888	-1.801565	-1.801565	-1.801565
Na	1s	0.997939	-0.245053	0.0	0.0	0.0
	2s	-0.047528	0.992269	0.0	0.0	0.0
	2s'	0.029848	0.019275	0.0	0.0	0.0
	3s	0.020016	0.015280	0.0	0.0	0.0
	3s'	0.042515	0.031979	0.0	0.0	0.0
	3s''	-0.030091	-0.023332	0.0	0.0	0.0
	2px	0.0	0.0	0.0	-1.000959	0.0
	2px'	0.0	0.0	0.0	0.006507	0.0
	3px	0.0	0.0	0.0	-0.002229	0.0
	3px'	0.0	0.0	0.0	-0.001276	0.0
	2py	0.0	0.0	-1.000959	0.0	0.0
	2py'	0.0	0.0	0.006507	0.0	0.0
	3py	0.0	0.0	-0.002229	0.0	0.0
	3py'	0.0	0.0	-0.001276	0.0	0.0
	2pz	0.0	0.0	0.0	0.0	-1.000959
	2pz'	0.0	0.0	0.0	0.0	0.006507
	3pz	0.0	0.0	0.0	0.0	-0.002229
	3pz'	0.0	0.0	0.0	0.0	-0.001276

Table 44. Basis B wavefunction and energy terms for Na+

Molecular Energy =	-161.6018052724	Elec-Elec Repulsion =	63.1748535046
Kinetic Energy =	161.5127492148	Elec-Nucl Attraction =	-386.2894079917
Potential Energy =	-323.1145544872	Nucl-Nucl Repulsion =	0.0
Virial Ratio =	1.9994489167	Wavefunction Norm =	1.0000000000

Coefficient Vectors and Eigenvalues

	Orbital	1s	2s	2py	2pz	2px
	Basis	-40.745661	-3.073127	-1.798230	-1.798230	-1.798230
Na	1s	0.999463	0.244073	0.0	0.0	0.0
	2s	-0.005212	-1.029041	0.0	0.0	0.0
	2s'	0.004205	0.001001	0.0	0.0	0.0
	3s	0.002578	-0.003088	0.0	0.0	0.0
	3s'	0.004816	0.002978	0.0	0.0	0.0
	3s''	0.007503	-0.000850	0.0	0.0	0.0
	2px	0.0	0.0	0.0	0.0	1.000604
	2px'	0.0	0.0	0.0	0.0	-0.000945
	3px	0.0	0.0	0.0	0.0	0.001258
	3px'	0.0	0.0	0.0	0.0	0.001574
	2py	0.0	0.0	1.000604	0.0	0.0
	2py'	0.0	0.0	-0.000945	0.0	0.0
	3py	0.0	0.0	0.001258	0.0	0.0
	3py'	0.0	0.0	0.001574	0.0	0.0
	2pz	0.0	0.0	0.0	1.000604	0.0
	2pz'	0.0	0.0	0.0	-0.000945	0.0
	3pz	0.0	0.0	0.0	0.001258	0.0
	3pz'	0.0	0.0	0.0	0.001574	0.0

Table 45. Basis A wavefunction and energy terms for NaH

Molecular Energy =	-162.0889363333	Elec-Elec Repulsion =	69.3754893377
Kinetic Energy =	161.8420560821	Elec-Nucl Attraction =	-396.4332583307
Potential Energy =	-323.9309924154	Nucl-Nucl Repulsion =	3.1267765776
Virial Ratio =	1.9984768840	Wavefunction Norm =	1.0000000000

Coefficient Vectors and Eigenvalues

	Orbital	1A1	2A1	1E1x	1E1y	3A1	4A1
	Basis	-40.432719	-2.773838	-1.489304	-1.489304	-1.487830	-0.247117
Na	1s	-0.997938	-0.244941	0.0	0.0	-0.006374	-0.026000
	2s	0.047602	0.991344	0.0	0.0	0.029465	0.110701
	2s'	-0.029885	0.019500	0.0	0.0	0.000164	0.010524
	3s	-0.019801	0.014906	0.0	0.0	0.000479	-0.316587
	3s'	-0.042627	0.032945	0.0	0.0	-0.006336	-0.011969
	3s''	0.030113	-0.023526	0.0	0.0	0.001222	-0.019698
	2px	0.0	0.0	0.999009	0.0	0.0	0.0
	2px'	0.0	0.0	-0.007181	0.0	0.0	0.0
	3px	0.0	0.0	-0.001674	0.0	0.0	0.0
	3px'	0.0	0.0	-0.001557	0.0	0.0	0.0
	2py	0.0	0.0	0.0	0.999009	0.0	0.0
	2py'	0.0	0.0	0.0	-0.007181	0.0	0.0
	3py	0.0	0.0	0.0	-0.001674	0.0	0.0
	3py'	0.0	0.0	0.0	-0.001557	0.0	0.0
	2pz	-0.000016	0.020443	0.0	0.0	-0.999066	-0.100012
	2pz'	-0.000380	-0.002628	0.0	0.0	0.006232	0.002847
	3pz	0.000511	-0.001867	0.0	0.0	0.009148	-0.130837
	3pz'	0.000206	-0.000728	0.0	0.0	0.003472	-0.028085
H	1s	-0.000598	0.004522	0.0	0.0	0.002407	-0.756513
	1s'	0.000281	-0.001455	0.0	0.0	0.006295	0.137725
	1s''	0.000078	-0.000388	0.0	0.0	0.000403	0.015362
	2px	0.0	0.0	-0.000468	0.0	0.0	0.0
	2px'	0.0	0.0	-0.000225	0.0	0.0	0.0
	2py	0.0	0.0	0.0	-0.000468	0.0	0.0
	2py'	0.0	0.0	0.0	-0.000225	0.0	0.0
	2pz	-0.000215	0.001871	0.0	0.0	0.011081	-0.021248
	2pz'	0.000025	-0.000352	0.0	0.0	-0.004244	0.023074

Table 46. Basis B wavefunction and energy terms for NaH

Molecular Energy =	-162.3141339130	Elec-Elec Repulsion =	69.3318129185
Kinetic Energy =	162.2451204983	Elec-Nucl Attraction =	-396.9440787092
Potential Energy =	-324.5592544113	Nucl-Nucl Repulsion =	3.0530113794
Virial Ratio =	1.9995748157	Wavefunction Norm =	1.0000000000

Coefficient Vectors and Eigenvalues

	Orbital	1A1	2A1	1E1x	1E1y	3A1	4A1
	Basis	-40.448084	-2.783071	-1.506296	-1.506296	-1.505019	-0.268901
Na	1s	0.999459	-0.244014	0.0	0.0	-0.005585	-0.022828
	2s	-0.005297	1.028395	0.0	0.0	0.024913	0.124813
	2s'	0.004216	-0.001016	0.0	0.0	0.000235	-0.000161
	3s	0.002214	0.001595	0.0	0.0	-0.001767	-0.323578
	3s'	0.004570	-0.004138	0.0	0.0	-0.006862	-0.018964
	3s''	0.007563	0.000936	0.0	0.0	-0.003214	0.011174
	2px	0.0	0.0	0.999476	0.0	0.0	0.0
	2px'	0.0	0.0	-0.001836	0.0	0.0	0.0
	3px	0.0	0.0	-0.001751	0.0	0.0	0.0
	3px'	0.0	0.0	-0.001406	0.0	0.0	0.0
	2py	0.0	0.0	0.0	0.999476	0.0	0.0
	2py'	0.0	0.0	0.0	-0.001836	0.0	0.0
	3py	0.0	0.0	0.0	-0.001751	0.0	0.0
	3py'	0.0	0.0	0.0	-0.001406	0.0	0.0
	2pz	0.000081	0.018313	0.0	0.0	-0.998915	-0.089687
	2pz'	0.000226	-0.002613	0.0	0.0	0.000666	0.001042
	3pz	-0.000273	-0.000894	0.0	0.0	0.004422	-0.124508
	3pz'	-0.000476	-0.002149	0.0	0.0	0.002590	-0.024923
H	1s	0.000375	0.002903	0.0	0.0	0.004345	-0.740228
	1s'	-0.000173	-0.000613	0.0	0.0	0.004525	0.149502
	1s''	0.000015	0.000188	0.0	0.0	0.000853	0.025058
	2px	0.0	0.0	0.000399	0.0	0.0	0.0
	2px'	0.0	0.0	-0.000845	0.0	0.0	0.0
	2py	0.0	0.0	0.0	0.000399	0.0	0.0
	2py'	0.0	0.0	0.0	-0.000845	0.0	0.0
	2pz	-0.000540	-0.003561	0.0	0.0	0.000864	0.028161
	2pz'	0.000272	0.001258	0.0	0.0	-0.002407	-0.002806

Table 47. Basis A wavefunction and energy terms for NaH_2^+

Molecular Energy =	-162.5280502590	Elec-Elec Repulsion =	67.8918816522
Kinetic Energy =	162.1415627885	Elec-Nucl Attraction =	-397.9055642254
Potential Energy =	-324.6696130475	Nucl-Nucl Repulsion =	5.3440695256
Virial Ratio =	1.9976220260	Wavefunction Norm =	1.0000000000

Coefficient Vectors and Eigenvalues

	Orbital	1A1	2A1	1B1	3A1	1B2	4A1
	Basis	-40.739771	-3.072715	-1.790389	-1.790319	-1.790305	-0.806620
H	1s	-0.000404	0.003141	-0.011044	-0.005176	0.0	-0.527327
	1s'	0.000305	-0.001943	0.004977	0.000744	0.0	-0.005072
	1s''	0.000054	-0.000254	0.000174	-0.000276	0.0	0.002200
	2px	0.000193	-0.001441	-0.004501	0.001797	0.0	-0.036655
	2px'	-0.000177	0.001107	0.002058	-0.001161	0.0	-0.003734
	2py	-0.000289	0.002021	0.001717	-0.001554	0.0	-0.021299
	2py'	0.000132	-0.000767	-0.000599	-0.000437	0.0	0.006945
	2pz	0.0	0.0	0.0	0.0	0.000754	0.0
	2pz'	0.0	0.0	0.0	0.0	-0.000451	0.0
H	1s	-0.000404	0.003141	0.011044	-0.005176	0.0	-0.527327
	1s'	0.000305	-0.001943	-0.004977	0.000744	0.0	-0.005072
	1s''	0.000054	-0.000254	-0.000174	-0.000276	0.0	0.002200
	2px	-0.000193	0.001441	-0.004501	-0.001797	0.0	0.036655
	2px'	0.000177	-0.001107	0.002058	0.001161	0.0	0.003734
	2py	-0.000289	0.002021	-0.001717	-0.001554	0.0	-0.021299
	2py'	0.000132	-0.000767	0.000599	-0.000437	0.0	0.006945
	2pz	0.0	0.0	0.0	0.0	0.000754	0.0
	2pz'	0.0	0.0	0.0	0.0	-0.000451	0.0
Na	1s	-0.997935	-0.245042	0.0	0.000439	0.0	-0.004542
	2s	0.047600	0.991590	0.0	-0.001657	0.0	0.021483
	2s'	-0.029685	0.019500	0.0	-0.000110	0.0	0.001685
	3s	-0.019561	0.012337	0.0	0.002087	0.0	-0.020797
	3s'	-0.042650	0.032832	0.0	0.000132	0.0	0.000975
	3s''	0.030103	-0.023665	0.0	0.000079	0.0	-0.002478
	2px	0.0	0.0	1.000837	0.0	0.0	0.0
	2px'	0.0	0.0	-0.006601	0.0	0.0	0.0
	3px	0.0	0.0	0.002740	0.0	0.0	0.0
	3px'	0.0	0.0	0.001033	0.0	0.0	0.0
	2py	0.000011	-0.001332	0.0	-1.000937	0.0	0.034279
	2py'	0.000020	0.000091	0.0	0.006525	0.0	-0.000565
	3py	-0.000681	0.004558	0.0	-0.004843	0.0	0.012450
	3py'	0.000021	0.000062	0.0	-0.001089	0.0	0.003401
	2pz	0.0	0.0	0.0	0.0	-1.000859	0.0
	2pz'	0.0	0.0	0.0	0.0	0.006582	0.0
	3pz	0.0	0.0	0.0	0.0	-0.002422	0.0
	3pz'	0.0	0.0	0.0	0.0	-0.001082	0.0

Table 48. Basis B wavefunction and energy terms for NaH_2^+

Molecular Energy =	-162.7395264268	Elec-Elec Repulsion =	68.1484448403
Kinetic Energy =	162.6468094894	Elec-Nucl Attraction =	-398.8740368164
Potential Energy =	-325.3863359162	Nucl-Nucl Repulsion =	5.3392560599
Virial Ratio =	1.9994302740	Wavefunction Norm =	1.0000000000

Coefficient Vectors and Eigenvalues

Orbital		1A1	2A1	1B1	1B2	3A1	4A1
	Basis	-40.734156	-3.062219	-1.787368	-1.787292	-1.787215	-0.806919
H	1s	0.000104	-0.000590	-0.003059	0.0	0.001668	0.532276
	1s'	0.000009	-0.000072	0.001308	0.0	-0.000075	0.001410
	1s''	0.000015	-0.000165	0.000028	0.0	-0.000152	-0.005520
	2px	-0.000200	0.001395	-0.000979	0.0	0.001002	0.033129
	2px'	0.000127	-0.000806	0.000297	0.0	-0.000352	0.007509
	2py	-0.000110	0.000720	-0.000375	0.0	0.000741	0.022947
	2py'	0.000078	-0.000534	0.000191	0.0	-0.000300	-0.008345
	2pz	0.0	0.0	0.0	0.000004	0.0	0.0
	2pz'	0.0	0.0	0.0	-0.000024	0.0	0.0
H	1s	0.000104	-0.000590	0.003059	0.0	0.001668	0.532276
	1s'	0.000009	-0.000072	-0.001308	0.0	-0.000075	0.001410
	1s''	0.000015	-0.000165	-0.000028	0.0	-0.000152	-0.005520
	2px	0.000200	-0.001395	-0.000979	0.0	-0.001002	-0.033129
	2px'	-0.000127	0.000806	0.000297	0.0	0.000352	-0.007509
	2py	-0.000110	0.000720	0.000375	0.0	0.000741	0.022947
	2py'	0.000078	-0.000534	-0.000191	0.0	-0.000300	-0.008345
	2pz	0.0	0.0	0.0	0.000004	0.0	0.0
	2pz'	0.0	0.0	0.0	-0.000024	0.0	0.0
Na	1s	-0.999461	-0.244067	0.0	0.0	-0.000436	0.004269
	2s	0.005242	1.028952	0.0	0.0	0.001838	-0.026479
	2s'	-0.004218	-0.001029	0.0	0.0	0.000003	0.000609
	3s	-0.002517	0.002658	0.0	0.0	-0.000924	0.009510
	3s'	-0.004749	-0.003471	0.0	0.0	-0.000883	0.007707
	3s''	-0.007546	0.000956	0.0	0.0	-0.000255	-0.001895
	2px	0.0	0.0	-1.000520	0.0	0.0	0.0
	2px'	0.0	0.0	0.001062	0.0	0.0	0.0
	3px	0.0	0.0	-0.001113	0.0	0.0	0.0
	3px'	0.0	0.0	-0.001398	0.0	0.0	0.0
	2py	-0.000010	-0.001358	0.0	0.0	1.000498	-0.033718
	2py'	0.000038	0.000146	0.0	0.0	-0.000882	0.000339
	3py	-0.000025	0.000093	0.0	0.0	0.001524	-0.000932
	3py'	-0.000165	0.000936	0.0	0.0	0.002006	-0.009632
	2pz	0.0	0.0	0.0	1.000529	0.0	0.0
	2pz'	0.0	0.0	0.0	-0.001040	0.0	0.0
	3pz	0.0	0.0	0.0	0.001071	0.0	0.0
	3pz'	0.0	0.0	0.0	0.001383	0.0	0.0

Table 49. Basis A wavefunction and energy terms for NaLi

Molecular Energy =	-168.9703983319	Elec-Elec Repulsion =	74.8971367794
Kinetic Energy =	168.7266968680	Elec-Nucl Attraction =	-418.9063972432
Potential Energy =	-337.6970951999	Nucl-Nucl Repulsion =	6.3121652640
Virial Ratio =	1.9985577269	Wavefunction Norm =	1.0000000000

Coefficient Vectors and Eigenvalues

	Orbital	1A1	2A1	3A1	1E1x	1E1y	4A1	5A1
	Basis	-40.430689	-2.770020	-2.390222	-1.484455	-1.484455	-1.484151	-0.148720
Na	1s	-0.997935	-0.245135	-0.000136	0.0	0.0	0.003388	-0.027968
	2s	0.047754	0.990983	0.000357	0.0	0.0	-0.014462	0.129785
	2s'	-0.029906	0.019640	0.000001	0.0	0.0	0.000020	0.017562
	3s	-0.018726	0.006644	-0.001462	0.0	0.0	0.009615	-0.267942
	3s'	-0.042676	0.032225	-0.000188	0.0	0.0	0.004606	0.019594
	3s''	0.030103	-0.023587	0.0	0.0	0.0	-0.000613	-0.028826
	2px	0.0	0.0	0.0	0.999220	0.0	0.0	0.0
	2px'	0.0	0.0	0.0	-0.006832	0.0	0.0	0.0
	3px	0.0	0.0	0.0	-0.001269	0.0	0.0	0.0
	3px'	0.0	0.0	0.0	-0.001084	0.0	0.0	0.0
	2py	0.0	0.0	0.0	0.0	0.999220	0.0	0.0
	2py'	0.0	0.0	0.0	0.0	-0.006832	0.0	0.0
	3py	0.0	0.0	0.0	0.0	-0.001269	0.0	0.0
	3py'	0.0	0.0	0.0	0.0	-0.001084	0.0	0.0
	2pz	-0.000037	0.010476	0.000325	0.0	0.0	0.999119	-0.046662
	2pz'	-0.000180	-0.001268	-0.000036	0.0	0.0	-0.006688	0.000174
	3pz	0.001193	-0.007663	-0.000585	0.0	0.0	0.002704	0.051830
	3pz'	0.000057	-0.000617	0.000086	0.0	0.0	-0.000935	0.003826
Li	1s	0.000075	-0.000757	0.991593	0.0	0.0	-0.001684	-0.128113
	1s'	-0.000030	0.000230	-0.036912	0.0	0.0	0.000046	0.003600
	2s	0.001384	-0.009805	0.003021	0.0	0.0	0.008544	0.828570
	2s'	-0.000127	0.000752	0.006364	0.0	0.0	0.001439	-0.043159
	2s''	0.000001	0.000061	0.007574	0.0	0.0	-0.000041	-0.006297
	2px	0.0	0.0	0.0	-0.002584	0.0	0.0	0.0
	2px'	0.0	0.0	0.0	0.000212	0.0	0.0	0.0
	2py	0.0	0.0	0.0	0.0	-0.002584	0.0	0.0
	2py'	0.0	0.0	0.0	0.0	0.000212	0.0	0.0
	2pz	0.001472	-0.010328	-0.002025	0.0	0.0	0.006748	0.250555
	2pz'	-0.000029	0.000142	-0.002400	0.0	0.0	0.001814	-0.003064

Table 50. Basis B wavefunction and energy terms for NaLi

Molecular Energy = -169.2124552969
Kinetic Energy = 169.1425396804
Potential Energy = -338.3549949773
Virial Ratio = 1.9995868176
Elec-Elec Repulsion = 74.4483564915
Elec-Nucl Attraction = -418.6983139554
Nucl-Nucl Repulsion = 5.8949624866
Wavefunction Norm = 1.0000000000

Coefficient Vectors and Eigenvalues

	Orbital	1A1	2A1	3A1	4A1	1E1x	1E1y	5A1
	Basis	-40.443180	-2.776407	-2.446015	-1.498893	-1.498766	-1.498766	-0.167503
Na	1s	-0.999476	-0.244085	-0.000044	-0.002415	0.0	0.0	-0.025185
	2s	0.005182	1.029719	0.000440	0.010822	0.0	0.0	0.138039
	2s'	-0.004206	-0.000946	-0.000022	0.000050	0.0	0.0	0.000448
	3s	-0.003648	0.010482	0.001029	0.000145	0.0	0.0	-0.408552
	3s'	-0.004691	-0.003888	-0.000373	-0.003848	0.0	0.0	-0.013347
	3s''	-0.007611	0.000890	0.000318	-0.001431	0.0	0.0	0.016002
	2px	0.0	0.0	0.0	0.0	0.999464	0.0	0.0
	2px'	0.0	0.0	0.0	0.0	-0.001351	0.0	0.0
	3px	0.0	0.0	0.0	0.0	-0.001856	0.0	0.0
	3px'	0.0	0.0	0.0	0.0	-0.001161	0.0	0.0
	2py	0.0	0.0	0.0	0.0	0.0	0.999464	0.0
	2py'	0.0	0.0	0.0	0.0	0.0	-0.001351	0.0
	3py	0.0	0.0	0.0	0.0	0.0	-0.001856	0.0
	3py'	0.0	0.0	0.0	0.0	0.0	-0.001161	0.0
	2pz	-0.000026	0.007790	-0.000080	-0.999227	0.0	0.0	-0.039085
	2pz'	-0.000108	-0.001140	0.000153	0.001202	0.0	0.0	0.000645
	3pz	-0.000687	0.004977	-0.000674	0.003722	0.0	0.0	0.000668
	3pz'	0.000137	-0.000422	-0.001289	0.001404	0.0	0.0	-0.020882
Li	1s	-0.000039	0.000314	0.997766	0.001313	0.0	0.0	-0.118911
	1s'	-0.000003	-0.000143	-0.039230	-0.000128	0.0	0.0	0.006022
	2s	-0.001068	0.007044	0.003832	0.001294	0.0	0.0	0.696118
	2s'	0.000230	-0.001632	-0.001210	-0.000802	0.0	0.0	-0.075160
	2s''	-0.000151	0.000765	0.002860	0.000413	0.0	0.0	0.003413
	2px	0.0	0.0	0.0	0.0	-0.000003	0.0	0.0
	2px'	0.0	0.0	0.0	0.0	-0.000191	0.0	0.0
	2py	0.0	0.0	0.0	0.0	0.0	-0.000003	0.0
	2py'	0.0	0.0	0.0	0.0	0.0	-0.000191	0.0
	2pz	-0.000752	0.005097	-0.000595	0.001294	0.0	0.0	0.162469
	2pz'	0.000281	-0.001840	-0.002390	-0.000934	0.0	0.0	0.007075

Table 51. Basis A wavefunction and energy terms for NaLi$_2^+$

Molecular Energy = -176.2794698430
Kinetic Energy = 175.8723279799
Potential Energy = -352.1517978229
Virial Ratio = 1.9976903614
Elec-Elec Repulsion = 80.2168346290
Elec-Nucl Attraction = -444.6589019225
Nucl-Nucl Repulsion = 12.2902694706
Wavefunction Norm = 1.0000000000

Coefficient Vectors and Eigenvalues

	Orbital	1A1	2A1	3A1	1B1	2B1	1B2	4A1	5A1
	Basis	-40.624468	-2.961253	-2.607688	-2.607596	-1.677540	-1.677212	-1.676845	-0.343851
Li	1s	0.0	-0.000164	0.701259	-0.701023	-0.000009	0.0	-0.000512	-0.111926
	1s'	0.000001	0.000082	-0.026025	0.025884	0.000089	0.0	0.000025	0.008003
	2s	-0.000497	-0.003588	0.002761	0.002093	-0.004740	0.0	0.003402	0.458529
	2s'	0.000206	0.001414	0.004552	-0.004954	0.000557	0.0	-0.000009	-0.010752
	2s''	-0.000020	0.000059	0.005317	-0.005262	0.000050	0.0	-0.000111	-0.004238
	2px	0.000253	0.001781	0.001024	-0.004490	0.002074	0.0	-0.001800	-0.138841
	2px'	-0.000069	-0.000402	0.001585	-0.001081	0.000097	0.0	-0.000475	-0.024521
	2py	0.000710	0.005053	0.000817	-0.000885	0.003541	0.0	-0.003370	-0.125696
	2py'	-0.000080	-0.000525	0.000693	-0.000758	-0.000181	0.0	-0.000949	-0.005258
	2pz	0.0	0.0	0.0	0.0	0.0	0.001302	0.0	0.0
	2pz'	0.0	0.0	0.0	0.0	0.0	-0.000338	0.0	0.0
Li	1s	0.0	-0.000164	0.701259	0.701023	0.000009	0.0	-0.000512	-0.111926
	1s'	0.000001	0.000082	-0.026025	-0.025884	-0.000089	0.0	0.000025	0.008003
	2s	-0.000497	-0.003588	0.002761	-0.002093	0.004740	0.0	0.003402	0.458529
	2s'	0.000206	0.001414	0.004552	0.004954	-0.000557	0.0	-0.000009	-0.010752
	2s''	-0.000020	0.000059	0.005317	0.005262	-0.000050	0.0	-0.000111	-0.004238
	2px	-0.000253	-0.001781	-0.001024	-0.004490	0.002074	0.0	0.001800	0.138841
	2px'	0.000069	0.000402	-0.001585	-0.001081	0.000097	0.0	0.000475	0.024521
	2py	0.000710	0.005053	0.000817	0.000885	-0.003541	0.0	-0.003370	-0.125696
	2py'	-0.000080	-0.000525	0.000693	0.000758	0.000181	0.0	-0.000949	-0.005258
	2pz	0.0	0.0	0.0	0.0	0.0	0.001302	0.0	0.0
	2pz'	0.0	0.0	0.0	0.0	0.0	-0.000338	0.0	0.0
Na	1s	0.997933	-0.245075	-0.000051	0.0	0.0	0.0	0.002679	-0.020363
	2s	-0.047696	0.991035	0.000078	0.0	0.0	0.0	-0.011493	0.094004
	2s'	0.029908	0.019625	-0.000018	0.0	0.0	0.0	-0.000010	0.011608
	3s	0.019052	0.008833	-0.001451	0.0	0.0	0.0	0.006992	-0.193187
	3s'	0.042704	0.032811	-0.000230	0.0	0.0	0.0	0.003491	0.009614
	3s''	-0.030102	-0.023719	-0.000002	0.0	0.0	0.0	-0.000468	-0.019261
	2px	0.0	0.0	0.0	0.000022	0.999817	0.0	0.0	0.0
	2px'	0.0	0.0	0.0	0.000010	-0.006860	0.0	0.0	0.0
	3px	0.0	0.0	0.0	-0.001131	0.002233	0.0	0.0	0.0
	3px'	0.0	0.0	0.0	-0.000167	-0.000358	0.0	0.0	0.0
	2py	-0.000032	-0.008315	-0.000053	0.0	0.0	0.0	-1.000196	0.054539
	2py'	-0.000144	0.001010	0.000001	0.0	0.0	0.0	0.006522	-0.001393
	3py	0.000925	0.005945	0.000683	0.0	0.0	0.0	-0.003746	0.039667
	3py'	0.000021	0.000334	0.000304	0.0	0.0	0.0	-0.000348	0.010224
	2pz	0.0	0.0	0.0	0.0	0.0	-0.999943	0.0	0.0
	2pz'	0.0	0.0	0.0	0.0	0.0	0.006777	0.0	0.0
	3pz	0.0	0.0	0.0	0.0	0.0	-0.000380	0.0	0.0
	3pz'	0.0	0.0	0.0	0.0	0.0	0.000159	0.0	0.0

Table 52. Basis B wavefunction and energy terms for $NaLi_2^+$

Molecular Energy =	-176.5156587092	Elec-Elec Repulsion =	80.1649101851
Kinetic Energy =	176.4100295343	Elec-Nucl Attraction =	-445.1242502822
Potential Energy =	-352.9256882435	Nucl-Nucl Repulsion =	12.0336518536
Virial Ratio =	1.9994015875	Wavefunction Norm =	1.0000000000

Coefficient Vectors and Eigenvalues

	Orbital	1A1	2A1	3A1	1B1	2B1	1B2	4A1	5A1
	Basis	-40.621456	-2.953082	-2.620740	-2.620664	-1.676880	-1.676542	-1.676352	-0.346484
Li	1s	-0.000010	-0.000166	-0.705395	-0.706045	-0.000220	0.0	-0.000475	-0.111951
	1s'	-0.000007	0.000061	0.027655	0.027870	0.000027	0.0	0.000048	0.010048
	2s	-0.000531	-0.003463	-0.002281	-0.010827	-0.000537	0.0	-0.000547	0.395255
	2s'	0.000115	0.000815	0.000673	0.003457	0.000309	0.0	0.000358	0.007601
	2s''	-0.000070	-0.000274	-0.001725	-0.002911	-0.000073	0.0	-0.000095	-0.007844
	2px	0.000162	0.001063	0.000109	0.003619	0.000239	0.0	0.000086	-0.130966
	2px'	-0.000042	-0.000261	-0.001092	-0.004056	-0.000116	0.0	-0.000262	-0.041112
	2py	0.000450	0.003020	-0.000005	0.000403	0.000383	0.0	0.000756	-0.079319
	2py'	-0.000087	-0.000518	-0.000958	-0.001043	-0.000264	0.0	-0.000207	-0.019134
	2pz	0.0	0.0	0.0	0.0	0.0	-0.000021	0.0	0.0
	2pz'	0.0	0.0	0.0	0.0	0.0	-0.000102	0.0	0.0
Li	1s	-0.000010	-0.000166	-0.705395	0.706045	0.000220	0.0	-0.000475	-0.111951
	1s'	-0.000007	0.000061	0.027655	-0.027870	-0.000027	0.0	0.000048	0.010048
	2s	-0.000531	-0.003463	-0.002281	0.010827	0.000537	0.0	-0.000547	0.395255
	2s'	0.000115	0.000815	0.000673	-0.003457	-0.000309	0.0	0.000358	0.007601
	2s''	-0.000070	-0.000274	-0.001725	0.002911	0.000073	0.0	-0.000095	-0.007844
	2px	-0.000162	-0.001063	-0.000109	0.003619	0.000239	0.0	-0.000086	0.130966
	2px'	0.000042	0.000261	0.001092	-0.004056	-0.000116	0.0	0.000262	0.041112
	2py	0.000450	0.003020	-0.000005	-0.000403	-0.000383	0.0	0.000756	-0.079319
	2py'	-0.000087	-0.000518	-0.000958	0.001043	0.000264	0.0	-0.000207	-0.019134
	2pz	0.0	0.0	0.0	0.0	0.0	-0.000021	0.0	0.0
	2pz'	0.0	0.0	0.0	0.0	0.0	-0.000102	0.0	0.0
Na	1s	-0.999470	0.244046	0.000007	0.0	0.0	0.0	0.002312	-0.019549
	2s	0.005196	-1.029532	-0.000289	0.0	0.0	0.0	-0.010324	0.107037
	2s'	-0.004219	0.001040	-0.000009	0.0	0.0	0.0	-0.000046	-0.000546
	3s	-0.003608	-0.010051	-0.001251	0.0	0.0	0.0	-0.000148	-0.297979
	3s'	-0.004651	0.004159	-0.000164	0.0	0.0	0.0	0.003773	-0.023310
	3s''	-0.007619	-0.001006	-0.000264	0.0	0.0	0.0	0.001412	0.011426
	2px	0.0	0.0	0.0	-0.000130	-0.999757	0.0	0.0	0.0
	2px'	0.0	0.0	0.0	0.000110	0.001389	0.0	0.0	0.0
	3px	0.0	0.0	0.0	0.001188	0.001367	0.0	0.0	0.0
	3px'	0.0	0.0	0.0	-0.000428	0.000471	0.0	0.0	0.0
	2py	0.000029	0.007496	-0.000209	0.0	0.0	0.0	-0.999808	0.050798
	2py'	0.000100	-0.001117	0.000181	0.0	0.0	0.0	0.000920	-0.001322
	3py	0.000716	0.005160	-0.000590	0.0	0.0	0.0	0.002351	0.101656
	3py'	-0.000130	-0.000406	-0.000606	0.0	0.0	0.0	0.000004	0.036995
	2pz	0.0	0.0	0.0	0.0	0.0	0.999571	0.0	0.0
	2pz'	0.0	0.0	0.0	0.0	0.0	-0.001308	0.0	0.0
	3pz	0.0	0.0	0.0	0.0	0.0	-0.000710	0.0	0.0
	3pz'	0.0	0.0	0.0	0.0	0.0	-0.000208	0.0	0.0

Table 53. Basis A wavefunction and energy terms for Na_2

Molecular Energy = -323.0565713457
Kinetic Energy = 322.8009575123
Potential Energy = -645.8575288580
Virial Ratio = 1.9992087645
Elec-Elec Repulsion = 156.0389785637
Elec-Nucl Attraction = -824.2542309989
Nucl-Nucl Repulsion = 22.3577235772
Wavefunction Norm = 1.0000000000

Coefficient Vectors and Eigenvalues

	Orbital	1A2u	1A1g	2A1g	2A2u	3A1g	1E1ux	1E1uy	1E1gx
	Basis	-40.357951	-40.357918	-2.700318	-2.700138	-1.414035	-1.413639	-1.413639	-1.413016
Na	1s	-0.705651	0.705660	-0.173308	-0.173387	-0.002355	0.0	0.0	0.0
	2s	0.033789	-0.033665	0.701710	0.701005	0.010476	0.0	0.0	0.0
	2s'	-0.021154	0.021124	0.013834	0.013963	0.000056	0.0	0.0	0.0
	3s	-0.013180	0.014346	0.012514	0.004315	-0.000442	0.0	0.0	0.0
	3s'	-0.030212	0.030162	0.022834	0.022713	-0.002502	0.0	0.0	0.0
	3s''	0.021315	-0.021305	-0.016371	-0.016679	0.000562	0.0	0.0	0.0
	2px	0.0	0.0	0.0	0.0	0.0	0.705527	0.0	0.706126
	2px'	0.0	0.0	0.0	0.0	0.0	-0.004873	0.0	-0.004946
	3px	0.0	0.0	0.0	0.0	0.0	-0.004121	0.0	-0.001494
	3px'	0.0	0.0	0.0	0.0	0.0	-0.001956	0.0	-0.001560
	2py	0.0	0.0	0.0	0.0	0.0	0.0	0.705527	0.0
	2py'	0.0	0.0	0.0	0.0	0.0	0.0	-0.004873	0.0
	3py	0.0	0.0	0.0	0.0	0.0	0.0	-0.004121	0.0
	3py'	0.0	0.0	0.0	0.0	0.0	0.0	-0.001956	0.0
	2pz	0.000002	0.000025	0.008401	0.008429	-0.704342	0.0	0.0	0.0
	2pz'	-0.000174	0.000148	-0.001124	-0.000997	0.004694	0.0	0.0	0.0
	3pz	0.001207	0.000017	0.000688	-0.007725	0.003758	0.0	0.0	0.0
	3pz'	0.000206	0.000038	0.000512	-0.001400	0.003255	0.0	0.0	0.0
Na	1s	0.705651	0.705660	-0.173308	0.173387	-0.002355	0.0	0.0	0.0
	2s	-0.033789	-0.033665	0.701710	-0.701005	0.010476	0.0	0.0	0.0
	2s'	0.021154	0.021124	0.013834	-0.013962	0.000056	0.0	0.0	0.0
	3s	0.013180	0.014346	0.012514	-0.004314	-0.000442	0.0	0.0	0.0
	3s'	0.030212	0.030162	0.022834	-0.022713	-0.002502	0.0	0.0	0.0
	3s''	-0.021315	-0.021305	-0.016371	0.016679	0.000562	0.0	0.0	0.0
	2px	0.0	0.0	0.0	0.0	0.0	0.705527	0.0	-0.706126
	2px'	0.0	0.0	0.0	0.0	0.0	-0.004873	0.0	0.004946
	3px	0.0	0.0	0.0	0.0	0.0	-0.004121	0.0	0.001494
	3px'	0.0	0.0	0.0	0.0	0.0	-0.001956	0.0	0.001560
	2py	0.0	0.0	0.0	0.0	0.0	0.0	0.705527	0.0
	2py'	0.0	0.0	0.0	0.0	0.0	0.0	-0.004873	0.0
	3py	0.0	0.0	0.0	0.0	0.0	0.0	-0.004121	0.0
	3py'	0.0	0.0	0.0	0.0	0.0	0.0	-0.001956	0.0
	2pz	0.000002	-0.000025	-0.008401	0.008429	0.704342	0.0	0.0	0.0
	2pz'	-0.000174	-0.000148	0.001124	-0.000997	-0.004694	0.0	0.0	0.0
	3pz	0.001207	-0.000017	-0.000688	-0.007725	-0.003758	0.0	0.0	0.0
	3pz'	0.000206	-0.000038	-0.000512	-0.001400	-0.003255	0.0	0.0	0.0

Table 53. (Continued)

	Orbital	1E1gy	3A2u	4A1g
	Basis	-1.413016	-1.410150	-0.093837
Na	1s	0.0	0.003048	-0.036936
	2s	0.0	-0.013399	0.140231
	2s'	0.0	0.000140	0.014733
	3s	0.0	0.009702	-0.608983
	3s'	0.0	0.004788	-0.031279
	3s''	0.0	-0.000586	-0.030949
	2px	0.0	0.0	0.0
	2px'	0.0	0.0	0.0
	3px	0.0	0.0	0.0
	3px'	0.0	0.0	0.0
	2py	0.706126	0.0	0.0
	2py'	-0.004946	0.0	0.0
	3py	-0.001494	0.0	0.0
	3py'	-0.001560	0.0	0.0
	2pz	0.0	0.707313	-0.045943
	2pz'	0.0	-0.004716	0.001067
	3pz	0.0	0.001865	-0.059661
	3pz'	0.0	0.000307	-0.013767
Na	1s	0.0	-0.003048	-0.036936
	2s	0.0	0.013399	0.140231
	2s'	0.0	-0.000140	0.014733
	3s	0.0	-0.009702	-0.608983
	3s'	0.0	-0.004788	-0.031279
	3s''	0.0	0.000586	-0.030949
	2px	0.0	0.0	0.0
	2px'	0.0	0.0	0.0
	3px	0.0	0.0	0.0
	3px'	0.0	0.0	0.0
	2py	-0.706126	0.0	0.0
	2py'	0.004946	0.0	0.0
	3py	0.001494	0.0	0.0
	3py'	0.001560	0.0	0.0
	2pz	0.0	0.707313	0.045943
	2pz'	0.0	-0.004716	-0.001067
	3pz	0.0	0.001865	0.059661
	3pz'	0.0	0.000307	0.013767

Table 54. Basis B wavefunction and energy terms for Na_2

Molecular Energy =	-323.5579633245	Elec-Elec Repulsion =	153.2715669623
Kinetic Energy =	323.4560968202	Elec-Nucl Attraction =	-820.8848780434
Potential Energy =	-647.0140601447	Nucl-Nucl Repulsion =	20.5992509363
Virial Ratio =	1.9996851677	Wavefunction Norm =	1.0000000000

Coefficient Vectors and Eigenvalues

	Orbital	1A2u	1A1g	2A1g	2A2u	3A1g	1E1ux	1E1uy	1E1gx
	Basis	-40.428816	-40.428807	-2.762316	-2.762251	-1.485405	-1.484614	-1.484614	-1.484337
Na	1s	-0.706737	0.706733	-0.172633	-0.172608	0.001460	0.0	0.0	0.0
	2s	0.003668	-0.003686	0.727640	0.728202	-0.006262	0.0	0.0	0.0
	2s'	-0.002980	0.002948	-0.000609	-0.000638	-0.000052	0.0	0.0	0.0
	3s	-0.002619	0.001746	0.001943	0.007582	0.000933	0.0	0.0	0.0
	3s'	-0.003353	0.003365	-0.002346	-0.002532	0.002260	0.0	0.0	0.0
	3s''	-0.005403	0.005269	0.000290	0.000683	0.001087	0.0	0.0	0.0
	2px	0.0	0.0	0.0	0.0	0.0	0.706533	0.0	0.706795
	2px'	0.0	0.0	0.0	0.0	0.0	-0.000947	0.0	-0.000968
	3px	0.0	0.0	0.0	0.0	0.0	-0.001466	0.0	-0.001438
	3px'	0.0	0.0	0.0	0.0	0.0	-0.001079	0.0	-0.000883
	2py	0.0	0.0	0.0	0.0	0.0	0.0	0.706533	0.0
	2py'	0.0	0.0	0.0	0.0	0.0	0.0	-0.000947	0.0
	3py	0.0	0.0	0.0	0.0	0.0	0.0	-0.001466	0.0
	3py'	0.0	0.0	0.0	0.0	0.0	0.0	-0.001079	0.0
	2pz	0.000008	0.000050	0.005283	0.005016	0.705669	0.0	0.0	0.0
	2pz'	-0.000101	0.000033	-0.000886	-0.000642	-0.000766	0.0	0.0	0.0
	3pz	-0.000598	0.000029	0.000394	0.004256	-0.001945	0.0	0.0	0.0
	3pz'	0.000105	0.000004	0.000158	-0.000256	-0.001533	0.0	0.0	0.0
Na	1s	0.706737	0.706733	-0.172633	0.172608	0.001460	0.0	0.0	0.0
	2s	-0.003668	-0.003686	0.727640	-0.728202	-0.006262	0.0	0.0	0.0
	2s'	0.002980	0.002948	-0.000609	0.000638	-0.000052	0.0	0.0	0.0
	3s	0.002619	0.001746	0.001943	-0.007582	0.000933	0.0	0.0	0.0
	3s'	0.003353	0.003365	-0.002346	0.002532	0.002260	0.0	0.0	0.0
	3s''	0.005403	0.005269	0.000290	-0.000683	0.001087	0.0	0.0	0.0
	2px	0.0	0.0	0.0	0.0	0.0	0.706533	0.0	-0.706795
	2px'	0.0	0.0	0.0	0.0	0.0	-0.000947	0.0	0.000968
	3px	0.0	0.0	0.0	0.0	0.0	-0.001466	0.0	0.001438
	3px'	0.0	0.0	0.0	0.0	0.0	-0.001079	0.0	0.000883
	2py	0.0	0.0	0.0	0.0	0.0	0.0	0.706533	0.0
	2py'	0.0	0.0	0.0	0.0	0.0	0.0	-0.000947	0.0
	3py	0.0	0.0	0.0	0.0	0.0	0.0	-0.001466	0.0
	3py'	0.0	0.0	0.0	0.0	0.0	0.0	-0.001079	0.0
	2pz	0.000008	-0.000050	-0.005283	0.005016	-0.705669	0.0	0.0	0.0
	2pz'	-0.000101	-0.000033	0.000886	-0.000642	0.000766	0.0	0.0	0.0
	3pz	-0.000598	-0.000029	-0.000394	0.004256	0.001945	0.0	0.0	0.0
	3pz'	0.000105	-0.000004	-0.000158	-0.000256	0.001533	0.0	0.0	0.0

Table 54. (Continued)

	Orbital	1E1gy	3A2u	4A1g
	Basis	-1.484337	-1.483743	-0.153585
Na	1s	0.0	0.001729	0.027109
	2s	0.0	-0.007871	-0.129977
	2s'	0.0	-0.000034	-0.002218
	3s	0.0	0.000143	0.579522
	3s'	0.0	0.002645	0.006062
	3s''	0.0	0.000841	-0.015154
	2px	0.0	0.0	0.0
	2px'	0.0	0.0	0.0
	3px	0.0	0.0	0.0
	3px'	0.0	0.0	0.0
	2py	0.706795	0.0	0.0
	2py'	-0.000968	0.0	0.0
	3py	-0.001438	0.0	0.0
	3py'	-0.000883	0.0	0.0
	2pz	0.0	0.707350	0.035611
	2pz'	0.0	-0.000968	-0.000893
	3pz	0.0	-0.003078	0.050904
	3pz'	0.0	-0.000917	0.015784
Na	1s	0.0	-0.001729	0.027109
	2s	0.0	0.007871	-0.129977
	2s'	0.0	0.000034	-0.002218
	3s	0.0	-0.000143	0.579522
	3s'	0.0	-0.002645	0.006062
	3s''	0.0	-0.000841	-0.015154
	2px	0.0	0.0	0.0
	2px'	0.0	0.0	0.0
	3px	0.0	0.0	0.0
	3px'	0.0	0.0	0.0
	2py	-0.706795	0.0	0.0
	2py'	0.000968	0.0	0.0
	3py	0.001438	0.0	0.0
	3py'	0.000883	0.0	0.0
	2pz	0.0	0.707350	-0.035611
	2pz'	0.0	-0.000968	0.000893
	3pz	0.0	-0.003078	-0.050904
	3pz'	0.0	-0.000917	-0.015784

Table 55. Basis A wavefunction and energy terms for Na_2H^+

Molecular Energy =	-323.5730299124	Elec-Elec Repulsion =	150.5254112128
Kinetic Energy =	322.8810075939	Elec-Nucl Attraction =	-819.2827739421
Potential Energy =	-646.4540375063	Nucl-Nucl Repulsion =	22.3033252230
Virial Ratio =	1.9978613103	Wavefunction Norm =	1.0000000000

Coefficient Vectors and Eigenvalues

	Orbital	1A2u	1A1g	2A2u	2A1g	1E1ux	1E1uy	1E1gx	1E1gy
	Basis	-40.619616	-40.619594	-2.956961	-2.956885	-1.673967	-1.673967	-1.673947	-1.673947
Na	1s	0.705651	0.705646	-0.173196	-0.173231	0.0	0.0	0.0	0.0
	2s	-0.033644	-0.033640	0.701089	0.701136	0.0	0.0	0.0	0.0
	2s'	0.021172	0.021109	0.014008	0.013630	0.0	0.0	0.0	0.0
	3s	0.014419	0.013800	0.012987	0.008953	0.0	0.0	0.0	0.0
	3s'	0.030370	0.030028	0.024668	0.022585	0.0	0.0	0.0	0.0
	3s''	-0.021313	-0.021280	-0.016939	-0.016548	0.0	0.0	0.0	0.0
	2px	0.0	0.0	0.0	0.0	0.706977	0.0	0.707031	0.0
	2px'	0.0	0.0	0.0	0.0	-0.004934	0.0	-0.004950	0.0
	3px	0.0	0.0	0.0	0.0	0.000120	0.0	0.000546	0.0
	3px'	0.0	0.0	0.0	0.0	-0.000199	0.0	-0.000327	0.0
	2py	0.0	0.0	0.0	0.0	0.0	0.706977	0.0	0.707031
	2py'	0.0	0.0	0.0	0.0	0.0	-0.004934	0.0	-0.004950
	3py	0.0	0.0	0.0	0.0	0.0	0.000120	0.0	0.000546
	3py'	0.0	0.0	0.0	0.0	0.0	-0.000199	0.0	-0.000327
	2pz	0.000025	-0.000011	0.008601	0.008755	0.0	0.0	0.0	0.0
	2pz'	0.000140	0.000176	-0.001045	-0.001114	0.0	0.0	0.0	0.0
	3pz	-0.000043	-0.000463	0.000270	-0.002333	0.0	0.0	0.0	0.0
	3pz'	0.000208	-0.000240	0.001171	-0.001128	0.0	0.0	0.0	0.0
Na	1s	-0.705651	0.705646	0.173196	-0.173231	0.0	0.0	0.0	0.0
	2s	0.033644	-0.033640	-0.701089	0.701136	0.0	0.0	0.0	0.0
	2s'	-0.021172	0.021109	-0.014008	0.013630	0.0	0.0	0.0	0.0
	3s	-0.014419	0.013800	-0.012987	0.008953	0.0	0.0	0.0	0.0
	3s'	-0.030370	0.030028	-0.024668	0.022585	0.0	0.0	0.0	0.0
	3s''	0.021313	-0.021280	0.016939	-0.016548	0.0	0.0	0.0	0.0
	2px	0.0	0.0	0.0	0.0	0.706977	0.0	-0.707031	0.0
	2px'	0.0	0.0	0.0	0.0	-0.004934	0.0	0.004950	0.0
	3px	0.0	0.0	0.0	0.0	0.000120	0.0	-0.000546	0.0
	3px'	0.0	0.0	0.0	0.0	-0.000199	0.0	0.000327	0.0
	2py	0.0	0.0	0.0	0.0	0.0	0.706977	0.0	-0.707031
	2py'	0.0	0.0	0.0	0.0	0.0	-0.004934	0.0	0.004950
	3py	0.0	0.0	0.0	0.0	0.0	0.000120	0.0	-0.000546
	3py'	0.0	0.0	0.0	0.0	0.0	-0.000199	0.0	0.000327
	2pz	0.000025	0.000011	0.008601	-0.008755	0.0	0.0	0.0	0.0
	2pz'	0.000140	-0.000176	-0.001045	0.001114	0.0	0.0	0.0	0.0
	3pz	-0.000043	0.000463	0.000270	0.002333	0.0	0.0	0.0	0.0
	3pz'	0.000208	0.000240	0.001171	0.001128	0.0	0.0	0.0	0.0
H	1s	0.0	0.001107	0.0	0.008383	0.0	0.0	0.0	0.0
	1s'	0.0	-0.000625	0.0	-0.003618	0.0	0.0	0.0	0.0
	1s''	0.0	-0.000137	0.0	-0.000641	0.0	0.0	0.0	0.0
	2px	0.0	0.0	0.0	0.0	-0.001542	0.0	0.0	0.0
	2px'	0.0	0.0	0.0	0.0	0.000233	0.0	0.0	0.0
	2py	0.0	0.0	0.0	0.0	0.0	-0.001542	0.0	0.0
	2py'	0.0	0.0	0.0	0.0	0.0	0.000233	0.0	0.0
	2pz	0.000684	0.0	0.005075	0.0	0.0	0.0	0.0	0.0
	2pz'	-0.000533	0.0	-0.003283	0.0	0.0	0.0	0.0	0.0

Table 55. (Continued)

	Orbital Basis	3A1g -1.673222	3A2u -1.672909	4A1g -0.480457
Na	1s	0.002689	-0.002686	0.016856
	2s	-0.012273	0.012887	-0.076105
	2s'	0.000208	0.000644	-0.007987
	3s	0.002345	0.007223	0.152918
	3s'	0.004135	0.000540	-0.002577
	3s''	-0.000836	-0.000117	0.013362
	2px	0.0	0.0	0.0
	2px'	0.0	0.0	0.0
	3px	0.0	0.0	0.0
	3px'	0.0	0.0	0.0
	2py	0.0	0.0	0.0
	2py'	0.0	0.0	0.0
	3py	0.0	0.0	0.0
	3py'	0.0	0.0	0.0
	2pz	0.706746	-0.707886	0.087769
	2pz'	-0.004343	0.004597	-0.002651
	3pz	-0.000948	0.007605	0.082671
	3pz'	0.000575	0.003886	0.016230
Na	1s	0.002689	0.002686	0.016856
	2s	-0.012273	-0.012887	-0.076105
	2s'	0.000208	-0.000644	-0.007987
	3s	0.002345	-0.007223	0.152918
	3s'	0.004135	-0.000540	-0.002577
	3s''	-0.000836	0.000117	0.013362
	2px	0.0	0.0	0.0
	2px'	0.0	0.0	0.0
	3px	0.0	0.0	0.0
	3px'	0.0	0.0	0.0
	2py	0.0	0.0	0.0
	2py'	0.0	0.0	0.0
	3py	0.0	0.0	0.0
	3py'	0.0	0.0	0.0
	2pz	-0.706746	-0.707886	-0.087769
	2pz'	0.004343	0.004597	0.002651
	3pz	0.000948	0.007605	-0.082671
	3pz'	-0.000575	0.003886	-0.016230
H	1s	-0.011308	0.0	0.774122
	1s'	-0.002454	0.0	-0.133253
	1s''	-0.000067	0.0	-0.012517
	2px	0.0	0.0	0.0
	2px'	0.0	0.0	0.0
	2py	0.0	0.0	0.0
	2py'	0.0	0.0	0.0
	2pz	0.0	0.020210	0.0
	2pz'	0.0	-0.011383	0.0

Table 56. Basis B wavefunction and energy terms for Na_2H^+

Molecular Energy =	-323.9979842976	Elec-Elec Repulsion =	150.3919009855
Kinetic Energy =	323.8169033912	Elec-Nucl Attraction =	-820.0148774927
Potential Energy =	-647.8148876888	Nucl-Nucl Repulsion =	21.8080888184
Virial Ratio =	1.9994411048	Wavefunction Norm =	1.0000000000

Coefficient Vectors and Eigenvalues

	Orbital	1A2u	1A1g	2A2u	2A1g	1E1ux	1E1uy	1E1gx	1E1gy
	Basis	-40.622111	-40.622101	-2.954032	-2.954004	-1.678562	-1.678562	-1.678532	-1.678532
Na	1s	-0.706715	-0.706725	0.172578	-0.172543	0.0	0.0	0.0	0.0
	2s	0.003633	0.003717	-0.727122	0.727362	0.0	0.0	0.0	0.0
	2s'	-0.003002	-0.002986	0.000868	-0.000714	0.0	0.0	0.0	0.0
	3s	-0.001459	-0.001644	-0.000644	0.001434	0.0	0.0	0.0	0.0
	3s'	-0.002861	-0.003377	0.005253	-0.002095	0.0	0.0	0.0	0.0
	3s''	-0.005412	-0.005345	-0.000732	0.000736	0.0	0.0	0.0	0.0
	2px	0.0	0.0	0.0	0.0	0.707061	0.0	-0.707107	0.0
	2pz'	0.0	0.0	0.0	0.0	-0.001112	0.0	0.001126	0.0
	3px	0.0	0.0	0.0	0.0	-0.000325	0.0	0.000171	0.0
	3px'	0.0	0.0	0.0	0.0	-0.000188	0.0	-0.000021	0.0
	2py	0.0	0.0	0.0	0.0	0.0	0.707061	0.0	-0.707107
	2py'	0.0	0.0	0.0	0.0	0.0	-0.001112	0.0	0.001126
	3py	0.0	0.0	0.0	0.0	0.0	-0.000325	0.0	0.000171
	3py'	0.0	0.0	0.0	0.0	0.0	-0.000188	0.0	-0.000021
	2pz	-0.000049	-0.000016	-0.008240	0.008091	0.0	0.0	0.0	0.0
	2pz'	-0.000087	-0.000122	0.001199	-0.001083	0.0	0.0	0.0	0.0
	3pz	0.000078	0.000187	-0.000231	-0.000742	0.0	0.0	0.0	0.0
	3pz'	0.000675	0.000203	0.003560	-0.000792	0.0	0.0	0.0	0.0
Na	1s	0.706715	-0.706725	-0.172578	-0.172543	0.0	0.0	0.0	0.0
	2s	-0.003333	0.003717	0.727122	0.727362	0.0	0.0	0.0	0.0
	2s'	0.003002	-0.002986	-0.000868	-0.000714	0.0	0.0	0.0	0.0
	3s	0.001459	-0.001644	0.000644	0.001434	0.0	0.0	0.0	0.0
	3s'	0.002861	-0.003377	-0.005253	-0.002095	0.0	0.0	0.0	0.0
	3s''	0.005412	-0.005345	0.000732	0.000736	0.0	0.0	0.0	0.0
	2px	0.0	0.0	0.0	0.0	0.707061	0.0	0.707107	0.0
	2px'	0.0	0.0	0.0	0.0	-0.001112	0.0	-0.001126	0.0
	3px	0.0	0.0	0.0	0.0	-0.000325	0.0	-0.000171	0.0
	3px'	0.0	0.0	0.0	0.0	-0.000188	0.0	0.000021	0.0
	2py	0.0	0.0	0.0	0.0	0.0	0.707061	0.0	0.707107
	2py'	0.0	0.0	0.0	0.0	0.0	-0.001112	0.0	-0.001126
	3py	0.0	0.0	0.0	0.0	0.0	-0.000325	0.0	-0.000171
	3py'	0.0	0.0	0.0	0.0	0.0	-0.000188	0.0	0.000021
	2pz	-0.000049	0.000016	-0.008240	-0.008091	0.0	0.0	0.0	0.0
	2pz'	-0.000087	0.000122	0.001199	0.001083	0.0	0.0	0.0	0.0
	3pz	0.000078	-0.000187	-0.000231	0.000742	0.0	0.0	0.0	0.0
	3pz'	0.000675	-0.000203	0.003560	0.000792	0.0	0.0	0.0	0.0
H	1s	0.0	-0.000372	0.0	0.002998	0.0	0.0	0.0	0.0
	1s'	0.0	0.000180	0.0	-0.000646	0.0	0.0	0.0	0.0
	1s''	0.0	-0.000033	0.0	0.000338	0.0	0.0	0.0	0.0
	2px	0.0	0.0	0.0	0.0	0.000112	0.0	0.0	0.0
	2px'	0.0	0.0	0.0	0.0	-0.000682	0.0	0.0	0.0
	2py	0.0	0.0	0.0	0.0	0.0	0.000112	0.0	0.0
	2py'	0.0	0.0	0.0	0.0	0.0	-0.000682	0.0	0.0
	2pz	0.001444	0.0	0.008560	0.0	0.0	0.0	0.0	0.0
	2pz'	-0.000865	0.0	-0.004247	0.0	0.0	0.0	0.0	0.0

Table 56. (Continued)

	Orbital	3A1g	3A2u	4A1g
	Basis	-1.677769	-1.677378	-0.485503
Na	1s	-0.002450	0.002523	0.014991
	2s	0.010731	-0.011396	-0.089750
	2s'	0.000098	-0.000073	0.000870
	3s	-0.001366	0.000173	0.131866
	3s'	-0.003267	0.003410	0.015149
	3s''	-0.001478	0.001374	-0.007585
	2px	0.0	0.0	0.0
	2px'	0.0	0.0	0.0
	3px	0.0	0.0	0.0
	3px'	0.0	0.0	0.0
	2py	0.0	0.0	0.0
	2py'	0.0	0.0	0.0
	3py	0.0	0.0	0.0
	3py'	0.0	0.0	0.0
	2pz	-0.706678	0.707246	0.079401
	2pz'	0.000451	-0.000441	-0.000885
	3pz	0.000857	-0.001999	0.058202
	3pz'	-0.000061	0.000104	0.020780
Na	1s	-0.002450	-0.002523	0.014991
	2s	0.010731	0.011396	-0.089750
	2s'	0.000098	0.000073	0.000870
	3s	-0.001366	-0.000173	0.131866
	3s'	-0.003267	-0.003410	0.015149
	3s''	-0.001478	-0.001374	-0.007585
	2px	0.0	0.0	0.0
	2px'	0.0	0.0	0.0
	3px	0.0	0.0	0.0
	3px'	0.0	0.0	0.0
	2py	0.0	0.0	0.0
	2py'	0.0	0.0	0.0
	3py	0.0	0.0	0.0
	3py'	0.0	0.0	0.0
	2pz	0.706678	0.707246	-0.079401
	2pz'	-0.000451	-0.000441	0.000885
	3pz	-0.000857	-0.001999	-0.058202
	3pz'	0.000061	0.000104	-0.020780
H	1s	0.007912	0.0	0.799930
	1s'	0.002951	0.0	-0.168462
	1s''	0.000963	0.0	-0.024971
	2px	0.0	0.0	0.0
	2px'	0.0	0.0	0.0
	2py	0.0	0.0	0.0
	2py'	0.0	0.0	0.0
	2pz	0.0	0.000245	0.0
	2pz'	0.0	0.002652	0.0

Table 57. Basis A wavefunction and energy terms for Na_2Li^+

Molecular Energy = -330.4249274273
Kinetic Energy = 329.7550846642
Potential Energy = -660.1800120915
Virial Ratio = 1.9979727838

Elec-Elec Repulsion = 160.2217542894
Elec-Nucl Attraction = -850.1796623848
Nucl-Nucl Repulsion = 29.7778960039
Wavefunction Norm = 1.0000000000

Coefficient Vectors and Eigenvalues

	Orbital	1B1	1A1	2B1	2A1	3A1	4A1	3B1	1B2
	Basis	-40.609319	-40.609296	-2.946750	-2.946683	-2.577761	-1.662930	-1.662632	-1.662442
Na	1s	0.705646	0.705646	0.173290	-0.173301	-0.000053	-0.000352	-0.000104	0.0
	2s	-0.033747	-0.033705	-0.700618	0.701008	0.000073	0.001905	0.000598	0.0
	2s'	0.021171	0.021126	-0.014036	0.013731	-0.000022	-0.000089	-0.000086	0.0
	3s	0.013481	0.013533	-0.006293	0.006799	-0.001451	0.001786	0.000663	0.0
	3s'	0.030307	0.030096	-0.023871	0.022533	-0.000250	-0.000705	-0.000441	0.0
	3s''	-0.021300	-0.021276	0.016949	-0.016564	0.000008	0.000245	0.000147	0.0
	2px	0.000020	0.000013	-0.005139	0.005268	0.000046	-0.520644	0.382589	0.0
	2px'	0.000092	0.000097	0.000591	-0.000702	-0.000005	0.003473	-0.002680	0.0
	3px	-0.000760	-0.000224	0.004976	-0.001133	-0.000382	0.001875	0.001932	0.0
	3px'	0.000031	-0.000063	0.000035	-0.000283	-0.000151	0.000537	-0.000115	0.0
	2py	0.000012	0.000020	-0.003831	0.003806	0.000073	0.477760	-0.594523	0.0
	2py'	0.000065	0.000060	0.000469	-0.000437	-0.000005	-0.003311	0.004104	0.0
	3py	-0.000287	-0.000640	0.001787	-0.004232	-0.000715	0.000067	-0.001147	0.0
	3py'	-0.000008	-0.000008	0.000118	-0.000250	-0.000179	-0.000322	0.000425	0.0
	2pz	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.706877
	2pz'	0.0	0.0	0.0	0.0	0.0	0.0	0.0	-0.004794
	3pz	0.0	0.0	0.0	0.0	0.0	0.0	0.0	-0.000581
	3pz'	0.0	0.0	0.0	0.0	0.0	0.0	0.0	-0.000245
Na	1s	-0.705646	0.705646	-0.173290	-0.173302	-0.000053	-0.000352	0.000104	0.0
	2s	0.033749	-0.033704	0.700630	0.700996	0.000073	0.001905	-0.000598	0.0
	2s'	-0.021172	0.021125	0.014028	0.013739	-0.000022	-0.000089	0.000086	0.0
	3s	-0.013481	0.013532	0.006289	0.006804	-0.001451	0.001786	-0.000663	0.0
	3s'	-0.030308	0.030095	0.023860	0.022544	-0.000250	-0.000705	0.000441	0.0
	3s''	0.021301	-0.021275	-0.016941	-0.016571	0.000008	0.000245	-0.000147	0.0
	2px	0.000020	-0.000013	-0.005139	-0.005268	-0.000046	0.520644	0.382589	0.0
	2px'	0.000092	-0.000097	0.000591	0.000702	0.000005	-0.003473	-0.002680	0.0
	3px	-0.000760	0.000224	0.004976	0.001133	0.000382	-0.001875	0.001932	0.0
	3px'	0.000031	0.000063	0.000035	0.000283	0.000151	-0.000537	-0.000115	0.0
	2py	-0.000012	0.000020	0.003831	0.003806	0.000073	0.477760	0.594523	0.0
	2py'	-0.000065	0.000060	-0.000469	-0.000437	-0.000005	-0.003311	-0.004104	0.0
	3py	0.000287	-0.000640	-0.001787	-0.004232	-0.000715	0.000067	0.001147	0.0
	3py'	0.000008	-0.000008	-0.000118	-0.000250	-0.000179	-0.000322	-0.000425	0.0
	2pz	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.706877
	2pz'	0.0	0.0	0.0	0.0	0.0	0.0	0.0	-0.004794
	3pz	0.0	0.0	0.0	0.0	0.0	0.0	0.0	-0.000581
	3pz'	0.0	0.0	0.0	0.0	0.0	0.0	0.0	-0.000245
Li	1s	0.0	-0.000043	0.0	-0.000540	0.991611	-0.000016	0.0	0.0
	1s'	0.0	0.000018	0.0	0.000228	-0.036804	-0.000045	0.0	0.0
	2s	0.0	-0.001339	0.0	-0.009488	0.002465	0.002599	0.0	0.0
	2s'	0.0	0.000319	0.0	0.002126	0.006612	-0.000429	0.0	0.0
	2s''	0.0	-0.000026	0.0	0.000100	0.007531	-0.000036	0.0	0.0
	2px	-0.000760	0.0	0.005408	0.0	0.0	0.0	-0.003407	0.0
	2px'	0.000021	0.0	-0.000155	0.0	0.0	0.0	0.000122	0.0
	2py	0.0	-0.001309	0.0	-0.009205	-0.002761	0.001449	0.0	0.0
	2py'	0.0	0.000147	0.0	0.000886	-0.002474	-0.000039	0.0	0.0
	2pz	0.0	0.0	0.0	0.0	0.0	0.0	0.0	-0.002577
	2pz'	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.000508

Table 57. (Continued)

Orbital	Basis	1A2 -1.662358	5A1 -1.662082	4B1 -1.661651	6A1 -0.326630
Na	1s	0.0	-0.001997	0.002121	0.022414
	2s	0.0	0.008723	-0.008952	-0.099679
	2s'	0.0	-0.000079	-0.000130	-0.011993
	3s	0.0	-0.004121	0.006511	0.245445
	3s'	0.0	-0.002924	0.002279	-0.004485
	3s''	0.0	0.000495	-0.000179	0.020734
	2px	0.0	-0.477801	0.595080	0.047759
	2px'	0.0	0.003037	-0.003950	-0.001532
	3px	0.0	-0.000217	0.004299	0.066821
	3px'	0.0	0.000061	0.000326	0.014082
	2py	0.0	-0.520930	0.382591	0.028823
	2py'	0.0	0.003449	-0.002494	-0.000244
	3py	0.0	-0.001787	0.001257	-0.012252
	3py'	0.0	0.000013	0.000040	0.001349
	2pz	-0.707006	0.0	0.0	0.0
	2pz'	0.004827	0.0	0.0	0.0
	3pz	-0.000486	0.0	0.0	0.0
	3pz'	0.000320	0.0	0.0	0.0
Na	1s	0.0	-0.001997	-0.002121	0.022414
	2s	0.0	0.008723	0.008952	-0.099676
	2s'	0.0	-0.000079	0.000129	-0.011995
	3s	0.0	-0.004121	-0.006511	0.245444
	3s'	0.0	-0.002923	-0.002279	-0.004488
	3s''	0.0	0.000494	0.000179	0.020736
	2px	0.0	0.477801	0.595080	-0.047759
	2px'	0.0	-0.003037	-0.003950	0.001532
	3px	0.0	0.000217	0.004299	-0.066821
	3px'	0.0	-0.000061	0.000326	-0.014082
	2py	0.0	-0.520930	-0.382591	0.028823
	2py'	0.0	0.003449	0.002494	-0.000244
	3py	0.0	-0.001787	-0.001257	-0.012252
	3py'	0.0	0.000013	-0.000040	0.001349
	2pz	0.707006	0.0	0.0	0.0
	2pz'	-0.004827	0.0	0.0	0.0
	3pz	0.000486	0.0	0.0	0.0
	3pz'	-0.000320	0.0	0.0	0.0
Li	1s	0.0	0.001013	0.0	0.113072
	1s'	0.0	-0.000021	0.0	-0.004464
	2s	0.0	-0.008019	0.0	-0.656361
	2s'	0.0	-0.000518	0.0	0.024590
	2s''	0.0	0.000183	0.0	0.004727
	2px	0.0	0.0	0.003189	0.0
	2px'	0.0	0.0	0.001242	0.0
	2py	0.0	-0.006294	0.0	-0.282548
	2py'	0.0	-0.001824	0.0	-0.006825
	2pz	0.0	0.0	0.0	0.0
	2pz'	0.0	0.0	0.0	0.0

Table 58. Basis B wavefunction and energy terms for Na_2Li^+

Molecular Energy =	-330.8679808772	Elec-Elec Repulsion =	159.0549888601
Kinetic Energy =	330.6841363883	Elec-Nucl Attraction =	-848.9490862812
Potential Energy =	-661.5521172655	Nucl-Nucl Repulsion =	28.3419801556
Virial Ratio =	1.9994443570	Wavefunction Norm =	1.0000000000

Coefficient Vectors and Eigenvalues

	Orbital	1B1	1A1	2A1	2B1	3A1	4A1	3B1	1B2
	Basis	-40.613631	-40.513631	-2.945360	-2.945340	-2.614430	-1.669108	-1.668938	-1.668743
Na	1s	-0.706732	-0.706731	-0.172576	-0.172576	0.000001	-0.000203	-0.000242	0.0
	2s	0.003672	0.003684	0.727891	0.728006	0.000270	0.000856	0.001074	0.0
	2s'	-0.002980	-0.002981	-0.000717	-0.000725	-0.000001	0.000010	0.000008	0.0
	3s	-0.002543	-0.002355	0.005771	0.007124	0.001630	-0.000111	0.000106	0.0
	3s'	-0.003300	-0.003291	-0.002916	-0.002866	0.000054	-0.000321	-0.000371	0.0
	3s''	-0.005375	-0.005381	0.000707	0.000647	0.000232	-0.000135	-0.000148	0.0
	2px	-0.000017	-0.000019	0.004387	0.004428	-0.000098	-0.454523	0.271107	0.0
	2px'	-0.000059	-0.000058	-0.000638	-0.000676	0.000084	0.000591	-0.000404	0.0
	3px	-0.000513	-0.000194	0.001484	0.003696	-0.000172	0.000488	-0.000279	0.0
	3px'	0.000029	0.000120	-0.000603	0.000124	-0.000267	0.000177	-0.000145	0.0
	2py	-0.000011	-0.000008	0.002723	0.002729	-0.000153	0.541304	-0.652917	0.0
	2py'	-0.000037	-0.000039	-0.000404	-0.000403	0.000135	-0.000768	0.000875	0.0
	3py	-0.000191	-0.000428	0.002964	0.001417	0.000126	-0.000507	0.000982	0.0
	3py'	0.000048	0.000057	-0.000177	-0.000166	-0.000533	-0.000334	0.000316	0.0
	2pz	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.706957
	2pz'	0.0	0.0	0.0	0.0	0.0	0.0	0.0	-0.000916
	3pz	0.0	0.0	0.0	0.0	0.0	0.0	0.0	-0.000593
	3pz'	0.0	0.0	0.0	0.0	0.0	0.0	0.0	-0.000239
Na	1s	0.706732	-0.706731	-0.172576	0.172576	0.000001	-0.000203	0.000242	0.0
	2s	-0.003672	0.003684	0.727891	-0.728006	0.000270	0.000856	-0.001074	0.0
	2s'	0.002980	-0.002981	-0.000717	0.000725	-0.000001	0.000010	-0.000008	0.0
	3s	0.002543	-0.002355	0.005771	-0.007124	0.001630	-0.000111	-0.000106	0.0
	3s'	0.003300	-0.003291	-0.002916	0.002866	0.000054	-0.000321	0.000371	0.0
	3s''	0.005375	-0.005381	0.000707	-0.000647	0.000232	-0.000135	0.000148	0.0
	2px	-0.000017	0.000019	-0.004387	0.004428	0.000098	0.454523	0.271107	0.0
	2px'	-0.000059	0.000058	0.000638	-0.000676	-0.000084	-0.000591	-0.000404	0.0
	3px	-0.000513	0.000194	-0.001484	0.003696	0.000172	-0.000488	-0.000279	0.0
	3px'	0.000029	-0.000120	0.000603	0.000124	0.000267	-0.000177	-0.000145	0.0
	2py	0.000011	-0.000008	0.002723	-0.002729	-0.000153	0.541304	0.652917	0.0
	2py'	0.000037	-0.000039	-0.000404	0.000403	0.000135	-0.000768	-0.000875	0.0
	3py	0.000191	-0.000428	0.002964	-0.001417	0.000126	-0.000507	-0.000982	0.0
	3py'	-0.000048	0.000057	-0.000177	0.000166	-0.000533	-0.000334	-0.000316	0.0
	2pz	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.706957
	2pz'	0.0	0.0	0.0	0.0	0.0	0.0	0.0	-0.000916
	3pz	0.0	0.0	0.0	0.0	0.0	0.0	0.0	-0.000593
	3pz'	0.0	0.0	0.0	0.0	0.0	0.0	0.0	-0.000239
Li	1s	0.0	-0.000032	0.000394	0.0	0.997821	-0.000165	0.0	0.0
	1s'	0.0	-0.000008	-0.000149	0.0	-0.039171	0.000008	0.0	0.0
	2s	0.0	-0.001163	0.007516	0.0	0.005030	0.000120	0.0	0.0
	2s'	0.0	0.000262	-0.001807	0.0	-0.001733	0.000162	0.0	0.0
	2s''	0.0	-0.000144	0.000596	0.0	0.002901	-0.000038	0.0	0.0
	2px	-0.000405	0.0	0.0	0.002763	0.0	0.0	0.000444	0.0
	2px'	0.000087	0.0	0.0	-0.000519	0.0	0.0	-0.000270	0.0
	2py	0.0	-0.000761	0.005017	0.0	0.000474	-0.000019	0.0	0.0
	2py'	0.0	0.000206	-0.001267	0.0	-0.002818	0.000085	0.0	0.0
	2pz	0.0	0.0	0.0	0.0	0.0	0.0	0.0	-0.000004
	2pz'	0.0	0.0	0.0	0.0	0.0	0.0	0.0	-0.000168

Table 53. (Continued)

Orbital		5A1	1A2	4B1	6A1
Basis		-1.668717	-1.668665	-1.668369	-0.332554
Na	1s	-0.001548	0.0	0.001622	0.020272
	2s	0.006867	0.0	-0.007252	-0.108564
	2s'	0.000035	0.0	-0.000031	0.000137
	3s	0.000069	0.0	0.000238	0.331075
	3s'	-0.002574	0.0	0.002597	0.020187
	3s''	-0.000943	0.0	0.000992	-0.011776
	2px	-0.541197	0.0	0.653107	0.041445
	2px'	0.000509	0.0	-0.000629	-0.001231
	3px	0.001069	0.0	-0.001533	0.089229
	3px'	-0.000107	0.0	-0.000204	0.027116
	2py	-0.454598	0.0	0.271086	0.025058
	2py'	0.000472	0.0	-0.000227	-0.000620
	3py	0.001440	0.0	-0.000526	0.040312
	3py'	0.000163	0.0	0.000052	0.017256
	2pz	0.0	-0.707030	0.0	0.0
	2pz'	0.0	0.000920	0.0	0.0
	3pz	0.0	0.000530	0.0	0.0
	3pz'	0.0	0.000160	0.0	0.0
Na	1s	-0.001548	0.0	-0.001622	0.020272
	2s	0.006867	0.0	0.007252	-0.108564
	2s'	0.000035	0.0	0.000031	0.000137
	3s	0.000069	0.0	-0.000238	0.331075
	3s'	-0.002574	0.0	-0.002597	0.020187
	3s''	-0.000943	0.0	-0.000992	-0.011776
	2px	0.541197	0.0	0.653107	-0.041445
	2px'	-0.000509	0.0	-0.000629	0.001231
	3px	-0.001069	0.0	-0.001533	-0.089229
	3px'	0.000107	0.0	-0.000204	-0.027116
	2py	-0.454598	0.0	-0.271086	0.025058
	2py'	0.000472	0.0	0.000227	-0.000620
	3py	0.001440	0.0	0.000526	0.040312
	3py'	0.000163	0.0	-0.000052	0.017256
	2pz	0.0	0.707030	0.0	0.0
	2pz'	0.0	-0.000920	0.0	0.0
	3pz	0.0	-0.000530	0.0	0.0
	3pz'	0.0	-0.000160	0.0	0.0
Li	1s	0.000801	0.0	0.0	0.109959
	1s'	-0.000093	0.0	0.0	-0.008481
	2s	0.001632	0.0	0.0	-0.468636
	2s'	-0.000765	0.0	0.0	0.013832
	2s''	0.000226	0.0	0.0	0.005399
	2px	0.0	0.0	-0.000701	0.0
	2px'	0.0	0.0	0.000047	0.0
	2py	0.001197	0.0	0.0	-0.167017
	2py'	-0.000691	0.0	0.0	-0.032078
	2pz	0.0	0.0	0.0	0.0
	2pz'	0.0	0.0	0.0	0.0

Table 59. Basis A wavefunction and energy terms for Na$_3^+$

Molecular Energy = -484.5483813124
Kinetic Energy = 483.7281094451
Potential Energy = -968.2764907575
Virial Ratio = 1.9983071415

Elec-Elec Repulsion = 252.9142048200
Elec-Nucl Attraction = -1280.3786949253
Nucl-Nucl Repulsion = 59.1879993478
Wavefunction Norm = 1.0000000000

Coefficient Vectors and Eigenvalues

	Orbital	1E'	1E'	1A1'	2E'	2E'	2A1'	3E'	3E'
	Basis	-40.574266	-40.574266	-40.574214	-2.913241	-2.913241	-2.913144	-1.628759	-1.628758
Na	1s	0.803039	0.138009	-0.576165	-0.019630	0.199145	0.141476	-0.000244	-0.000421
	2s	-0.038421	-0.006603	0.027445	0.079362	-0.805138	-0.573019	0.001211	0.002093
	2s'	0.024097	0.004141	-0.017231	0.001593	-0.016158	-0.011132	-0.000041	-0.000071
	3s	0.015277	0.002625	-0.011757	0.000679	-0.006891	-0.010556	0.000744	0.001296
	3s'	0.034502	0.005930	-0.024545	0.002700	-0.027391	-0.018328	-0.000416	-0.000720
	3s''	-0.024252	-0.004168	0.017378	-0.001919	0.019470	0.013316	0.000136	0.000236
	2px	-0.000013	-0.000002	0.000019	-0.000711	0.007639	0.005540	0.416565	-0.077866
	2px'	-0.000146	-0.000026	0.000095	0.000044	-0.000909	-0.000764	-0.002824	0.000604
	3px	0.000868	0.000447	0.000079	0.002630	-0.005700	0.001003	-0.001524	-0.000416
	3px'	0.000044	0.000007	0.000004	0.000157	-0.000401	0.000208	-0.000838	-0.000082
	2py	0.000008	0.000002	-0.000011	0.000507	-0.004400	-0.003198	0.559069	-0.415755
	2py'	0.000085	0.000013	-0.000055	-0.000129	0.000515	0.000441	-0.003866	0.002819
	3py	-0.000616	0.000411	-0.000046	0.003212	0.003758	-0.000579	-0.001349	0.001525
	3py'	-0.000025	-0.000005	-0.000002	0.000178	0.000258	-0.000120	-0.000888	0.000838
	2pz	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
	2pz'	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
	3pz	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
	3pz'	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Na	1s	-0.282000	-0.764456	-0.576165	0.182280	-0.082573	0.141476	-0.000242	0.000421
	2s	0.013492	0.036575	0.027445	-0.736951	0.333839	-0.573019	0.001204	-0.002093
	2s'	-0.008462	-0.022939	-0.017231	-0.014790	0.006700	-0.011132	-0.000041	0.000071
	3s	-0.005365	-0.014543	-0.011757	-0.006307	0.002857	-0.010556	0.000752	-0.001293
	3s'	-0.012116	-0.032845	-0.024545	-0.025071	0.011357	-0.018328	-0.000415	0.000720
	3s''	0.008517	0.023087	0.017378	0.017821	-0.008073	0.013316	0.000136	-0.000236
	2px	-0.000004	-0.000013	-0.000019	-0.007005	0.003127	-0.005540	-0.415868	-0.078444
	2px'	-0.000052	-0.000139	-0.000095	0.000847	-0.000334	0.000764	0.002820	0.000608
	3px	0.000598	0.000772	-0.000079	0.004553	-0.004322	-0.001003	0.001528	-0.000413
	3px'	0.000015	0.000041	-0.000004	0.000330	-0.000278	-0.000208	0.000839	-0.000081
	2py	-0.000003	-0.000007	-0.000011	-0.004004	0.001894	-0.003198	0.558645	0.416761
	2py'	-0.000028	-0.000081	-0.000055	0.000446	-0.000288	0.000441	-0.003863	-0.002826
	3py	-0.000292	0.000681	-0.000046	0.004590	0.001834	-0.000579	-0.001345	-0.001527
	3py'	0.000009	0.000024	-0.000002	0.000302	0.000085	-0.000120	-0.000886	-0.000839
	2pz	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
	2pz'	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
	3pz	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
	3pz'	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Na	1s	-0.521038	0.626448	-0.576165	-0.162650	-0.116573	0.141476	0.000486	0.0
	2s	0.024929	-0.029972	0.027445	0.657589	0.471299	-0.573019	-0.002416	0.0
	2s'	-0.015635	0.018798	-0.017231	0.013197	0.009458	-0.011131	0.000082	0.0
	3s	-0.009912	0.011917	-0.011757	0.005628	0.004034	-0.010556	-0.001496	-0.000003
	3s'	-0.022386	0.026915	-0.024545	0.022371	0.016034	-0.018328	0.000831	0.0
	3s''	0.015736	-0.018919	0.017378	-0.015902	-0.011397	0.013316	-0.000272	0.0
	2px	0.0	0.0	0.0	0.000049	-0.000068	0.0	0.000715	-0.799135
	2px'	-0.000002	-0.000001	0.0	-0.000053	0.000073	0.0	-0.000005	0.005494
	3px	0.000452	0.000376	0.0	0.002398	-0.003345	0.0	-0.000001	0.002228
	3px'	0.0	0.0	0.0	0.000136	-0.000190	0.0	-0.000001	0.001371
	2py	0.000010	-0.000012	0.000022	-0.007200	-0.005160	0.006397	-0.162051	0.000002
	2py'	0.000110	-0.000132	0.000110	0.000853	0.000612	-0.000882	0.001023	0.0
	3py	-0.000688	0.000827	0.000091	0.005567	0.003989	0.001159	0.001297	0.000002
	3py'	-0.000033	0.000039	0.000004	0.000389	0.000279	0.000240	0.000565	0.0
	2pz	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
	2pz'	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
	3pz	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
	3pz'	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0

Table 59. (Continued)

Orbital		1A2''	3A1'	1E''	1E''	1A2'	4E'	4E'	4A1'
Basis		-1.628537	-1.628415	-1.628279	-1.628279	-1.627985	-1.626832	-1.626832	-0.296041
Na	1s	0.0	-0.001854	0.0	0.0	0.0	0.000780	-0.002835	-0.027563
	2s	0.0	0.008521	0.0	0.0	0.0	-0.003318	0.012062	0.107031
	2s'	0.0	-0.000102	0.0	0.0	0.0	-0.000031	0.000111	0.010204
	3s	0.0	0.000287	0.0	0.0	0.0	0.002511	-0.009124	-0.432207
	3s'	0.0	-0.002582	0.0	0.0	0.0	0.000928	-0.003373	-0.024843
	3s''	0.0	0.000618	0.0	0.0	0.0	-0.000079	0.000289	-0.021572
	2px	0.0	0.499071	0.0	0.0	-0.288619	-0.262231	0.646780	0.051078
	2px'	0.0	-0.003181	0.0	0.0	0.002029	0.001786	-0.004270	-0.001630
	3px	0.0	-0.002107	0.0	0.0	-0.000928	-0.002342	0.004054	0.106087
	3px'	0.0	-0.001091	0.0	0.0	0.000221	-0.000325	0.000449	0.023033
	2py	0.0	-0.288139	0.0	0.0	-0.499903	-0.029523	-0.423498	-0.029490
	2py'	0.0	0.001837	0.0	0.0	0.003515	0.000282	0.002829	0.000941
	3py	0.0	0.001216	0.0	0.0	-0.001607	-0.001280	-0.003064	-0.061249
	3py'	0.0	0.000630	0.0	0.0	0.000383	-0.000244	-0.000378	-0.013298
	2pz	-0.576748	0.0	-0.703178	0.414059	0.0	0.0	0.0	0.0
	2pz'	0.003938	0.0	0.004873	-0.002869	0.0	0.0	0.0	0.0
	3pz	0.002173	0.0	0.000036	-0.000021	0.0	0.0	0.0	0.0
	3pz'	0.000553	0.0	0.000766	-0.000451	0.0	0.0	0.0	0.0
Na	1s	0.0	-0.001854	0.0	0.0	0.0	-0.002845	0.000742	-0.027563
	2s	0.0	0.008521	0.0	0.0	0.0	0.012105	-0.003157	0.107031
	2s'	0.0	-0.000102	0.0	0.0	0.0	0.000112	-0.000029	0.010204
	3s	0.0	0.000287	0.0	0.0	0.0	-0.009157	0.002388	-0.432207
	3s'	0.0	-0.002582	0.0	0.0	0.0	-0.003385	0.000883	-0.024843
	3s''	0.0	0.000618	0.0	0.0	0.0	0.000290	-0.000076	-0.021572
	2px	0.0	-0.499071	0.0	0.0	-0.288619	-0.650525	0.253766	-0.051078
	2px'	0.0	0.003181	0.0	0.0	0.002029	0.004295	-0.001731	0.001630
	3px	0.0	0.002107	0.0	0.0	-0.000928	-0.004085	0.002286	-0.106087
	3px'	0.0	0.001091	0.0	0.0	0.000221	-0.000453	0.000318	-0.023033
	2py	0.0	-0.288139	0.0	0.0	0.499903	-0.422612	-0.035459	-0.029490
	2py'	0.0	0.001837	0.0	0.0	-0.003515	0.002821	0.000321	0.000941
	3py	0.0	0.001216	0.0	0.0	0.001607	-0.003048	-0.001321	-0.061249
	3py'	0.0	0.000630	0.0	0.0	-0.000383	-0.000375	-0.000249	-0.013298
	2pz	-0.576748	0.0	0.710175	0.401941	0.0	0.0	0.0	0.0
	2pz'	0.003938	0.0	-0.004922	-0.002786	0.0	0.0	0.0	0.0
	3pz	0.002173	0.0	-0.000036	-0.000020	0.0	0.0	0.0	0.0
	3pz'	0.000653	0.0	-0.000774	-0.000438	0.0	0.0	0.0	0.0
Na	1s	0.0	-0.001854	0.0	0.0	0.0	0.002065	0.002093	-0.027563
	2s	0.0	0.008521	0.0	0.0	0.0	-0.008787	-0.008904	0.107032
	2s'	0.0	-0.000102	0.0	0.0	0.0	-0.000081	-0.000082	0.010204
	3s	0.0	0.000287	0.0	0.0	0.0	0.006646	0.006736	-0.432208
	3s'	0.0	-0.002582	0.0	0.0	0.0	0.002458	0.002490	-0.024843
	3s''	0.0	0.000618	0.0	0.0	0.0	-0.000211	-0.000213	-0.021572
	2px	0.0	0.0	0.0	0.0	0.577239	-0.115953	0.114221	0.0
	2px'	0.0	0.0	0.0	0.0	-0.004059	0.000841	-0.000829	0.0
	3px	0.0	0.0	0.0	0.0	0.001856	-0.001682	0.001660	0.0
	3px'	0.0	0.0	0.0	0.0	-0.000443	-0.000275	0.000272	0.0
	2py	0.0	0.576277	0.0	0.0	0.0	-0.562340	-0.569839	0.058980
	2py'	0.0	-0.003674	0.0	0.0	0.0	0.003724	0.003774	-0.001883
	3py	0.0	-0.002432	0.0	0.0	0.0	-0.003673	-0.003724	0.122499
	3py'	0.0	-0.001259	0.0	0.0	0.0	-0.000421	-0.000427	0.026596
	2pz	-0.576748	0.0	-0.006997	-0.816000	0.0	0.0	0.0	0.0
	2pz'	0.003938	0.0	0.000049	0.005655	0.0	0.0	0.0	0.0
	3pz	0.002173	0.0	0.0	0.000042	0.0	0.0	0.0	0.0
	3pz'	0.000653	0.0	0.000008	0.000889	0.0	0.0	0.0	0.0

Table 60. Basis B wavefunction and energy terms for Na$_3^+$

Molecular Energy = -485.2201602420
Kinetic Energy = 484.9678757404
Potential Energy = -970.1880359824
Virial Ratio = 1.9994800618
Elec-Elec Repulsion = 247.4564043191
Elec-Nucl Attraction = -1271.6462254845
Nucl-Nucl Repulsion = 54.0017851830
Wavefunction Norm = 1.0000000000

Coefficient Vectors and Eigenvalues

Orbital		1E'	1E'	1A1'	2A1'	2E'	2E'	3E'	3E'
Basis		-40.604840	-40.604840	-40.604836	-2.936659	-2.936637	-2.936637	-1.660296	-1.660296
Na	1s	-0.037298	-0.815211	0.577041	0.140933	0.077603	-0.183551	-0.000289	-0.000045
	2s	0.000194	0.004239	-0.003033	-0.594017	-0.327344	0.774249	0.001253	0.000195
	2s'	-0.000157	-0.003436	0.002424	0.000550	0.000319	-0.000756	0.000013	0.000002
	3s	-0.000131	-0.002859	0.001366	-0.001104	-0.003011	0.007122	0.000065	0.000009
	3s'	-0.000175	-0.003818	0.002702	0.002261	0.001258	-0.002975	-0.000429	-0.000067
	3s''	-0.000283	-0.006193	0.004344	-0.000453	-0.000279	0.000661	-0.000188	-0.000029
	2px	0.000002	-0.000018	0.000023	-0.003626	-0.001994	0.004724	-0.063173	-0.416151
	2px'	-0.000006	-0.000070	0.000039	0.000539	0.000295	-0.000709	0.000043	0.000562
	3px	-0.000171	-0.000514	0.000024	-0.000312	-0.000542	0.003880	0.000226	0.000447
	3px'	-0.000012	0.000049	-0.000096	0.000571	0.000122	0.000083	0.000002	0.000253
	2py	-0.000005	-0.000010	0.000013	-0.002093	-0.001158	0.002725	-0.180992	0.675351
	2py'	0.000003	-0.000041	0.000022	0.000311	0.000180	-0.000405	0.000222	-0.000927
	3py	0.000241	-0.000312	0.000014	-0.000180	-0.002465	0.001330	0.000277	-0.000672
	3py'	0.000025	0.000027	-0.000056	0.000330	-0.000237	-0.000082	0.000091	-0.000422
	2pz	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
	2pz'	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
	3pz	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
	3pz'	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Na	1s	0.724643	0.375305	0.577041	0.140933	0.120158	0.158982	0.000184	-0.000228
	2s	-0.003768	-0.001951	-0.003033	-0.594017	-0.506847	-0.670613	-0.000796	0.000988
	2s'	0.003054	0.001582	0.002424	0.000550	0.000495	0.000654	-0.000008	0.000010
	3s	0.002541	0.001316	0.001366	-0.001104	-0.004662	-0.006169	-0.000041	0.000051
	3s'	0.003394	0.001758	0.002702	0.002261	0.001948	0.002577	0.000273	-0.000338
	3s''	0.005505	0.002851	0.004344	-0.000453	-0.000433	-0.000572	0.000119	-0.000148
	2px	-0.000017	-0.000006	-0.000023	0.003626	0.003089	0.004093	0.232109	0.351514
	2px'	-0.000061	-0.000035	-0.000039	-0.000539	-0.000459	-0.000615	-0.000345	-0.000446
	3px	-0.000395	-0.000371	-0.000024	0.000312	0.001475	0.003630	-0.000133	-0.000485
	3px'	0.000049	0.000010	0.000096	-0.000571	-0.000098	0.000110	-0.000168	-0.000188
	2py	0.000007	0.000009	0.000013	-0.002093	-0.001789	-0.002358	0.586683	0.380029
	2py'	0.000038	0.000015	0.000022	0.000311	0.000274	0.000349	-0.000786	-0.000539
	3py	0.000385	-0.000088	0.000014	-0.000180	-0.002716	-0.000687	-0.000655	-0.000313
	3py'	-0.000014	-0.000034	-0.000056	0.000330	-0.000209	0.000137	-0.000350	-0.000253
	2pz	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
	2pz'	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
	3pz	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
	3pz'	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Na	1s	-0.687345	0.439907	0.577041	0.140933	-0.197761	0.024569	0.000105	0.000273
	2s	0.003574	-0.002287	-0.003033	-0.594017	0.834191	-0.103636	-0.000457	-0.001183
	2s'	-0.002897	0.001854	0.002424	0.000550	-0.000814	0.000101	-0.000005	-0.000013
	3s	-0.002410	0.001543	0.001366	-0.001104	0.007674	-0.000953	-0.000024	-0.000061
	3s'	-0.003220	0.002061	0.002702	0.002261	-0.003205	0.000398	0.000156	0.000405
	3s''	-0.005222	0.003342	0.004344	-0.000453	0.000712	-0.000088	0.000068	0.000177
	2px	0.000003	0.000004	0.0	0.0	0.000001	0.000006	0.749293	-0.288075
	2px'	-0.000003	-0.000005	0.0	0.0	-0.000001	-0.000009	-0.001024	0.000394
	3px	-0.000159	-0.000248	0.0	0.0	0.000249	0.002009	-0.000761	0.000293
	3px'	-0.000015	-0.000023	0.0	0.0	0.000035	0.000286	-0.000465	0.000179
	2py	0.000018	-0.000011	-0.000026	0.004186	-0.005875	0.000730	-0.052876	-0.137127
	2py'	0.000069	-0.000044	-0.000045	-0.000622	0.000880	-0.000109	0.000054	0.000140
	3py	0.000507	-0.000324	-0.000028	0.000361	-0.004337	0.000538	0.000122	0.000315
	3py'	-0.000047	0.000030	0.000111	-0.000659	-0.000033	0.000004	0.000017	0.000044
	2pz	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
	2pz'	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
	3pz	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
	3pz'	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0

Table 60. (Continued)

	Orbital	3A1'	1A2''	1A2'	1E''	1E''	4E'	4E'	4A1'
	Basis	-1.660114	-1.660010	-1.659988	-1.659878	-1.659878	-1.659506	-1.659506	-0.318850
Na	1s	0.001227	0.0	0.0	0.0	0.0	0.001803	0.000426	0.021278
	2s	-0.005277	0.0	0.0	0.0	0.0	-0.008060	-0.001904	-0.107359
	2s'	-0.000039	0.0	0.0	0.0	0.0	-0.000035	-0.000008	-0.000518
	3s	0.000854	0.0	0.0	0.0	0.0	0.000413	0.000097	0.397607
	3s'	0.002054	0.0	0.0	0.0	0.0	0.002872	0.000678	0.017608
	3s''	0.000780	0.0	0.0	0.0	0.0	0.001090	0.000257	-0.011556
	2px	0.499584	0.0	-0.288648	0.0	0.0	0.693950	0.088276	0.039627
	2px'	-0.000500	0.0	0.000391	0.0	0.0	-0.000677	-0.000066	-0.001225
	3px	-0.000818	0.0	0.000462	0.0	0.0	-0.001671	-0.000014	0.090818
	3px'	0.000004	0.0	0.000167	0.0	0.0	-0.000242	0.000097	0.024041
	2py	0.288435	0.0	0.499953	0.0	0.0	0.361359	0.216349	0.022879
	2py'	-0.000289	0.0	-0.000677	0.0	0.0	-0.000342	-0.000243	-0.000707
	3py	-0.000472	0.0	-0.000800	0.0	0.0	-0.000767	-0.000841	0.052434
	3py'	0.000002	0.0	-0.000289	0.0	0.0	-0.000060	-0.000280	0.013880
	2pz	0.0	-0.577166	0.0	-0.816372	-0.003133	0.0	0.0	0.0
	2pz'	0.0	0.000747	0.0	0.001064	0.000004	0.0	0.0	0.0
	3pz	0.0	0.000539	0.0	0.000706	0.000003	0.0	0.0	0.0
	3pz'	0.0	0.000298	0.0	0.000265	0.000001	0.0	0.0	0.0
Na	1s	0.001227	0.0	0.0	0.0	0.0	-0.001270	0.001349	0.021278
	2s	-0.005277	0.0	0.0	0.0	0.0	0.005679	-0.006028	-0.107359
	2s'	-0.000039	0.0	0.0	0.0	0.0	0.000024	-0.000026	-0.000518
	3s	0.000854	0.0	0.0	0.0	0.0	-0.000291	0.000309	0.397607
	3s'	0.002054	0.0	0.0	0.0	0.0	-0.002024	0.002148	0.017608
	3s''	0.000780	0.0	0.0	0.0	0.0	-0.000768	0.000815	-0.011556
	2px	-0.499584	0.0	-0.288648	0.0	0.0	0.530433	-0.455781	-0.039627
	2px'	0.000500	0.0	0.000391	0.0	0.0	-0.000529	0.000428	0.001225
	3px	0.000818	0.0	0.000462	0.0	0.0	-0.001387	0.000931	-0.090818
	3px'	-0.000004	0.0	0.000167	0.0	0.0	-0.000255	0.000052	-0.024041
	2py	0.288435	0.0	-0.499953	0.0	0.0	-0.182680	0.379807	0.022879
	2py'	-0.000289	0.0	0.000677	0.0	0.0	0.000152	-0.000392	-0.000707
	3py	-0.000472	0.0	0.000800	0.0	0.0	0.000178	-0.001125	0.052434
	3py'	0.000002	0.0	0.000289	0.0	0.0	-0.000104	-0.000267	0.013880
	2pz	0.0	-0.577166	0.0	0.410899	-0.705432	0.0	0.0	0.0
	2pz'	0.0	0.000747	0.0	-0.000535	0.000919	0.0	0.0	0.0
	3pz	0.0	0.000539	0.0	-0.000355	0.000610	0.0	0.0	0.0
	3pz'	0.0	0.000298	0.0	-0.000133	0.000229	0.0	0.0	0.0
Na	1s	0.001227	0.0	0.0	0.0	0.0	-0.000533	-0.001774	0.021278
	2s	-0.005277	0.0	0.0	0.0	0.0	0.002381	0.007932	-0.107359
	2s'	-0.000039	0.0	0.0	0.0	0.0	0.000010	0.000034	-0.000518
	3s	0.000854	0.0	0.0	0.0	0.0	-0.000122	-0.000406	0.397607
	3s'	0.002054	0.0	0.0	0.0	0.0	-0.000848	-0.002826	0.017608
	3s''	0.000780	0.0	0.0	0.0	0.0	-0.000322	-0.001072	-0.011556
	2px	0.0	0.0	0.577296	0.0	0.0	0.141040	-0.042193	0.0
	2px'	0.0	0.0	-0.000782	0.0	0.0	-0.000175	0.000052	0.0
	3px	0.0	0.0	-0.000924	0.0	0.0	-0.000710	0.000213	0.0
	3px'	0.0	0.0	-0.000333	0.0	0.0	-0.000287	0.000086	0.0
	2py	-0.576870	0.0	0.0	0.0	0.0	0.230949	0.769245	-0.045757
	2py'	0.000578	0.0	0.0	0.0	0.0	-0.000224	-0.000746	0.001414
	3py	0.000945	0.0	0.0	0.0	0.0	-0.000541	-0.001802	-0.104868
	3py'	-0.000005	0.0	0.0	0.0	0.0	-0.000071	-0.000235	-0.027760
	2pz	0.0	-0.577166	0.0	0.405473	0.708565	0.0	0.0	0.0
	2pz'	0.0	0.000747	0.0	-0.000528	-0.000923	0.0	0.0	0.0
	3pz	0.0	0.000539	0.0	-0.000350	-0.000612	0.0	0.0	0.0
	3pz'	0.0	0.000298	0.0	-0.000131	-0.000230	0.0	0.0	0.0

Table 61. Mulliken population analyses for H_2

	Basis A			Basis B		
			Net Atom Population			
Atom	Core	Valence	Total	Core	Valence	Total
H	0.0	0.57519	0.57519	0.0	0.57578	0.57578
H	0.0	0.57519	0.57519	0.0	0.57578	0.57578
			Overlap Population			
Bond	Core	Valence	Total	Core	Valence	Total
H-H	0.0	0.84963	0.84963	0.0	0.84844	0.84844
			Gross Atom Population			
Atom	Core	Valence	Total	Core	Valence	Total
H	0.0	1.0	1.0	0.0	1.0	1.0
H	0.0	1.0	1.0	0.0	1.0	1.0

Table 62. Mulliken population analyses for H_3^+

	Basis A			Basis B		
			Net Atom Population			
Atom	Core	Valence	Total	Core	Valence	Total
H	0.0	0.29569	0.29569	0.0	0.30142	0.30142
H	0.0	0.29569	0.29569	0.0	0.30142	0.30142
H	0.0	0.29569	0.29569	0.0	0.30142	0.30142
			Overlap Population			
Bond	Core	Valence	Total	Core	Valence	Total
H-H	0.0	0.37097	0.37097	0.0	0.36524	0.36524
H-H	0.0	0.37097	0.37097	0.0	0.36524	0.36524
H-H	0.0	0.37097	0.37097	0.0	0.36524	0.36524
			Gross Atom Population			
Atom	Core	Valence	Total	Core	Valence	Total
H	0.0	0.66667	0.66667	0.0	0.66667	0.66667
H	0.0	0.66667	0.66667	0.0	0.66667	0.66667
H	0.0	0.66667	0.66667	0.0	0.66667	0.66667

Table 63. Mulliken population analyses for LiH

	Basis A			Basis B		
			Net Atom Population			
Atom	Core	Valence	Total	Core	Valence	Total
Li	1.99707	0.34537	2.34244	1.97967	0.29600	2.27567
H	0.00006	0.91118	0.91125	0.00083	0.97418	0.97501
			Overlap Population			
Bond	Core	Valence	Total	Core	Valence	Total
Li-H	0.00287	0.74344	0.74631	0.01950	0.72982	0.74932
			Gross Atom Population			
Atom	Core	Valence	Total	Core	Valence	Total
Li	1.99850	0.71709	2.71560	1.98942	0.66091	2.65033
H	0.00150	1.28291	1.28440	0.01058	1.33909	1.34967

Table 64. Mulliken population analyses for LiH_2^+

	Basis A			Basis B		
			Net Atom Population			
Atom	Core	Valence	Total	Core	Valence	Total
H	0.00000	0.55180	0.55181	0.00001	0.55157	0.55159
H	0.00000	0.55180	0.55181	0.00001	0.55157	0.55159
Li	2.00019	0.00627	2.00646	1.99746	0.00676	2.00422
			Overlap Population			
Bond	Core	Valence	Total	Core	Valence	Total
H-H	0.00000	0.83503	0.83503	0.00002	0.82450	0.82452
Li-H	-0.00010	0.02755	0.02745	0.00125	0.03279	0.03404
Li-H	-0.00010	0.02755	0.02745	0.00125	0.03279	0.03404
			Gross Atom Population			
Atom	Core	Valence	Total	Core	Valence	Total
H	-0.00005	0.98309	0.98305	0.00065	0.98022	0.98087
H	-0.00005	0.98309	0.98305	0.00065	0.98022	0.98087
Li	2.00009	0.03381	2.03390	1.99871	0.03956	2.03826

Table 65. Mulliken population analyses for Li_2

	Basis A			Basis B		
			Net Atom Population			
Atom	Core	Valence	Total	Core	Valence	Total
Li	1.99704	0.62619	2.62323	2.00465	0.59796	2.60261
Li	1.99704	0.62619	2.62323	2.00465	0.59796	2.60261
			Overlap Population			
Bond	Core	Valence	Total	Core	Valence	Total
Li-Li	0.00592	0.74763	0.75355	-0.00930	0.80407	0.79477
			Gross Atom Population			
Atom	Core	Valence	Total	Core	Valence	Total
Li	2.00000	1.00000	3.00000	2.00000	1.00000	3.00000
Li	2.00000	1.00000	3.00000	2.00000	1.00000	3.00000

Table 66. Mulliken population analyses for Li_2H^+

	Basis A			Basis B		
			Net Atom Population			
Atom	Core	Valence	Total	Core	Valence	Total
Li	1.99643	0.06685	2.06328	1.98925	0.07809	2.06815
Li	1.99643	0.06685	2.06328	1.98925	0.07809	2.06815
H	0.00005	1.16203	1.16208	0.00100	1.06040	1.06140
			Overlap Population			
Bond	Core	Valence	Total	Core	Valence	Total
Li-Li	0.00193	0.05964	0.06157	-0.00520	0.06524	0.06004
Li-H	0.00258	0.32232	0.32490	0.01204	0.35909	0.37113
Li-H	0.00258	0.32232	0.32490	0.01204	0.35909	0.37113
			Gross Atom Population			
Atom	Core	Valence	Total	Core	Valence	Total
Li	1.99868	0.25783	2.25651	1.99347	0.29026	2.28373
Li	1.99868	0.25783	2.25651	1.99347	0.29026	2.28373
H	0.00263	1.48435	1.48698	0.01305	1.41948	1.43253

Table 67. Mulliken population analyses for Li_3^+

	Basis A			Basis B		
			Net Atom Population			
Atom	Core	Valence	Total	Core	Valence	Total
Li	1.99733	0.29819	2.29552	2.00610	0.29288	2.29898
Li	1.99733	0.29819	2.29552	2.00610	0.29288	2.29898
Li	1.99733	0.29819	2.29552	2.00610	0.29288	2.29898
			Overlap Population			
Bond	Core	Valence	Total	Core	Valence	Total
Li-Li	0.00268	0.36847	0.37115	-0.00610	0.37379	0.36769
Li-Li	0.00268	0.36847	0.37115	-0.00610	0.37379	0.36769
Li-Li	0.00268	0.36847	0.37115	-0.00610	0.37379	0.36769
			Gross Atom Population			
Atom	Core	Valence	Total	Core	Valence	Total
Li	2.00000	0.66667	2.66667	2.00000	0.66667	2.66667
Li	2.00000	0.66667	2.66667	2.00000	0.66667	2.66667
Li	2.00000	0.66667	2.66667	2.00000	0.66667	2.66667

Table 68. Mulliken population analyses for NaH

	Basis A			Basis B		
			Net Atom Population			
Atom	Core	Valence	Total	Core	Valence	Total
Na	10.00923	0.25114	10.26037	9.99792	0.25672	10.25464
H	0.00043	1.18404	1.18447	0.00015	1.14231	1.14246
			Overlap Population			
Bond	Core	Valence	Total	Core	Valence	Total
Na-H	-0.00966	0.56482	0.55516	0.00194	0.60096	0.60290
			Gross Atom Population			
Atom	Core	Valence	Total	Core	Valence	Total
Na	10.00440	0.53355	10.53795	9.99889	0.55720	10.55609
H	-0.00440	1.46645	1.46205	0.00111	1.44280	1.44391

Table 69. Mulliken population analyses for NaH_2^+

	Basis A			Basis B		
			Net Atom Population			
Atom	Core	Valence	Total	Core	Valence	Total
H	0.00046	0.55995	0.56041	0.00005	0.57020	0.57025
H	0.00046	0.55995	0.56041	0.00005	0.57020	0.57025
Na	9.99644	0.00388	10.00032	9.99785	0.00338	10.00123
			Overlap Population			
Bond	Core	Valence	Total	Core	Valence	Total
H-H	-0.00062	0.84511	0.84449	-0.00004	0.85498	0.85494
Na-H	0.00163	0.01555	0.01718	0.00105	0.00062	0.00167
Na-H	0.00163	0.01555	0.01718	0.00105	0.00062	0.00167
			Gross Atom Population			
Atom	Core	Valence	Total	Core	Valence	Total
H	0.00097	0.99028	0.99125	0.00055	0.99800	0.99855
H	0.00097	0.99028	0.99125	0.00055	0.99800	0.99855
Na	9.99806	0.01944	10.01750	9.99890	0.00400	10.00290

Table 70. Mulliken population analyses for NaLi

	Basis A			Basis B		
			Net Atom Population			
Atom	Core	Valence	Total	Core	Valence	Total
Na	9.98669	0.18755	10.17424	10.00684	0.34337	10.35021
Li	2.00023	1.47378	3.47401	2.00057	1.01244	3.01301
			Overlap Population			
Bond	Core	Valence	Total	Core	Valence	Total
Na-Li	0.01308	0.33867	0.35175	-0.00742	0.64420	0.63678
			Gross Atom Population			
Atom	Core	Valence	Total	Core	Valence	Total
Na	9.99323	0.35688	10.35011	10.00313	0.66547	10.66860
Li	2.00677	1.64312	3.64989	1.99687	1.33453	3.33140

Table 71. Mulliken population analyses for $NaLi_2^+$

	Basis A			Basis B		
			Net Atom Population			
Atom	Core	Valence	Total	Core	Valence	Total
Li	1.99823	0.48316	2.48139	2.00425	0.35762	2.36187
Li	1.99823	0.48316	2.48139	2.00425	0.35762	2.36187
Na	9.99014	0.09671	10.08685	10.00594	0.20507	10.21101
			Overlap Population			
Bond	Core	Valence	Total	Core	Valence	Total
Li-Li	0.00371	0.60699	0.61070	-0.00777	0.46918	0.46141
Na-Li	0.00485	0.16499	0.16984	-0.00334	0.30526	0.30192
Na-Li	0.00485	0.16499	0.16984	-0.00334	0.30526	0.30192
			Gross Atom Population			
Atom	Core	Valence	Total	Core	Valence	Total
Li	2.00250	0.86915	2.87165	1.99870	0.74483	2.74353
Li	2.00250	0.86915	2.87165	1.99870	0.74483	2.74353
Na	9.99498	0.26171	10.25669	10.00260	0.51033	10.51293

Table 72. Mulliken population analyses for Na_2

	Basis A			Basis B		
			Net Atom Population			
Atom	Core	Valence	Total	Core	Valence	Total
Na	9.99475	0.74963	10.74438	10.00332	0.67130	10.67462
Na	9.99475	0.74963	10.74438	10.00332	0.67130	10.67462
			Overlap Population			
Bond	Core	Valence	Total	Core	Valence	Total
Na-Na	0.01050	0.50074	0.51124	-0.00663	0.65739	0.65076
			Gross Atom Population			
Atom	Core	Valence	Total	Core	Valence	Total
Na	10.00000	1.00000	11.00000	10.00000	1.00000	11.00000
Na	10.00000	1.00000	11.00000	10.00000	1.00000	11.00000

Table 73. Mulliken population analyses for Na_2H^+

	Basis A			Basis B		
			Net Atom Population			
Atom	**Core**	**Valence**	**Total**	**Core**	**Valence**	**Total**
Na	10.01131	0.07737	10.08868	9.99493	0.05950	10.05443
Na	10.01131	0.07737	10.08868	9.99493	0.05950	10.05443
H	0.00159	1.23342	1.23501	0.00037	1.33642	1.33679
			Overlap Population			
Bond	**Core**	**Valence**	**Total**	**Core**	**Valence**	**Total**
Na-Na	-0.00091	0.03041	0.02950	-0.00173	0.03572	0.03399
Na-H	-0.01165	0.29071	0.27906	0.00575	0.25443	0.26018
Na-H	-0.01165	0.29071	0.27906	0.00575	0.25443	0.26018
			Gross Atom Population			
Atom	**Core**	**Valence**	**Total**	**Core**	**Valence**	**Total**
Na	10.00502	0.23794	10.24296	9.99694	0.20457	10.20151
Na	10.00502	0.23794	10.24296	9.99694	0.20457	10.20151
H	-0.01005	1.52413	1.51408	0.00612	1.59085	1.59697

Table 74. Mulliken population analyses for Na_2Li^+

	Basis A			Basis B		
			Net Atom Population			
Atom	Core	Valence	Total	Core	Valence	Total
Na	9.99126	0.14692	10.13818	10.00490	0.24329	10.24819
Na	9.99126	0.14692	10.13818	10.00490	0.24329	10.24819
Li	2.00020	1.00278	3.00298	2.00111	0.48786	2.48897
			Overlap Population			
Bond	Core	Valence	Total	Core	Valence	Total
Na-Na	0.00247	0.07423	0.07670	-0.00132	0.23413	0.23281
Na-Li	0.00741	0.31458	0.32199	-0.00479	0.39571	0.39092
Na-Li	0.00741	0.31458	0.32199	-0.00479	0.39571	0.39092
			Gross Atom Population			
Atom	Core	Valence	Total	Core	Valence	Total
Na	9.99620	0.34132	10.33752	10.00185	0.55821	10.56006
Na	9.99620	0.34132	10.33752	10.00185	0.55821	10.56006
Li	2.00761	1.31736	3.32497	1.99632	0.88357	2.87989

Table 75. Mulliken population analyses for Na_3^+

	Basis A			Basis B		
			Net Atom Population			
Atom	Core	Valence	Total	Core	Valence	Total
Na	9.99513	0.40413	10.39926	10.00253	0.33824	10.34077
Na	9.99513	0.40413	10.39926	10.00253	0.33824	10.34077
Na	9.99513	0.40413	10.39926	10.00253	0.33824	10.34077
			Overlap Population			
Bond	Core	Valence	Total	Core	Valence	Total
Na-Na	0.00486	0.26254	0.26740	-0.00254	0.32843	0.32589
Na-Na	0.00486	0.26254	0.26740	-0.00254	0.32843	0.32589
Na-Na	0.00486	0.26254	0.26740	-0.00254	0.32843	0.32589
			Gross Atom Population			
Atom	Core	Valence	Total	Core	Valence	Total
Na	10.00000	0.66667	10.66667	10.00000	0.66667	10.66667
Na	10.00000	0.66667	10.66667	10.00000	0.66667	10.66667
Na	10.00000	0.66667	10.66667	10.00000	0.66667	10.66667

Table 76. Energy of $Li_2 \cdots Li^+$ system (Basis A)

		Gross Population	
h	Energy	Li_2	Li^+
10.0	-22.0813	5.694	2.305
12.5	-22.0660	5.808	2.193
15.0	-22.0588	5.890	2.110
20.0	-22.0564	6.000	2.000
25.0	-22.0559	6.000	2.000
30.0	-22.0557	6.000	2.000
limit of infinite separation	-22.0555	6.0	2.0

Table 77. Triatomic ion dissociation energies

Reaction	D (kcal/mole)	
	Basis A	Basis B
$H_3^+ \longrightarrow H^+ + H_2$	103.7	103.7
$LiH_2^+ \longrightarrow Li^+ + H_2$	5.7	5.2
$Li_2H^+ \longrightarrow Li^+ + LiH$	58.3	57.2
$Li_3^+ \longrightarrow Li^+ + Li_2$	45.0	41.8
$NaH_2^+ \longrightarrow Na^+ + H_2$	3.3	2.9
$NaLi_2^+ \longrightarrow Na^+ + Li_2$	33.4	31.2
$\longrightarrow Li^+ + NaLi$	54.9	44.0
$Na_2H^+ \longrightarrow Na^+ + NaH$	57.7	51.4
$Na_2Li^+ \longrightarrow Na^+ + NaLi$	39.2	33.6
$\longrightarrow Li^+ + Na_2$	92.1	48.3
$Na_3^+ \longrightarrow Na^+ + Na_2$	62.5	37.8

SUMMARY

The concept of an even-tempered atomic orbital basis has been introduced. The basis is shown to be a practical, as well as accurate replacement for traditional atomic orbital bases which depend on many non-linear parameters in an awkward and uneconomical manner. In SCF calculations on atoms, near Hartree-Fock accuracy, as well as calculational efficiency and speed has been obtained. For a wide variety of atoms, full optimization of the few even-tempered basis parameters was carried out economically.

For use in molecular calculations, "contracted" even-tempered Gaussian bases, i.e. linear combinations of even-tempered Gaussians are formed. An efficient method of assembling contracted two-electron integrals made possible the use of a new scheme for the definition of the contracted Gaussian atomic orbitals. It was shown to be energetically very competitive with the best prior method. Using the new contracted even-tempered Gaussian atomic orbital bases, several calculations on positive triatomic alkali ions were made and their significance discussed. The performance of the new basis in the molecular calculations was found to be excellent, showing economy and efficiency and causing no convergence problems.

APPENDIX A: DESCRIPTION OF THE ATOMIC SCF PROGRAM

General Specifications

The program used for all atomic calculations employing exponential basis functions is based on the well-known open-shell matrix Hartree-Fock procedure in terms of symmetry orbitals as given by Roothaan (9) and described following the introduction. It was of interest to find the best even-tempered bases for the atoms and so an optimization of the SCF atomic energy in terms of the even-tempered basis parameters of Eq. 22 was included. A modified version of Powell's program VA04A (124) for minimization of a non-linear function (125) was used and the accuracy of each parameter x was required to be $2 \cdot 10^{-3} \cdot x(\text{initial})$. The optimization of each symmetry was carried out independently beginning with s and proceeding through the p, d, and f shells before returning to s. Each symmetry proved to be largely independent of the next and often only one pass through each was necessary to achieve a stable energy with an accompanying good virial coefficient V/E.

A set of subroutines is incorporated to compute several atomic properties from the wavefunctions obtained. At completion, the wavefunction is punched onto cards which may be used as input for future runs. A restart feature was incorporated in order that system failure or a poor estimate of running time on the user's part would result in loss of a minimum amount of computation. Current information is stored on a peripheral device (disk file) at given time intervals and the supervisor program has an optional entry point which permits recovery of this information.

The basis size is limited so that main core size is kept at 128K bytes. This limitation only affects the section which carries out the formation of the $\mathcal{J}$ and $\underline{\mathcal{K}}$ symmetry averaged supermatrices. The consequence is that the largest basis for a given symmetry is fifteen exponential-type functions. If fifteen are used for one symmetry, all other symmetries must be twelve or less. A certain array is adjusted to 9260 elements which is $[n(n+1)/2]\bullet[m(m+1)/2]$ where $n=15$ and $m=12$. A basis of 195 primitives is possible if all four symmetries (s,p,d,f), with degeneracies (1,3,5,7), are used and if the numbers per symmetry are (15,12,12,12).

Sample running times for some typical atoms on an IBM 360/65 are:

Atom	State	Basis	Time/Energy (sec.)
O	^3P	(4,3)	5
Kr	^1S	(8,6,3)	13
S	^3P	(9,6)	18
Gd^{+3}	^8S	(10,8,5,4)	68
Ga	^2P	(12,9,4)	75
Rn	^1S	(12,10,6,3)	92

Matrix Elements

The integrals which represent the matrix elements in the procedure were programmed by this author. The one-electron integrals which are expectation values of one-electron operators $\hat{O}$, with respect to the primitive exponential basis functions defined in Eq. 19, (p=1).,

$$\langle X(klm)|\hat{O}|X(k'l'm')\rangle = \int dV\; X(klm)\;\hat{O}\;X(k'l'm')$$

are easily derived and are quite simple by virtue of the limitation to 1s, 2p, 3d, and 4f orbitals. The formulae are; overlap,

$$\langle X(klm)|X(k'l'm')\rangle = (\zeta_p/\zeta_a)^{2l+3}\;\delta(l,l')\;\delta(m,m')$$

nuclear attraction,

$$\langle X(klm)|-Z/r|X(k'l'm')\rangle = -Z\zeta_a\langle X(klm)|X(k'l'm')\rangle/(l+1)$$

and kinetic energy,

$$\langle X(klm)|-\Delta/2|X(k'l'm')\rangle = \zeta_p^2\langle X(klm)|X(k'l'm')\rangle/2$$

with

$$\zeta_a = (\zeta_k+\zeta_{k'})/2 \qquad \text{and} \qquad \zeta_p = (\zeta_k\zeta_{k'})^{1/2} \quad .$$

The symbol $\delta(i,j)$ is the ordinary Kronecker delta.

The expectation values of various powers of r comprise a set of one-electron integrals which form the essential part of several atomic properties. They can be expressed in a general form. If

$$I(l,n) = \langle X(klm)|r^n|X(k'lm)\rangle$$

it is easily shown that

$$I(l,n) = I(l,0)\,(\zeta_k+\zeta_{k'})^{-n}(2l+k+2)!/(2l+2)!, \quad (2l+k+2)\geq 0$$

where I(l,0) is the overlap integral given previously.

The two-electron integrals which are the expectation values of the two-electron operator r_{12}^{-1} were programmed from a formula derived from the more general one given by Silver (126). Because of the symmetry restriction in the SCF procedure and because the primitive basis functions X(klm) are carriers for the irreducible representations of the three-dimensional orthogonal group, only integrals

$$[X_1X_2|X_3X_4] = [X(k_1l_1m_1)X(k_2l_2m_2)|X(k_3l_3m_3)X(k_4l_4m_4)]$$

where the pairs of quantum numbers $q\nu = (l_\nu, m_\nu)$ have a specific relationship must be computed. Either q1=q2 and q3=q4 or q1=q3 and q2=q4 (equivalently q1=q4 and q2=q3) must be satisfied. All other possibilities lead to integrals which are not required in the present SCF formalism. The special case q1=q2=q3=q4 is of course included. The two cases above must be provided for, with the special case treated best using formulae for the second.

Case 1: q1=q2 and q3=q4

$$[X_1X_2|X_3X_4] = \left[\frac{\left(\zeta_p^{\,12}\right)^{2l_1+3}\left(\zeta_p^{\,34}\right)^{2l_3+3}}{\zeta_a^{\,2l_1+2}\,\zeta_{a'}^{\,2l_3+2}\left(\zeta_a+\zeta_{a'}\right)}\right]$$

$$\times\left\{\tau_{a'}^{2l_3+2}\sum_{s=0}^{2l_1+1}\tau_a^s\;B_s+\tau_a^{2l_1+2}\sum_{t=0}^{2l_3+1}\tau_{a'}^t\;B_t{}'\right\}$$

with

$B_s = (n'+s+1)!\ A(s,n)$, $\qquad n = 2l_1+1$,

$B_t{}' = (n+t+1)!\ A(t,n')$, $\qquad n' = 2l_3+1$.

Case 2: q1=q3 and q2=q4

$$[X_1X_2|X_3X_4] = \left[\frac{\left(\zeta_p^{\,13}\right)^{2l_1+3}\left(\zeta_p^{\,24}\right)^{2l_2+3}}{\left(\zeta_a\zeta_{a'}\right)^{l_1+l_2+2}\left(\zeta_a+\zeta_{a'}\right)}\right]$$

$$\times\left\{\tau_{a'}^{l_1+l_2+2}\sum_{s=s^o}^{l_1+l_2+1}\tau_a^s\;B_s+\tau_a^{l_1+l_2+2}\sum_{s=s^o}^{l_1+l_2+1}\tau_{a'}^s\;B_s\right\}$$

with

$B_s = (n+s+1)!\ A(s,n)$, $\qquad n=l_1+l_2+1$.

The following definitions serve to complete the two-electron integral formulae:

$$\zeta_p^{ij} = (\zeta i \zeta j)^{1/2}$$

$$\zeta_a = (\zeta 1 + \zeta 2)/2, \qquad \zeta_{a'} = (\zeta 3 + \zeta 4)/2 ,$$

$$\tau_a = [\zeta_a/(\zeta_a+\zeta_{a'})] , \qquad \tau_{a'} = [\zeta_{a'}/(\zeta_a+\zeta_{a'})] ,$$

$$A(s,n) = P \sum_{l=l^o}^{l(max)} \frac{(n-l)!}{(n-s)!} \sum_{m,m'} \delta(m,m') \; Q(lmq1q2) \; Q(lmq3q4) ,$$

$$P = \prod_{\mu=1}^{4} (-1)^{\mu} \; (2l_{\mu}+1)^{1/2} ,$$

$$s^o = l^o = \max\{|l_1-l_2|,|l_3-l_4|,m^*\} ,$$

$$m^* = \min\{|m-|,|m+|\} ,$$

$$m\pm = \mathrm{sign}(m_1) \; \mathrm{sign}(m_2) \; ||m_1|\pm|m_2|| ,$$

$$m\pm' = \mathrm{sign}(m_3) \; \mathrm{sign}(m_4) \; ||m_3|\pm|m_4|| ,$$

$$\mathrm{sign}(m) = m/|m| , \qquad \mathrm{sign}(0) = +1 ,$$

$$l(max) = \min\{l_1+l_2, l_3+l_4, s\} ,$$

and $(l+l_1+l_2)$ must be even. The remaining quantities are:

$$Q(lm+q1q2) = e^{+}(m_1,m_2)(-1)^{m_1+m_2}[(1+\delta(0,m_1m_2))/2]^{1/2} \times \begin{pmatrix} l_1 & l_2 & l \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} l_1 & l_2 & l \\ |m_1| & |m_2| & -(|m_1|+|m_2|) \end{pmatrix}$$

$$Q(lm-q1q2) = e^{-}(m_1,m_2)(-1)^{M}[(1+\delta(m_1,m_2))/2]^{1/2} \times \begin{pmatrix} l_1 & l_2 & l \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} l_1 & l_2 & l \\ -|m_1| & |m_2| & (|m_1|-|m_2|) \end{pmatrix}$$

where $M = \max\{|m_1|,|m_2|\}$, the symbol

$$\begin{pmatrix} l & l' & l'' \\ m & m' & m'' \end{pmatrix}$$

is the Wigner 3j coefficient (127), and e^+ and e^- depend upon the signs of the product, (m_1m_2), and the sum, (m_1+m_2), according to

(m_1m_2)	(m_1+m_2)	e^+	e^-
+	+	1	1
+	-	-1	1
-	+	1	-1
-	-	1	1
-	0	1	0
0	+,0,-	1	0

The sums on m and m' in the definition of A(s,n) are each over the two values m+ and m-. The B's are considered constants and were computed once and for all for each set of possible basis parameters l and m where $0\le l\le 3$ and $-l\le m\le l$.

The basic integrals were computed in blocks with respect to the pairs of quantum numbers l and m, the cycles within the blocks being over the zetas. Because of this, it was easy to include a feature whereby only blocks of integrals which change in successive energy calculations are recomputed. In successive calculations, during an energy optimization, only the parameters of a single symmetry, are changed at one time. Thus only integrals over basis functions belonging to that symmetry will change. This may involve a relatively small fraction of the total number of basic integrals and consequently a large percentage of the integral computation time is saved.

After computation of the necessary basic integrals, a transformation of the naturally symmetry adapted two-electron integral supermatrices to "symmetry averaged" supermatrices

$$\mathcal{J}(lpql'rs) = (d_l d_{l'})^{-1} \sum_{mm'} \mathcal{J}(lmpql'm'rs)$$

and

$$\mathcal{K}(lpql'rs) = (d_l d_{l'})^{-1} \sum_{mm'} \mathcal{K}(lmpql'm'rs)$$

is carried out where $d_l=2l+1$ and the m summations run over all partners in the irrep l ($-l \leq m \leq l$). This serves to condense the number of integrals which must be handled during SCF iterations. Then the symmetry averaged supermatrices

$\mathcal{P}(ll')$ and $\mathcal{Q}(ll')$ as defined in Eqs. 17 and 18 are found. The coupling coefficients $A(ll')$ and $B(ll')$ in Eq. 18 are required for the open-shell calculations. Single open-shell coefficients used in this work are recorded in Table 78. All double open-shells were double half-filled shells for which the off-diagonal $(l' \neq l)$ coefficients are: $A(ll')=0$ and $B(ll')=-1$.

SCF Specifications

The Restricted Hartree-Fock program used is a highly revised version of Wahl's programs which form a part of the BISON system (11). It consists of the procedure which was described in the text and is essentially that of Roothaan and Bagus (9). The Fock equations are formed and solved separately for each symmetry l for both open and closed shells.

In order to aid convergence, a density extrapolation procedure was used. Unlike vector extrapolation, orthonormalization of extrapolated densities is not required. Along with the extrapolation, a density averaging technique was used. In the case where intermediate energies undergo an oscillatory behavior, convergence may often not be obtained. Averaging the prior two density matrices aids in damping the oscillation. The density extrapolation techniques were found satisfactory in all cases except one in which even a prior vector extrapolation technique failed. The atomic state under consideration, a ^1S state of carbon, was not important in this investigation and so the solution of this convergence problem was not pursued.

Table 78. Single open-shell coupling coefficients

l	Configu-ration	State	A	B
0	s^1	^2S	0	-1
1	p^1	^2P	1	1
1	p^2	^3P	1/4	-1/2
		^1D	11/20	13/10
		^1S	1	4
1	p^3	^4S	0	-1
		^2D	1/5	1/5
		^2P	1/3	1
1	p^4	^3P	1/16	-1/8
		^1D	11/80	13/40
		^1S	1/4	1
1	p^5	^2P	1/25	1/25
2	d^1	^2D	1	1
2	d^5	^6S	0	-1
3	f^1	^2F	1	1
3	f^7	^8S	0	-1

APPENDIX B: NON-ORTHOGONAL SCF ATOMIC ORBITALS

Discussion

The atomic orbitals of hydrogen can be formed by a Schmidt orthogonalization process. The 1s, 2s, 3s,... orbitals result from carrying out this process on the nodeless radial functions $\exp(-r)$, $r \exp(-r/2)$, $r^2\exp(-r/3)$, etc. Similarly, approximations to canonical SCF atomic orbitals of larger atoms formed from a minimal basis set can be expressed as the result of successive Schmidt orthogonalizations of certain Slater-type atomic orbitals; $\exp(-\zeta_1 r)$, $r \exp(-\zeta_2 r)$, $r^2\exp(-\zeta_3 r)$, etc. An inspection of the accurate canonical SCF atomic orbitals reveals that they too have similar character with respect to the functional form. The number of nodes increases with the quantum number, the inner lobes appearing to represent those admixtures of orbitals with lower quantum number required for Schmidt orthogonality.

Molecular calculations employing unscaled minimal basis set Slater-type atomic orbitals may be carried out with either these non-orthogonal functions or with the orthogonalized atomic functions. The result is the same. It is most convenient to work with a non-orthogonal basis since such a basis is composed of single analytic functions in terms of which the necessary integrals are usually computed. Hence, an additional transformation of integrals is avoided. If independent scale factors are to be introduced, then there exists two choices: (1) introduce a scale parameter for each of the non-orthogonal Slater-type atomic orbitals of the minimal basis set, or (2) introduce a scale parameter for each orthogonal canonical SCF atomic orbital. If the latter were done, then the orthogonality between orthogonal functions would not be preserved. Furthermore, this would result in an increase in the number of primitive basis orbitals, because the function comprising an inner lobe of some scaled outer atomic orbital will be different from that comprising the innermost scaled atomic orbital. Linear dependence problems would arise unless the scale factors were made sufficiently different. Moreover, the two scaling procedures would end up energetically different. It is believed here that the first scaling procedure, which is the one usually adopted for practical reasons, would also yield better energies.

A similar situation is to be expected when accurate SCF atomic orbitals are used as basis for minimal basis set molecular calculations, and it seems desirable to be able to form non-orthogonal nodeless radial functions whose Schmidt orthogonalization reproduces the exact canonical SCF atomic orbitals. Any one of these nodeless functions should represent one lobe with the same qualitative character as a term $r^{l}\exp(-\zeta r)$. Moreover one would expect that each of these non-orthogonal, nodeless, single-lobe functions would cover a much smaller domain of the radial coordinate than the original canonical SCF atomic orbitals. Consequently, if accurate SCF atomic orbitals are expressed as linear combinations of primitive exponentials or Gaussians, a smaller number of these primitives will be required to represent the nodeless SCF atomic orbitals to an accuracy equivalent to that in the case of the canonical SCF atomic orbitals. This will lead to a savings in computation time for the calculation of integrals between the SCF atomic orbitals. It stands to reason, that the mentioned advantages will also persist if the minimal basis set is expanded to a larger basis.

Inversion of the Schmidt Process

The desired "deorthogonalization" of the canonical SCF atomic orbitals is conceptually the inverse of the Schmidt orthogonalization. Since the deorthogonalization need only be carried out within a symmetry, only the radial part of the SCF atomic orbital has to be considered. Hence, if $q_i^o(r)$ are the radial parts of the orthogonal canonical orbitals and $q_k(r)$ those of the desired non-orthogonal orbitals, the inverse Schmidt process is expressed by

$$q_k(r) = \sum_{i=1}^{k} q_i^o(r)\ c_{ik} \qquad (k=2,3,\dots).$$

where the sum extends only up to k. This implies that the inverse Schmidt matrix $\underline{c}$ is triangular. The process is however not unique. There are infinitely many non-orthogonal bases whose Schmidt orthogonalization yields the same orthogonal basis. For this reason, some criterion must be introduced.

Criterion

In view of the stated objective, it seems reasonable to demand that each of the nodeless SCF atomic orbitals should have as little absolute overlap as possible with all nodeless SCF atomic orbitals with lower quantum number. Therefore, the radial part of the k-th non-orthogonal SCF atomic orbital $q_k(r)$ is chosen such that

$$(31) \qquad D(f) = \int_0^\infty r^2 dr \, |q_k(r)|^2 \, f(r)$$

is a minimum where f(r) is a function of the inner shell density. In order to maintain normalization, the usual constraint

$$\int_0^\infty r^2 dr |q_k(r)|^2 = 1$$

is imposed. Several likely functions of the inner shell density were tested for f(r). That one chosen was simply

$$f(r) = r^{-2} \sum_{j=1}^{k-1} |q_j(r)|^2 \quad .$$

The sum above is over all non-orthogonal SCF atomic orbitals of the same symmetry and inner to that one being deorthogonalized (viz. that in Eq. 31). Since the part of the orthogonal orbital which is to be removed in deorthogonalization is that closest to the origin, the factor r^{-2} diminishes the deemphasis of that region caused by the volume element r^2dr of Eq. 31.

Computational method

The method is recursive in nature. One proceeds to determine the k-th non-orthogonal atomic orbital after the previous ones $q_2(r)\ldots q_{k-1}(r)$ have already been found. Minimization of the integral $D(f)$ of Eq. 31 to determine the k-th non-orthogonal SCF atomic orbital $q_k(r)$ is equivalent to diagonalizing the k-dimensional matrix $\underline{D}^k$ which is the matrix of expectation values of $f(r)$ computed with respect to the orthogonal SCF atomic orbitals

$$(32) \qquad D_{ij}{}^k = \int r^2dr\; q_i{}^o(r)\; q_j{}^o(r)\; f(r).$$

That eigenvector corresponding to the smallest eigenvalue of $\underline{D}^k$ is the k-th non-orthogonal orbital which satisfies the proposed criterion. Hence for each non-orthogonal atomic orbital a new matrix diagonalization is required, which yields one additional non-orthogonal orbital. The procedure consists therefore of a sequence of diagonalizations of matrices whose orders successively increase by one.

The matrix elements of $\underline{D}^k$ are found by substituting expressions for $q_i^o(r)$ and $f(r)$ into Eq. 32. If

$$q_i^o(r) = \sum_l R_l(r)\ a_{il}^o \qquad (l=1,2,\ldots,m)$$

and

$$q_i(r) = \sum_l R_l(r)\ a_{il} \qquad (l=1,2,\ldots,m)$$

and $R_l(r)$ is the normalized radial part of the primitive basis functions, then

$$D_{ij}^{\ k} = \sum_{stuv} a_{is}^o\ a_{jt}^o\ \left(\sum_{l=1}^{k-1} a_{lu}\ a_{lv} \right) I(stuv)$$

with

$$I(stuv) = \int R_s(r)\ R_t(r)\ R_u(r)\ R_v(r)\ dr \quad .$$

A closed form expression for this integral is readily found for $R(r)$ of either exponential or Gaussian form using standard integral tables.

Origin adjustment

The procedure outlined above forms non-orthogonal orbitals which are very much like those desired. However, in most cases some residual nodal behavior still exists near the origin, and furthermore, the quantities $q_k(r)/r^l$ (l being the symmetry quantum number) do not go to zero at the origin. By further forcing the condition

$$(d/dr)^l q_k(r) = 0 \qquad (k=2,3,\ldots)$$

at the origin, even more acceptable orbitals which have this property may be formed. This is accomplished by adding enough of the innermost SCF atomic orbital of the particular symmetry to bring the value of $q_k(r)/r^l$ to zero at the origin for each new non-orthogonal orbital. Often some slight nodes persist, but the result is quite sufficient for the purposes outlined.

Example

The result of applying this process is illustrated in Table 79. The orthogonal orbitals shown are the three canonical SCF s-atomic orbitals of aluminum in ^2P ground state as given by Clementi (46). Each column corresponds to a linear combination of Slater-type orbitals characterized by exponents (zeta) and the principal quantum number n. The non-orthogonal orbitals were formed according to the above process and are expressed in terms of the same Slater-type orbitals. The inverse Schmidt matrix which effects the transformation is given. Note that the 1s SCF atomic orbital is left unchanged as prescribed. Radial plots of these orbitals are shown in Figures 3 and 4. These show clearly how much the orbitals are changed by the process and also how much the non-orthogonal orbitals resemble non-orthogonal Slater-type orbitals.

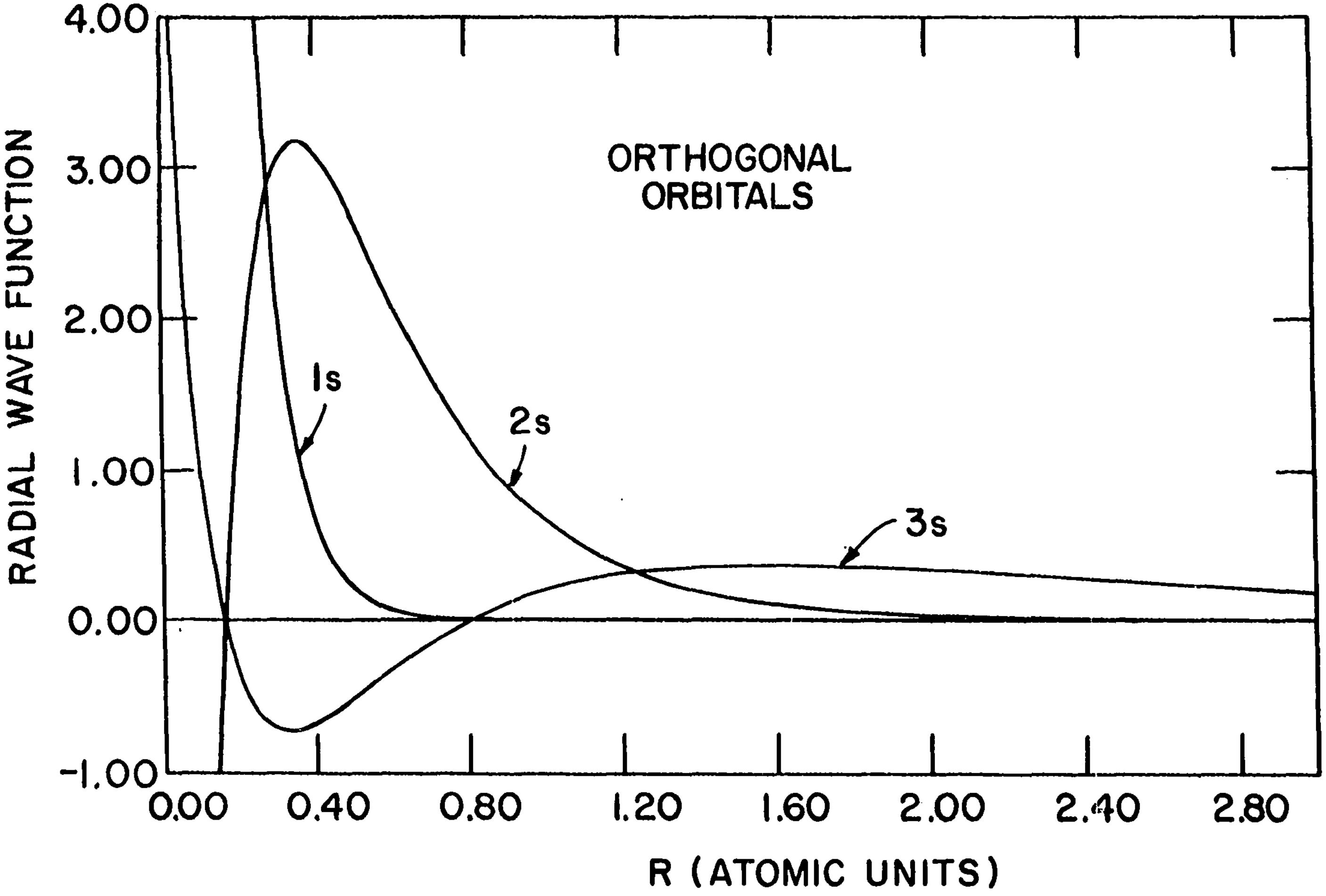

Figure 3. Orthogonal SCF s-atomic orbitals of aluminum

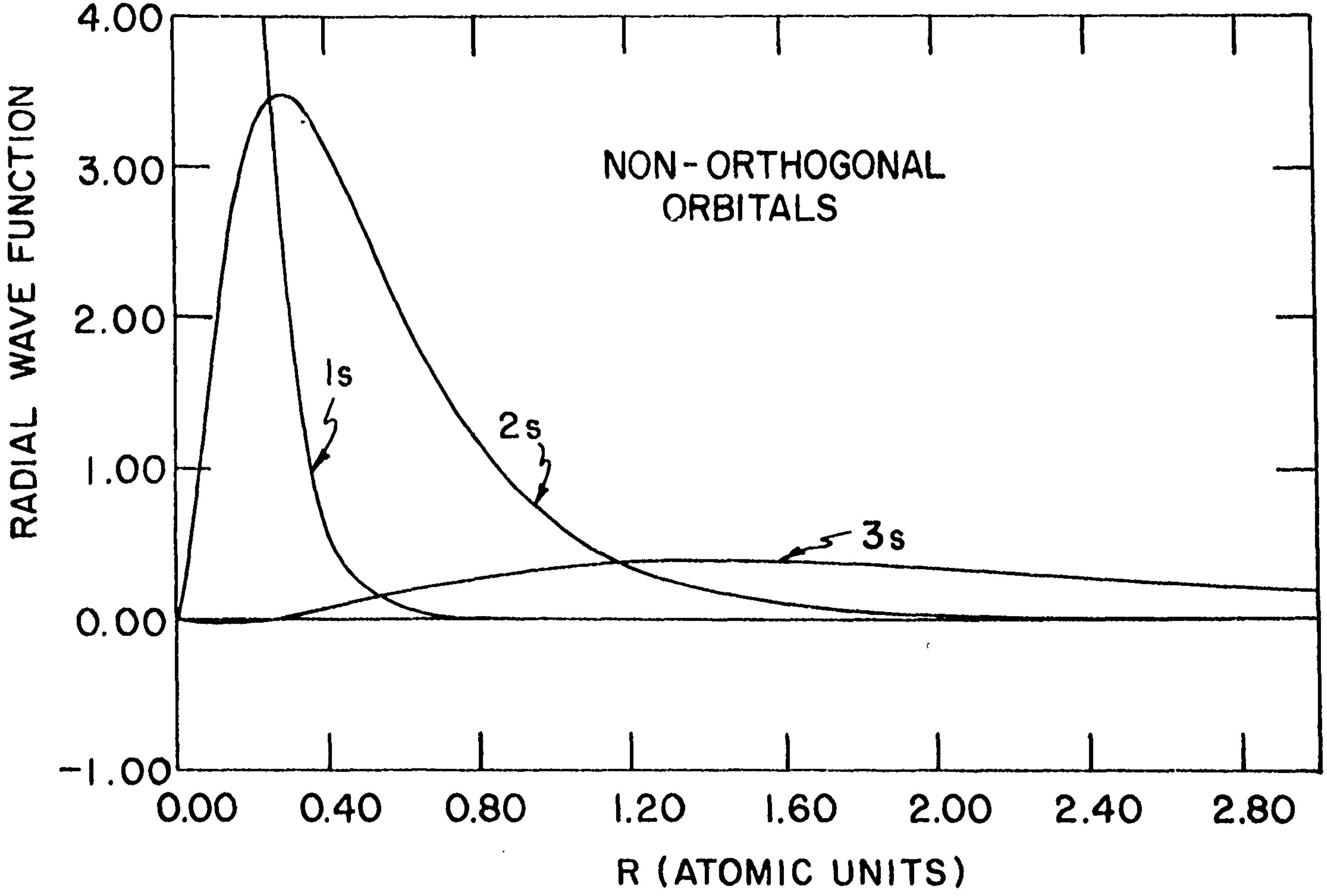

Figure 4. Non-orthogonal SCF s-atomic orbitals of aluminum

Table 79. Orthogonal and non-orthogonal aluminum orbitals

Primitives		Orthogonal	Orbitals	
n	Zeta	$a^{o}(1s)$	$a^{o}(2s)$	$a^{o}(3s)$
1	13.00000	0.96741	-0.25135	0.05804
3	14.71120	0.03493	-0.00465	0.00047
3	9.90000	0.01691	0.12045	-0.02622
3	7.10880	-0.00304	0.37640	-0.10400
3	4.74670	0.00178	0.55297	-0.13670
3	2.87680	-0.00048	0.05379	-0.10971
3	1.90290	0.00020	-0.01021	0.57002
3	1.11400	-0.00004	0.00178	0.59412

	Inverse	Schmidt Matrix	
	1s	2s	3s
$1s^{o}$	1.00000	0.25173	0.00279
$2s^{o}$		0.96888	0.23516
$3s^{o}$			0.97195

Primitives		Non-Orthogonal	Orbitals	
n	Zeta	a(1s)	a(2s)	a(3s)
1	13.00000	0.96741	0.0	0.00000
3	14.71120	0.03493	0.00429	-0.00054
3	9.90000	0.01691	0.12096	0.00289
3	7.10880	-0.00304	0.36392	-0.01258
3	4.74670	0.00178	0.53621	-0.00282
3	2.87680	-0.00048	0.05199	-0.09399
3	1.90290	0.00020	-0.00984	0.55163
3	1.11400	-0.00004	0.00171	0.57788

APPENDIX C: DESCRIPTION OF THE MOLECULAR SCF PROGRAM

In order to test the even-tempered Gaussian basis for molecular calculations, a new integral program, which takes into account certain properties of the basis, had to be designed. The most important and unique feature of the present basis is that several of the contracted functions forming the computational basis have contributions from the same even-tempered Gaussian primitive functions. This fact requires that integrals over contracted functions are formed by a general transformation of the integrals over primitive functions. Transformations of this sort are notoriously time consuming and must be carried out efficiently or else this scheme cannot be competitive with those in which segmented basis contractions are used. Certain algorithmic advantages accrue from the use of an even-tempered basis but all of these have not been provided for here in order that time would not be wasted "tooling up" for an approach which could turn out to be fruitless. Happily this was shown not to be the case. Certain advantages which were left out had been kept in mind so that appropriate modifications can easily be introduced into the programs as time permits.

Matrix Elements

Basic integrals

This package of subroutines was designed to provide integrals over Gaussians of only s and p symmetry. This limited set of Gaussians is alternately represented by normalized "cartesian" Gaussian functions

$$X(\underline{A},\zeta,l,m,n) = N(\zeta,l,m,n)\ x_A^{\,l} y_A^{\,m} z_A^{\,n} \exp(-\zeta r_A^2)$$

with

$$0 \le (l+m+n) \le 1, \qquad r_A^2 = x_A^2 + y_A^2 + z_A^2,$$

$$x_A = x - A_x, \qquad y_A = y - A_y, \qquad z_A = z - A_z,$$

and

$$N(\zeta,l,m,n) = (2/\pi)^{3/4} \left[\frac{\zeta^{l+m+n+3/2}}{(2l-1)!!(2m-1)!!(2n-1)!!} \right]^{\frac{1}{2}}$$

(in contrast to the real, normalized, "solid spherical" Gaussians of Eq. 19, p=2) and hence, the integral formulae, as given by Taketa et al. (64) and Huzinaga (128) for cartesian Gaussians were employed. In order that computation speed might be a maximum, the formulae were decomposed into special cases as far as was deemed worthwhile.

Contracted integrals

The transformation of primitive to contracted integrals required for use of the contracted functions as calculational basis need not involve all primitive integrals at once. Primitive functions with distinct values of the set of parameters ($\underline{A}$,l,m,n) contribute only to contracted functions which may be characterized by the same parameters. Moreover, the relation is also inverse. The integrals then can be divided into groups according to the atomic center (denoted by $\underline{A}$) and the orbital parameters (l,m,n) which are equivalent to the ordinary angular quantum numbers (l,m). For example, the most general electron repulsion integral would involve orbitals from four centers and four sets of orbital parameters. If each group or "block" of integrals so designated is not overly large, the calculation of primitive integrals and the transformation to contracted integrals may be efficiently done. Each primitive integral is computed and its contribution to each contracted integral in which it appears is made. The primitive integrals are not stored or recomputed. The calculations of blocks of integrals is done within cycles over the atomic centers and orbital parameters of such groups of primitives located on those centers. These cycles also take into account the index symmetries which prevail in one- and two-electron integrals so that only unique blocks are computed.

Because of the quantum number and atomic center cycling, it is easy to administer simple tests in order to determine whether an entire block is identically zero by symmetry. If such is the case, one simply skips the calculation and proceeds to the next block. This results of course, in a savings of considerable computation time.

It is apparent that the algorithm for contracting or transforming the primitive integrals is a very important feature. The procedure used is easiest to describe for the case of one-electron integrals which require a two-index transformation. The generalization to four indices is straightforward.

Suppose that the contracted functions involved are

$$G_i = \sum_{k=1}^{m_i} X_k \quad A_{ki} \qquad (i=1,2,\ldots,n_i)$$

and

$$G_j = \sum_{l=1}^{m_j} X_l \quad B_{lj} \qquad (j=1,2,\ldots,n_j)$$

Integrals over primitive functions X with a one-electron operator $\hat{O}$ are

$$O_{kl} = \int dV \; X_k \; \hat{O} \; X_l \quad .$$

The contracted integrals may be expressed by

$$(33)\qquad O_{ij}' = \int dV\, G_i\, \hat{O}\, G_j$$
$$= \sum_{kl} A_{ki}\, B_{lj}\, O_{kl} \quad .$$

This is the form of a general two index transformation, with the matrices $\underline{A}$ and $\underline{B}$ rectangular with $m_i \geq n_i$ and $m_j \geq n_j$. Given the matrix of primitive integrals, $\underline{O}$, it would be eminently simple to sum Eq. 33 for each element of $\underline{O}'$ separately. This would involve $2 \bullet m_i \bullet m_j$ multiplications for each element of $\underline{O}'$ or $2 \bullet m_i \bullet m_j \bullet n_i \bullet n_j$ multiplications altogether, independent of other operations which in general require less time than a multiplication. This method would be highly inefficient timewise and would require keeping the $m_i \bullet m_j$ elements of the matrix $\underline{O}$ available until all $n_i \bullet n_j$ elements of $\underline{O}'$ were computed.

The procedure developed for this work is based on the rearrangement of Eq. 33, namely

$$O_{ij}' = \sum_{k} T_{kj}\, A_{ki}$$

and

$$T_{kj} = \sum_{l} B_{lj}\, O_{kl} \quad .$$

Now, in computing, the order of operations is important. The program structure is given in Figure 5. Two outer program loops on k and l define the indices of $\underline{O}$. As soon as O_{kl} is computed, it is used to form values of T_j. Note that T_j need not be indexed by k in the algorithm since k is defined by an outer loop. When the index l is exhausted, the elements of the intermediate vector $\underline{T}$ are used to form their contribution to $\underline{O}'$. From the figure it is easy to see that $n_i \bullet n_j \bullet m_i$ + $n_j \bullet m_i \bullet m_j$ multiplications and $n_j(1+n_i)$ words of storage are required. A comparison to the simple approach mentioned previously shows a tremendous savings in multiplications and likewise in storage. The value of n_i or n_j is typically ≤6

```
Zero array $\underline{O}'$
    $k=1,2,\ldots,m_i$
        Zero array T
        $l=1,2,\ldots,m_j$
            Compute $O_{kl}$
            $j=1,2,\ldots,n_j$
                $T_j = T_j + B_{lj} \bullet O_{kl}$
        $i=1,2,\ldots,n_i$
            $j=1,2,\ldots,n_j$
                $O_{ij}' = O_{ij}' + A_{ki} \bullet T_j$
```

Figure 5. Program structure for a general two-index transformation

while m_i or m_j is ordinarily of the order of 10 for first row atoms to obtain fair accuracy (so-called double-zeta accuracy).

The generalization of this procedure to a four-index transformation

$$I(ijkl)' = \sum_{i'j'k'l'} A_{ii'}B_{jj'}C_{kk'}D_{ll'}I(i'j'k'l')$$

with

$$i=1,2,\ldots,n_i\ , \qquad i'=1,2,\ldots,m_i\ , \qquad m_i \geq n_i\ ,$$

etc., requires $n_l(1+n_k(1+n_j(1+n_i)))$ words of storage and $n_l \bullet m_l \bullet m_k \bullet m_j \bullet m_i + n_l \bullet n_k \bullet m_k \bullet m_j \bullet m_i + n_l \bullet n_k \bullet n_j \bullet m_j \bullet m_i +$ $n_l \bullet n_k \bullet n_j \bullet n_i \bullet m_i$ multiplications. A diagram of the program flow is shown in Figure 6. Arrays I1, I2, and I3 are temporary and correspond to $\underline{T}$ in the two index procedure. The space necessary for typical values of n is easily allocated in the main or fast core storage area. As a result, no input/output operations other than writing of the finished block of contracted integrals themselves are needed. This must be done in any case.

```
Zero array $I'$
$i'=1,2,..,m_i$
    Zero array $I3$
    $j'=1,2,..,m_j$
        Zero array $I2$
        $k'=1,2,..,m_k$
            Zero array $I1$
            $l'=1,2,..,m_l$
                Compute $I0 = I(i'j'k'l')$
                $l=1,2,..,n_l$
                    $I1(l) = I1(l) + D_{ll'} \cdot I0$
            $k=1,2,..,n_k$
                $l=1,2,..,n_l$
                    $I2(kl) = I2(kl) + C_{kk'} \cdot I1(l)$
        $j=1,2,..,n_j$
            $k=1,2,..,n_k$
                $l=1,2,..,n_l$
                    $I3(jkl) = I3(jkl) + B_{jj'} \cdot I2(kl)$
    $i=1,2,..,n_i$
        $j=1,2,..,n_j$
            $k=1,2,..,n_k$
                $l=1,2,..,n_l$
                    $I(ijkl)' = I(ijkl)' + A_{ii'} \cdot I3(jkl)$
```

Figure 6. Program structure for a general four-index transformation

Integral storage

The size of typical molecular bases requires calculation of large numbers of integrals which must be reused. Core sizes exclude the possibility of keeping these numbers close at hand and they must be stored on peripheral devices. There has recently been debate concerning the storage of two-electron integrals. On the one hand, if all integrals are computed and stored, then their order is defined by the order of calculation. Detractors of this method say that it requires the storage of zero integrals which are not used and of which there are often very many (perhaps as much as 25% or more of all unique integrals necessary for a molecule of high symmetry). Furthermore, programs which use the integrals are tied to the specific ordering pattern used. On the other hand, there are those who would store each non-zero integral in arbitrary order along with a label or word giving the four orbital indices and a code for the integral type. The type refers to index symmetries and tells how the integral is used in the calculation. This alleviates the order dependence of programs using the integrals. Detractors of this method would argue that an effectively random order is bad since the use of program loops, which often permit computational code optimization, is <u>not possible</u>. Any non-random ordering of the integrals is a lost advantage. Moreover, additional storage and input/output is needed for the labels. The labels must also be decoded, requiring the separation of one word into five and is often accomplished by using four division operations. The present program uses the best features of both methods. The ordering of the blocks of integrals is defined by loops and the blocks are stored and retrieved in this order. Zero blocks are not computed, stored, or otherwise used. Furthermore, a set of just ten integers is stored with a block of up to 6^4 integrals. Eight of these integers provide program loop limits to define basis function indices of a block. One integer specifies a particular set of loops to be used for specifying the indices. The last integer is the number of integrals in the block. This is in order to read the block from storage. Although the blocks may be randomly ordered, the integrals in each block are identified by use of a set of loops, allowing the possibility of explicit program optimization. A large share of the zeroes are eliminated and very little space is required for the index information. Integrals stored which are not needed are the ones which are not exactly zero but negligible. These occur most often for large molecules having several non-bonded atoms and are not a consideration in this work. A satisfactory method of storing just part of a block is not directly available with this technique. However, when integrals are used, their values are tested to determine if they are negligible with respect to the required accuracy. If so, work done with them is avoided.

SCF Specifications

The SCF program used for the molecular calculations is based on the standard Roothaan closed-shell method (7). It differs from the atomic programs by a direct formation of the Fock matrix $\underline{F}$ from the contracted basis function integrals as opposed to forming the symmetry adapted integrals described in Appendix A. This is sufficient since the program is just for closed-shell calculations.

In order to save computation time, a novel technique was introduced to separate the eigenvalue problem into subproblems according to the point group symmetry. In the case where no symmetry exists, a fast Givens algorithm is used to diagonalize the Fock matrix (Wilkinson, 129). When symmetry allows the problem to be broken up, a Jacobi technique is used because of the possible multiple degeneracies which occur (Greenstadt, 130). With the Jacobi diagonalization, no explicit orthogonalization of degenerate eigenvectors must be done. Though the Jacobi technique is slower, the sizes of matrices corresponding to each subproblem are smaller than the entire basis. This also compensates for its use.

Automatic construction of symmetry adapted basis functions

The Hamiltonian operator describing the interactions of particles comprising a molecule has the symmetry of the point group to which the molecule belongs. This symmetry is a consequence of the spatial configuration of the atomic nuclei. As a result, the canonical SCF orbitals, which form a solution to the Hartree-Fock equations, belong to irreducible representations or irreps of the point group. It is possible to make linear combinations of certain atomic orbital basis functions which are symmetry adapted functions and which therefore belong to irreps of the point group. If these symmetry adapted functions are used as basis for a molecular calculation, there will be no subsequent mixing among those basis functions belonging to separate irreps. Thus a molecular problem may be broken up into several smaller, largely independent sub-problems, one for each irrep. This is an advantage first of all because each sub-problem requires handling of smaller matrices and hence, less computation time and storage space is needed. For the full problem, all the matrices would be the size of the full basis, but would have many zeroes. Another advantage is that having broken the problem into symmetry species, one may easily select the electronic configuration or state to be determined by assigning electrons to orbitals belonging to the proper irreps.

This investigation makes use of a novel fully automatic scheme for constructing the symmetry adapted basis functions from the atomic orbital basis. It could fail if the original atomic basis were linearly dependent. Such bases are excluded for other obvious reasons.

The method is based on a general numerical approach to the construction of symmetry orbitals. It requires two operators which are invariant against the symmetry group. Diagonalization of the first yields symmetry adapted functions. Diagonalization or examination of the block diagonal form of the second in the symmetry adapted basis is necessary to recognize those functions belonging to the same irreps.

In the present approach the first operator is taken to be the projection operator in the space of all basis functions, i.e.

$$\rho(x|x') = \sum_{kl} |X_k\rangle\, S_{kl}^{-1} \langle X_l| \quad .$$

This operator is invariant with respect to all symmetry operations of the molecule since the set of all X's is naturally assumed to form a basis for a (reducible) representation of the symmetry group, i.e.

$$\hat{\rho}\,\hat{R} = \hat{R}\,\hat{\rho}$$

for all symmetry operators $\hat{R}$. The matrix of this operator becomes

$$\langle X_i | \hat{\rho} | X_j\rangle = \langle X_i | X_j\rangle = S_{ij} \quad ,$$

the overlap matrix. Thus the eigenvectors of the overlap matrix represent symmetry adapted orbitals. We modify these slightly by normalizing them to unity. Thus, they are defined by

$$|X'\rangle = |X\rangle \underline{T}$$

where

$$\underline{T} = \underline{U}\,\underline{S}^{-1/2}$$

with $\underline{U}$ being the orthogonal matrix ($\underline{U}^{+}=\underline{U}^{-1}$) that diagonalizes $\underline{S}$, i.e.

$$\underline{U}^{+}\underline{S}\,\underline{U} = \underline{S}_D,$$

with $\underline{S}_D$ being the resulting diagonal matrix.

It is apparent that the transformation of the basis, $|X\rangle$, with $\underline{T}$ is identical with Löwdin's canonical orthogonalization (89). Thus the resulting functions are not only symmetry adapted but also mutually orthogonal. Diagonalization of the matrix, $\langle X|\hat{O}|X\rangle$, of other symmetry invariant operators would in general not give orbitals, $|X'\rangle$, which are orthogonal with respect to the overlap.

In order to be able to handle the new functions, $|X'\rangle$, belonging to separate irreps together for each subproblem, they must be grouped with respect to that classification. Now, in the symmetry adapted basis $|X'\rangle$, the matrix of another specific operator $\hat{O}(\neq\hat{I})$, having the same molecular point group symmetry is,

$$\underline{O}' = \langle X'|O|X'\rangle = \underline{T}^{+}\langle X|O|X\rangle\underline{T} = \underline{T}^{+}\underline{O}\,\underline{T}\,.$$

This matrix will now have block form. In general the block form will *not* be that simple one in which the blocks all lie along the main diagonal. If the new matrix $\underline{O}'$ is now diagonalized, then each eigenvector belongs to an irrep and hence, has contributions from the symmetry adapted functions, $|X'\rangle$, belonging to that irrep. The eigenvectors may therefore be classified into groups with respect to irreps by use of the observation that those belonging to one irrep all have zeroes in the same rows while others have zeroes elsewhere. Finally, the eigenvectors of the matrix which diagonalizes $\underline{O}'$, i.e. its columns, are permuted so that those associated with a particular irrep are adjacent. This represents a new transformation $\underline{V}$ whose product with $\underline{T}$, i.e. $(\underline{TV})$, when applied to the matrix $\underline{U}$ of *any* operator $\hat{U}$ computed with respect to the original basis, produces a block diagonal matrix in which the blocks fall along the main diagonal:

$$(\underline{TV})^{+}\underline{U}\;(\underline{TV}) = \left[\begin{array}{c|c|c} \underline{U}_1 & & 0 \\ \hline & \underline{U}_2 & \\ \hline 0 & & \underline{U}_3 \end{array}\right]$$

In particular, if $\underline{U}$ is the Fock matrix, the problem of Eq. 7

is directly transformed to an ordinary eigenvalue equation and to convenient block form.

The operator $\hat{O}=\hat{H}_1$ was used here to gain another advantage. Since $\hat{H}_1$ can be considered as a very rough approximation to the Fock operator, its eigenvectors can be used as starting vectors for the self-consistent-field process. The ordering of the eigenvalues of $\hat{H}_1$ enable one to make an automatic assignment of a ground state configuration. This facility has proved useful in most cases. However, the omission of the important electron repulsion term and the resulting lack of nuclear screening by inner electrons has the consequence that the valence shells in particular are not well approximated. This leads to incorrect ground state configuration assignments and as such, the assignments must be adjusted.

It is apparent that because of the block diagonal form, one does not need a very precise diagonalization of $\underline{O}$ in order to recognize orbitals of the same irrep. In practice, diagonalization of the matrix of $\hat{O}$ was carried out by a Jacobi technique such that off-diagonal elements were brought to values approximately $10^{-3}\cdot$(average diagonal element).

General Specifications

The programs were designed to require a small amount of core storage so that under the present multiprogramming environment, short runs could be made frequently rather than only during periods of light work load. The program and primary I/O (read/write) buffers require 128K bytes of main core. Secondary I/O buffers are allocated to slow core. Large buffers are used to maintain efficiency and therefore 96K of slow core is required. This requirement is flexible however, since it is defined by job control input rather than the programs themselves. The efficiency of the program (central processor time, CPU, versus real or system residence time) depends on the number of electrons in a molecule, the number of primitive basis functions, and the number of contracted functions. For example, in typical runs on H_3^+ and Na_3^+ in the B bases, the total Real:CPU time ratios were 5.2:1 and 1.3:1 respectively. The efficiency increases as the amount of information processed increases. Table 80 includes more complete information on the program performance. Processing time is given for all molecule calculations for both integral and SCF steps and total run time is the sum of these. Integral time is highly dependent on the number of primitive basis functions used, and is therefore different for the A and B bases. The SCF times depend on the numbers of contracted functions and the number of iterations needed for convergence. Since both bases contain equal numbers of contracted functions and since the numbers of SCF iterations were essentially the same for both bases, the SCF times differ little.

The integrals section of the program has some restrictions on the amount of input data which can be processed, e.g. number of atom centers, total number of contraction coefficients, and total number of primitive orbital zetas. Information for each kind of atom is entered only once unless an inhomogeniety is required. Redimensioning certain small arrays alleviates this with little change in core requirements. The main restrictions however are the maximum number of primitives per contracted orbital (ten), and the maximum number of contracted orbitals per symmetry (six) in one atom. These restrictions highly influence the size of core needed for processing integrals and changes here will require drastic changes in core requirements. These restrictions may be avoided by the trick of including dummy atoms with nuclear charge zero, at the site of real atoms in order to increase the basis size in an artificial way. However, contraction of functions on real atoms with those on dummy atoms is not possible.

Because of the practical restriction of the integrals to a 128K region, the SCF step was adjusted to admit a maximum of 54 variational basis functions. The source of this restriction is not the integral program since many more contracted integrals than this could be computed using it with no change. In order to do larger basis calculations, only the SCF segment dimensions need be changed. If necessary, all the size restrictions are easily modified but the integral program ought to be made still more efficient. Work on more efficient integrals programs which make heavier use of even-tempered basis simplifications is under way.

Special Features

The programs have a number of optional features which may be selected. Two of the most important are the restarts available during integral computation and during the SCF iterations. Essential information may be copied to a peripheral device if the run terminates because of a time underestimate. Options are then chosen to take up where the calculation left off.

Using the integral restart feature one may do efficient brute force geometry optimizations. Atoms in a molecule to be left stationary are treated first as a separate molecule or molecule fragment. These integrals are calculated and stored separately. Then the molecule data is augmented by addition of the atoms which are to be moved during a series of SCF runs. The stored integrals are copied into the two-integral data set and the integral restart is opted for. The program will automatically add the new integrals involving the fragment and the new atoms to the end of the set which was already computed for just the molecule fragment. The SCF step is subsequently carried out and one energy is obtained. The same process may be repeated using the same separate fragment integrals as often as the new atoms need be moved. Rearrangement of the fragment nuclei of course requires recomputation of the fragment integrals.

An advantage is gained if the molecule has a particular orientation in the external coordinate system with respect to which atom coordinates are designated. The orientation is that one in which the most pairs of atom x-, y-, and z-coordinates are equal (especially for those atoms with more basis functions). The consequence of this is that more blocks of integrals are zero by symmetry. Since it is often easier to find atom coordinates which do not conform to the above criterion, a facility has been incorporated whereby the molecule may be rotated in order to reorient it to gain efficiency.

Other options are mainly print options, allowing one to increase the amount of printed output for debugging purposes. The standard punched output may be suppressed if desired.

Table 80. Molecule calculation times

			Basis A			Basis B			
				Time (CPU min.)			Time (CPU min.)		
Molecule	Num. Orbitals	Num. Contr. Functions	Prim. Functions	Integrals	SCF	Prim. Functions	Integrals	SCF	Num. SCF Iterations
H_2	1	18	26	0.6	0.3	36	1.8	0.3	6
H_3^+	1	27	39	4.5	1.0	54	13.7	1.0	4
Li^+	1	11	18	0.2	0.1	23	0.4	0.1	6
LiH	2	20	31	1.4	0.6	41	3.1	0.5	9
LiH_2^+	2	29	44	7.2	2.0	59	19.2	2.0	7
Li_2	3	22	36	2.1	0.7	46	4.5	0.7	10
Li_2H^+	3	31	49	6.0	2.0	64	15.1	1.8	8
Li_3^+	4	33	54	13.0	3.5	69	31.5	3.4	8

Table 80. (Continued)

Molecule	Num. Orbitals	Num. Contr. Functions	Basis A			Basis B			Num. SCF Iterations
			Prim. Functions	Time (CPU min.)		Prim. Functions	Time (CPU min.)		
				Integrals	SCF		Integrals	SCF	
Na^+	5	18	23	0.5	0.3	31	1.3	0.4	11
NaH	6	27	36	2.4	1.8	49	5.9	1.9	17
NaH_2^+	6	36	49	10.7	8.2	67	29.9	9.0	16
NaLi	7	29	41	3.1	2.6	54	8.4	2.9	20
$NaLi_2^+$	8	40	59	18.3	16.6	77	46.1	16.7	21
Na_2	11	36	46	5.2	4.5	62	12.0	4.3	15
Na_2H^+	11	45	59	11.6	10.1	80	31.3	10.6	16
Na_2Li^+	12	47	64	23.4	23.2	85	57.3	21.9	18
Na_3^+	16	54	69	32.7	33.4	93	70.5	32.0	15

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ACKNOWLEDGEMENTS

The author wishes to thank Professor Klaus Ruedenberg for the guidance and encouragement given him during the pursuance of this work and in the preparation of the dissertation.

Special thanks also go to Dr. Arnold Wahl of Argonne National Laboratories for his interest in the even-tempered exponential atomic bases and for his open-shell SCF programs which were used as a model for the final general atomic programs.

Appreciation is extended to the programming and operating staffs of the ISU Computation Center for the special considerations and for the service programs which were provided.