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A GAUSSIAN WAVEFUNCTION FOR THE
ISOELECTRONIC SEQUENCE OF
TWO-ELECTRON HOMONUCLEAR
DIATOMIC MOLECULES

S. L. BRENNER

A thesis submitted in partial fulfillment
of the requirements for honors
in Science and Mathematics

Granted the Honor:

Distinguished Independent Work in the
Division of Science and Mathematics

on May 29, 1969.

Charles J. Houghton
Chairman, Science and Mathematics
Honors Committee

A GAUSSIAN WAVEFUNCTION FOR THE
ISOELECTRONIC SEQUENCE OF TWO-ELECTRON
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by

STEPHEN LOUIS BRENNER

A Thesis submitted in Partial Fulfillment
of the Requirements for the Degree of
BACHELOR OF ARTS

WITH

HONORS

IN SCIENCE AND MATHEMATICS

1969

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TABLE OF CONTENTS

	Page
1. Abstract	i
2. Statement of the Problem	1
3. Background information	4
4. Method and Results	7
5. Discussion	9
a. The H_2 molecule	9
1. Figure 1 - H_2 binding energy	9A
2. Figure 2 - Scaled H_2 energy	10A
3. Figure 3 - Slopes of H_2 potential curves	10B
b. The He_2^{+2} , Li_2^{+4} , and Be_2^{+6} systems	11
1. Figure 4 - Binding energy of He_2^{+2}	11A
2. Table F - Scaled H_2 parameters	13A
3. Figure 5 - Scaled orbital exponents	13B
4. Figure 6 - Scaled pz coefficient	13C
5. Figure 7 - Scaled px,py coefficient	13D
6. Conclusions	15
7. Bibliography	16
8. Appendix A - Gaussian Integrals	17
a. Figure 8 - The Gaussian	19
b. Proof of Hirschfelder-Kim error	35
9. Appendix B(- Computer programs	38
10. A tables (see pp. 8 for content of tables)	120
11. B tables	134
12. C tables	148
13. D tables	162
14. E tables	172

Abstract

The Gaussian wavefunctions recently reported by Kim and Hirschfelder were found to be in error due to incorrect formulas for two integrals. The interaction potentials calculated in terms of the corrected wavefunctions are found to be in reasonable accord with the exact results of Kolos and Wolniewicz near the equilibrium separation but in relatively poor accord at moderately large internuclear separations. A scaling of the energy and length to fit the exact curve at its minimum did not ameliorate the situation. For the H_2 isoelectronic sequence it was found that scaling the H_2 optimized orbital exponent by Z^2 and the internuclear distance by Z allowed the prediction of the fully optimized energy of other members of the sequence to within (at worst) 1%.

Statement of the Problem

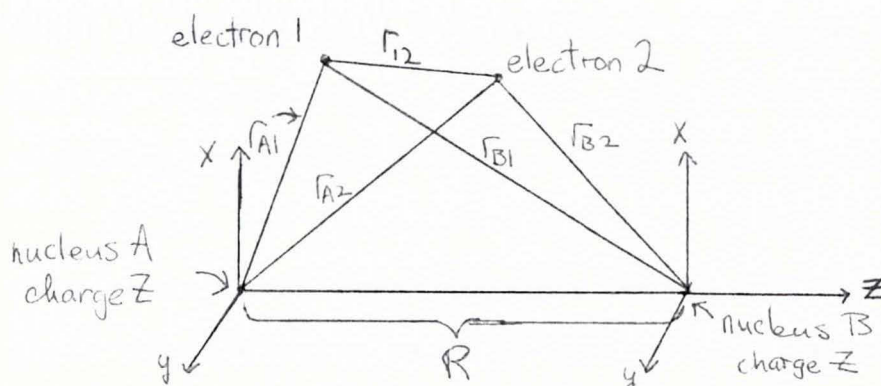
The study of intermolecular forces is undergoing a renaissance.¹ In principle, one can study the interactions of atoms and molecules in terms of solutions to the Schrödinger equation

$$\hat{H}\psi = E\psi, \quad (1)$$

where \hat{H} is the Hamiltonian operator for the system, ψ is the wavefunction, and E is the total energy. For example, the non-relativistic, time-independent Hamiltonian for two H atoms separated by a distance R is (in atomic units*)

$$\hat{H} = -\frac{\nabla_1^2}{2} - \frac{\nabla_2^2}{2} - Z \left(\frac{1}{r_{A1}} + \frac{1}{r_{A2}} + \frac{1}{r_{B1}} + \frac{1}{r_{B2}} \right) + \frac{1}{r_{12}} + \frac{Z^2}{R},$$

where ∇^2 is the Laplacian and the coordinate system is defined as below.



The first two terms of the Hamiltonian are the kinetic energy operators for electron 1 and electron 2 respectively. The third term is the nucleus-electron attraction operator and the last term is the nucleus-nucleus repulsion operator.

* atomic units will be used consistently in this paper:

$$1 \text{ a.u. of length} = \hbar^2/m_e e^2 = 0.52917 \text{ \AA} = a_0$$

$$1 \text{ a.u. of energy} = e^2/a_0 = 27.210 \text{ eV}$$

where \hbar = Planck's constant/ 2π ; m_e = mass of electron;
 e = electronic charge; a_0 = radius of first Bohr orbit of H_2

The practical difficulty is that the Schrödinger equation is soluble analytically for only a very few systems.

As noted by Kim and Hirschfelder² (hereafter referred to as HK) there exist several calculations for the system of two H atoms which agree with experiment for a limited range of the internuclear separation R . However, there are very few theoretical treatments which are good both for small and large separations. Especially with a small number of basis functions there is only the work of Hirschfelder and Linnett³ which falls into this category. Thus, KH investigated the interaction of two H atoms using a Gaussian counterpart of the Hirschfelder-Linnett function. They hoped to find whether the errors in the molecular energy might be essentially constant over the whole range of internuclear separations R . In fact, their results were not too promising, especially in the long range situation.

It was our initial intention to consider a more flexible variational function than the KH function to learn whether their disappointing results were due to the simplicity of their wavefunction. Consider the trial function

$$\psi = (1 \pm P_{12}) \left\{ \sum_{i=1}^l \alpha_i S_A^{(i)}(1) S_B^{(i)}(2) + \sum_{j=1}^m \beta_j P_{2A}^{(j)}(1) P_{2B}^{(j)}(2) + \sum_{k=1}^n \gamma_k (P_{1A}^{(k)}(1) P_{1B}^{(k)}(2) + P_{2A}^{(k)}(1) P_{2B}^{(k)}(2)) \right\} \quad (2)$$

where P_{12} is the permutation operator, (see footnote next page)

$S_A^{(i)} = \exp(-J_{1i} r_A^2)$; $P_{2A} = Z_A \exp(-J_{2i} r_A^2)$, etc and $J_{1i}, J_{2i}, J_{3i}, \alpha_i, \beta_i$, and γ_i are ^{*} variational parameters and $l=8$, $m=3$, and $n=3$. The HK function is obtained by setting

* The variational theorem for trial wavefunctions states that, in general, any trial function (which is normalizable) leads to a value of the energy which is never lower than the true ground state energy of the system.⁴

$l=m=n=1$ and $J_1=J_2=J_3$. KH considered the subcases

$$\psi_0 \text{ (where } \gamma = \beta = 0 \text{)}$$

$$\psi_1 \text{ (where } \gamma = 0 \text{)}$$

In the course of treating the wavefunction of Eq.(2) a serious error was discovered in the KH work.* Therefore, we redirected our efforts to the reconsideration of the simple KH wavefunction rather than the expanded wavefunction of Eq.(2). It is important to have correct results for the KH function in order to assess the improvements obtained by using the more complex function of Eq.(2).

Our motivation is also to explore scaling of the wavefunction for an isoelectronic sequence of molecules (H_2 , He_2^{+2} , Li_2^{+4} , and Be_2^{+6}). We also wish to examine the usefulness of the Gaussian s, pz, px, and py basis set in the prediction of ground state energies for the H_2 and He_2^{+2} systems. Finally, we wish to see if the Gaussian basis set will yield the proper shape for the interaction potential curve of two H atoms as a measure of the usefulness of Gaussians in intermolecular and interatomic force problems.

footnote for page 2: The $(1+P_{12})$ term permits the calculation of the $^1\Sigma_u^+$ (ground) state of the system and the $(1-P_{12})$ term the $^3\Sigma_u^+$ (first excited state) state of the system.

* In fact, when the error was found we were well along in the problem using the wavefunction of Eq.(2) as can be seen from much of the discussion in Appendices A, B, and C.

Background Information

In this section we review some background material (available in standard Quantum Mechanics texts, see, for example, ref. 4) largely to establish notation used in succeeding sections of the paper.

The problem of computing an approximate energy eigenvalue of the Schrödinger equation may be formulated as follows

$$E = \frac{\int \psi^* \hat{H} \psi d\tau}{\int \psi^* \psi d\tau} = \frac{\langle \psi | \hat{H} | \psi \rangle}{\langle \psi | \psi \rangle}, \quad (3)$$

The problem of computing E thus involves the evaluation of integrals, the most complex of which involve the $1/r_{12}$ operator. With Slater orbitals *such integrals often provide a major roadblock to the computation of molecular properties.

Boys⁵ has proposed the Gaussian basis set

$$x^i y^j z^k \exp(-\alpha r^2)$$

where i , j , and k are integers and where the exponent α may be varied or fixed. In general, it requires several Gaussian orbitals to represent a Slater orbital. The Gaussians, however, possess certain transformation properties which make them convenient in the evaluation of multi-center integrals (see Appendix A). Several calculations of molecular

* One electron wavefunctions of any sort are called orbitals. Slater type orbitals are eigenfunctions of the H atom Hamiltonian and have the form

$$r^n e^{-\alpha r}$$

The majority of molecular wavefunctions used to date and built up in some way from Slater type functions.

properties using a Gaussian basis set have been carried out to date (see the compendium by Krauss⁶ for recent references).

The Valence-Bond wavefunction of Eq.(2) is of such a form that it may dissociate properly to the wavefunction for 2 H atoms as $R \rightarrow \infty$. The pz, px, and py functions are introduced to help take into account the correlation energy of the systems. The correlation energy^{*} reflects the fact that in many approximate wavefunctions the coulombic interaction between electrons (especially those with anti-parallel spins) is not properly accounted for. The spatial correlation of electrons in a two-electron diatomic molecule may be thought of as consisting of three parts:⁴

(1) "in-out" or "radial" correlation, where, when one electron is close to the bond axis, the other is far away.

(2) "angular" correlation, where the two electrons tend to stay on opposite sides of the axial plane.

(3) "left-right" correlation, where the two electrons tend to stay near different nuclei.

The pz functions should help take into account the left-right correlation and the px and py should take into account the in-out and angular correlation. It was hoped that the extension of the basis set to eight s, three pz, and three each of px and py with the consequent increase from 2 to 14

* The correlation energy is properly defined as

$$E_{\text{corr}} = \langle H \rangle_{\text{EXACT}} - \langle H \rangle_{\text{HARTREE-FOCK}}$$

linear and from 1 to 3 non-linear parameters (see Appendix B) would produce significant improvement in the potential curve computed using the Gaussian basis set. All integrals required to compute the energy have been evaluated and are listed in appendix A. The computer programs to compute the eigenvalue and eigenvector are in the final testing stage (see appendix C).

Method and Results

The three subcases are treated following the method of KH,

$$\left. \begin{aligned} \psi_0 &= (1 + P_{12}) S_A(1) S_B(2) \\ \psi_1 &= (1 + P_{12}) [S_A(1) S_B(2) + \alpha P_{ZA}(1) P_{ZB}(2)] \\ \psi_L &= (1 + P_{12}) [S_A(1) S_B(2) + \beta P_{ZA}(1) P_{ZB}(2) + \gamma (P_{XA}(1) P_{XB}(2) + P_{YA}(1) P_{YB}(2))] \end{aligned} \right\} (4)$$

The use of these three forms allows one to assess the improvement obtained by adding pz and then px and py functions to the simple s wavefunction.

Details of the formulation of the problem are presented in Appendix B. The computer programs used to calculate integrals and minimize the energy are presented in Appendix C. For the three wavefunctions of Eq.(4) we minimized the energy functional

$$E = \frac{\langle \psi | \hat{H} | \psi \rangle}{\langle \psi | \psi \rangle}$$

with respect to the parameters α, β, γ as appropriate. Both the energy and the wavefunction itself are fixed by these means. In order to assess the various qualities of the wavefunction, we calculated ~~several~~ expectation values other than the energy (the expectation value of any dynamical variable is defined to be $\langle a \rangle = \frac{\langle \psi | a | \psi \rangle}{\langle \psi | \psi \rangle}$).

First let us consider the Virial Theorem which may be stated in its general form for diatomic molecules as⁴

$$2\langle \hat{T} \rangle = -\langle \hat{V} \rangle - R \frac{dE(R)}{dR} \quad (5)$$

where $\langle \hat{T} \rangle$ is the expectation value of the kinetic energy,

$\langle \hat{V} \rangle$ is the expectation value of the potential energy.

Knowing $\langle \hat{T} \rangle$ and $\langle \hat{V} \rangle$ one can calculate dE/dR which gives a picture of the shape of the energy curve.

The $\langle \frac{1}{r_{12}} \rangle$ gives a measure of the average separation between the electrons while $\langle \frac{1}{r} \rangle$ gives a measure of the average separation between a nucleus and an electron.

The results are presented in the following tables:

TABLE	Page	CONTENTS
A	120	R, Energy, \mathcal{I} , α or β and γ for ψ_0, ψ_1, ψ_2 ; the H_2 molecule. $R, E, \mathcal{I}, \beta, \gamma$ for ψ_2 ; $He_2^{+2}, Li_2^{+4}, Be_2^{+6}$
B	134	R, Binding Energy, $\langle V \rangle, -\langle V \rangle/2\langle T \rangle$, dE/dR for $H_2, He_2^{+2}, Li_2^{+4}, Be_2^{+6}$
C	148	$R, \langle \frac{1}{r_{12}} \rangle, \langle \frac{1}{r} \rangle$ for $H_2, He_2^{+2}, Li_2^{+4}, Be_2^{+6}$
D	162	Scaled R, Scaled binding energy, scaled dE/dR (see discussion).
E	172	$ZR, \mathcal{I}/Z^2, \beta/Z$ and γ/Z for He_2^{+2}, Li_2^{+4} , and Be_2^{+6}
F	13A	Initial guess \mathcal{I} used to test scaling of \mathcal{I} and E for H_2 isoelectronic sequence (see discussion).

Many of the results are also summarized in Figs.(1-8).

The binding energy is defined as

$$\Delta E = B.E. = E_{R=R} - E_{R=\infty}$$

At infinite separation the E_{∞} for Eq.(4) is given by

$$E_{\infty} = 2 \left(-\frac{4Z^2}{3\pi} \right) a.u.$$

with

$$\mathcal{I}_{\infty} = \frac{8Z^2}{9\pi} \text{ bohr}^{-2}$$

That is, E_{∞} is twice the variational energy of the hydrogen atom (when $Z=1$) calculated with the s Gaussian function.

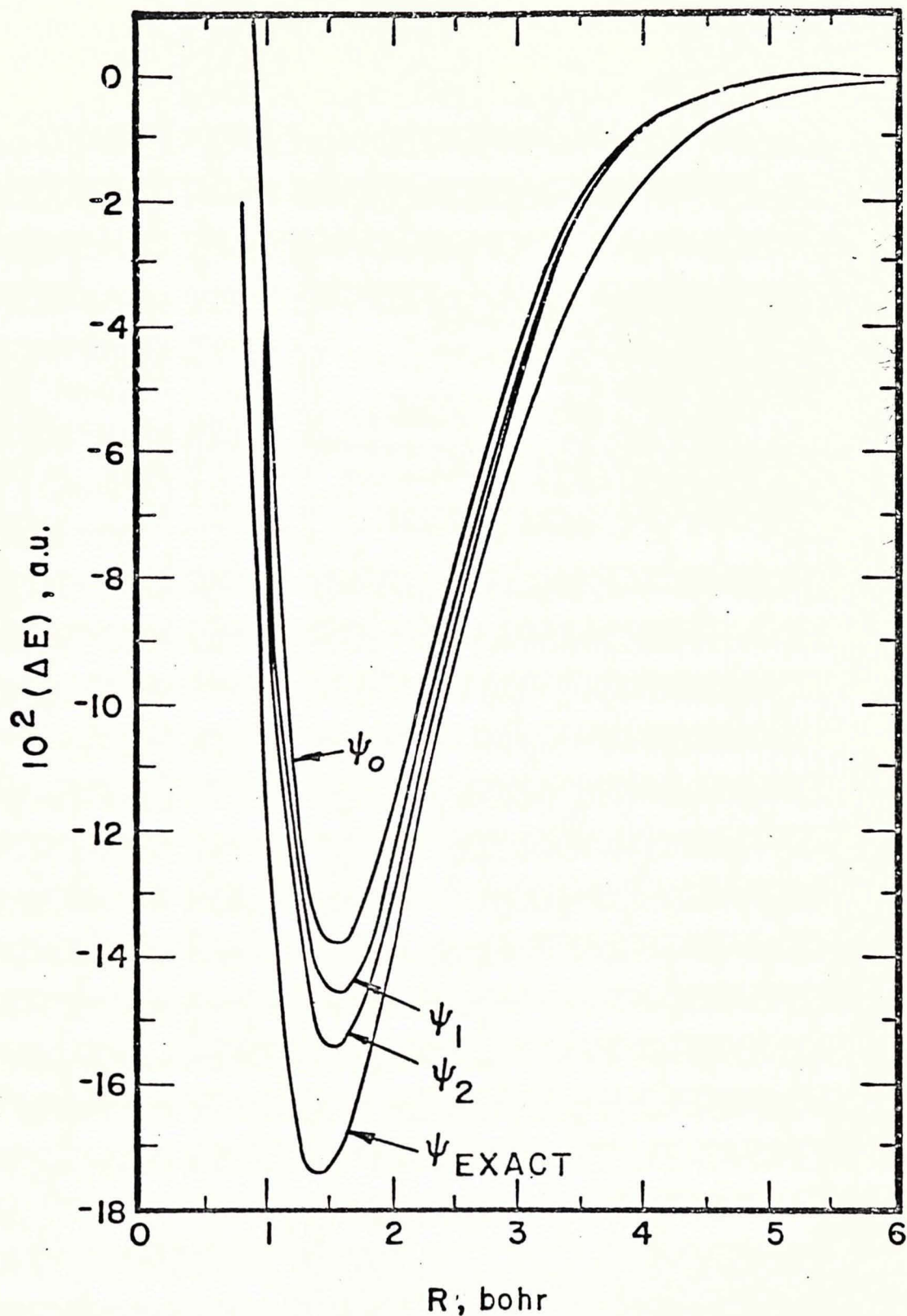
Discussion

In this section we discuss the approximate ground-state wavefunctions and energies of the first four members of the H_2 isoelectronic sequence in order of increasing atomic number.

The H_2 Molecule

The binding energies for the wavefunction of Eq.(4) for H_2 over the range $0.1 \leq R \leq 6$ bohrs are plotted in Fig.(1). There they are compared with the exact results of Kolos and Wolniewicz⁷ who used an 80 term correlated wavefunction. A comparison of the results for ψ_0 and ψ_1 in Fig.(1) shows that the addition of pz character to ψ_0 improves the binding energy by .00766 a.u. at the calculated equilibrium separation $R=1.55$ a.u. The addition of px and py character to ψ_1 further improves the binding energy at $R=R_e$ by an additional 0.00842 a.u. and also shifts the minimum from $R=1.55$ bohr to $R=1.53$ bohr. This significant energy improvement due to the addition of px and py functions is in direct contradiction to the statement by KH that "...the addition of px and py functions gives very little influence to the overall picture of the potential curve."

One should also note that ^{by} using the wrong integral formulas (see Appendix A) KH obtained binding energies for ψ_1 and ψ_2 at the equilibrium separation of -.282953 and -.290025 respectively, values very far below the true binding energy reported by Kolos and Wolniewicz⁷, of -.1744 a.u. This fact alone shows the great discrepancy introduced into the KH results by using the improper integrals.



- Figure 1 -

Binding energy for H_2 for ψ_0 , ψ_1 and ψ_2
compared to the exact results.

A central question is whether the potential curves obtained from the simple KH wavefunctions are of the proper shape. It is difficult to answer this question on the basis of Fig.(1) alone. Following KH we scaled the units of length and energy as follows

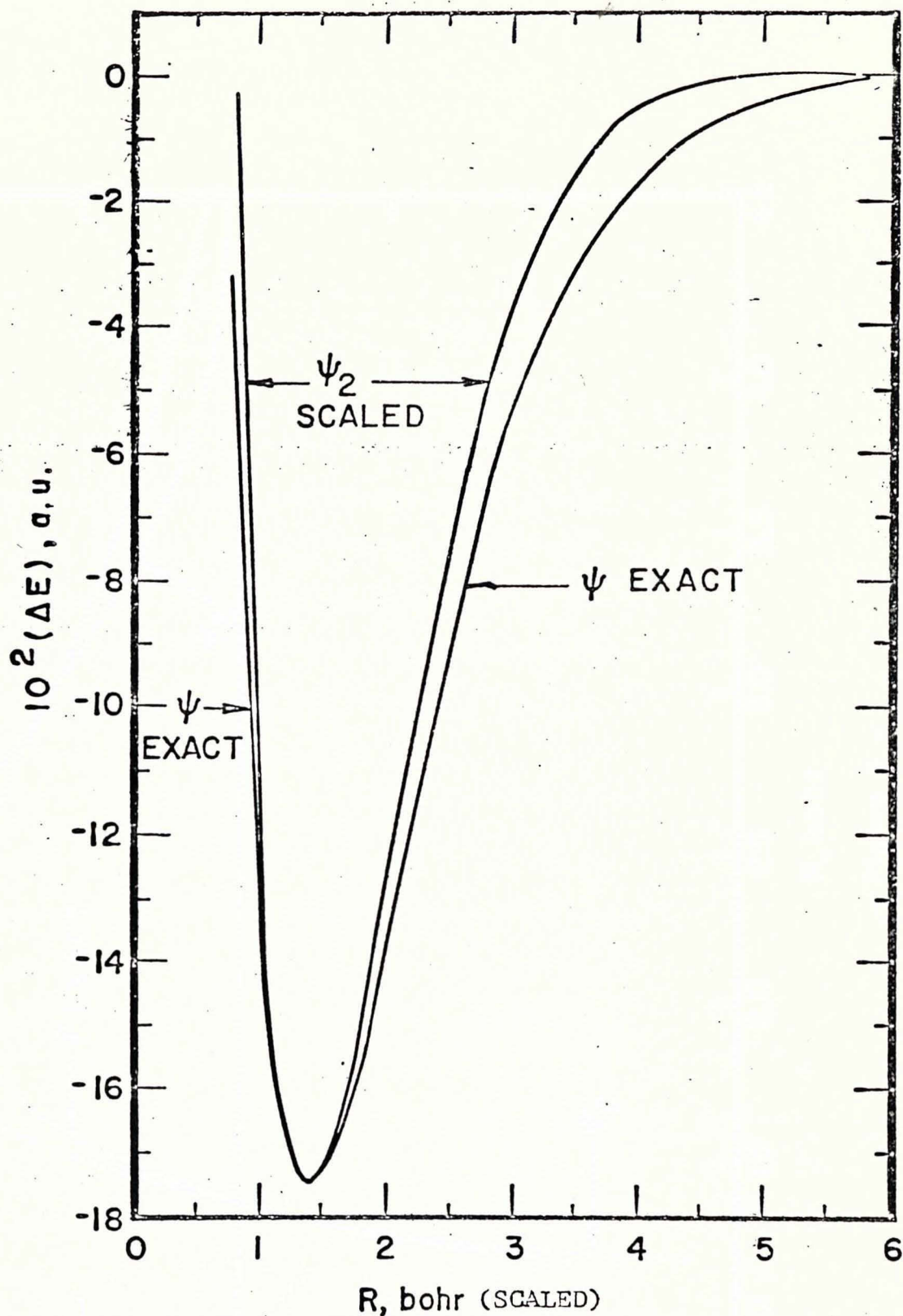
$$R_{\text{SCALED}}^{\psi_L} = R^{\psi_L} \left(\frac{R^{\psi_{\text{EXACT}}}_{\text{MINIMUM ENERGY}}}{R^{\psi_L}_{\text{MINIMUM ENERGY}}} \right) \quad (6)$$

$$\Delta E_{\text{SCALED}}^{\psi_L} = \Delta E^{\psi_L} \left(\frac{\Delta E^{\psi_{\text{EXACT}}}_{\text{MINIMUM}}}{\Delta E^{\psi_L}_{\text{MINIMUM}}} \right).$$

The results of the scaling for ψ_L are presented in Fig.(2).

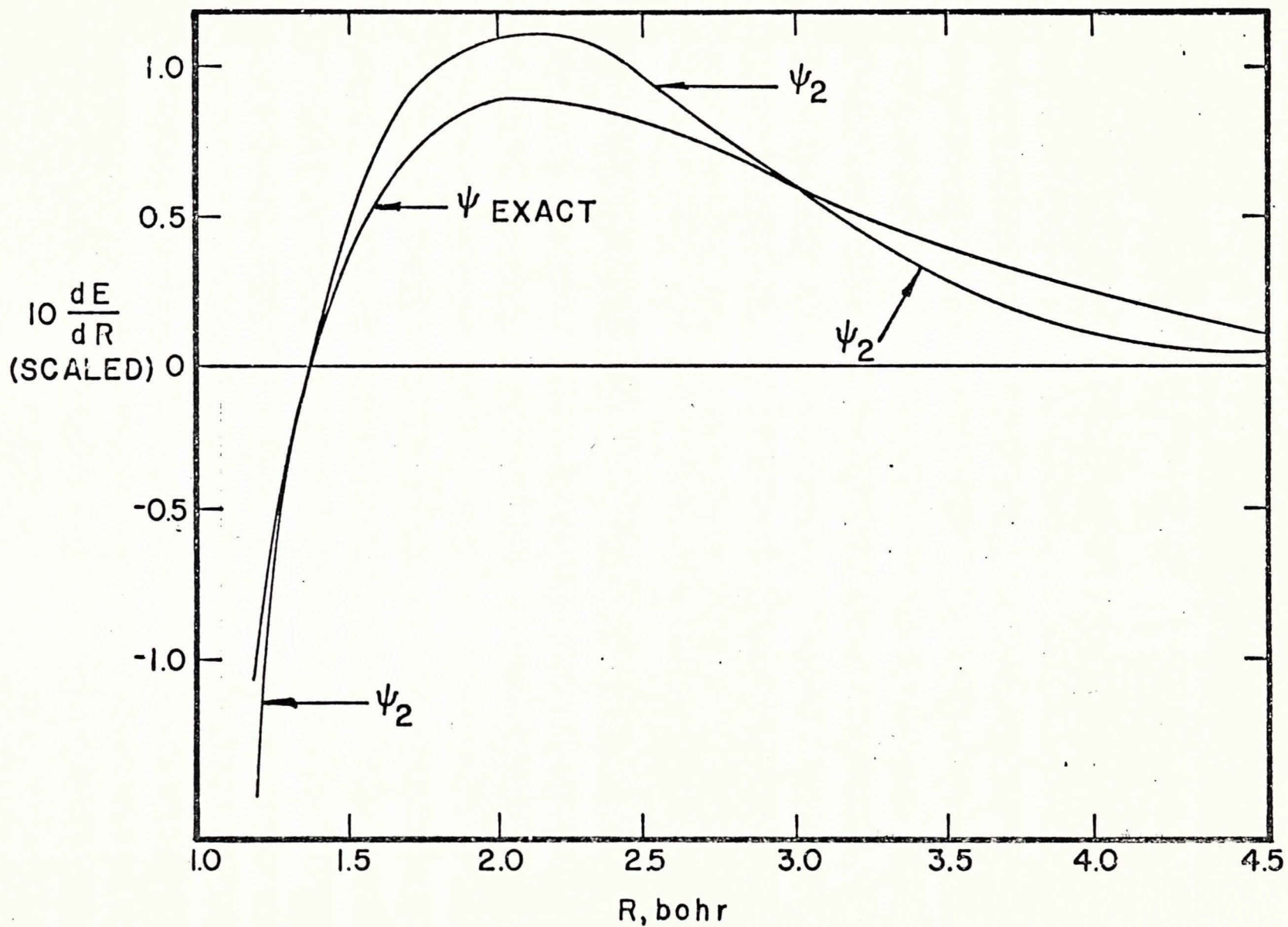
According to Eq.(5) it is easy to calculate the slope of the potential curve from Virial theorem considerations. Values of dE/dR are listed in Tables B1-B3. Values of dE/dR for ψ_L scaled according to Eqs.(6) are compared graphically with the Kolos-Wolniewicz exact values.⁷ in Fig.(3). There it is seen that ψ_L yields a potential curve of the incorrect shape (as seen in Figs(1) and (2) as well), especially at intermediate to large separations. It is not certain whether one should ascribe this defect entirely to the use of a Gaussian basis set (as KH appear to imply) or whether the form of the wavefunction may be partially at fault. Note that none of the KH functions contain ionic terms ($A(1)A(2) + B(1)B(2)$) which are known to be important at small separations.³

It is immediately obvious from Fig.(2) that the two-parameter scaling scheme of KH is inadequate, since the scaled $\Delta E(\psi_L)$ is not sufficiently "fat". For the sake of argument let us assume that both $\Delta E(\psi)$ and $\Delta E(\psi_{\text{EXACT}})$ are represent-



- Figure 2 -

Scaled Binding energy for H_2 (ψ_2). Also included in this figure is the exact curve of Kolos and Wolniewicz (not scaled).



- Figure 3 -

Comparison of the slopes of the H_2 potential curves using ψ_{EXACT} and scaled ψ_2

ed by the Morse potential⁸

$$\Delta E = e(x^2 - 2x)$$

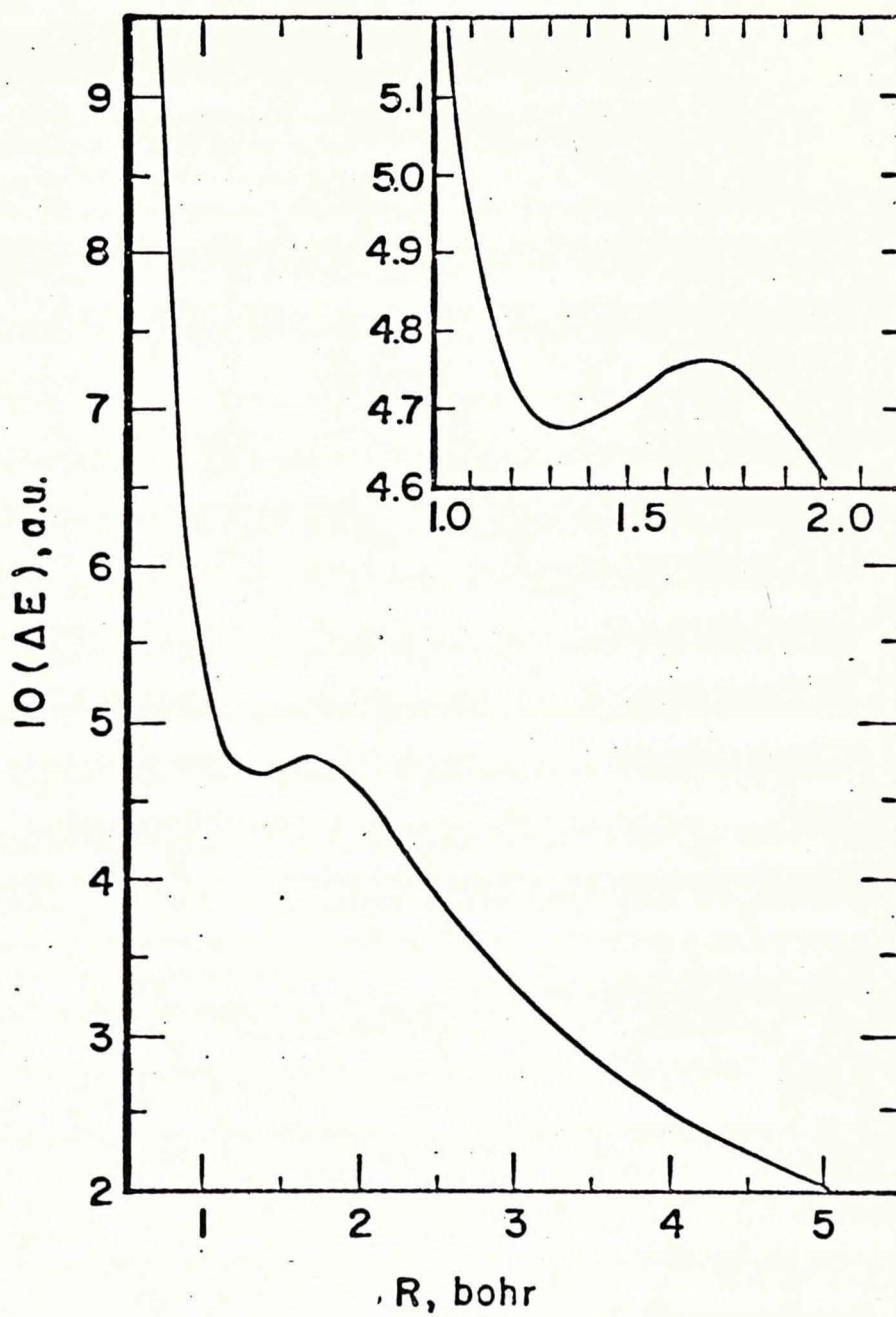
$$x = \exp \left\{ -a \left[\left(R/R_m \right) - 1 \right] \right\}$$

As plotted in Fig.(2), both curves have the same values (respectively) of the equilibrium separation R_m and e , the binding energy at $R=R_m$. Clearly, however, $a(\psi_L) > a(\text{exact})$. Thus to make the two curves coincide, $a(\psi_L)$ would need to be scaled by a factor $a(\text{exact})/a(\psi_L)$. The investigation of such a scaling scheme is beyond the scope of the present work and so will not be pursued further here.

The He_2^{+2} , Li_2^{+4} , and Be_2^{+6} Molecular Ions

The results for the He_2^{+2} system which was treated in terms of the HK ψ_L are reported in Tables A4, B4, C4, E1. The binding energy curve is plotted in Fig.(4).

It is known that the He_2^{+2} molecule is metastably bound.⁹ Thus, the binding energy curve shown in Fig.(4) is qualitatively correct. Its shortcomings are revealed by a comparison of our calculation with a more nearly exact configuration interaction calculation⁹ (in terms of Slater orbitals) summarized on page 12. R_{\min} and R_{\max} refer to the R values at which the curve exhibits a maximum and a minimum respectively.



- Figure 4 -

Binding energy of He_2^{+2} calculated using ψ_{L}

Inset provides additional detail of potential well.

Summary of He₂⁺² System

	<u>CI Calc.^a</u>	<u>Gaussian ψ_2 Calc.^b</u>
R_{\min}	1.34 a.u.	1.35 a.u.
R_{\max}	2.10 a.u.	1.70 a.u.
$E(R_{\min})$	-3.6622 a.u.	-2.9278 a.u.
$E(R_{\max})$	-3.6162 a.u.	-2.9195 a.u.
^a ref. 9		
^b this work		

If we were to scale the binding energy and distances (the latter according to R_{\min} or R_{\max}) we should find the "potential well" for the ψ_2 curve to be too narrow compared to the CI curve (this is evident by comparing the R_{\min} and R_{\max} values for the CI and Gaussian calculations). Recall that the Gaussian functions gave too narrow a scaled potential curve for the H₂ system as well.

No stable species are predicted for Li₂⁺⁴ and Be₂⁺⁶. However, the real reason for studying higher members of the isoelectronic sequence was to search for a relationship between the H₂ wavefunction parameters and those for systems with higher Z values. We attempted to predict γ values for high Z cases by scaling the H₂ minimized γ by Z² and the internuclear distance by Z so that

$$\begin{aligned} \gamma(Z) &= Z^2 \gamma(Z=1) \\ \text{and } R(Z) &= Z R(Z=1) \end{aligned} \quad (7)$$

The justification for this attempt is that if all distances were scaled by Z then

$$\exp(-\mathfrak{J}r^{-2}) = \exp(-Z^2 \mathfrak{J} r^{-2})$$

The scaled $\mathfrak{J}(Z)$ calculated as in Eq.(7) were given as input to the energy minimization program. The initial value of the energy computed was noted and the minimization was allowed to proceed. A comparison of the initial guess \mathfrak{J} , final \mathfrak{J} , initial E and final E is given in Table F. It can be seen that evenⁱⁿ the worst cases (very low R), the predicted energies using scaled \mathfrak{J} 's are correct to within 1% of the final minimized values. As one approaches $ZR=6$ bohr, the energy can be predicted to 5-7 places and the final \mathfrak{J} can be predicted to 2-3 places. The increase in the accuracy of the scaled \mathfrak{J} as R becomes large is expected because for the separated atoms \mathfrak{J} scales exactly as Z^2 :

$$\mathfrak{J}_{R \rightarrow \infty} = \frac{8Z^2}{9\pi}$$

It was unexpected that this Z -scaling of \mathfrak{J} should persist to such small separations.

The behavior of the \mathfrak{J} parameters corresponding to the fully optimized ψ_L is seen in Fig.(5) to indicate Z^2 scaling for the majority of R values shown. Also note that the scaling between higher members of the sequence is better than the scaling for any high member with H_2 .

We also investigated possible scaling of the linear parameters of ψ_L . The numerical results are given in Tables E, and are presented graphically in Figs.(6,7). It is clear that simple Z scaling works quite adequately for \mathfrak{Y} , the

TABLE F

Scaled H_2 parameters for He_2^{+2} , Li_2^{+4} , and Be_2^{+6}
 $HE2+2$ ($z=2$)

<u>ZR</u>	<u>$J(z)=Z^2 J(z=1)$</u>	<u>Final J</u>	<u>Initial E</u>	<u>Final E</u>
0.1	3.061	3.734	68.827	68.726
0.2	2.991	3.642	28.936	28.838
0.5	2.621	3.168	5.565	5.480
1.0	1.988	2.310	-1.069	-1.117
1.2	1.777	2.009	-1.877	-1.908
1.4	1.592	1.759	-2.339	-2.359
2.0	1.206	1.288	-2.848	-2.855
3.0	1.005	1.027	-2.92319	-2.92359
5.0	1.1186	1.1169	-2.9999944	-2.9999961
7.0	1.13146	1.13163	-3.1096376	-3.1096368

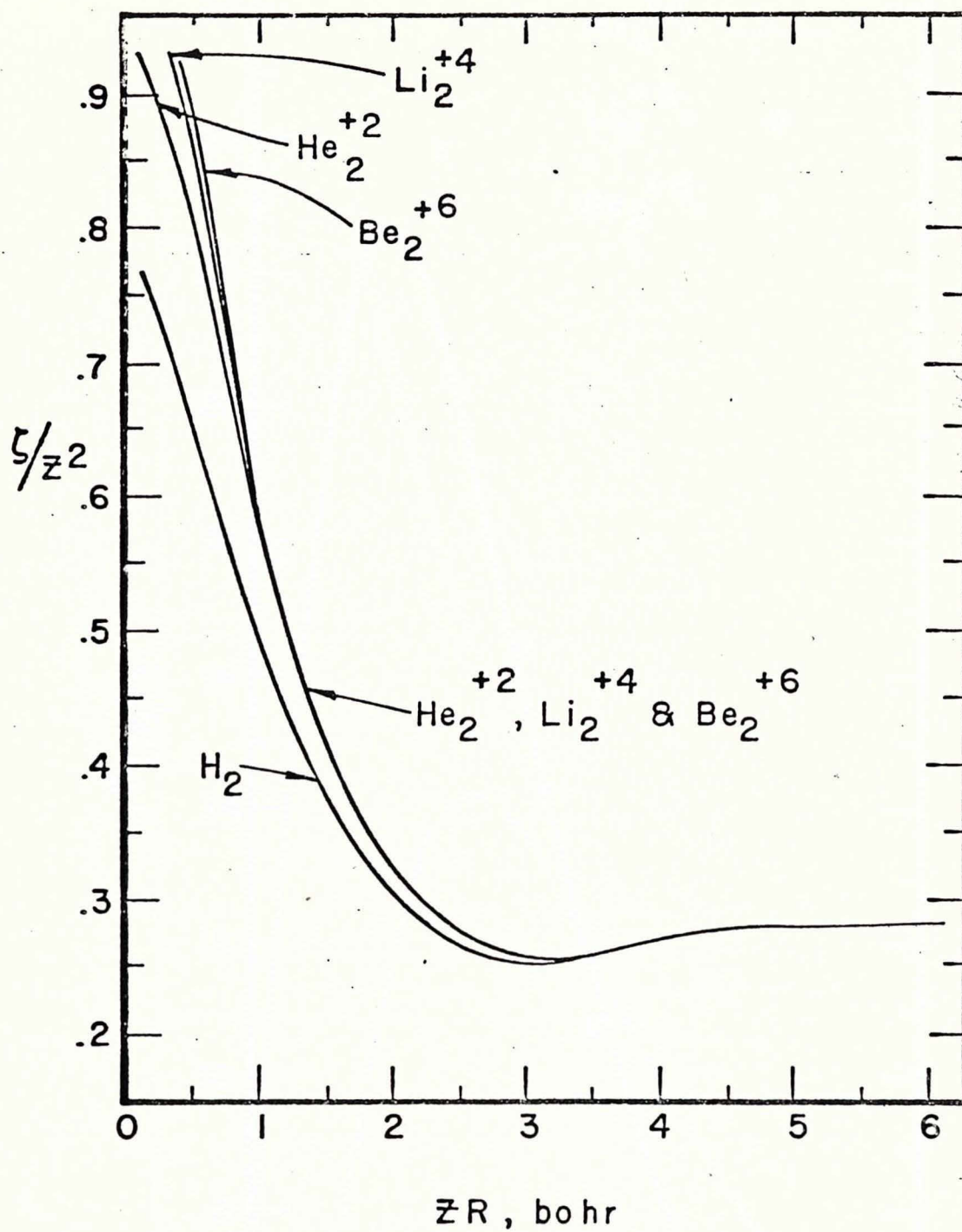
 $LI2+4$ ($z=3$)

0.3	6.492	8.387	64.086	63.707
0.6	5.586	7.133	20.844	20.528
1.2	3.999	4.671	2.281	2.164
1.8	2.940	3.234	-1.979	-2.013
2.4	2.411	2.576	-3.4316	-3.4434
3.0	2.261	2.323	-4.0894	-4.0908
6.0	2.5422	2.5428	-5.64020262	-5.64020272

 $BE2+6$ ($z=4$)

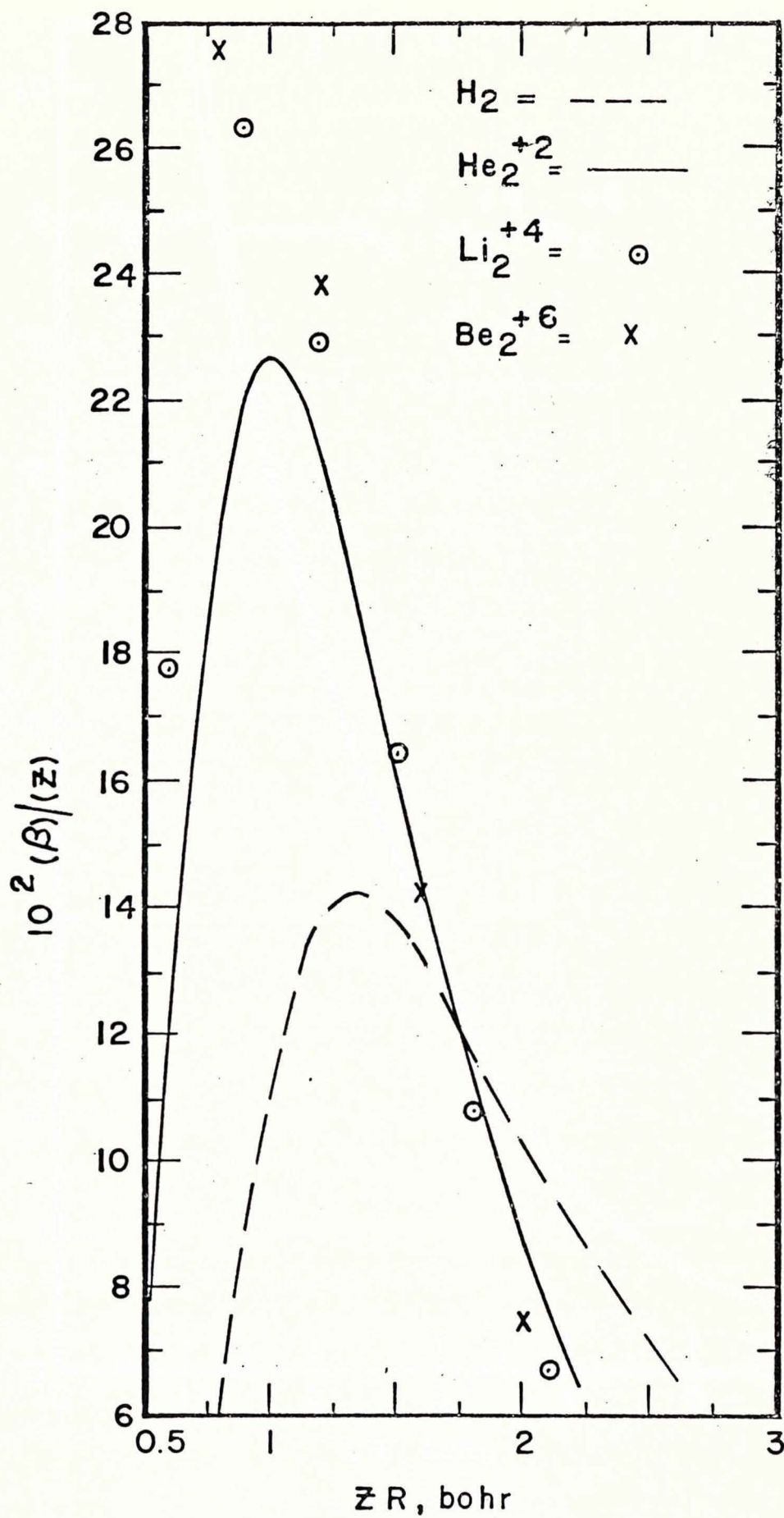
0.4	11.032	14.634	113.639	112.826
0.8	8.885	11.409	38.372	37.804
1.2	7.109	8.430	16.500	16.243
2.8	4.046	4.237	-1.7289	-1.7373
4.0	4.294	4.229	-4.75800	-4.75869
6.0	4.5194	4.5204	-7.58254419	-7.58254435

Note: Scaled J is obtained by multiplying the H_2 minimized J by Z^2 . The initial E is obtained by computing the energy using the initial guess scaled H_2 with no minimization.



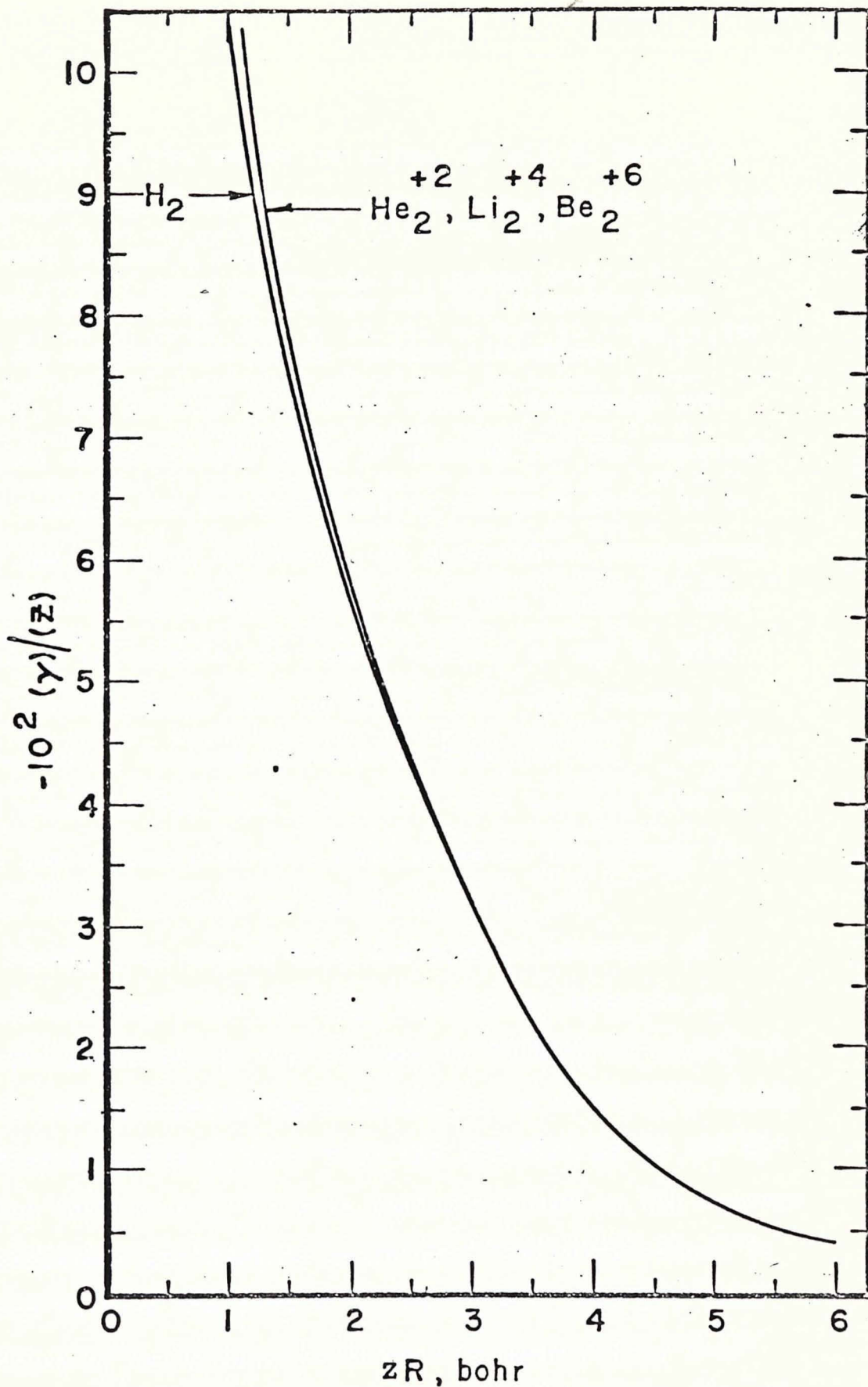
- Figure 5 -

Scaling of the orbital exponents for the H_2
Isoelectronic Sequence



- Figure 6 -

Attempted scaling of optimized pz coefficient



- Figure 7 -

Scaling of the optimized coefficient of the
px and py terms.

coefficient of the p_x and p_y terms, at all R . However, it appears that β (coefficient of p_z terms) fails to scale very well at any R shown.

The ZR scaling is not new and has recently been noted by several authors in various situations.^{10,11,12} However, the ability to predict orbital exponents and energies so accurately using Z^2 scaling for the exponent and Z scaling for the internuclear distance seems to be an ~~new and~~ exciting discovery. As a practical consequence it enables a significant decrease in the length of time necessary to compute the energy minimum at any R . With large wavefunctions such as Eq.(2) this will result in a substantial savings of computer time. (if the Z^2 scaling still persists for this function). Such scaling also enables the computation of a good guess at the energy (to within about 1%) with no minimization at all.

Finally, we should note the general behavior of the expectation value of $1/r_{12}$ for the H_2 molecule as reported in Table C. One can see by looking at these tables that generally the addition of p_z to the ψ_0 produces a decrease in the $\langle \frac{1}{r_{12}} \rangle$ and that the addition of p_x and p_y further decreases $\langle \frac{1}{r_{12}} \rangle$. This indicates that on the average the electrons are farther apart when the wavefunction is assumed to have the form of ψ_2 vs. ψ_1 or ψ_1 vs. ψ_0 . Thus our hopes of being able to account to some degree for electron correlation by addition of p character appear to have a foundation in fact.

Conclusions

The Gaussian wavefunction for the ground $1\Sigma_g^+$ state of H_2 recently reported by Kim and Hirschfelder² was found to be in error due to errors in two of their integrals. The interaction potential calculated in terms of the corrected approximate wavefunction is now found to be in reasonable accord with the (essentially) exact results of Kolos and Wolniewicz⁷ near the equilibrium separation but in relatively poor accord at moderately large separations. A scaling of the energy and length to fit the exact curve at its minimum did not ameliorate that situation.

For the H_2 isoelectronic sequence scaling of a different sort was investigated. We found that scaling J and R as follows allows one to predict the ground-state energy of a member of the sequence to at worst 1% of the fully optimized result

$$J(Z) = J(Z=1)Z^2$$

and $R(Z) = R(Z=1)Z$.

We note that the addition of p character to a simple s-type Gaussian wavefunction appears to increase the wavefunctions ability to correlate the motions of the two-electrons in the H_2 molecule.

Future work is planned to finish the study of the wavefunction of Eq.(2) which provides an increased flexibility in the number of variational parameters and the representation of the long range potential curve. We also hope to assess the usefulness of simply adding an ionic term to the Kim-Hirschfelder wavefunction.

BIBLIOGRAPHY

1. J. O. Hirschfelder, Intermolecular Forces, Advances in Chemical Physics, Interscience, New York (1967).
2. H. Kim and J. O. Hirschfelder, J. Chem. Phys. 47, 1005 (1967).
3. J. O. Hirschfelder and W. Linnett, J. Chem. Phys. 18, 130 (1950).
4. F. L. Pilar, Elementary Quantum Chemistry, McGraw-Hill, Inc., New York (1968).
5. S. F. Boys, Proc. Roy. Soc. A201, 125 (1950)
6. M. Krauss, National Bureau of Standards Technical Note number 438, Washington, D.C. (1967).
7. W. Kolos and L. Wolniewicz, J. Chem. Phys. 43, 2429 (1965).
8. P. M. Morse, Phys. Rev. 34, 57 (1929).
9. S. Fraga and B. Ransil, J. Chem. Phys. 37, 1112 (1962).
10. D. D. Konowalow, W. H. Barker, and R. Mandel, J. Chem. Phys. 49, 5137 (1968).
11. M. Cohen, B. H. Dorrell, R. P. McEachran, Theor. Chim. Acta. 9, 324 (1968).
12. S. K. Luke, G. Hunter, R. P. McEachran, and M. Cohen, J. Chem. Phys. 50, 1644 (1969).
13. I. Shavitt in: Methods in Computational Physics, 2, 1 (1963).
14. E. Clementi and D. R. Davis, J. Comp. Phys. 1, 223 (1966).
15. R. K. Nesbet, J. Chem. Phys. 43, 311 (1965).
16. P. O. Lowdin, J. Math. Phys. 3, 969 (1962).
17. J. A. Nedler and R. Mead, Computer Journal 7, 308 (1965).
18. J. V. L. Longstaff and K. Singer, Proc. Roy. Soc. A258, 421 (1960).

- APPENDIX A -

Introduction

The following section is based in large part on an article by Shavitt.¹³ This section is presented to familiarize the reader with notation and to develop some of the basic integral formulas involving Gaussian-type functions.

The reader should note that no further reference to Shavitt will be given in this appendix although much of the material is taken from his paper.

Some Properties of the Gaussian Function

Consider the three-dimensional Gaussian function which we will write in any one of the equivalent forms

$$G_i(r_A) = G(\alpha_i; r_A) = \exp(-\alpha_i r_A^2). \quad (A1)$$

Here α_i is a parameter ($\alpha_i > 0$), the index i referring to its position in an independently specified ordered list of α 's. The argument r_A is the magnitude of the vector \vec{r}_A from a given fixed point A to the variable point $P(x,y,z)$. The fixed point A , having the Cartesian coordinates A_x, A_y, A_z , is referred to as the "center" of the Gaussian. Different subscripts A, B, \dots will be used to distinguish different centers; thus $G_i(r_A)$ is a Gaussian centered on the point A and having the parameter α_i . It can be written as a function of the coordinates of $P(x,y,z)$,

$$G_i(r_A) = \exp\{-\alpha_i [(x-A_x)^2 + (y-A_y)^2 + (z-A_z)^2]\} \quad (A2)$$

We shall also use the abbreviations

$$x_A = x - A_x, \quad y_A = y - A_y, \quad \text{and} \quad z_A = z - A_z. \quad (A3)$$

When the center designation (the A of r_A) is omitted, it can be assumed that the Gaussian is centered on the origin of the coordinate system.

We derive the following theorem:

THEOREM. The product of two Gaussians having different centers A and B is itself a Gaussian (apart from a constant factor) with a center somewhere on the line segment \overline{AB} .

Specifically

$$G_i(r_A)G_j(r_B) = kG_k(r_C), \quad (A4)$$

where k is the constant

$$k = \exp\left(-\frac{\alpha_i \alpha_j}{\alpha_i + \alpha_j} \overline{AB}^2\right) \quad (A5)$$

and

$$\alpha_k = \alpha_i + \alpha_j ; \quad (A6)$$

$$C_x = \frac{\alpha_i A_x + \alpha_j B_x}{\alpha_i + \alpha_j} ; \quad C_y = \frac{\alpha_i A_y + \alpha_j B_y}{\alpha_i + \alpha_j} ; \quad C_z = \frac{\alpha_i A_z + \alpha_j B_z}{\alpha_i + \alpha_j} . \quad (A7)$$

PROOF:(refer to figure 8) If the point C is placed in accordance with eqs.(A7), then

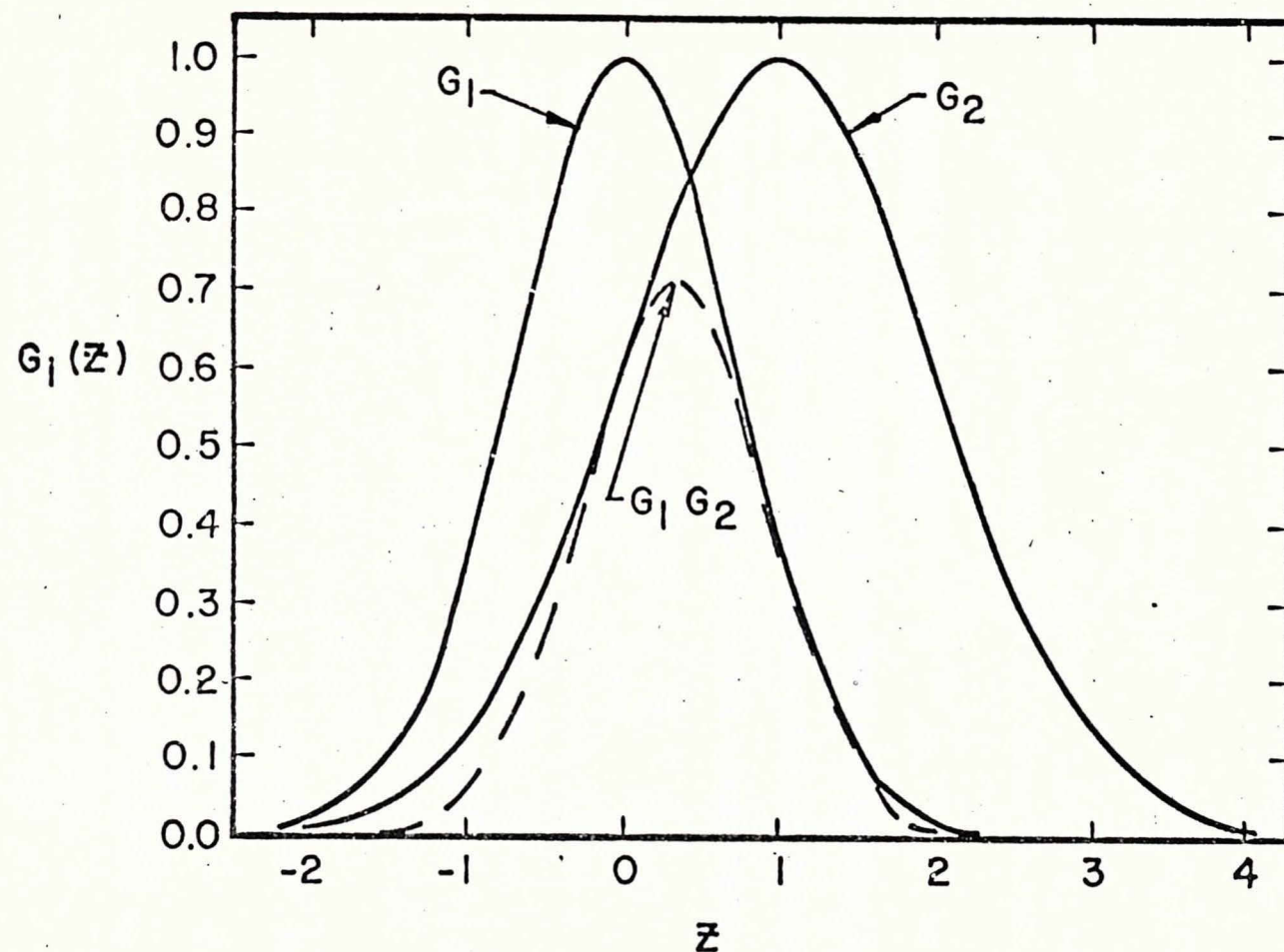
$$\begin{aligned} \overline{AC} &= \left(\frac{\alpha_j}{\alpha_i + \alpha_j}\right)R \\ \overline{CB} &= \left(\frac{\alpha_i}{\alpha_i + \alpha_j}\right)R \end{aligned} \quad (A8)$$

where $R = \overline{AB}$. Using the law of cosines we have

$$r_A^2 = \overline{AC}^2 + r_C^2 + 2\overline{AC}r_C \cos \theta$$

$$r_B^2 = \overline{CB}^2 + r_C^2 - 2\overline{CB}r_C \cos \theta$$

and thus



- Figure 8 -

The values of the following Gaussians along the z axis:

$$G_1 = \exp(-z^2)$$

$$G_2 = \exp(-0.5(z-1)^2)$$

$$G_3 = G_1 G_2$$

$$\begin{aligned}\overline{CB}^2 \Gamma_A^2 + \overline{AC}^2 \Gamma_B^2 &= \overline{AC}^2 \overline{CB} + \overline{CB}^2 \overline{AC} + (\overline{AC} + \overline{CB}) \Gamma_C^2 \\ &= R(\overline{AC} \overline{CB} + \Gamma_C^2)\end{aligned}$$

Substituting for \overline{AC} and \overline{CB} from eqs.(A8) and multiplying throughout by $(\alpha_i + \alpha_j)/R$ we get

$$\left(\frac{\alpha_i}{\alpha_i + \alpha_j}\right) R \Gamma_A^2 + \left(\frac{\alpha_j}{\alpha_i + \alpha_j}\right) R \Gamma_B^2 = R \left(\frac{\alpha_i \alpha_j}{\alpha_i + \alpha_j}\right) R^2 + \Gamma_C^2$$

$$\alpha_i \Gamma_A^2 + \alpha_j \Gamma_B^2 = \left(\frac{\alpha_i \alpha_j}{\alpha_i + \alpha_j}\right) R^2 + (\alpha_i + \alpha_j) \Gamma_C^2$$

or

$$e^{-\alpha_i \Gamma_A^2} e^{-\alpha_j \Gamma_B^2} = e^{-\left(\frac{\alpha_i \alpha_j}{\alpha_i + \alpha_j}\right) R^2} e^{-(\alpha_i + \alpha_j) \Gamma_C^2} \quad \text{Q.E.D.}$$

Integrals of Gaussians

We will now consider some basic Gaussian integrals which are necessary for the evaluation of the matrix elements in the energy calculation. The most elementary of these is

$$\int_0^\infty \exp(-\alpha x^2) dx = \frac{1}{2} \sqrt{\frac{\pi}{\alpha}} \quad (\alpha > 0) \quad (A9)$$

The proof is

$$\begin{aligned}\left\{ \int_0^\infty \exp(-\alpha x^2) dx \right\}^2 &= \int_0^\infty \int_0^\infty \exp(-\alpha x^2) \exp(-\alpha y^2) dx dy \\ &= \int_0^\infty \int_0^{\pi/2} \exp(-\alpha r^2) r d\theta dr \\ &= \frac{\pi}{2} \int_0^\infty r e^{-\alpha r^2} dr\end{aligned}$$

Putting $r^2=s$, $2rdr=ds$, we get

$$\left\{ \int_0^\infty \exp(-\alpha x^2) dx \right\}^2 = \frac{\pi}{4} \int_0^\infty e^{-\alpha s} ds = \frac{\pi}{4} \left[-\frac{e^{-\alpha s}}{\alpha} \right]_0^\infty \\ = \frac{\pi}{4\alpha}.$$

So

$$\int_0^\infty e^{-\alpha x^2} dx = \sqrt{\frac{\pi}{4\alpha}} = \frac{1}{2} \sqrt{\frac{\pi}{\alpha}}. \quad \text{Q.E.D.}$$

We shall now consider the class of integrals

$$F_m(t) = \int_0^1 u^{2m} e^{-tu^2} du \quad (t>0; m=0,1,2,\dots) \quad (\text{A10})$$

which can be considered as a reduced form of the incomplete gamma function,

$$F_m(t) = \frac{1}{2t^{m+1/2}} \gamma(m+\frac{1}{2}, t)$$

They are closely related to the error function and its derivatives, for by making the substitution $tu^2=v^2$, we find

$$F_0(t) = \frac{1}{\sqrt{t}} \int_0^{\sqrt{t}} \exp(-v^2) dv = \frac{1}{2} \sqrt{\frac{\pi}{t}} \operatorname{erf}(\sqrt{t}), \quad (\text{A11})$$

where $\operatorname{erf}(x)$ is the error function,

$$\operatorname{erf}(x) = \int_0^x e^{-u^2} du$$

Furthermore, by differentiating with respect to t under the integral sign of Eq.(A10), we get

$$\begin{aligned}\frac{d}{dt} F_m(t) &= \int_0^1 u^{2m} (-u^2) e^{-tu^2} du \\ &= - \int_0^1 u^{2(m+1)} e^{-tu^2} du\end{aligned}$$

$$\frac{d}{dt} F_m(t) = -F_{m+1}(t) \quad (A12)$$

Integration by parts yields the following recurrence relation,

$$\begin{aligned}F_m(t) &= \left[\frac{u^{2m+1}}{2m+1} e^{-tu^2} \right]_{u=0}^{u=1} - \int_0^1 \frac{-2tu^{2m+2}}{2m+1} e^{-tu^2} du \\ &= \frac{1}{2m+1} e^{-t} + \frac{2t}{2m+1} F_{m+1}(t)\end{aligned}$$

$$F_m(t) = \frac{1}{2m+1} [2t F_{m+1}(t) + e^{-t}] \quad (A13)$$

Eq.(A13) provides a way of computing $F_m(t)$ for a sequence of values of m . Choosing $F_m(t) = 0$ for some large m , and uses Eq.(A13) to go from high to low m with accuracy increasing as you proceed. For our purposes it is more profitable to compute $F_0(t)$ from Eq.(A11) using an I.B.M. function subroutine to compute $\text{erf}(x)$ to sixteen places. The backward recursion formula is particularly useful for a large sequence of m , but necessitates special formulas for very large and very small t . As a test, the values of $F_m(t)$, $m = 0, 1, 2, 3, 4$ were computed by the backward recursion method assuming $F_{100}(t)$ equal to 0 and by using the recursion formula from low to high m computing $F_0(t)$ by Eq.(A11). For $50 > t > 10^{-3}$ both

methods yielded identical results to at least ten places.
For $t > 50$ the backward recursion yielded 0 for all $F_m(t)$.

We will now derive the transformation

$$\frac{1}{r^\lambda} = \frac{1}{\Gamma(\lambda/2)} \int_0^\infty \alpha^{\lambda/2-1} e^{-\alpha r^2} d\alpha \quad \lambda > 0, r > 0 \quad (A14)$$

which will be useful in evaluating basic nuclear-attraction and electron repulsion integrals.

Proof: Consider the integral representation of the Gamma function

$$\Gamma(x) = \int_0^\infty e^{-s} s^{x-1} ds$$

Let $x = \lambda/2$

$$\Gamma(\lambda/2) = \int_0^\infty e^{-s} s^{\lambda/2-1} ds$$

Let $s = \alpha r^2$, $ds = r^2 d\alpha$

$$\Gamma(\lambda/2) = \int_0^\infty e^{-\alpha r^2} (\alpha r^2)^{\lambda/2-1} r^2 d\alpha$$

$$\Gamma(\lambda/2) = \int_0^\infty e^{-\alpha r^2} \alpha^{\lambda/2-1} r^\lambda d\alpha$$

Rearranging yields Eq.(A14).

Energy Integrals

The following formulas were derived by Boys⁵ for the integrals between basic (1s-type) Gaussian orbitals,
(aA) = $\exp(-ar_{1A}^2)$, etc.,

$$(aA|bB) = \int \exp(-ar_A^2 - br_B^2) dr_1 = \left(\frac{\pi}{a+b}\right)^{3/2} \exp\left(-\frac{ab}{a+b} \overline{AB}^2\right) \quad (A15)$$

$$\begin{aligned} (aA|K|bB) &= \int \exp(-ar_A^2) \left(-\frac{1}{2} \nabla_1^2\right) \exp(-br_B^2) dr_1 \\ &= \frac{ab}{a+b} \left(3 - \frac{2ab}{a+b} \overline{AB}^2\right) \left(\frac{\pi}{a+b}\right)^{3/2} \exp\left(-\frac{ab}{a+b} \overline{AB}^2\right) \end{aligned} \quad (A16)$$

$$\begin{aligned} (aA|V_c|bB) &= \int \left(\frac{1}{r_c}\right) \exp(-ar_A^2 - br_B^2) dr_1 \\ &= \frac{2\pi}{a+b} F_0 \left[(a+b) \overline{CP}^2\right] \exp\left(-\frac{ab}{a+b} \overline{AB}^2\right) \end{aligned} \quad (A17)$$

$$\begin{aligned} (aABB|cCD) &= \iint \left(\frac{1}{r_{12}}\right) \exp(-ar_A^2 - br_B^2 - cr_C^2 - dr_D^2) dr_1 dr_2 \\ &= \frac{2\pi^{5/2}}{(a+b)(c+d)(a+b+c+d)^{3/2}} F_0 \left[\frac{(a+b)(c+d)}{(a+b+c+d)} \overline{PQ}^2\right] \\ &\quad \times \exp\left(-\frac{ab}{a+b} \overline{AB}^2 - \frac{cd}{c+d} \overline{CD}^2\right) \end{aligned} \quad (A18)$$

The points P and Q lie on \overline{AB} and \overline{CD} respectively, and are given by

$$P_x = \frac{aA_x + bB_x}{a+b}, \quad Q_x = \frac{cC_x + dD_x}{c+d}, \text{ etc.} \quad (A19)$$

All formulas are valid when two or more centers coincide.

As examples, we shall now derive Eq.(A15) and Eq.(A18).

Eq.(A16) is a straightforward integral which may be evaluated

using Eq.(A4) and Eq.(A9):

$$(aA|bB) = \int \exp(-ar_{1A}^2 - br_{1B}^2) dr_1$$

using Eq.(A4)

$$\exp(-ar_{1A}^2 - br_{1B}^2) = \exp(-(a+b)r_{1C}^2) \exp(-\frac{ab}{a+b}\bar{AB}^2)$$

let $c = a + b$

$$\begin{aligned} (aA|bB) &= \exp(-\frac{ab}{a+b}\bar{AB}^2) \iiint_{-\infty}^{+\infty} e^{-cx_1^2} e^{-cy_1^2} e^{-cz_1^2} dx_1 dy_1 dz_1 \\ &= \exp(-\frac{ab}{a+b}\bar{AB}^2) (8) \int_0^\infty \int_0^\infty \int_0^\infty e^{-cx_1^2} e^{-cy_1^2} e^{-cz_1^2} dx_1 dy_1 dz_1 \\ &= \exp(-\frac{ab}{a+b}\bar{AB}^2) \left(\frac{\pi}{a+b}\right)^{3/2} \quad \text{Q.E.D.} \end{aligned}$$

To derive Eq.(A18) we consider the transform of Eq.(A14) with $\lambda = 1$,

$$\frac{1}{r_{12}} = \frac{1}{\sqrt{\pi}} \int_0^\infty s^{-1/2} e^{-sr_{12}^2} ds$$

Introducing this transform into the integral of Eq.(A18) and factoring the integral into x, y, and z parts gives

$$(aAB|cCdD) = \frac{1}{\sqrt{\pi}} e^{-\left(\frac{ab}{a+b}\bar{AB}^2 + \frac{cd}{c+d}\bar{CD}^2\right)} \int_0^\infty I_x I_y I_z s^{-1/2} ds$$

where

$$I_x = \iint_{-\infty}^{+\infty} e^{-[p(x_1 - p_x)^2 - q(x_2 - q_x)^2 - s(x_1 - x_2)^2]} dx_1 dx_2, \text{ etc.}$$

Putting $u = x_1 - P_x$, $v = x_2 - Q_x$, $X = P_x - Q_x$ and using Eq.(A9),

$$\begin{aligned}
 I_X &= \exp(-s\bar{X}^2) \int_{-\infty}^{\infty} d\mu \exp(-(p+s)u^2 - 2\bar{X}s\mu) \int_{-\infty}^{\infty} dv \\
 &\quad \times \exp(-(q+s)v^2 + 2(\bar{X}+\mu)sv) \\
 &= \sqrt{\frac{\pi}{q+s}} \exp(-s\bar{X}^2) \int_{-\infty}^{\infty} \exp(-(p+s)u^2 - 2\bar{X}s\mu + (\bar{X}+\mu)^2 s^2 / (q+s)) d\mu \\
 &= \sqrt{\frac{\pi}{q+s}} \exp\left(-\frac{qs}{q+s} \bar{X}^2\right) \int_{-\infty}^{\infty} \exp\left(-\frac{p+(p+q)s}{q+s} u^2 - 2\frac{qs}{q+s} \bar{X}u\right) d\mu \\
 &= \sqrt{\frac{\pi^2}{pq+(p+q)s}} \exp\left(-\frac{qs}{q+s} \bar{X}^2\right) \exp\left(\frac{q^2 s^2 \bar{X}^2}{(q+s)(pq+(p+q)s)}\right)
 \end{aligned}$$

$$I_X = \frac{\pi}{\sqrt{pq}} \left(1 + \frac{p+q}{pq} s\right)^{-1/2} \exp\left(-\frac{s\bar{X}^2}{1+s(p+q)/pq}\right)$$

therefore

$$\begin{aligned}
 (aAbB|cCdD) &= \frac{\pi^{5/2}}{(pq)^{3/2}} \exp\left(-\frac{ab}{a+b} \bar{AB}^2 - \frac{cd}{c+d} \bar{CD}^2\right) \\
 &\quad \times \int_0^{\infty} \left(1 + \frac{p+q}{pq} s\right)^{-3/2} \exp\left(-\frac{s\bar{PQ}^2}{1+s(p+q)/pq}\right) ds
 \end{aligned}$$

Now making the substitution

$$1 + \frac{p+q}{pq} s = \frac{1}{1-t^2}$$

we find

$$\left(1 + \frac{p+q}{pq} s\right)^{-3/2} s^{-1/2} ds = 2 \sqrt{\frac{pq}{p+q}} dt,$$

therefore

$$\begin{aligned} (aA b B | cC d D) &= \frac{2\pi^{5/2}}{pq\sqrt{p+q}} \exp\left(-\frac{ab}{a+b} \bar{AB}^2 - \frac{cd}{c+d} \bar{CD}^2\right) \\ &\times \int_0^1 \exp\left(-\frac{pq}{p+q} \bar{PQ}^2 t^2\right) dt \end{aligned}$$

which is equivalent to Eq.(A18).

The basis set proposed by Boys⁵ is made up of the class of functions

$$x_A^l y_A^m z_A^n \exp(-ar_A^2)$$

where l , m , and n are integers and a is positive. Integral formulas for which not all l , m , and n are zero can be derived from the basic formulas, Eqs.(A15-A18), by differentiations with respect to parameters, i. e.,

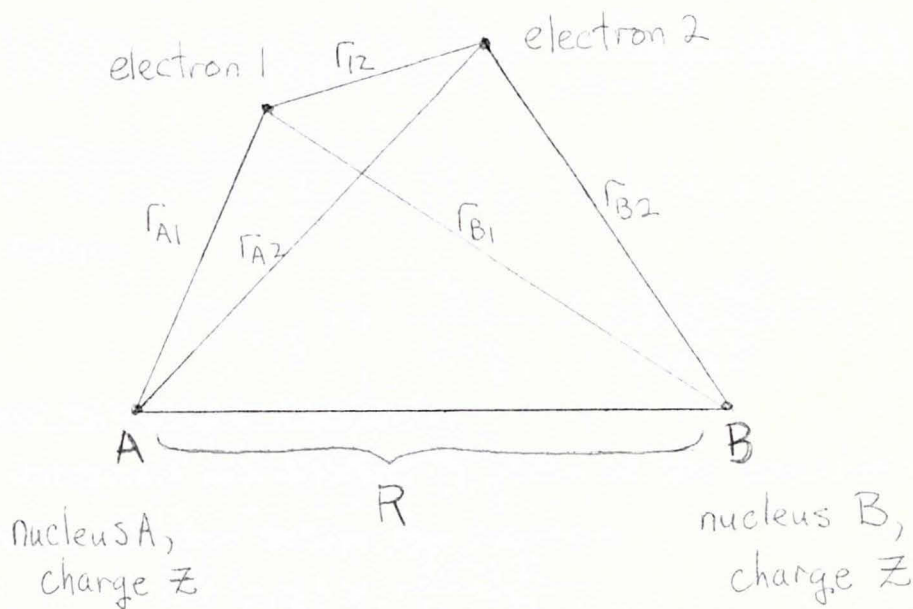
$$x_A \exp(-ar_A^2) = \frac{1}{2a} \frac{\partial}{\partial A_x} \exp(-ar_A^2), \text{ etc.}$$

where A_x is defined in Eq.(A3). For example

$$\begin{aligned} \langle P_{XA} | \frac{1}{c} | S_B \rangle &= \int \left(\frac{1}{r_{1c}} \right) \chi_{1A} \exp(-a r_{1A}^2 - b r_{1B}^2) dr_1 \\ &= \frac{\pi}{a(a+b)} \frac{\partial}{\partial A_x} \left[F_0 \left[(a+b) \bar{CP}^2 \right] \exp\left(-\frac{ab}{a+b} \bar{AB}^2\right) \right] \end{aligned}$$

$$= \frac{2\pi}{a+b} \left\{ (C_X - P_X) F_1 [(a+b) \overline{CP}^2] - \frac{b}{a+b} (A_X - B_X) \right. \\ \left. \times F_0 [(a+b) \overline{CP}^2] \right\} \exp \left(-\frac{ab}{a+b} \overline{AB}^2 \right)$$

A collection of formulas for overlap, kinetic energy, nuclear attraction, and electron repulsion integrals over s and p type Gaussians is presented by Clementi and Davis.¹⁴ The integrals in the following table are derived from the Clementi-Davis expressions by introducing the coordinate system below.



Integral Formulas

Overlap Integrals

$$(a S_A | b S_A) = N(a, b) = \left(\frac{\pi}{a+b} \right)^{3/2}$$

$$(a S_A | b S_B) = W(a, b) = N(a, b) \exp\left(-\frac{ab}{a+b} R^2\right)$$

$$(a p_{zA} | b p_{zA}) = (a p_{xA} | b p_{xA}) = (a p_{yA} | b p_{yA}) = \frac{1}{2(a+b)} N(a, b)$$

$$(a S_B | b p_{zA}) = -(a S_A | b p_{zB}) = \left(\frac{a}{a+b} \right) R W(a, b)$$

$$(a p_{zA} | b p_{zB}) = \left(\frac{1}{2(a+b)} - \frac{ab R^2}{(a+b)^2} \right) W(a, b)$$

$$(a p_{xA} | b p_{xB}) = (a p_{yA} | b p_{yB}) = \frac{1}{2(a+b)} W(a, b)$$

Kinetic Energy Integrals

Define

$$K1(x, y) = \frac{3xy}{x+y} - \frac{2x^2 y^2 R^2}{(x+y)^2}$$

$$K2(x, y) = \frac{3xy}{x+y}$$

$$K3(x, y) = \frac{2x^2 y R}{(x+y)^2}$$

$$K4(x, y) = \frac{xy}{(x+y)^2}$$

then

$$(a S_A | K | b S_A) = K2(a, b) N(a, b)$$

$$(aS_A|K|bS_B) = K1(a,b)W(a,b)$$

$$(aS_A|K|bP_{zB}) = K3(a,b)W(a,b) + K1(a,b)W(a,b)R\left(\frac{a}{a+b}\right)$$

$$(aS_B|K|bP_{zA}) = -(aS_A|K|bP_{zB})$$

$$(aP_{zA}|K|bP_{zB}) = K4(a,b)W(a,b) - R\left(\frac{a}{a+b}\right)(K3(a,b) + K3(b,a)) \\ + W(a,b) + K1(a,b)W(a,b)\left(\frac{1}{2(a+b)} - \frac{abR^2}{(a+b)^2}\right)$$

$$(aP_{zA}|K|bP_{zA}) = K4(a,b)N(a,b) + K2(a,b)N(a,b)\frac{1}{2(a+b)}$$

$$(aP_{xA}|K|bP_{xA}) = (aP_{yA}|K|bP_{yA}) = (aP_{zA}|K|bP_{zA})$$

$$(aP_{xA}|K|bP_{xB}) = (aP_{yA}|K|bP_{yB}) = K4(a,b)W(a,b) \\ + K1(a,b)W(a,b)\frac{1}{2(a+b)}$$

Nuclear Attraction Integrals

Integrals are defined in terms of the function $F_m(t)$ of Eq.(A10). We also define the function

$$\Theta(x,y) = \frac{2}{\pi^{1/2}} (x+y)^{1/2}$$

and the quantities

$$t = (x+y)\bar{P}C^2$$

where $P_x = \frac{aA_x + bB_x}{a+b}$, etc.

$$(a S_A | \frac{1}{r_A} | b S_A) = \Theta(a, b) N(a, b)$$

$$(a S_A | \frac{1}{r_B} | b S_A) = (a S_B | \frac{1}{r_A} | b S_B) = \Theta(a, b) N(a, b) F_0((a+b)R^2)$$

$$(a S_A | \frac{1}{r_A} | b S_B) = \Theta(a, b) W(a, b) F_0\left(\frac{b^2 R^2}{a+b}\right)$$

$$(a S_A | \frac{1}{r_B} | b S_B) = \Theta(a, b) W(a, b) F_0\left(\frac{a^2 R^2}{a+b}\right)$$

$$(a p_{ZA} | \frac{1}{r_A} | b p_{ZA}) = \Theta(a, b) N(a, b) \frac{1}{3(a+b)}$$

$$(a p_{ZA} | \frac{1}{r_B} | b p_{ZA}) = \Theta(a, b) N(a, b) \left\{ R^2 F_2(t) - \frac{1}{2(a+b)} F_1(t) + F_0(t) \frac{1}{2(a+b)} \right\}$$

$$\text{where } t = (a+b)R^2$$

$$(a p_{ZA} | \frac{1}{r_A} | b p_{ZE}) = \frac{\Theta(a, b) W(a, b)}{a+b} \left\{ \frac{(bR)^2}{a+b} F_2(t) - \frac{1}{2} F_1(t) + \left(\frac{1}{2} - \frac{abR^2}{a+b} \right) F_0(t) \right\}$$

$$\text{where } t = \frac{(bR)^2}{a+b}$$

$$(a p_{XA} | \frac{1}{r_A} | b p_{XB}) = \frac{\Theta(a, b) W(a, b)}{2(a+b)} \left\{ F_0(t) - F_1(t) \right\}$$

$$\text{where } t = \frac{(bR)^2}{a+b}$$

$$(a p_{xA} | \frac{1}{r_B} | b p_{xA}) = \frac{\Theta(a,b) N(a,b)}{2(a+b)} \{ F_0(t) - F_1(t) \}$$

$$\text{where } t = (a+b)R^2$$

$$(a S_A | \frac{1}{r_B} | b p_{zA}) = -(a S_B | \frac{1}{r_A} | b p_{zB}) = \Theta(a,b) N(a,b) R F_1(t)$$

$$\text{where } t = (a+b)R^2$$

$$(b p_{zA} | \frac{1}{r_B} | a S_B) = -(a S_A | \frac{1}{r_A} | b p_{zB}) = \frac{\Theta(a,b) W(a,b) R}{(a+b)} (a F_0(t) + b F_1(t))$$

$$\text{where } t = \frac{(bR)^2}{a+b}$$

$$(b p_{zA} | \frac{1}{r_A} | a S_B) = -(a S_A | \frac{1}{r_B} | b p_{zB}) = \Theta(a,b) W(a,b) \left(\frac{aR}{a+b} \right) (F_0(t) - F_1(t))$$

$$\text{where } t = \frac{(aR)^2}{a+b}$$

Electron Repulsion Integrals

Define

$$G(a,b) = 2 \left(\frac{a+b}{2\pi} \right)^{1/2}$$

$$t = \left(\frac{a+b}{2} \right) \overline{PQ}^2$$

$$P_i = \frac{aA_i + bB_i}{a+b}$$

$$Q_i = \frac{cC_i + dD_i}{a+b} \quad i=x,y,z.$$

$$(a S_A b S_A | a S_A b S_A) = G(a, b) N^2(a, b)$$

$$(a S_A b S_B | a S_B b S_A) = G(a, b) N^2(a, b) F_0\left(\frac{a+b}{2} R^2\right)$$

$$(b S_B a S_A | b S_A a S_B) = G(a, b) W^2(a, b)$$

$$(a p_{zA} b p_{zA} | a p_{zB} b p_{zA}) = G(a, b) \left\{ (SAA)^2 F_0(t) + 2(SAA)(G\phi Z Z) N(a, b) + N^2(a, b) G Z Z Z \right\}$$

$$\text{where } SAA = \frac{1}{2(a+b)} N(a, b)$$

$$G\phi Z Z = \frac{1}{4} \left\{ R^2 F_2(t) - \frac{1}{a+b} F_1(t) \right\}$$

$$G Z Z Z = \frac{1}{4(a+b)} \left\{ \frac{(a+b)^2}{4} R^4 F_4(t) - \frac{3(a+b)}{2} R^2 F_3(t) + \frac{3}{4} F_2(t) \right\}$$

$$t = \left(\frac{a+b}{2}\right) R^2$$

$$(a p_{zA} b p_{zB} | a p_{zB} b p_{zA}) = G(a, b) \left\{ SAB^2 F_0(t) + 2W(a, b) G\phi Z Z + W^2(a, b) G Z Z Z \right\}$$

$$\text{where } SAB = \left(\frac{1}{2(a+b)} - \frac{abR^2}{(a+b)^2} \right) W(a, b)$$

and $t = \left(\frac{a+b}{2}\right) \bar{\rho}^2$

$$\bar{\rho} = \left(\frac{b-a}{b+a}\right) R$$

$$G_{\phi\phi z z} = \frac{1}{2} \left\{ \frac{1}{2} \bar{\rho}^2 F_2(t) - \frac{1}{2(a+b)} F_1(t) \right\}$$

$$G_{zzzz} = \frac{1}{4(a+b)^2} \left\{ \frac{(a+b)^2 \bar{\rho}^4}{4} F_4(t) - \frac{3(a+b)}{2} \bar{\rho}^2 F_3(t) + \frac{3}{4} F_2(t) \right\}$$

$$(a\rho_{zA} b\rho_{zA} | a\rho_{zA} b\rho_{zA}) = G(a,b) N^2(a,b) \frac{196}{960(a+b)^2}$$

$$(a\rho_{xA} b\rho_{xA} | a\rho_{xB} b\rho_{xB}) = \frac{G(a,b) N^2(a,b)}{2(a+b)^2} \left\{ \frac{F_0(t)}{2} - F_1(t) + \frac{3}{8} F_2(t) \right\}$$

where $t = \left(\frac{a+b}{2}\right) R^2$

$$(a\rho_{xA} b\rho_{yA} | a\rho_{xB} b\rho_{yB}) = G(a,b) N^2(a,b) \frac{1}{16(a+b)^2} F_2(t)$$

where $t = \left(\frac{a+b}{2}\right) R^2$

$$(a\rho_{xA} b\rho_{xB} | a\rho_{xB} b\rho_{xA}) = \frac{G(a,b) W^2(a,b)}{4(a+b)^2} \left\{ F_0(t) - F_1(t) + \frac{3}{4} F_2(t) \right\}$$

where $t = \left(\frac{a+b}{2}\right) R^2 \left(\frac{b-a}{b+a}\right)^2$

$$(a\rho_{xA} b\rho_{yB} | a\rho_{xB} b\rho_{yA}) = G(a,b) W^2(a,b) \frac{1}{16(a+b)^2} F_2(t)$$

$$\text{where } t = \left(\frac{a+b}{2}\right) R^2 \left(\frac{b-a}{b+a}\right)^2$$

$$(a\rho_{xA} bS_A | a\rho_{xB} bS_B) = G(a,b) N^2(a,b) \frac{1}{4(a+b)} F_1(t)$$

$$\text{where } t = \left(\frac{a+b}{2}\right) R^2$$

$$(a\rho_{xA} bS_B | a\rho_{xB} bS_A) = G(a,b) W^2(a,b) \frac{1}{4(a+b)} F_1(t)$$

$$\text{where } t = \left(\frac{a+b}{2}\right) R^2 \left(\frac{b-a}{b+a}\right)^2$$

$$(a\rho_{zA} b\rho_{xA} | a\rho_{zB} b\rho_{xB}) = G(a,b) N^2(a,b) \left\{ \frac{1}{4(a+b)^2} \left(\frac{1}{4} F_2(t) - \frac{(a+b)R^2}{4} F_3(t) \right) \right\}$$

$$\text{where } t = \left(\frac{a+b}{2}\right) R^2$$

$$(a\rho_{zA} bS_A | a\rho_{zB} bS_B) = G(a,b) N^2(a,b) \frac{1}{2(a+b)} \left\{ \frac{F_1(t)}{2} - \frac{(a+b)R^2}{2} F_2(t) \right\}$$

$$\text{where } t = \left(\frac{a+b}{2}\right) R^2$$

$$(a\rho_{zA} bS_B | a\rho_{zB} bS_A) = G(a,b) W^2(a,b) \left\{ \frac{F_1(t)}{4(a+b)} - \frac{\overline{PQ}^2}{4} F_2(t) - \left(\frac{aR}{a+b}\right)^2 F_0(t) \right\}$$

$$\text{where } t = \left(\frac{a+b}{2}\right) R^2 \left(\frac{b-a}{b+a}\right)^2$$

$$(a\rho_{zAB}\rho_{xB}|a\rho_{zEB}\rho_{xA}) = G(a,b)W^2(a,b) \left\{ \frac{1}{16(a+b)^2} \left(F_2(t) - (a+b)\overline{PQ}^2 F_3(t) \right) - \left(\frac{bR}{a+b} \right)^2 \frac{1}{4(a+b)} F_1(t) \right\}$$

$$\text{where } t = \left(\frac{a+b}{2} \right) \overline{PQ}^2$$

$$\overline{PQ} = R \left(\frac{b-a}{b+a} \right)$$

Error in Kim-Hirschfelder Integral Tables

An error has been found in the computation of Kim and Hirschfelder,² which changes the major part of the results reported in their paper. The error involves the integrals

$$(aS_A|\frac{1}{r_B}|b\rho_{zB})$$

and

$$(aS_A|\frac{1}{r_A}|b\rho_{zB})$$

which are given to be equal in the Kim-Hirschfelder paper.

One may evaluate these integrals in a simple manner by considering Eq.(A17) and the fact that

$$z_A e^{-a r_A^2} = \frac{1}{2a} \frac{\partial}{\partial A_3} e^{-a r_A^2}$$

yielding

$$(aS_A|\frac{1}{r_C}|b\rho_{zB}) = \frac{2\pi}{a+b} \left\{ (C_3 - P_3) F_1((a+b)C\overline{P}^2) - \frac{b}{a+b} (A_3 - B_3) F_0((a+b)C\overline{P}^2) \right\} \times e^{-\frac{ab}{a+b} \overline{AB}^2}$$

In both cases $\overline{AB}=R$ so

$$\text{Case I: } C=A, C_A=C_y=C_3=0$$

$$B_x=B_y=0$$

$$B_3=R$$

$$P_A=P_y=0$$

$$P_3 = \frac{bR}{a+b}$$

$$C\overline{P} = -\frac{bR}{a+b}$$

$$\text{so } (aS_A | \frac{1}{r_A} | bP_{zB}) = \left(\frac{2\pi}{a+b} \right) \left\{ -\left(\frac{bR}{a+b} \right) F_1 \left(\frac{b^2 R^2}{a+b} \right) + \left(\frac{bR}{a+b} \right) F_0 \left(\frac{b^2 R^2}{a+b} \right) \right\} \times e^{-\frac{ab}{a+b} R^2}$$

Consider $J=a=b$ (Kim-Hirschfelder case)

$$(aS_A | \frac{1}{r_A} | bP_{zB}) = \frac{\pi R}{2J} \left\{ F_0 \left(\frac{JR^2}{2} \right) - F_1 \left(\frac{JR^2}{2} \right) \right\} e^{-JR^2/2}$$

noting that (Eq. (A13))

$$F_1(t) = (F_0(t) - e^{-2t}) / (2t)$$

$$\begin{aligned} (aS_A | \frac{1}{r_A} | bP_{zB}) &= \frac{\pi R}{2J} \left\{ F_0 \left(\frac{JR^2}{2} - \frac{F_0 \left(\frac{JR^2}{2} \right) - e^{-JR^2/2}}{JR^2} \right) \right\} e^{-JR^2/2} \\ &= \left(\frac{\pi}{J} \right) \left(\frac{1}{2JR} \right) \left\{ F_0 \left(\frac{JR^2}{2} \right) (JR^2 - 1) + e^{-JR^2/2} \right\} e^{-JR^2/2} \quad (\text{A20}) \end{aligned}$$

which is equivalent to the Kim-Hirschfelder result.
However,

$$\text{CASE II: } C=B, C_x=C_y=0, C_z=R$$

$$B_x=B_y=0$$

$$B_z=R$$

$$P_z = \frac{bR}{a+b}$$

$$\overline{CP} = R - \frac{bR}{a+b} = \frac{aR}{a+b}$$

$$\text{so } (aS_A | \frac{1}{r_B} | bP_{zB}) = \left(\frac{2\pi}{a+b} \right) \left\{ \left(\frac{aR}{a+b} \right) F_1 \left(\frac{a^2 R^2}{a+b} \right) + \left(\frac{bR}{a+b} \right) F_0 \left(\frac{b^2 R^2}{a+b} \right) \right\}$$

again let $J=a=b$

$$(aS_A | \frac{1}{r_B} | bP_{zB}) = \left(\frac{\pi}{J} \right) \left(\frac{1}{2JR} \right) \left\{ F_0 \left(\frac{JR^2}{2} \right) + F_1 \left(\frac{JR^2}{2} \right) \right\} e^{-JR^2/2}$$

$$0.9 \quad (aS_A | \frac{1}{R_B} | bP_{ZB}) = \left(\frac{\pi}{J} \right) \left(\frac{1}{2JR} \right) \left\{ F_0 \left(\frac{JR^2}{2} \right) (JR^2 + 1) - e^{-JR^2/2} \right\} e^{-JR^2/2} \quad (A21)$$

which is not equivalent to Eq.(A21). The recomputation and extension of the Kim-Hirschfelder work with the correct integral forms is a major topic of discussion in this thesis.

APPENDIX B

Computer Programs (Program listings are found in Appendix C)

The problem of computing the lowest eigenvalue and its corresponding eigenvector was programmed in FORTRAN IV for the I.B.M. System 360/Model 40 at the State University of New York at Binghamton Data Processing Center. Several subroutines were obtained from the Quantum Chemistry Program Exchange, Indiana University, Bloomington, Indiana (Q.C.P.E.). A description of these routines follows (also see comments within the program listings in Appendix C):

SUBROUTINE CEIG, Q.C.P.E. Program # 97.

Authors: H.H.Michels, C.P.VanDine, and P.Elliot, United Aircraft Research Laboratories.

Purpose: This routine solves the secular equations of the form

$$(H - \lambda S)C = 0$$

where H and S are real symmetric matrices. The procedure is;

define A by $S = A^T A$

then $(H A^{-1} - \lambda A^T) A C = 0$

and $(A^{-T} H A^{-1} - \lambda I) A C = 0$

but $B = A^{-T} H A^{-1}$ is symmetric therefore

$(B - \lambda I) A C = 0$ is a symmetric eigenvalue problem which is diagonalized by SUBROUTINE NESBET.

Comments: The program was transformed from single-precision to double-precision floating point arithmetic.

SUBROUTINE NESBET, Q.C.P.E. Program # 93.

Authors: H.H.Michels, P. Elliot, United Aircraft Research Laboratories.

Purpose: This subroutine is a FORTRAN coding of a FAP routine due to R.K. Nesbet.¹⁵ The routine

computes the lowest eigenvalue and eigenvector of a real symmetric matrix using the second order matrix diagonalization algorithm of Lowdin.¹⁶ The procedure involves fixing one eigenvector component at unity while the other components c_u are incremented as follows:

$$\nabla_u = \sum_i H_{ui} c_i - E \sum_i S_{ui} c_i,$$

$$\Delta c_u = \nabla_u / (E S_{uu} - H_{uu}),$$

$$\Delta D = (2 \sum_i S_{ui} c_i + S_{uu} \Delta c_u) \Delta c_u$$

$$\Delta E = \nabla_u \Delta c_u / (D + \Delta D)$$

This unit step computes $c_u + \Delta c_u$ as an exact solution of the linear equation of index u , given current values of E and the coefficients (c_i), and computes $E + \Delta E$ as the current second order eigenvalue estimate. The Eqs. above are repeated for the index u in increasing sequence with appropriate convergence criteria. After a complete iteration (all values of u), the computation terminates if the largest increment $|\Delta c_u|_{\text{MAX}}$ is less than a preset tolerance.

The program is particularly suited for large matrices because

- (a) the time required to compute a single eigenvector of an $n \times n$ matrix is proportional to n^2 not n^3 as in most standard diagonalization methods.
- (b) the eigenvalue convergence is 2nd order.
- (c) the lowest eigenvalue converges monotonically.

Comments: The program was transformed from single-precision to double-precision floating point arithmetic. The tolerance for the eigenvalue convergence was set at 10^{-12} .

SUBROUTINE SIMPLEX, Q.C.P.E. program # 67.

Author: J.P.Chandler, Physics Department, Indiana University, Bloomington, Indiana. 47401.

Purpose: Simplex is called to find the local minima of real functions of several variables (up to 20).

The program is a coding of the method of Nedler and Mead.¹⁷ The only requirement is that the function to be minimized is continuous and is defined on a continuous domain, and that all of its derivatives are continuous.

The first derivatives do not have to be computed explicitly.

Comments: A double precision version of Simplex prepared by Mr. W.H. Barker, Science Division Programmer, S.U.N.Y. at Binghamton was used. Convergence criteria for Simplex will be discussed below.

Formulation of the Problem

The wavefunction we use in its most general form is

$$\psi = (1 + P_{12}) \left\{ \sum_i \alpha_i S_A^{(i)} S_B^{(i)} + \sum_j \beta_j P_{ZA}^{(j)} P_{ZB}^{(j)} + \sum_k \gamma_k (P_{XA}^{(k)} P_{XB}^{(k)} + P_{YA}^{(k)} P_{YB}^{(k)}) \right\} \quad (B.1)$$

There are a total of 14 linear ($8\alpha_i, 3\beta_j, 3\gamma_k$) and 14 non-linear ($8J_{1i}, 3J_{2i}, 3J_{3i}$). The ratios $J_{in}/J_{1(N+1)}$ are fixed at

$$\begin{aligned} J_{12} &= 2J_{11} \\ J_{13} &= 3J_{11} \\ J_{14} &= 5J_{11} \\ J_{15} &= 10J_{11} \\ J_{16} &= 50J_{11}, J_{17} = 100J_{11}, J_{18} = 500J_{11} \end{aligned}$$

These ratios were determined by considering the orbital exponents found by Longstaff and Singer¹⁸, who used an eight term Gaussian s expansion to treat the H atom. Fixing the $J_{in}/J_{1(N+1)}$ ratios at the Longstaff-Singer final H atom results (leaving J_{11} free) should then provide a wavefunction which dissociates to give the Longstaff and Singer H atom result of -0.4999 Hartrees as $R \rightarrow \infty$ (exact = -0.5000 Hartrees). The J_{2N} and J_{3N} were fixed as follows to give a good spread in the p_z and p_x, p_y Gaussians; \leftarrow

$$\begin{aligned} J_{22} &= 10J_{21}, J_{23} = 100J_{21} \\ J_{32} &= 10J_{31}, J_{33} = 100J_{31} \end{aligned}$$

We therefore now only have 3 non-linear parameters. The minimization of the energy with respect to these parameters will take from 1-3 hrs./R value on the I.B.M. 360/40. The comp-

utation is carried out as follows.

We write the wavefunction in the form

$$\psi = \sum_{i=1}^{14} c_i \phi_i$$

We need to determine the 14 linear c_i and the three non-linear λ . The (c_i) are the eigenvector components corresponding to the lowest eigenvalue of the Schrödinger equation in matrix form

$$(H - E_1 S) C_i = 0$$

where H is the matrix representation of the Hamiltonian in terms of the basis (ϕ_i) and is given by

$$H = \langle \phi | \hat{H} | \phi \rangle \text{ and}$$

$$S = \langle \phi | \phi \rangle$$

where

$$\phi = [\phi_1, \phi_2, \dots]$$

and

$$C_i = \begin{bmatrix} c_{i1} \\ c_{i2} \\ \vdots \\ \vdots \end{bmatrix}$$

With the Q.C.P.E. programs available, it is only necessary to compute the matrices H and S in order to determine E_1 (lowest eigenvalue) and C_1 (corresponding eigenvector). The problem is further simplified by noting that for our wavefunction of Eq.(B1) and Hamiltonian of Eq.(I), the H and S matrices are real and symmetric. Therefore, one needs to compute only $n(n+1)/2$ elements of the $n \times n$ matrix rather than n^2 elements.

The S matrix is computed in SUBROUTINE OVERLA (see appendix C for listings of computer programs). Special attention was given to preventing exponential underflows which occur when $e^{-x} < 16^{-65}$.

A cutoff criterion of $e^{-x} < 10^{-25}$ was used such that when $e^{-x} < 10^{-25}$ we set $e^{-x} = 0$. This criterion was found not to effect the energy until the 15th place and increased the speed of the computation (especially at large R).

The computation of the H matrix was divided for convenience into three separate steps

$$H = H_A + H_B + H_C$$

where

$$H_A = \langle \phi | -\frac{\nabla_1^2}{2} - \frac{\nabla_2^2}{2} | \phi \rangle$$

$$H_B = \langle \phi | \frac{1}{r_{12}} | \phi \rangle$$

$$H_C = -Z \langle \phi | \frac{1}{r_{A1}} + \frac{1}{r_{B1}} + \frac{1}{r_{A2}} + \frac{1}{r_{B2}} | \phi \rangle + \langle \phi | \frac{Z^2}{R} | \phi \rangle$$

the speed of the computation is further improved by noting that

$$\langle \phi | -\frac{\nabla_1^2}{2} - \frac{\nabla_2^2}{2} | \phi \rangle = 2 \langle \phi | -\frac{\nabla_1^2}{2} | \phi \rangle$$

$$\langle \phi | \frac{1}{r_{A1}} + \frac{1}{r_{B1}} + \frac{1}{r_{A2}} + \frac{1}{r_{B2}} | \phi \rangle = 2 \langle \phi | \frac{1}{r_{A1}} + \frac{1}{r_{B1}} | \phi \rangle$$

The matrices H_A, H_B, H_C are computed in SUBROUTINES HAMTRX, HBMTRX, and HCMTRX respectively.

In order to compute the minimum energy it was found that for 3 non-linear parameters it takes Simplex about 200 energy computations, and with 1 non-linear parameter (the Kim-Hirschfelder function) about 60-70 computations. (For the Kim-Hirschfelder function this involved about 80 seconds per R value).

The final accuracy of the non-linear parameter of the Kim-Hirschfelder function was set at 10^{-5} for Simplex which

gives ten figures in the energy.

Once the energy minimization is complete, the normalized eigenvector is returned to the calling program and several other quantities of interest are computed. They are:

$$\langle V \rangle = 2 \langle \phi | -Z \left(\frac{1}{r_{A1}} + \frac{1}{r_{B1}} \right) | \phi \rangle + Z^2/R$$

$$\langle T \rangle = \langle \phi | -\frac{\nabla_1^2}{2} - \frac{\nabla_2^2}{2} | \phi \rangle$$

$$-\langle V \rangle / 2 \langle T \rangle$$

$$\frac{dE}{dR} = - \frac{2 \langle T \rangle + \langle V \rangle}{R}$$

$$\langle \frac{1}{r_{12}} \rangle = \langle \phi | \frac{1}{r_{12}} | \phi \rangle$$

$$\langle \frac{1}{r_{A1}} \rangle = \frac{1}{4} \langle \phi | -Z \left(\frac{1}{r_{A1}} + \frac{1}{r_{A2}} + \frac{1}{r_{B1}} + \frac{1}{r_{B2}} \right) | \phi \rangle$$

$$\Delta E_R(\text{binding energy}) = E_R - E_{R=\infty}$$

All computed quantities are printed out and punched on cards. The cards may then be fed into PROGRAM OUTPUT and the various tables in the thesis are produced.

- APPENDIX C -

PROGRAM TO COMPUTE ENERGY EIGENVALUE
AND EIGENVECTOR FOR THE WAVEFUNCTION
OF EQUATION

2

LEVEL 1, MOD 3

MAIN

DATE = 69131

17/11/31

IMPLICIT REAL*8(A-H,O-Z)
EXTERNAL TOTAL

MAIN INPUT AND OUTPUT ROUTINE
GAUSSIAN WAVEFUNCTION FOR H2 ISOELECTRONIC SEQUENCE
ENERGY CALCULATION AND MINIMIZATION

COMMON/S1/CHISQ,X(20)
COMMON/S2/XMAX(20),XMIN(20),DELTAX(20),DELMIN(20),NV,NTRACE,
1 MASK(20)
COMMON/A1/PI,R,S(14,14),H(14,14),XP1(8),XP2(3),XP3(3),COF(14),Z,
1 ISTATE
COMMON/A2/HA(14,14),HB(14,14),HC(14,14)
DIMENSION KP(20),COFN(20),SMAT(105)

SET DSIMPX PARAMETERS

500 READ(5,500)CUTOFF
FORMAT(D20.10)
NTRACE=1
NV=3
DO 11 I=1,3
XMAX(I)=2500
XMIN(I)=1D-5
DELMIN(I)=CUTOFF
11 MASK(I)=0

READ NUCLEAR CHARGE, INTERNUCLEAR DISTANCE, AND GROUND OR TRIPLET STATE

2000 READ(5,1)Z,R,ISTATE
IF(Z.LT.0D0)GO TO 999
1 FORMAT(2F10.0,I2)
WRITE(6,5)
WRITE(6,6)Z,R
IF(ISTATE.EQ.0)GO TO 7
WRITE(6,9)
GO TO 10
7 WRITE(6,8)
10 CONTINUE

READ ORBITAL EXPONENTS

2 READ(5,2)(X(I),I=1,3)
FORMAT(3F10.0)

READ INITIAL STEP SIZES ON EXPONENTS

READ(5,2)(DELTAX(I),I=1,3)

CALL SIMPLEX TO MINIMIZE ENERGY FUNCTION

CALL DSIMPX(TOTAL)

LEVEL 1, MOD 3

MAIN

DATE = 69131

17/11/31

COMPUTE THE OVERLAP INTEGRAL - INTEGRAL OF $\Psi I * \Psi I$

SUM1=0D0

SUM2=0D0

SUM3=0D0

SUM4=0D0

DO 100 I=1,8

DO 100 J=1,8

SUM1 = SUM1 + COF(I)*COF(J)*S(I,J)

DO 101 I=1,8

DO 101 J=9,11

SUM2= SUM2 + COF(I)*COF(J)*S(I,J)

SUM2=2D0*SUM2

DO 102 I=9,11

DO 102 J=9,11

SUM3 = SUM3 + COF(I)*COF(J)*S(I,J)

DO 103 I=12,14

DO 103 J=12,14

SUM4 = SUM4 + COF(I)*COF(J)*S(I,J)

PSISQ= SUM1 + SUM2 + SUM3 + SUM4

OUTPUT SECTION

WRITE(6,6)Z,R

IF(ISTATE.EQ.0)GO TO 77

WRITE(6,9)

GO TO 80

77 WRITE(6,8)

80 CONTINUE

5 FORMAT('1',4X,' GAUSSIAN WAVEFUNCTION FOR THE',/5X,' H2 ISOELECTRO
1NIC SEQUENCE',//5X,' S.L.BRENNER',/5X,' SUNY AT BINGHAMTON',/5X,'
2NEW YORK')

6 FORMAT(/6X,'NUCLEAR CHARGE',F10.0,/5X,' INTERNUCLEAR DISTANCE',F10
1.5)

8 FORMAT(5X,' GROUND STATE')

9 FORMAT(5X,' TRIPLET STATE')

WRITE(6,301)

WRITE(6,300)(COF(I),I=1,14)

300 FORMAT(/(3D25.16))

310 FORMAT(3D25.16)

301 FORMAT(14H0 EIGENVECTORS//)

WRITE(6,401)

WRITE(6,300)(X(I),I=1,3)

401 FORMAT(11H0 EXPONENTS//)

WRITE(6,303)

303 FORMAT(19H0 LOWEST EIGENVALUE//)

WRITE(6,304)CHISQ

304 FORMAT(10X,D25.16)

WRITE(6,110)PSISQ

110 FORMAT(21H0 INTEGRAL OF $\Psi I * \Psi I$,/D25.16)

WRITE(6,1000)

LEVEL 1, MOD 3

MAIN

DATE = 69131

17/11/31

```
1000 FORMAT('1')  
GO TO 2000  
999 STOP  
END
```

LEVEL 1, MOD 3

TOTAL

DATE = 69131

17/11/31

SUBROUTINE TOTAL

IMPLICIT REAL*8(A-H,O-Z)

COMMON/A1/PI,R,S(14,14),H(14,14),XP1(8),XP2(3),XP3(3),COF(14),Z,

1 ISTATE

13 COMMON/A2/HA(14,14),HB(14,14),HC(14,14)

COMMON/S1/CHISQ,X(20)

DIMENSION KP(14),HMAT(105),SMAT(105),E(14),COET(14,14),VEC(14,5),

1 ITIME(2)

PI=3.1415926535897932D0

N1=1

NN=14

N=14

INITIALIZE EXPONENTS WITH CURRENT X VALUES

XP1(1)= X(1)

XP1(2)= 2D0 *X(1)

XP1(3)= 3D0 *X(1)

XP1(4)= 5D0 *X(1)

XP1(5)= 10D0 *X(1)

XP1(6)= 20D0 *X(1)

XP1(7)= 100D0 *X(1)

XP1(8)= 500D0 *X(1)

XP2(1)=X(2)

XP2(2)=10D0*X(2)

XP2(3)=100D0*X(2)

XP3(1)=X(3)

XP3(2)=10D0*X(3)

XP3(3)=100D0*X(3)

CALL ENERGY MATRIX ROUTINES

CALL OVERLA

CALL HAMTRX

CALL HBMTRX

CALL HCMTRX

COMPUTE HAMILTONIAN MATRIX

DO 10 J=1,N

DO 10 I=1,J

H(I,J)= HA(I,J) + HB(I,J) + HC(I,J)

10 CONTINUE

DO 12 I=1,N

12 KP(I)=(I*(I-1))/2

TAKE MATRIX WHICH IS STORED IN UPPER TRIANGULAR FORM AND
STORE IN A VECTOR COLUMN BY COLUMN

DO 13 J=1,N

DO 13 I=1,J

III=KP(J)+I

G LEVEL 1, MOD 3

TOTAL

DATE = 69131

17/11/31

HMAT(III)=H(I,J)

SMAT(III)=S(I,J)

IF(DABS(HMAT(III)).LT.1D-10)HMAT(III)=0D0

IF(DABS(SMAT(III)).LT.1D-10)SMAT(III)=0D0

13 CONTINUE

C
C
C

OBTAIN EIGENVLAUE AND EIGENVECTOR

C
C
C

CALL CEIG(N,N1,NN,HMAT,SMAT,E,COET,VEC,KP)

TOTAL ENERGY = ELECTRONIC ENERGY + NUCLEAR REPULSION ENERGY

CHISQ=E(1) + Z**2/R

DO 15 I=1,N

15 COF(I)=COET(I,1)

RETURN

END


```
SUBROUTINE FT
IMPLICIT REAL*8(A-H,N-Z)
COMMON/A1/PI,R,S(14,14),H(14,14),XP1(8),XP2(3),XP3(3),COF(14),Z,
1  ISTATE
COMMON/F/T,FT1,FT2,FT3,FT4,FT0
IF(T.LT.1.D-15)GO TO 10
FT0=(1D0/2D0)*DSQRT(PI/T)*DERF(DSQRT(T))
YY=DEXP(-T)
FT1=(FT0-YY      )/(2D0*T)
FT2=(3D0*FT1-YY  )/(2D0*T)
FT3=(5D0*FT2-YY  )/(2D0*T)
FT4=(7D0*FT3-YY  )/(2D0*T)
RETURN
10 FT0=1D0
FT1=1D0/3D0
FT2=1D0/5D0
FT3=1D0/7D0
FT4=1D0/9D0
RETURN
END
```

G LEVEL 1, MOD 3

OVERLA

DATE = 69132

10/45/24

SUBROUTINE OVERLA

C
C
C
COMPUTE OVERLAP MATRIX S(I,J)

IMPLICIT REAL*8(A-H,N-Z)

COMMON/A1/PI,R,S(14,14),H(14,14),XP1(8),XP2(3),XP3(3),COF(14),Z,
1 ISTATE

DIMENSION VLAP(8)

N(X,Y)=(PI/(X+Y))**(3D0/2D0)

IF(ISTATE.NE.0)GO TO 1000

C
C
C
COMPUTE S-S ELEMENTS

DO 10 I=1,8

DO 10 J=1,I

A=XP1(I)

B=XP1(J)

VLAP(1) = N(A,B)

TEST= A*B*R**2/(A+B)

IF(TEST.GE.25D0)GO TO 30

VLAP(2)=VLAP(1)*DEXP(-TEST)

GO TO 40

30 VLAP(2)=0D0

40 CONTINUE

S(I,J)=2D0*(VLAP(1)**2 + VLAP(2)**2)

S(J,I)=S(I,J)

10 CONTINUE

C
C
C
COMPUTE S-PZ ELEMENTS

DO 11 I=1,8

DO 11 J=1,3

A=XP1(I)

U=XP2(J)

TEST=A*U*R**2/(A+U)

IF(TEST.GE.25D0)GO TO 31

VLAP(5)=(A/(A+U))*R*N(A,U)*DEXP(-TEST)

GO TO 41

31 VLAP(5)=0D0

41 CONTINUE

IJ=J+8

S(I,IJ) = 2D0*(- VLAP(5)**2)

S(IJ,I)=S(I,IJ)

11 CONTINUE

C
C
C
COMPUTE S-PX ELEMENTS

DO 12 I=1,8

DO 12 J=12,14

S(I,J)=0D0

S(J,I)=0D0

12 CONTINUE

G LEVEL 1, MOD 3

OVERLA

DATE = 69132

10/45/24

C
C 10 COMPUTE PZ-PX ELEMENTS
CDO 13 I=12,14
DO 13 J=9,11
S(I,J)=0D0
S(J,I)=0D0
13 CONTINUEC
C COMPUTE PZ-PZ ELEMENTS
CDO 14 I=1,3
DO 14 J=1,I
II=I+8
JJ=J+8
U=XP2(I)
D=XP2(J)
VLAP(3) = N(U,D) * (1D0/(2D0*(U+D)))
TEST=U*D*R**2/(U+D)
IF(TEST.GE.25D0)GO TO 33
VLAP(7)=N(U,D)*DEXP(-TEST)*(1D0/(2D0*(U+D))-U*D*R**2/((U+D)**2))
GO TO 43
33 VLAP(7)=0D0
43 CONTINUE
S(II,JJ)= 2D0 * (VLAP(3)**2 + VLAP(7)**2)
S(JJ,II)=S(II,JJ)
14 CONTINUEC
C COMPUTE PX-PX ELEMENTS
CDO 15 I=1,3
DO 15 J=1,I
E=XP3(I)
F=XP3(J)
VLAP(4) = N(E,F)*(1D0/(2D0*(E+F)))
TEST=E*F*R**2/(E+F)
IF(TEST.GE.25D0)GO TO 35
VLAP(8)=VLAP(4)*DEXP(-TEST)
GO TO 45
35 VLAP(8)=0D0
45 CONTINUE
II=I+11
JJ=J+11
S(II,JJ) = 4D0 * (VLAP(4)**2 + VLAP(8)**2)
S(JJ,II)=S(II,JJ)
15 CONTINUEC
C RETURN AFTER GROUND STATE CALCULATION
C

RETURN

C
C EXCITED STATE SECTION - ELEMENTS COMPUTED IN SAME ORDER AS ABOVE

LEVEL 1, MOD 3

OVERLA

DATE = 69132

10/45/24

C

```
1000 CONTINUE
DO 20 I=1,8
DO 20 J=1,I
A=XP1(I)
B=XP1(J)
VLAP(1) = N(A,B)
TEST= A*B*R**2/(A+B)
IF(TEST.GE.2500)GO TO 50
VLAP(2)=VLAP(1)*DEXP(-TEST)
GO TO 60
50 VLAP(2)=0D0
60 CONTINUE
S(I,J)=2D0*(VLAP(1)**2 - VLAP(2)**2)
S(J,I)=S(I,J)
20 CONTINUE
DO 21 I=1,8
DO 21 J=1,3
A=XP1(I)
U=XP2(J)
TEST=A*U*R**2/(A+U)
IF(TEST.GE.2500)GO TO 51
VLAP(5)=(A/(A+U))*R*N(A,U)*DEXP(-TEST)
GO TO 61
51 VLAP(5)=0D0
61 CONTINUE
IJ=J+8
S(I,IJ) = 2D0*( + VLAP(5)**2)
S(IJ,I)=S(I,IJ)
21 CONTINUE
DO 22 I=1,8
DO 22 J=12,14
S(I,J)=0D0
S(J,I)=0D0
22 CONTINUE
DO 23 I=12,14
DO 23 J=9,11
S(I,J)=0D0
S(J,I)=0D0
23 CONTINUE
DO 24 I=1,3
DO 24 J=1,I
II=I+8
JJ=J+8
U=XP2(I)
D=XP2(J)
VLAP(3) = N(U,D) * (1D0/(2D0*(U+D)))
TEST=U*D*R**2/(U+D)
IF(TEST.GE.2500)GO TO 53
VLAP(7)=N(U,D)*DEXP(-TEST)*(1D0/(2D0*(U+D))-U*D*R**2/((U+D)**2))
GO TO 63
53 VLAP(7)=0D0
```

LEVEL 1, MOD 3

OVERLA

DATE = 69132

10/45/24

```
63 CONTINUE
S(II,JJ)= 2D0 * ( VLAP(3)**2 - VLAP(7)**2 )
S(JJ,II)=S(II,JJ)
24 CONTINUE
DO 25 I=1,3
DO 25 J=1,I
E=XP3(I)
F=XP3(J)
VLAP(4) = N(E,F)*(1D0/(2D0*(E+F)))
TEST=E*F*R**2/(E+F)
IF(TEST.GE.25D0)GO TO 55
VLAP(8)=VLAP(4)*DEXP(-TEST)
GO TO 65
55 VLAP(8)=0D0
65 CONTINUE
II=I+11
JJ=J+11
S(II,JJ) = 4D0 * (VLAP(4)**2 - VLAP(8)**2 )
S(JJ,II)=S(II,JJ)
25 CONTINUE
RETURN
END
```

LEVEL 1, MOD 3

MAIN

DATE = 69132

10/45/24

C
C
C

KINETIC ENERGY MATRIX

C
C
C

SUBROUTINE HAMTRX

IMPLICIT REAL*8(A-H,N-Z)

REAL*8 K1,K2,K3,K4

COMMON/A1/PI,R,S(14,14),H(14,14),XP1(8),XP2(3),XP3(3),COF(14),Z,
1 ISTATE

COMMON/A2/HA(14,14),HB(14,14),HC(14,14)

DIMENSION VLAP(8),EKIN(10)

N(X,Y)=(PI/(X+Y))**(3D0/2D0)

C
C
C

DEFINE AUXILIARY K FUNCTIONS

 $K1(X,Y) = 3D0 * X * Y / (X + Y) - 2D0 * (X * Y * R) ** 2 / ((X + Y) ** 2)$ $K2(X,Y) = 3D0 * X * Y / (X + Y)$ $K3(X,Y) = 2D0 * Y * R * X ** 2 / ((X + Y) ** 2)$ $K4(X,Y) = X * Y / ((X + Y) ** 2)$

IF(ISTATE.NE.0)GO TO 1000

C
C
C

S-S ELEMENTS

DO 10 I=1,8

DO 10 J=1,I

A=XP1(I)

B=XP1(J)

VLAP(1)=N(A,B)

EKIN(1)=K2(A,B)*N(A,B)

TEST=A*B*R**2/(A+B)

IF(TEST.GE.25D0)GO TO 20

VLAP(2)=VLAP(1)*DEXP(-TEST)

EKIN(2)=K1(A,B)*VLAP(2)

GO TO 30

20 EKIN(2)=0D0

VLAP(2)=0D0

30 CONTINUE

HA(I,J)=4D0*(EKIN(1)*VLAP(1) + EKIN(2)*VLAP(2))

HA(J,I)=HA(I,J)

10 CONTINUE

C
C
C

S-PZ ELEMENTS

DO 11 I=1,8

DO 11 J=1,3

A=XP1(I)

C=XP2(J)

TEST=A*C*R**2/(A+C)

IF(TEST.GE.25D0)GO TO 21

W=N(A,C)*DEXP(-TEST)

VLAP(5)=(A/(A+C))*R*W

EKIN(3)=W*K3(A,C)+K1(A,C)*VLAP(5)

GO TO 31

LEVEL 1, MOD 3

HAMTRX

DATE = 69132

10/45/24

21 VLAP(5)=0D0

EKIN(3)=0D0

31 CONTINUE

JJ=J+8

HA(I,JJ)= - 4D0*EKIN(3)*VLAP(5)

HA(JJ,I)=HA(I,JJ)

11 CONTINUE

S-PX ELEMENTS

DO 12 I=1,8

DO 12 J=12,14

HA(I,J)=0D0

HA(J,I)=0D0

12 CONTINUE

PZ-PX ELEMENTS

DO 43 I=9,11

DO 43 J=12,14

HA(I,J)=0D0

HA(J,I)=0D0

43 CONTINUE

PZ-PZ ELEMENTS

DO 14 I=1,3

DO 14 J=1,I

II=I+8

JJ=J+8

C=XP2(I)

D=XP2(J)

NN=N(C,D)

VLAP(3)=NN*(1D0/(2D0*(C+D)))

EKIN(6)=K4(C,D)*NN+K2(C,D)*VLAP(3)

TEST=C*D*R**2/(C+D)

IF(TEST.GE.25D0)GO TO 24

W=NN*DEXP(-TEST)

VLAP(7)=W*(1D0/(2D0*(C+D))-C*D*R**2/((C+D)**2))

EKIN(5)=W*K4(C,D)-W*R*(C/(C+D))*K3(C,D)+K3(D,C)+K1(C,D)*VLAP(7)

GO TO 34

24 VLAP(7)=0D0

EKIN(5)=0D0

34 CONTINUE

HA(II,JJ)=4D0*(EKIN(6)*VLAP(3) + VLAP(7)*EKIN(5))

HA(JJ,II)=HA(II,JJ)

14 CONTINUE

PX-PY ELEMENTS

DO 15 I=1,3

DO 15 J=1,I

LEVEL 1, MOD 3

HAMTRX

DATE = 69132

10/45/24

II=I+11

JJ=J+11

E=XP3(I)

F=XP3(J)

NN=N(E,F)

VLAP(4)=NN*(1D0/(2D0*(E+F)))

EKIN(7)=K4(E,F)*NN+K2(E,F)*VLAP(4)

TEST=E*F*R**2/(E+F)

IF(TEST.GE.25D0)GO TO 25

W=NN*DEXP(-TEST)

VLAP(8)=W*(1D0/(2D0*(E+F)))

EKIN(9)=K4(E,F)*W+K1(E,F)*VLAP(8)

GO TO 35

25 VLAP(8)=0D0

EKIN(9)=0D0

35 CONTINUE

HA(II,JJ)=8D0*(EKIN(7)*VLAP(4) + EKIN(9)*VLAP(8))

HA(JJ,II)=HA(II,JJ)

15 CONTINUE

RETURN AFTER GROUND STATE CALCULATION

RETURN

EXCITED STATE - MATRIX ELEMENTS COMPUTED IN SAME ORDER AS ABOVE

1000 CONTINUE

DO 40 I=1,8

DO 40 J=1,I

A=XP1(I)

B=XP1(J)

VLAP(1)=N(A,B)

EKIN(1)=K2(A,B)*N(A,B)

TEST=A*B*R**2/(A+B)

IF(TEST.GE.25D0)GO TO 50

VLAP(2)=VLAP(1)*DEXP(-TEST)

EKIN(2)=K1(A,B)*VLAP(2)

GO TO 60

50 VLAP(2)=0D0

EKIN(2)=0D0

60 CONTINUE

HA(I,J)=4D0*(EKIN(1)*VLAP(1) - EKIN(2)*VLAP(2))

HA(J,I)=HA(I,J)

40 CONTINUE

DO 41 I=1,8

DO 41 J=1,3

A=XP1(I)

C=XP2(J)

TEST=A*C*R**2/(A+C)

IF(TEST.GE.25D0)GO TO 51

W=N(A,C)*DEXP(-TEST)

LEVEL 1, MOD 3

HAMTRX

DATE = 69132

10/45/24

```

      VLAP(5)=(A/(A+C))*R*W
      EKIN(3)=W*K3(A,C)+K1(A,C)*VLAP(5)
      GO TO 61
51  VLAP(5)=0D0
      EKIN(3)=0D0
61  CONTINUE
      JJ=J+8
      HA(I,JJ)= + 4D0*EKIN(3)*VLAP(5)
      HA(JJ,I)=HA(I,JJ)
41  CONTINUE
      DO 42 I=1,8
      DO 42 J=12,14
      HA(I,J)=0D0
      HA(J,I)=0D0
42  CONTINUE
      DO 13 I=9,11
      DO 13 J=12,14
      HA(I,J)=0D0
      HA(J,I)=0D0
13  CONTINUE
      DO 44 I=1,3
      DO 44 J=1,I
      II=I+8
      JJ=J+8
      C=XP2(I)
      D=XP2(J)
      NN=N(C,D)
      VLAP(3)=NN*(1D0/(2D0*(C+D)))
      EKIN(6)=K4(C,D)*NN+K2(C,D)*VLAP(3)
      TEST=C*D*R**2/(C+D)
      IF(TEST.GE.25D0)GO TO 54
      W=NN*DEXP(-TEST)
      VLAP(7)=W*(1D0/(2D0*(C+D))-C*D*R**2/((C+D)**2))
      EKIN(5)=W*K4(C,D)-W*R*(C/(C+D))*(K3(C,D)+K3(D,C))+K1(C,D)*VLAP(7)
      GO TO 64
54  VLAP(7)=0D0
      EKIN(5)=0D0
64  CONTINUE
      HA(II,JJ)=4D0*(EKIN(6)*VLAP(3) - VLAP(7)*EKIN(5))
      HA(JJ,II)=HA(II,JJ)
44  CONTINUE
      DO 45 I=1,3
      DO 45 J=1,I
      II=I+11
      JJ=J+11
      E=XP3(I)
      F=XP3(J)
      NN=N(E,F)
      VLAP(4)=NN*(1D0/(2D0*(E+F)))
      EKIN(7)=K4(E,F)*NN+K2(E,F)*VLAP(4)
      TEST=E*F*R**2/(E+F)
      IF(TEST.GE.25D0)GO TO 55

```


LEVEL 1, MOD 3

HAMTRX

DATE = 69132

10/45/24

W=NN*DEXP(-TEST)

VLAP(8)=W*(1D0/(2D0*(E+F)))

EKIN(9)=K4(E,F)*W+K1(E,F)*VLAP(8)

GO TO 65

55 VLAP(8)=0D0

EKIN(9)=0D0

65 CONTINUE

HA(II,JJ)=8D0*(EKIN(7)*VLAP(4) - EKIN(9)*VLAP(8))

HA(JJ,II)=HA(II,JJ)

45 CONTINUE

RETURN

END

G LEVEL 1, MOD 3

HBMTRX

DATE = 69131

17/11/31

SUBROUTINE HBMTRX
IMPLICIT REAL*8(A-H,N-Z)

ELECTRON REPULSION MATRIX

COMMON/A1/PI,R,S(14,14),H(14,14),XP1(8),XP2(3),XP3(3),COF(14),Z,
1 ISTATE
COMMON/A2/HA(14,14),HB(14,14),HC(14,14)
COMMON/F/T,FT1,FT2,FT3,FT4,FTO
DIMENSION REP1(4),REP2(4),REP3(4),REP4(4),REP5(4),REP6(4)
N(X,Y)=(PI/(X+Y))**((3DO/2DO)
G(W,X,Y,Z)=2DO*DSQRT((W+X)*(Y+Z)/(PI*(W+X+Y+Z)))

TEST FOR GROUND OR EXCITED STATE

IF(ISTATE.NE.0)GO TO 1000

COMPUTE S-S ELEMENTS

DO 10 I=1,8
DO 10 J=1,I
A=XP1(I)
B=XP1(J)
C=A
D=B
S1=A+B
S2=S1
S4=S1+S2
T=S1*S2*R**2/S4
CALL FT
NN=N(A,B)
GG=G(A,B,C,D)
REP1(2)=GG*NN**2*FTO
TEST=A*B*R**2/(A+B)
IF(TEST.GE.25DO)GO TO 11
REP1(3)=GG*(NN*DEXP(-TEST))**2
GO TO 12
11 REP1(3)=0DO
12 CONTINUE
HB(I,J)=2DO*(REP1(2) + REP1(3))
HB(J,I)=HB(I,J)
10 CONTINUE

COMPUTE S-PZ ELEMENTS

DO 20 I=1,8
DO 20 J=1,3
JJ=J+8
B=XP1(I)
A=XP2(J)
C=A

G LEVEL 1, MOD 3

HBMTRX

DATE = 69131

17/11/31

```
D=B
S1=A+B
S2=S1
S4=S1+S2
T=S1*S2*R**2/S4
CALL FT
NN=N(A,B)
GG=G(A,B,C,D)
REP6(1)=GG*NN**2/S4*(FT1/2D0-S1*S2*FT2*R**2/S4)
TEST=A*B*R**2/(A+B)
IF(TEST.GE.25D0)GO TO 21
PQ=R*(B/(A+B)-C/(C+D))
T=S1*S2*PQ**2/S4
CALL FT
W=NN*DEXP(-TEST)
REP6(3)=GG*W**2*((B*R/(A+B))*(-B*R/(C+D)*FT0+S1*PQ*FT1/S4)+FT1/(2D
1 0*S4)-S1*S2*PQ**2*FT2/S4**2 - B*R*S1*PQ*FT1/((A+B)*S4))
GO TO 22
21 REP6(3)=0D0
22 CONTINUE
HB(I,JJ)=2D0*(REP6(1) + REP6(3))
HB(JJ,I)=HB(I,JJ)
20 CONTINUE

C
C
C
COMPUTE S-PX ELEMENTS

DO 30 I=1,8
DO 30 J=1,3
JJ=J+11
A=XP3(J)
B=XP1(I)
C=A
D=B
S1=A+B
S2=S1
S4=S1+S2
NN=N(A,B)
GG=G(A,B,C,D)
T=S1*S2*R**2/S4
CALL FT
REP5(1)=GG*NN**2*FT1/(2D0*S4)
TEST=A*B*R**2/(A+B)
IF(TEST.GE.25D0)GO TO 31
T=S1*S2*R**2/S4*(B/(A+B) -C/(C+D))**2
CALL FT
W=NN*DEXP(-TEST)
REP5(2)= GG*W**2*FT1/(2D0*S4)
GO TO 32
31 REP5(2)=0D0
32 CONTINUE
HB(I,JJ)=4D0*(REP5(1) + REP5(2))
HB(JJ,I)=HB(I,JJ)
```


G LEVEL 1, MOD 3

HBMTRX

DATE = 69131

17/11/31

30 CONTINUE

C
C
C

COMPUTE PZ-PZ ELEMENTS

DO 40 I=1,3

DO 40 J=1,I

II=I+8

JJ=J+8

A=XP2(I)

B=XP2(J)

C=A

D=B

S1=A+B

S2=C+D

S4=S1+S2

T=S1*S2*R**2/S4

CALL FT

NN=N(A,B)

GG=G(A,B,C,D)

SAA=NN/(2D0*(A+B))

SBB=SAA

GOZZ=(S1/S4)*((S1/S4)*FT2*R**2-(1D0/(2D0*S2))*FT1)

GZZO=GOZZ

GZZZ=(1D0/(S4**2))*((S1*S2*R**2/S4)**2*FT4-S1*S2*3D0*FT3*R**2/S4
1 +3D0*FT2/4D0)

REP2(1)=GG*(SAA*(SBB*FTO+NN*GOZZ)+NN*(SBB*GZZO+NN*GZZZ))

TEST=A*B*R**2/(A+B)

IF(TEST.GE.25D0)GO TO 41

W=NN*DEXP(-TEST)

SAB1=(1D0/(2D0*(A+B))-A*B*R**2/((A+B)**2))*W

PQ=(B-C)/(B+C)*R

T=S1*S2*PQ**2/S4

CALL FT

G0000=FTO

G00ZZ=S1/S4*(S1/S4*PQ**2*FT2-1D0/(2D0*S2)*FT1)

GZZZZ=1D0/S4**2*(S1**2*S2**2*PQ**4*FT4/S4**2-3D0*S1*S2*PQ**2*FT3/
1 S4 +3D0*FT2/4D0)

REP2(2)=GG*(SAB1**2*G0000+2D0*W*SAB1*G00ZZ+W**2*GZZZZ)

GO TO 42

41 REP2(2)=0D0

42 CONTINUE

HB(II,JJ)=2D0*(REP2(1) + REP2(2))

HB(JJ,II)=HB(II,JJ)

40 CONTINUE

C
C
C

COMPUTE PZ-PX ELEMENTS

DO 50 I=1,3

DO 50 J=1,3

II=I+8

JJ=J+11

A=XP2(I)

G LEVEL 1, MOD 3

HBMTRX

DATE = 69131

17/11/31

```

B=XP3(J)
C=A
D=B
S1=A+B
S2=S1
S4=S1+S2
T=S1*S2*R**2/S4
CALL FT
NN=N(A,B)
GG=G(A,B,C,D)
REP4(1)=GG*NN**2*(1D0/S4**2*(FT2/4D0-S1*S2*R**2*FT3/(2D0*S4)))
TEST=A*B*R**2/(A+B)
IF(TEST.GE.25D0)GO TO 51
PQ=R*(B/(A+B)-C/(C+D))
T=S1*S2*PQ**2/S4
CALL FT
W=NN*DEXP(-TEST)
REP4(2)=GG*W**2*(1D0/(16D0*S1**2)*(-S1*PQ**2*FT3+FT2)-(B*R/(A+B))*
1  *2*FT1/(2D0*S4))
GO TO 52
51 REP4(2)=0D0
52 CONTINUE
HB(II,JJ)= 4D0*(REP4(1) + REP4(2))
HB(JJ,II)=HB(II,JJ)
50 CONTINUE

C
C
C
COMPUTE PX-PY ELEMENTS

DO 60 I=1,3
DO 60 J=1,I
II=I+11
JJ=J+11
A=XP3(I)
B=XP3(J)
C=A
D=B
S1=A+B
S2=S1
S4=S1+S2
T=S1*S2*R**2/S4
CALL FT
NN=N(A,B)
GG=G(A,B,C,D)
REP3(1)=GG*NN**2*(FT0/(4D0*S1*S2)-FT1*( S1      /{(2D0*S1*S2*S4)})+
1  3D0*FT2/(4D0*S4**2))
REP3(2)=GG*NN**2*FT2/(4D0*S4**2)
TEST=A*B*R**2/(A+B)
IF(TEST.GE.25D0)GO TO 61
W=NN*DEXP(-TEST)
T=S1*S2*R**2/S4*(B/(A+B)-C/(C+D))**2
CALL FT
REP3(3)=GG*W**2*((1D0/(2D0*(A+B)))*{FT0/(2D0*(C+D))-S1*FT1/(2D0*S2

```

G LEVEL 1, MOD 3

HBMTRX

DATE = 69131

17/11/31

```

1    *S4)) + 3D0*FT2/(4D0*S4**2) - FT1/(4D0*S1*S4))
    REP3(4) = GG*W**2*FT2*(1D0/(4D0*S4**2))
    GO TO 62
61   REP3(3) = 0D0
    REP3(4) = 0D0
62   CONTINUE
    HB(II,JJ) = 4D0*(REP3(1)+REP3(2) + REP3(3) + REP3(4))
    HB(JJ,II) = HB(II,JJ)
60   CONTINUE

C
C   RETURN AFTER GROUND STATE CALCULATION
C
C   RETURN
1000 CONTINUE

C
C   EXCITED STATE CALCULATION
C
C   COMPUTATION OF MATRIX ELEMENTS IN SAME ORDER AS FOR GROUND STATE
C
C
DO 70 I=1,8
DO 70 J=1,I
A=XP1(I)
B=XP1(J)
C=A
D=B
S1=A+B
S2=S1
S4=S1+S2
T=S1*S2*R**2/S4
CALL FT
NN=N(A,B)
GG=G(A,B,C,D)
REP1(2) = GG*NN**2*FT0
TEST = A*B*R**2/(A+B)
IF(TEST.GE.25D0) GO TO 71
REP1(3) = GG*(NN*DEXP(-TEST))**2
GO TO 72
71   REP1(3) = 0D0
72   CONTINUE
    HB(I,J) = 2D0*(REP1(2) - REP1(3))
    HB(J,I) = HB(I,J)
70   CONTINUE

C
DO 80 I=1,8
DO 80 J=1,3
JJ=J+8
B=XP1(I)
A=XP2(J)
C=A
D=B
S1=A+B

```


G LEVEL 1, MOD 3

HBMTRX

DATE = 69131

17/11/31

```

S2=S1
S4=S1+S2
T=S1*S2*R**2/S4
CALL FT
NN=N(A,B)
GG=G(A,B,C,D)
REP6(1)=GG*NN**2/S4*(FT1/2D0-S1*S2*FT2*R**2/S4)
TEST=A*B*R**2/(A+B)
IF(TEST.GE.25D0)GO TO 81
PQ=R*(B/(A+B)-C/(C+D))
T=S1*S2*PQ**2/S4
CALL FT
W=NN*DEXP(-TEST)
REP6(3)=GG*W**2*((B*R/(A+B))*(-B*R/(C+D)*FT0+S1*PQ*FT1/S4)+FT1/(2D
1 0*S4)-S1*S2*PQ**2*FT2/S4**2 - B*R*S1*PQ*FT1/((A+B)*S4))
GO TO 82
81 REP6(3)=0D0
82 CONTINUE
HB(I,JJ)=2D0*(REP6(1) - REP6(3))
HB(JJ,I)=HB(I,JJ)
80 CONTINUE

C
DO 90 I=1,8
DO 90 J=1,3
JJ=J+11
A=XP3(J)
B=XP1(I)
C=A
D=B
S1=A+B
S2=S1
S4=S1+S2
NN=N(A,B)
GG=G(A,B,C,D)
T=S1*S2*R**2/S4
CALL FT
REP5(1)=GG*NN**2*FT1/(2D0*S4)
TEST=A*B*R**2/(A+B)
IF(TEST.GE.25D0)GO TO 91
T=S1*S2*R**2/S4*(B/(A+B) -C/(C+D))**2
CALL FT
W=NN*DEXP(-TEST)
REP5(2)= GG*W**2*FT1/(2D0*S4)
GO TO 92
91 REP5(2)=0D0
92 CONTINUE
HB(I,JJ)=4D0*(REP5(1) - REP5(2))
HB(JJ,I)=HB(I,JJ)
90 CONTINUE

C
DO 100 I=1,3
DO 100 J=1,I

```

G LEVEL 1, MOD 3

HBMTRX

DATE = 69131

17/11/31

```

II=I+8
JJ=J+8
A=XP2(I)
B=XP2(J)
C=A
D=B
S1=A+B
S2=C+D
S4=S1+S2
T=S1*S2*R**2/S4
CALL FT
NN=N(A,B)
GG=G(A,B,C,D)
SAA=NN/(2D0*(A+B))
SBB=SAA
GOZZ=(S1/S4)*((S1/S4)*FT2*R**2-(1D0/(2D0*S2))*FT1)
GZZO=GOZZ
GZZZ=(1D0/(S4**2))*((S1*S2*R**2/S4)**2*FT4-S1*S2*3D0*FT3*R**2/S4
1      +3D0*FT2/4D0)
REP2(1)=GG*(SAA*(SBB*FTO+NN*GOZZ)+NN*(SBB*GZZO+NN*GZZZ))
TEST=A*B*R**2/(A+B)
IF(TEST.GE.25D0)GO TO 101
W=NN*DEXP(-TEST)
SAB1=(1D0/(2D0*(A+B))-A*B*R**2/((A+B)**2))*W
PQ=(B-C)/(B+C)*R
T=S1*S2*PQ**2/S4
CALL FT
G0000=FTO
G00ZZ=S1/S4*(S1/S4*PQ**2*FT2-1D0/(2D0*S2)*FT1)
GZZZZ=1D0/S4**2*(S1**2*S2**2*PQ**4*FT4/S4**2-3D0*S1*S2*PQ**2*FT3/
1      S4 +3D0*FT2/4D0)
REP2(2)=GG*(SAB1**2*G0000+2D0*W*SAB1*G00ZZ+W**2*GZZZZ)
GO TO 102
101 REP2(2)=0D0
102 CONTINUE
HB(II,JJ)=2D0*(REP2(1) - REP2(2))
HB(JJ,II)=HB(II,JJ)
100 CONTINUE
C
DO 110 I=1,3
DO 110 J=1,3
II=I+8
JJ=J+11
A=XP2(I)
B=XP3(J)
C=A
D=B
S1=A+B
S2=S1
S4=S1+S2
T=S1*S2*R**2/S4
CALL FT

```

LEVEL 1, MOD 3

HBMTRX

DATE = 69131

17/11/31

```

NN=N(A,B)
GG=G(A,B,C,D)
REP4(1)=GG*NN**2*(1D0/S4**2*(FT2/4D0-S1*S2*R**2*FT3/(2D0*S4)))
TEST=A*B*R**2/(A+B)
IF(TEST.GE.25D0)GO TO 111
PQ=R*(B/(A+B)-C/(C+D))
T=S1*S2*PQ**2/S4
CALL FT
W=NN*DEXP(-TEST)
REP4(2)=GG*W**2*(1D0/(16D0*S1**2)*(-S1*PQ**2*FT3+FT2)-(B*R/(A+B))*
1  *2*FT1/(2D0*S4))
GO TO 112
111 REP4(2)=0D0
112 CONTINUE
HB(II,JJ)= 4D0*(REP4(1) - REP4(2))
HB(JJ,II)=HB(II,JJ)
110 CONTINUE
C
DO 120 I=1,3
DO 120 J=1,I
II=I+1
JJ=J+1
A=XP3(I)
B=XP3(J)
C=A
D=B
S1=A+B
S2=S1
S4=S1+S2
T=S1*S2*R**2/S4
CALL FT
NN=N(A,B)
GG=G(A,B,C,D)
REP3(1)=GG*NN**2*(FT0/(4D0*S1*S2)-FT1*(S1/(2D0*S1*S2*S4))+
1  3D0*FT2/(4D0*S4**2))
REP3(2)=GG*NN**2*FT2/(4D0*S4**2)
TEST=A*B*R**2/(A+B)
IF(TEST.GE.25D0)GO TO 121
W=NN*DEXP(-TEST)
T=S1*S2*R**2/S4*(B/(A+B)-C/(C+D))**2
CALL FT
REP3(3)=GG*W**2*((1D0/(2D0*(A+B)))*(FT0/(2D0*(C+D))-S1*FT1/(2D0*S2
1  *S4))+3D0*FT2/(4D0*S4**2)-FT1/(4D0*S1*S4))
REP3(4)=GG*W**2*FT2*(1D0/(4D0*S4**2))
GO TO 122
121 REP3(3)=0D0
REP3(4)=0D0
122 CONTINUE
HB(II,JJ) = 4D0*(REP3(1)+REP3(2) - REP3(3) - REP3(4))
HB(JJ,II)=HB(II,JJ)
120 CONTINUE
RETURN

```


LEVEL 1, MOD 3

HCMTRX

DATE = 69131

17/11/31

SUBROUTINE HCMTRX

C
C
C
COMPUTE NUCLEAR ATTRACTION MATRAIX

IMPLICIT REAL*8(A-H,N-Z)

COMMON/A1/PI,R,S(14,14),H(14,14),XP1(8),XP2(3),XP3(3),COF(14),Z,

1 ISTATE

COMMON/A2/HA(14,14),HB(14,14),HC(14,14)

COMMON/F/T,FT1,FT2,FT3,FT4,FT0

DIMENSION VLAP(8),ATRAC(16)

N(X,Y)=(PI/(X+Y))**(3D0/2D0)

TH(X,Y)=Q*DSQRT(X+Y)

Q=(2D0/DSQRT(PI))

IF(ISTATE.NE.0)GO TO 1000

C
C
C
COMPUTE S-S ELEMENTS

DO 10 I=1,8

DO 10 J=1,I

A=XP1(I)

B=XP1(J)

NN=N(A,B)

VLAP(1)=NN

THETA=TH(A,B)

ATRAC(1)=THETA*NN

T=(A+B)*R**2

CALL FT

ATRAC(2)=ATRAC(1)*FT0

TEST=A*B*R**2/(A+B)

IF(TEST.GE.25D0)GO TO 11

W=NN*DEXP(-TEST)

VLAP(2)=W

T=(B*R)**2/(A+B)

CALL FT

ATRAC(4)=THETA*W*FT0

T=(A*R)**2/(A+B)

CALL FT

DTRAC=THETA*W*FT0

GO TO 12

11 VLAP(2)=0D0

ATRAC(4)=0D0

DTRAC=0D0

12 CONTINUE

HC(I,J)=4D0*(VLAP(1)*(ATRAC(1)+ATRAC(2))+VLAP(2)*(ATRAC(4)+DTRAC))

HC(J,I)=HC(I,J)

10 CONTINUE

C
C
C
COMPUTE S-PZ ELEMENTS

DO 20 I=1,8

DO 20 J=1,3

JJ=J+8

LEVEL 1, MOD 3

HCMTRX

DATE = 69131

17/11/31

```
A=XP1(I)
C=XP2(J)
TEST=A*C*R**2/(A+C)
IF(TEST.GE.2500)GO TO 21
NN=N(A,C)
THETA=TH(A,C)
W=NN*DEXP(-TEST)
VLAP(6)=- (A/(A+C))*R*W
T=(A*R)**2/(A+C)
CALL FT
ATRAC(13)=THETA*W*(A*R/(A+C))*(FT0-FT1)
T=(C*R)**2/(A+C)
CALL FT
```

```
ATRAC(15)=THETA*W*R/(A+C)*(A*FT0+C*FT1)
```

```
GO TO 22
21 VLAP(6)=0D0
   ATRAC(13)=0D0
   ATRAC(15)=0D0
22 CONTINUE
   HC(I,JJ)=+ 4D0*VLAP(6)*(ATRAC(13)+ATRAC(15))
   HC(JJ,I)=HC(I,JJ)
20 CONTINUE
```

```
COMPUTE S-PX ELEMENTS
```

```
DO 30 I=1,8
DO 30 J=12,14
HC(I,J)=0D0
HC(J,I)=0D0
30 CONTINUE
```

```
COMPUTE PZ-PX ELEMENTS
```

```
DO 31 I=9,11
DO 31 J=12,14
HC(I,J)=0D0
HC(J,I)=0D0
31 CONTINUE
```

```
COMPUTE PZ/PZ ELEMENTS
```

```
DO 40 I=1,3
DO 40 J=1,I
JJ=J+8
II=I+8
C=XP2(I)
```

LEVEL 1, MOD 3

HCMTRX

DATE = 69131

17/11/31

```
D=XP2(J)
NN=N(C,D)
VLAP(3)=NN*(1D0/(2D0*(C+D)))
THETA=TH(C,D)
THN=THETA*NN
ATRAC(6)=THN*(1D0/(3D0*(C+D)))
T=(C+D)*R**2
CALL FT
ATRAC(7)=THN*(FT2*R**2-1D0/(2D0*(C+D))*FT1+1D0/(2D0*(C+D))*FT0)
TEST=C*D*R**2/(C+D)
IF(TEST.GE.25D0)GO TO 41
W=NN*DEXP(-TEST)
T=(D*R)**2/(C+D)
CALL FT
ATRAC(8)=THETA*W/(C+D)*(((D*R)**2/(C+D))*FT2-FT1/2D0+(1D0/2D0-C*D
1 *R**2/(C+D))*FT0)
VLAP(7)=W*(1D0/(2D0*(C+D))-C*D*R**2/((C+D)**2))
GO TO 42
41 ATRAC(8)=0D0
VLAP(7)=0D0
42 CONTINUE
HC(II,JJ)=4D0*(VLAP(3)*(ATRAC(6)+ATRAC(7)) + VLAP(7)*2D0*ATRAC(8))
HC(JJ,II)=HC(II,JJ)
40 CONTINUE

C
C
C COMPUTE PX-PX ELEMENTS

DO 50 I=1,3
DO 50 J=1,I
JJ=J+11
II=I+11
E=XP3(I)
F=XP3(J)
NN=N(E,F)
THETA=TH(E,F)
THN=THETA*NN
VLAP(4)=NN*(1D0/(2D0*(E+F)))
ATRAC(6)=THN*(1D0/(3D0*(E+F)))
T=(E+F)*R**2
CALL FT
ATRAC(10)=THN/(2D0*(E+F))*(FT0-FT1)
TEST=E*F*R**2/(E+F)
IF(TEST.GE.25D0)GO TO 51
W=NN*DEXP(-TEST)
VLAP(8)=W*(1D0/(2D0*(E+F)))
T=(F*R)**2/(E+F)
CALL FT
ATRAC(9)=THETA*W/(2D0*(E+F))*(FT0-FT1)
GO TO 52
51 VLAP(8)=0D0
ATRAC(9)=0D0
52 CONTINUE
```


LEVEL 1, MOD 3

HCMTRX

DATE = 69131

17/11/31

```
HC(II,JJ)=8DO*(VLAP(4)*(ATRAC(6)+ATRAC(10))+VLAP(8)*2DO*ATRAC(9))
HC(JJ,II)=HC(II,JJ)
```

50 CONTINUE

MULTIPLY MATRIX BY -Z(NUCLEAR CHARGE)

DO 200 I=1,14

DO 200 J=1,I

HC(I,J)=-Z*HC(I,J)

HC(J,I)=HC(I,J)

200 CONTINUE

RETURN AFTER GROUND STATE CALCULATION

RETURN

EXCITED STATE COMPUTATION - ELEMENTS COMPUTED IN SAME ORDER AS ABOVE

1000 CONTINUE

DO 60 I=1,8

DO 60 J=1,I

A=XP1(I)

B=XP1(J)

NN=N(A,B)

VLAP(1)=NN

THETA=TH(A,B)

ATRAC(1)=THETA*NN

T=(A+B)*R**2

CALL FT

ATRAC(2)=ATRAC(1)*FTO

TEST=A*B*R**2/(A+B)

IF(TEST.GE.25DO)GO TO 61

W=NN*DEXP(-TEST)

VLAP(2)=W

T=(B*R)**2/(A+B)

CALL FT

ATRAC(4)=THETA*W*FTO

T=(A*R)**2/(A+B)

CALL FT

DTRAC=THETA*W*FTO

GO TO 62

61 VLAP(2)=ODO

ATRAC(4)=ODO

DTRAC=ODO

62 CONTINUE

HC(I,J)=4DO*(VLAP(1)*(ATRAC(1)+ATRAC(2))-VLAP(2)*(ATRAC(4)+DTRAC))

HC(J,I)=HC(I,J)

60 CONTINUE

DO 70 I=1,8

DO 70 J=1,3

LEVEL 1, MOD 3

HCMTRX

DATE = 69131

17/11/31

```
JJ=J+8
A=XP1(I)
C=XP2(J)
TEST=A*C*R**2/(A+C)
IF(TEST.GE.2500)GO TO 71
NN=N(A,C)
THETA=TH(A,C)
W=NN*DEXP(-TEST)
VLAP(6)=-(A/(A+C))*R*W
T=(A*R)**2/(A+C)
CALL FT
ATRAC(13)=THETA*W*(A*R/(A+C))*(FT0-FT1)
T=(C*R)**2/(A+C)
CALL FT
```

```
ATRAC(15)=THETA*W*R/(A+C)*(A*FT0+C*FT1)
```

```
GO TO 72
71 VLAP(6)=0D0
   ATRAC(13)=0D0
   ATRAC(15)=0D0
72 CONTINUE
   HC(I,JJ)=- 4D0*VLAP(6)*(ATRAC(13)+ATRAC(15))
   HC(JJ,I)=HC(I,JJ)
70 CONTINUE

DO 80 I=1,8
DO 80 J=12,14
   HC(I,J)=0D0
   HC(J,I)=0D0
80 CONTINUE

DO 81 I=9,11
DO 81 J=12,14
   HC(I,J)=0D0
   HC(J,I)=0D0
81 CONTINUE

DO 90 I=1,3
DO 90 J=1,I
   JJ=J+8
   II=I+8
   C=XP2(I)
   D=XP2(J)
   NN=N(C,D)
   VLAP(3)=NN*(1D0/(2D0*(C+D)))
   THETA=TH(C,D)
   THN=THETA*NN
```

LEVEL 1, MOD 3

HCMTRX

DATE = 69131

17/11/31

```

      ATRAC(6)=THN*(1D0/(3D0*(C+D)))
      T=(C+D)*R**2
      CALL FT
      ATRAC(7)=THN*(FT2*R**2-1D0/(2D0*(C+D))*FT1+1D0/(2D0*(C+D))*FT0)
      TEST=C*D*R**2/(C+D)
      IF(TEST.GE.25D0) GO TO 91
      W=NN*DEXP(-TEST)
      T=(D*R)**2/(C+D)
      CALL FT
      ATRAC(8)=THETA*W/(C+D)*(((D*R)**2/(C+D))*FT2-FT1/2D0+(1D0/2D0-C*D
1      *R**2/(C+D))*FT0)
      VLAP(7)=W*(1D0/(2D0*(C+D))-C*D*R**2/((C+D)**2))
      GO TO 92
91  ATRAC(8)=0D0
      VLAP(7)=0D0
92  CONTINUE
      HC(II,JJ)=4D0*(VLAP(3)*(ATRAC(6)+ATRAC(7)) - VLAP(7)*2D0*ATRAC(8))
      HC(JJ,II)=HC(II,JJ)
90  CONTINUE

C
      DO 100 I=1,3
      DO 100 J=1,I
      JJ=J+11
      II=I+11
      E=XP3(I)
      F=XP3(J)
      NN=N(E,F)
      THETA=TH(E,F)
      THN=THETA*NN
      VLAP(4)=NN*(1D0/(2D0*(E+F)))
      ATRAC(6)=THN*(1D0/(3D0*(E+F)))
      T=(E+F)*R**2
      CALL FT
      ATRAC(10)=THN/(2D0*(E+F))*{FT0-FT1}
      TEST=E*F*R**2/(E+F)
      IF(TEST.GE.25D0) GO TO 101
      W=NN*DEXP(-TEST)
      VLAP(8)=W*(1D0/(2D0*(E+F)))
      T=(F*R)**2/(E+F)
      CALL FT
      ATRAC(9)=THETA*W/(2D0*(E+F))*{FT0-FT1}
      GO TO 102
101 VLAP(8)=0D0
      ATRAC(9)=0D0
102 CONTINUE
      HC(II,JJ)=8D0*(VLAP(4)*{ATRAC(6)+ATRAC(10)}-VLAP(8)*2D0*ATRAC(9))
      HC(JJ,II)=HC(II,JJ)
100 CONTINUE

C
      DO 300 I=1,14
      DO 300 J=1,I
      HC(I,J)=-Z*HC(I,J)

```


G LEVEL 1, MOD 3

HCMTRX

DATE = 69131

17/11/31

```
HC(J,I)=HC(I,J)
300 CONTINUE
RETURN
END
```

PROGRAM TO COMPUTE THE
KIM - HIRSCHFELDER SUB-
CASES OF THE FUNCTION IN
EQUATION 2

LEVEL 1, MOD 3

MAIN

DATE = 69133

15/33/50

C
C
C
MAIN INPUT ROUTINE

IMPLICIT REAL*8(A-H,O-Z)

COMMON/NEW/CUTOFF,NN,N

DIMENSION NCSE(100),ISTE(100),ZCHAR(100),RDISTC(100),XVAL(100),

1 DXVAL(100)

DIMENSION IDATE(3),ITIME(2)

CALL DATEA(IDATE)

CALL TIMEA(ITIME)

WRITE(6,1122)

1122 FORMAT('1')

WRITE(6,345) IDATE,ITIME

345 FORMAT(50X,' DATE ',3A4,/50X,' TIME ',2A4)

C
C
C
READ INPUT DATA FOR TOTAL RUN

READ(5,9)CUTOFF

9 FORMAT(F10.0)

DO 100 I=1,500

READ(5,10)NCASE,ISTAT,ZCHG,RDIST,XVALU,DXVALU

NCASE=NCASE+1

10 FORMAT(2I5,4F10.0)

NCSE(I)=NCASE

ISTE(I)=ISTAT

ZCHAR(I)=ZCHG

RDISTC(I)=RDIST

XVAL(I)=XVALU

DXVAL(I)=DXVALU

IF(NCASE.LT.0)GO TO 11

100 CONTINUE

11 J=I-1

C
C
C
J IS THE TOTAL NUMBER OF CASES FOR THIS RUN

WRITE(6,12)J

12 FORMAT(//5X,' NUMBER OF CASES THIS RUN',I4,/5X,' CASE',2X,' ST
1ATE',2X,' NUC. CHG.',4X,' R',//)

WRITE(6,13)(NCSE(M),ISTE(M),ZCHAR(M),RDISTC(M),M=1,J)

13 FORMAT(5X,I4,6X,I4,2X,F5.2,4X,F10.5)

C
C
C
DO EACH CASE IN TURN

DO 101 K=1,J

N=NCSE(K)

NM=ISTE(K)

CG=ZCHAR(K)

RD=RDISTC(K)

XVALI=XVAL(K)

DXVALI=DXVAL(K)

CALL MAINS (N,NM,CG,RD,XVALI,DXVALI)

101 CONTINUE

G LEVEL 1, MOD 3

MAIN

DATE = 69133

15/33/50

STOP
END

15/33/50

```
CALL SIMPLEX TO MINIMIZE ENERGY FUNCTION
COF(1)=0D0
```

15/33/50

$$EXPV = EXPV1 + EXPV2$$

$$EXPV = EXPV / PSISQ + 7**2 / R$$

LEVEL 1, MOD 3

MAINS

DATE = 69133

15/33/50

```

VIRIAL=-EXPV/(2D0*EXPT)
DEDR=- (2D0*EXPT+EXPV)/R
BINDEN=CHISQ+8D0/(3D0*PI)
EXPR12=EXPV2/PSISQ
EXPRA=(1D0/4D0)*(EXPV-EXPV2-Z**2/R)
CNF(1)=0D0
CNF(2)=0D0
CNF(3)=0D0
DO 602 I=1,N
602 CNF(I)=COF(I)/COF(1)
WRITE(6,301)
IF(NNN.EQ.0)WRITE(6,300)CNF(1)
IF(NNN.EQ.1)WRITE(6,300)CNF(1),CNF(2)
IF(NNN.EQ.2)WRITE(6,300)CNF(1),CNF(2),CNF(3)
300 FORMAT(/(5X,3D25.16))
310 FORMAT(3D25.16)
301 FORMAT(/5X,' EIGENVECTOR COMPONENTS')
WRITE(6,401)
WRITE(6,300)X(1)
401 FORMAT(/5X,' ORBITAL EXPONENT')
WRITE(6,303)
303 FORMAT(/5X,' LOWEST EIGENVALUE')
WRITE(6,300)CHISQ
WRITE(6,6007)EXPV,EXPT,VIRIAL
6007 FORMAT(/5X,' POTENTIAL ENERGY:',F15.10,' HARTREES',/5X,' KINETIC E
2ENERGY:',F15.10,' HARTREES',/5X,' VIRIAL THEOREM; -V/2T:',F15.10)
WRITE(6,603)BINDEN,EXPR12,EXPRA,DEDR
603 FORMAT(5X,' BINDING ENERGY',F15.10,/5X,' EXPECT. VALUE OF 1/R12',
1F15.10,/5X,' EXPECTATION VALUE OF 1/RA',F15.10,/5X,' DE/DR',F15.10
1)
WRITE(7,600)Z,R,ISTATE,N,X(1), VIRIAL,BINDEN,EXPT,EXPV,EXPR12,DEDR
1,CNF(1),CNF(2),CNF(3),EXPRA,CHISQ
600 FORMAT(F10.5,F15.10,2I5,D25.16,/3D25.16,/3D25.16,/3D20.10,D15.8,
1/D25.16)
CALL DATEA(IDATE)
CALL TIMEA(ITIME)
WRITE(6,345)IDATE,ITIME
345 FORMAT(50X,' DATE ',3A4,/50X,' TIME ',2A4)
RETURN
END

```

LEVEL 1, MOD 3

TOTAL

DATE = 69133

15/33/50

SUBROUTINE TOTAL

IMPLICIT REAL*8(A-H,O-Z)

COMMON/A1/PI,R,S(14,14),H(14,14),XP1(8),XP2(3),XP3(3),COF(14),Z,

1 ISTATE

COMMON/A2/HA(14,14),HB(14,14),HC(14,14)

COMMON/NEW/CUTOFF,NN,N

COMMON/S1/CHISQ,X(20)

DIMENSION KP(14),HMAT(105),SMAT(105),E(14),COET(14,14),VEC(14,5),

1 ITIME(2)

PI=3.1415926535897932D0

N1=1

INITIALIZE EXPONENTS WITH CURRENT X VALUES

XP1(1)= X(1)

XP2(1)=X(1)

XP3(1)=X(1)

CALL ENERGY MATRIX ROUTINES

CALL OVERLA

CALL HAMTRX

CALL HBMTRX

CALL HCMTRX

SMAT(1)=S(1,1)

SMAT(2)=S(1,9)

SMAT(3)=S(9,9)

SMAT(4)=S(1,12)

SMAT(5)=S(9,12)

SMAT(6)=S(12,12)

HMAT(1)=HA(1,1)+HB(1,1)+HC(1,1)

HMAT(2)=HA(1,9)+HB(1,9)+HC(1,9)

HMAT(3)=HA(9,9)+HB(9,9)+HC(9,9)

HMAT(4)=HA(1,12)+HB(1,12)+HC(1,12)

HMAT(5)=HA(9,12)+HB(9,12)+HC(9,12)

HMAT(6)=HA(12,12)+HB(12,12)+HC(12,12)

DO 897 I=1,6

IF(DABS(SMAT(I)).LT.1D-10)SMAT(I)=0D0

IF(DABS(HMAT(I)).LT.1D-10)HMAT(I)=0D0

897 CONTINUE

OBTAIN EIGENVLAUE AND EIGENVECTOR

CALL CEIG(N,N1,NN,HMAT,SMAT,E,COET,VEC,KP)

TOTAL ENERGY = ELECTRONIC ENERGY + NUCLEAR REPULSION ENERGY

CHISQ=E(1) + Z**2/R

DO 15 I=1,N

15 COF(I)=COET(I,1)

RETURN

END

G LEVEL 1, MOD 3

OVERLA

DATE = 69133

15/33/50

SUBROUTINE OVERLA

C
C
C
COMPUTE OVERLAP MATRIX S(I,J)

IMPLICIT REAL*8(A-H,N-Z)

COMMON/A1/PI,R,S(14,14),H(14,14),XP1(8),XP2(3),XP3(3),CDF(14),Z,

1 ISTATE

COMMON/NEW/CUTOFF,LL,LLL

DIMENSION VLAP(8)

N(X,Y)=(PI/(X+Y))**(3D0/2D0)

I=1

J=1

IF(ISTATE.NE.0)GO TO 1000

C
C
C
COMPUTE S-S ELEMENTS

A=XP1(I)

B=XP1(J)

VLAP(1) = N(A,B)

TEST= A*B*R**2/(A+B)

IF(TEST.GE.25D0)GO TO 30

VLAP(2)=VLAP(1)*DEXP(-TEST)

GO TO 40

30 VLAP(2)=0D0

40 CONTINUE

S(I,J)=2D0*(VLAP(1)**2 + VLAP(2)**2)

S(J,I)=S(I,J)

IF(LLL.EQ.1)GO TO 2000

C
C
C
COMPUTE S-PZ ELEMENTS

A=XP1(I)

U=XP2(J)

TEST=A*U*R**2/(A+U)

IF(TEST.GE.25D0)GO TO 31

VLAP(5)=(A/(A+U))*R*N(A,U)*DEXP(-TEST)

GO TO 41

31 VLAP(5)=0D0

41 CONTINUE

IJ=J+8

S(I,IJ) = 2D0*(- VLAP(5)**2)

S(IJ,I)=S(I,IJ)

C
C
C
COMPUTE S-PX ELEMENTS

S(1,12)=0D0

S(9,12)=0D0

S(12,1)=0D0

S(12,9)=0D0

C
C
C
COMPUTE PZ-PZ ELEMENTS

LEVEL 1, MOD 3

OVERLA

DATE = 69133

15/33/50

```
II=I+8
JJ=J+8
U=XP2(I)
D=XP2(J)
VLAP(3) = N(U,D) * (1D0/(2D0*(U+D)))
TEST=U*D*R**2/(U+D)
IF(TEST.GE.25D0)GO TO 33
VLAP(7)=N(U,D)*DEXP(-TEST)*(1D0/(2D0*(U+D))-U*D*R**2/((U+D)**2))
GO TO 43
33 VLAP(7)=0D0
43 CONTINUE
S(II,JJ)= 2D0 * ( VLAP(3)**2 + VLAP(7)**2 )
S(JJ,II)=S(II,JJ)
IF(LLL.EQ.2)GO TO 2001
```

C
C
C
COMPUTE PX-PX ELEMENTS

```
E=XP3(I)
F=XP3(J)
VLAP(4) = N(E,F)*(1D0/(2D0*(E+F)))
TEST=E*F*R**2/(E+F)
IF(TEST.GE.25D0)GO TO 35
VLAP(8)=VLAP(4)*DEXP(-TEST)
GO TO 45
35 VLAP(8)=0D0
45 CONTINUE
II=I+11
JJ=J+11
S(II,JJ) = 4D0 * (VLAP(4)**2 + VLAP(8)**2 )
S(JJ,II)=S(II,JJ)
```

C
C
C
RETURN AFTER GROUND STATE CALCULATIONC
C
C
GO TO 2003C
C
C
EXCITED STATE SECTION - ELEMENTS COMPUTED IN SAME ORDER AS ABOVE

```
1000 CONTINUE
A=XP1(I)
B=XP1(J)
VLAP(1) = N(A,B)
TEST= A*B*R**2/(A+B)
IF(TEST.GE.25D0)GO TO 50
VLAP(2)=VLAP(1)*DEXP(-TEST)
GO TO 60
50 VLAP(2)=0D0
60 CONTINUE
S(I,J)=2D0*(VLAP(1)**2 - VLAP(2)**2)
S(J,I)=S(I,J)
A=XP1(I)
U=XP2(J)
TEST=A*U*R**2/(A+U)
```

LEVEL 1, MOD 3

OVERLA

DATE = 69133

15/33/50

```
IF(TEST.GE.25D0)GO TO 51
VLAP(5)=(A/(A+U))*R*N(A,U)*DEXP(-TEST)
GO TO 61
51 VLAP(5)=0D0
61 CONTINUE
IJ=J+8
S(I,IJ) = 2D0*( + VLAP(5)**2)
S(IJ,I)=S(I,IJ)
S(1,12)=0D0
S(9,12)=0D0
S(12,1)=0D0
S(12,9)=0D0
II=I+8
JJ=J+8
U=XP2(I)
D=XP2(J)
VLAP(3) = N(U,D) * (1D0/(2D0*(U+D)))
TEST=U*D*R**2/(U+D)
IF(TEST.GE.25D0)GO TO 53
VLAP(7)=N(U,D)*DEXP(-TEST)*(1D0/(2D0*(U+D))-U*D*R**2/((U+D)**2))
GO TO 63
53 VLAP(7)=0D0
63 CONTINUE
S(II,JJ)= 2D0 * ( VLAP(3)**2 - VLAP(7)**2 )
S(JJ,II)=S(II,JJ)
E=XP3(I)
F=XP3(J)
VLAP(4) = N(E,F)*(1D0/(2D0*(E+F)))
TEST=E*F*R**2/(E+F)
IF(TEST.GE.25D0)GO TO 55
VLAP(8)=VLAP(4)*DEXP(-TEST)
GO TO 65
55 VLAP(8)=0D0
65 CONTINUE
II=I+11
JJ=J+11
S(II,JJ) = 4D0 * (VLAP(4)**2 - VLAP(8)**2 )
S(JJ,II)=S(II,JJ)
2000 S(1,9)=0D0
S(9,1)=0D0
S(9,9)=0D0
2001 S(9,12)=0D0
S(12,9)=0D0
S(1,12)=0D0
S(21,1)=0D0
S(12,12)=0D0
2003 RETURN
END
```

G LEVEL 1, MOD 3

MAIN

DATE = 69133

15/33/50

KINETIC ENERGY MATRIX

SUBROUTINE HAMTRX

IMPLICIT REAL*8(A-H,N-Z)

REAL*8 K1,K2,K3,K4

COMMON/A1/PI,R,S(14,14),H(14,14),XP1(8),XP2(3),XP3(3),COF(14),Z,
1 ISTATE

COMMON/A2/HA(14,14),HB(14,14),HC(14,14)

COMMON/NEW/CUTOFF,LL,LLL

DIMENSION VLAP(8),EKIN(10)

N(X,Y)=(PI/(X+Y))**((3D0/2D0)

DEFINE AUXILIARY K FUNCTIONS

 $K1(X,Y) = 3D0 * X * Y / (X+Y) - 2D0 * (X * Y * R) ** 2 / ((X+Y) ** 2)$ $K2(X,Y) = 3D0 * X * Y / (X+Y)$ $K3(X,Y) = 2D0 * Y * R * X ** 2 / ((X+Y) ** 2)$ $K4(X,Y) = X * Y / ((X+Y) ** 2)$

I=1

J=1

IF(ISTATE.NE.0)GO TO 1000

S-S ELEMENTS

A=XP1(I)

B=XP1(J)

VLAP(1)=N(A,B)

EKIN(1)=K2(A,B)*N(A,B)

TEST=A*B*R**2/(A+B)

IF(TEST.GE.25D0)GO TO 20

VLAP(2)=VLAP(1)*DEXP(-TEST)

EKIN(2)=K1(A,B)*VLAP(2)

GO TO 30

20 EKIN(2)=0D0

VLAP(2)=0D0

30 CONTINUE

HA(I,J)=4D0*(EKIN(1)*VLAP(1) + EKIN(2)*VLAP(2))

HA(J,I)=HA(I,J)

IF(LLL.EQ.1)GO TO 2000

S-PZ ELEMENTS

A=XP1(I)

C=XP2(J)

TEST=A*C*R**2/(A+C)

IF(TEST.GE.25D0)GO TO 21

W=N(A,C)*DEXP(-TEST)

VLAP(5)=(A/(A+C))*R*W

EKIN(3)=W*K3(A,C)+K1(A,C)*VLAP(5)

GO TO 31

21 VLAP(5)=0D0

LEVEL 1, MOD 3

HAMTRX

DATE = 69133

15/33/50

```
EKIN(3)=0D0
31 CONTINUE
JJ=J+8
HA(I,JJ)= - 4D0*EKIN(3)*VLAP(5)
HA(JJ,I)=HA(I,JJ)
HA(1,12)=0D0
HA(12,1)=0D0
HA(9,12)=0D0
HA(12,9)=0D0

C
C
C
PZ-PZ ELEMENTS

II=I+8
JJ=J+8
C=XP2(I)
D=XP2(J)
NN=N(C,D)
VLAP(3)=NN*(1D0/(2D0*(C+D)))
EKIN(6)=K4(C,D)*NN+K2(C,D)*VLAP(3)
TEST=C*D*R**2/(C+D)
6 IF(TEST.GE.25D0)GO TO 24
W=NN*DEXP(-TEST)
VLAP(7)=W*(1D0/(2D0*(C+D))-C*D*R**2/((C+D)**2))
EKIN(5)=W*K4(C,D)-W*R*(C/(C+D))*(K3(C,D)+K3(D,C))+K1(C,D)*VLAP(7)
GO TO 34
24 VLAP(7)=0D0
EKIN(5)=0D0
34 CONTINUE
HA(II,JJ)=4D0*(EKIN(6)*VLAP(3) + VLAP(7)*EKIN(5))
HA(JJ,II)=HA(II,JJ)
IF(LLL.EQ.2)GO TO 2001

C
C
C
PX-PY ELEMENTS

II=I+11
JJ=J+11
E=XP3(I)
F=XP3(J)
NN=N(E,F)
VLAP(4)=NN*(1D0/(2D0*(E+F)))
EKIN(7)=K4(E,F)*NN+K2(E,F)*VLAP(4)
TEST=E*F*R**2/(E+F)
IF(TEST.GE.25D0)GO TO 25
W=NN*DEXP(-TEST)
VLAP(8)=W*(1D0/(2D0*(E+F)))
EKIN(9)=K4(E,F)*W+K1(E,F)*VLAP(8)
GO TO 35
25 VLAP(8)=0D0
EKIN(9)=0D0
35 CONTINUE
HA(II,JJ)=8D0*(EKIN(7)*VLAP(4) + EKIN(9)*VLAP(8))
HA(JJ,II)=HA(II,JJ)
```

LEVEL 1, MOD 3

HAMTRX

DATE = 69133

15/33/50

```
C
C RETURN AFTER GROUND STATE CALCULATION
C
C 5 GO TO 2003
C
C 6 EXCITED STATE - MATRIX ELEMENTS COMPUTED IN SAME ORDER AS ABOVE
C
C
1000 CONTINUE
A=XP1(I)
B=XP1(J)
VLAP(1)=N(A,B)
EKIN(1)=K2(A,B)*N(A,B)
TEST=A*B*R**2/(A+B)
IF(TEST.GE.2500)GO TO 50
VLAP(2)=VLAP(1)*DEXP(-TEST)
EKIN(2)=K1(A,B)*VLAP(2)
GO TO 60
50 VLAP(2)=0D0
EKIN(2)=0D0
60 CONTINUE
HA(I,J)=4D0*(EKIN(1)*VLAP(1) - EKIN(2)*VLAP(2))
HA(J,I)=HA(I,J)
A=XP1(I)
C=XP2(J)
TEST=A*C*R**2/(A+C)
IF(TEST.GE.2500)GO TO 51
W=N(A,C)*DEXP(-TEST)
VLAP(5)=(A/(A+C))*R*W
EKIN(3)=W*K3(A,C)+K1(A,C)*VLAP(5)
GO TO 61
51 VLAP(5)=0D0
EKIN(3)=0D0
61 CONTINUE
JJ=J+8
HA(I,JJ)= + 4D0*EKIN(3)*VLAP(5)
HA(JJ,I)=HA(I,JJ)
HA(1,12)=0D0
HA(12,1)=0D0
HA(9,12)=0D0
HA(12,9)=0D0
II=I+8
JJ=J+8
C=XP2(I)
D=XP2(J)
NN=N(C,D)
VLAP(3)=NN*(1D0/(2D0*(C+D)))
EKIN(6)=K4(C,D)*NN+K2(C,D)*VLAP(3)
TEST=C*D*R**2/(C+D)
IF(TEST.GE.2500)GO TO 54
W=NN*DEXP(-TEST)
VLAP(7)=W*(1D0/(2D0*(C+D))-C*D*R**2/((C+D)**2))
```

LEVEL 1, MOD 3

HAMTRX

DATE = 69133

15/33/50

 $EKIN(5) = W * K4(C, D) - W * R * (C / (C + D)) * (K3(C, D) + K3(D, C)) + K1(C, D) * VLAP(7)$

GO TO 64

54 VLAP(7)=0D0

EKIN(5)=0D0

64 CONTINUE

 $HA(II, JJ) = 4D0 * (EKIN(6) * VLAP(3) - VLAP(7) * EKIN(5))$ $HA(JJ, II) = HA(II, JJ)$

II=I+11

JJ=J+11

E=XP3(I)

F=XP3(J)

NN=N(E, F)

 $VLAP(4) = NN * (1D0 / (2D0 * (E + F)))$ $EKIN(7) = K4(E, F) * NN + K2(E, F) * VLAP(4)$ $TEST = E * F * R ** 2 / (E + F)$

IF(TEST.GE.25D0)GO TO 55

W=NN*DEXP(-TEST)

 $VLAP(8) = W * (1D0 / (2D0 * (E + F)))$ $EKIN(9) = K4(E, F) * W + K1(E, F) * VLAP(8)$

GO TO 65

55 VLAP(8)=0D0

EKIN(9)=0D0

65 CONTINUE

 $HA(II, JJ) = 8D0 * (EKIN(7) * VLAP(4) - EKIN(9) * VLAP(8))$ $HA(JJ, II) = HA(II, JJ)$

2000 HA(1,9)=0D0

HA(9,1)=0D0

HA(9,9)=0D0

2001 HA(9,12)=0D0

HA(12,9)=0D0

HA(1,12)=0D0

HA(12,1)=0D0

HA(12,12)=0D0

2003 RETURN

END

LEVEL 1, MOD 3

HBMTRX

DATE = 69133

15/33/50

SUBROUTINE HBMTRX
IMPLICIT REAL*8(A-H,N-Z)

ELECTRON REPULSION MATRIX

COMMON/A1/PI,R,S(14,14),H(14,14),XP1(8),XP2(3),XP3(3),COF(14),Z,
1 ISTATE
COMMON/A2/HA(14,14),HB(14,14),HC(14,14)
COMMON/F/T,FT1,FT2,FT3,FT4,FT0
COMMON/NEW/CUTOFF,LL,LLL
DIMENSION REP1(4),REP2(4),REP3(4),REP4(4),REP5(4),REP6(4)
N(X,Y)=(PI/(X+Y))*{(3D0/2D0)
G(W,X,Y,Z)=2D0*DSQRT((W+X)*(Y+Z)/(PI*(W+X+Y+Z)))

TEST FOR GROUND OR EXCITED STATE

I=1

J=1

IF(ISTATE.NE.0)GO TO 1000

COMPUTE S-S ELEMENTS

A=XP1(I)

B=XP1(J)

C=A

D=B

S1=A+B

S2=S1

S4=S1+S2

T=S1*S2*R**2/S4

CALL FT

NN=N(A,B)

GG=G(A,B,C,D)

REP1(2)=GG*NN**2*FT0

TEST=A*B*R**2/(A+B)

IF(TEST.GE.25D0)GO TO 11

REP1(3)=GG*(NN*DEXP(-TEST))**2

GO TO 12

11 REP1(3)=0D0

12 CONTINUE

HB(I,J)=2D0*(REP1(2) + REP1(3))

HB(J,I)=HB(I,J)

IF(LLL.EQ.1)GO TO 2000

COMPUTE S-PZ ELEMENTS

JJ=J+8

B=XP1(I)

A=XP2(J)

C=A

D=B

LEVEL 1, MOD 3

HBMTRX

DATE = 69133

15/33/50

```

S1=A+B
S2=S1
S4=S1+S2
T=S1*S2*R**2/S4
CALL FT
NN=N(A,B)
GG=G(A,B,C,D)
REP6(1)=GG*NN**2/S4*(FT1/2D0-S1*S2*FT2*R**2/S4)
TEST=A*B*R**2/(A+B)
IF(TEST.GE.25D0)GO TO 21
PQ=R*(B/(A+B)-C/(C+D))
T=S1*S2*PQ**2/S4
CALL FT
W=NN*DEXP(-TEST)
REP6(3)=GG*W**2*((B*R/(A+B))*(-B*R/(C+D)*FT0+S1*PQ*FT1/S4)+FT1/(2D
1 0*S4)-S1*S2*PQ**2*FT2/S4**2 - B*R*S1*PQ*FT1/((A+B)*S4))
GO TO 22
21 REP6(3)=0D0
22 CONTINUE
HB(I,JJ)=2D0*(REP6(1) + REP6(3))
HB(JJ,I)=HB(I,JJ)

COMPUTE PZ-PZ ELEMENTS

II=I+8
JJ=J+8
A=XP2(I)
B=XP2(J)
C=A
D=B
S1=A+B
S2=C+D
S4=S1+S2
T=S1*S2*R**2/S4
CALL FT
NN=N(A,B)
GG=G(A,B,C,D)
SAA=NN/(2D0*(A+B))
SBB=SAA
GOZZ=(S1/S4)*((S1/S4)*FT2*R**2-(1D0/(2D0*S2))*FT1)
GZZD=GOZZ
GZZZ=(1D0/(S4**2))*((S1*S2*R**2/S4)**2*FT4-S1*S2*3D0*FT3*R**2/S4
1 +3D0*FT2/4D0)
REP2(1)=GG*(SAA*(SBB*FT0+NN*GOZZ)+NN*(SBB*GZZD+NN*GZZZ))
TEST=A*B*R**2/(A+B)
IF(TEST.GE.25D0)GO TO 41
W=NN*DEXP(-TEST)
GZZZZ=1D0/S4**2*(S1**2*S2**2*PQ**4*FT4/S4**2-3D0*S1*S2*PQ**2*FT3/
1 S4 +3D0*FT2/4D0)
REP2(2)=GG*(SAB1**2*G0000+2D0*W*SAB1*G00ZZ+W**2*GZZZZ)
G00ZZ=S1/S4*(S1/S4*PQ**2*FT2-1D0/(2D0*S2)*FT1)
T=S1*S2*PQ**2/S4

```

LEVEL 1, MOD 3

HBMTRX

DATE = 69133

15/33/50

```
CALL FT
G0000=FT0
SAB1=(1D0/(2D0*(A+B))-A*B*R**2/((A+B)**2))*W
PQ=(B-C)/(B+C)*R
GO TO 42
41 REP2(2)=0D0
42 CONTINUE
HB(II,JJ)=2D0*(REP2(1) + REP2(2))
HB(JJ,II)=HB(II,JJ)
```

```
C
IF(LLL.EQ.2)GO TO 2001
```

```
C
C
C
C
COMPUTE S-PX ELEMENTS
```

```
JJ=J+11
A=XP3(J)
B=XP1(I)
C=A
D=B
S1=A+B
S2=S1
S4=S1+S2
NN=N(A,B)
GG=G(A,B,C,D)
T=S1*S2*R**2/S4
CALL FT
REP5(1)=GG*NN**2*FT1/(2D0*S4)
TEST=A*B*R**2/(A+B)
IF(TEST.GE.25D0)GO TO 31
T=S1*S2*R**2/S4*(B/(A+B) -C/(C+D))**2
CALL FT
W=NN*DEXP(-TEST)
REP5(2)= GG*W**2*FT1/(2D0*S4)
GO TO 32
31 REP5(2)=0D0
32 CONTINUE
HB(I,JJ)=4D0*(REP5(1) + REP5(2))
HB(JJ,I)=HB(I,JJ)
COMPUTE PZ-PX ELEMENTS
```

```
C
C
II=I+8
JJ=J+11
A=XP2(I)
B=XP3(J)
C=A
D=B
S1=A+B
S2=S1
S4=S1+S2
T=S1*S2*R**2/S4
CALL FT
NN=N(A,B)
```


LEVEL 1, MOD 3

HBMTRX

DATE = 69133

15/33/50

```

1000 GG=G(A,B,C,D)
      REP4(1)=GG*NN**2*(1D0/S4**2*(FT2/4D0-S1*S2*R**2*FT3/(2D0*S4)))
      TEST=A*B*R**2/(A+B)
      IF(TEST.GE.25D0)GO TO 51
      PQ=R*(B/(A+B)-C/(C+D))
      T=S1*S2*PQ**2/S4
      CALL FT
      W=NN*DEXP(-TEST)
      REP4(2)=GG*W**2*(1D0/(16D0*S1**2)*(-S1*PQ**2*FT3+FT2)-(B*R/(A+B))*
1      *2*FT1/(2D0*S4))
      GO TO 52
51 REP4(2)=0D0
52 CONTINUE
      HB(II,JJ)= 4D0*(REP4(1) + REP4(2))
      HB(JJ,II)=HB(II,JJ)

C
C
C      COMPUTE PX-PY ELEMENTS

      II=I+11
      JJ=J+11
      A=XP3(I)
      B=XP3(J)
      C=A
      D=B
      S1=A+B
      S2=S1
      S4=S1+S2
      T=S1*S2*R**2/S4
      CALL FT
      NN=N(A,B)
      GG=G(A,B,C,D)
      REP3(1)=GG*NN**2*(FT0/(4D0*S1*S2)-FT1*(S1/(2D0*S1*S2*S4))+
1      3D0*FT2/(4D0*S4**2))
      REP3(2)=GG*NN**2*FT2/(4D0*S4**2)
      TEST=A*B*R**2/(A+B)
      IF(TEST.GE.25D0)GO TO 61
      W=NN*DEXP(-TEST)
      T=S1*S2*R**2/S4*(B/(A+B)-C/(C+D))**2
      CALL FT
      REP3(3)=GG*W**2*((1D0/(2D0*(A+B)))*(FT0/(2D0*(C+D))-S1*FT1/(2D0*S2
1      *S4))+3D0*FT2/(4D0*S4**2)-FT1/(4D0*S1*S4))
      REP3(4)=GG*W**2*FT2*(1D0/(4D0*S4**2))
      GO TO 62
61 REP3(3)=0D0
      REP3(4)=0D0
62 CONTINUE
      HB(II,JJ) = 4D0*(REP3(1)+REP3(2) + REP3(3) + REP3(4))
      HB(JJ,II)=HB(II,JJ)

C
C
C      RETURN AFTER GROUND STATE CALCULATION

87 GO TO 2003

```

LEVEL 1, MOD 3

HBMTRX

DATE = 69133

15/33/50

1000 CONTINUE

C
C
C
C
C
C

EXCITED STATE CALCULATION

COMPUTATION OF MATRIX ELEMENTS IN SAME ORDER AS FOR GROUND STATE

A=XP1(I)

B=XP1(J)

C=A

D=B

S1=A+B

S2=S1

S4=S1+S2

T=S1*S2*R**2/S4

CALL FT

NN=N(A,B)

GG=G(A,B,C,D)

REP1(2)=GG*NN**2*FT0

TEST=A*B*R**2/(A+B)

IF(TEST.GE.25D0)GO TO 71

REP1(3)=GG*(NN*DEXP(-TEST))**2

GO TO 72

71 REP1(3)=0D0

72 CONTINUE

HB(I,J)=2D0*(REP1(2) - REP1(3))

HB(J,I)=HB(I,J)

JJ=J+8

B=XP1(I)

A=XP2(J)

C=A

D=B

S1=A+B

S2=S1

S4=S1+S2

T=S1*S2*R**2/S4

CALL FT

NN=N(A,B)

GG=G(A,B,C,D)

REP6(1)=GG*NN**2/S4*(FT1/2D0-S1*S2*FT2*R**2/S4)

TEST=A*B*R**2/(A+B)

IF(TEST.GE.25D0)GO TO 81

PQ=R*(B/(A+B)-C/(C+D))

T=S1*S2*PQ**2/S4

CALL FT

W=NN*DEXP(-TEST)

REP6(3)=GG*W**2*((B*R/(A+B))*(-B*R/(C+D)*FT0+S1*PQ*FT1/S4)+FT1/(2D

1 0*S4)-S1*S2*PQ**2*FT2/S4**2 - B*R*S1*PQ*FT1/((A+B)*S4))

GO TO 82

81 REP6(3)=0D0

82 CONTINUE

HB(I,JJ)=2D0*(REP6(1) - REP6(3))

LEVEL 1, MOD 3

HBMTRX

DATE = 69133

15/33/50

HB(JJ,I)=HB(I,JJ)

JJ=J+11

A=XP3(J)

B=XP1(I)

C=A

D=B

S1=A+B

S2=S1

S4=S1+S2

NN=N(A,B)

GG=G(A,B,C,D)

T=S1*S2*R**2/S4

CALL FT

REP5(1)=GG*NN**2*FT1/(2D0*S4)

TEST=A*B*R**2/(A+B)

IF(TEST.GE.25D0)GO TO 91

T=S1*S2*R**2/S4*(B/(A+B) -C/(C+D))**2

CALL FT

W=NN*DEXP(-TEST)

REP5(2)= GG*W**2*FT1/(2D0*S4)

GO TO 92

91 REP5(2)=0D0

92 CONTINUE

HB(I,JJ)=4D0*(REP5(1) - REP5(2))

HB(JJ,I)=HB(I,JJ)

II=I+8

JJ=J+8

A=XP2(I)

B=XP2(J)

C=A

D=B

S1=A+B

S2=C+D

S4=S1+S2

T=S1*S2*R**2/S4

CALL FT

NN=N(A,B)

GG=G(A,B,C,D)

SAA=NN/(2D0*(A+B))

SBB=SAA

GOZZ=(S1/S4)*((S1/S4)*FT2*R**2-(1D0/(2D0*S2))*FT1)

GZZ0=GOZZ

GZZZ=(1D0/(S4**2))*((S1*S2*R**2/S4)**2*FT4-S1*S2*3D0*FT3*R**2/S4
+3D0*FT2/4D0)

REP2(1)=GG*(SAA*(SBB*FT0+NN*GOZZ)+NN*(SBB*GZZ0+NN*GZZZ))

TEST=A*B*R**2/(A+B)

IF(TEST.GE.25D0)GO TO 101

W=NN*DEXP(-TEST)

SAB1=(1D0/(2D0*(A+B))-A*B*R**2/((A+B)**2))*W

PQ=(B-C)/(B+C)*R

T=S1*S2*PQ**2/S4

LEVEL 1, MOD 3

HBMTRX

DATE = 69133

15/33/50

```

CALL FT
G0000=FT0
G00ZZ=S1/S4*(S1/S4*PQ**2*FT2-1D0/(2D0*S2)*FT1)
GZZZZ=1D0/S4**2*(S1**2*S2**2*PQ**4*FT4/S4**2-3D0*S1*S2*PQ**2*FT3/
1  S4+3D0*FT2/4D0)
REP2(2)=GG*(SAB1**2*G0000+2D0*W*SAB1*G00ZZ+W**2*GZZZZ)
GO TO 102
101 REP2(2)=0D0
102 CONTINUE
HB(II,JJ)=2D0*(REP2(1) - REP2(2))
HB(JJ,II)=HB(II,JJ)
II=I+8
JJ=J+11
A=XP2(I)
B=XP3(J)
C=A
D=B
S1=A+B
S2=S1
S4=S1+S2
T=S1*S2*R**2/S4
CALL FT
NN=N(A,B)
GG=G(A,B,C,D)
REP4(1)=GG*NN**2*(1D0/S4**2*(FT2/4D0-S1*S2*R**2*FT3/(2D0*S4)))
TEST=A*B*R**2/(A+B)
IF(TEST.GE.25D0)GO TO 111
PQ=R*(B/(A+B)-C/(C+D))
T=S1*S2*PQ**2/S4
CALL FT
W=NN*DEXP(-TEST)
REP4(2)=GG*W**2*(1D0/(16D0*S1**2)*(-S1*PQ**2*FT3+FT2)-(B*R/(A+B))*
1  *2*FT1/(2D0*S4))
GO TO 112
111 REP4(2)=0D0
112 CONTINUE
HB(II,JJ)=4D0*(REP4(1) - REP4(2))
HB(JJ,II)=HB(II,JJ)
II=I+11
JJ=J+11
A=XP3(I)
B=XP3(J)
C=A
D=B
S1=A+B
S2=S1
S4=S1+S2
T=S1*S2*R**2/S4
CALL FT
NN=N(A,B)
GG=G(A,B,C,D)
REP3(1)=GG*NN**2*(FT0/(4D0*S1*S2)-FT1*(S1/(2D0*S1*S2*S4))+

```

G LEVEL 1, MOD 3

HBMTRX

DATE = 69133

15/33/50

```
1 3D0*FT2/(4D0*S4**2))
  REP3(2)=GG*NN**2*FT2/(4D0*S4**2)
  TEST=A*B*R**2/(A+B)
  IF(TEST.GE.25D0)GO TO 121
  W=NN*DEXP(-TEST)
  T=S1*S2*R**2/S4*(B/(A+B)-C/(C+D))**2
  CALL FT
  REP3(3)=GG*W**2*((1D0/(2D0*(A+B)))*(FT0/(2D0*(C+D))-S1*FT1/(2D0*S2
1  *S4))+3D0*FT2/(4D0*S4**2)-FT1/(4D0*S1*S4))
  REP3(4)=GG*W**2*FT2*(1D0/(4D0*S4**2))
  GO TO 122
121 REP3(3)=0D0
    REP3(4)=0D0
122 CONTINUE
    HB(II,JJ) = 4D0*(REP3(1)+REP3(2) - REP3(3) - REP3(4))
    HB(JJ,II)=HB(II,JJ)
2000 HB(1,9)=0D0
    HB(9,1)=0D0
    HB(9,9)=0D0
2001 HB(9,12)=0D0
    HB(12,9)=0D0
    HB(1,12)=0D0
    HB(12,1)=0D0
    HB(12,12)=0D0
2003 RETURN
    END
```

LEVEL 1, MOD 3

HCMTRX

DATE = 69133

15/33/50

SUBROUTINE HCMTRX

C
C
C
COMPUTE NUCLEAR ATTRACTION MATRAIX

IMPLICIT REAL*8(A-H,N-Z)

COMMON/A1/PI,R,S(14,14),H(14,14),XP1(8),XP2(3),XP3(3),CDF(14),Z,

1 ISTATE

COMMON/A2/HA(14,14),HB(14,14),HC(14,14)

COMMON/F/T,FT1,FT2,FT3,FT4,FT0

COMMON/NEW/CUTOFF,LL,LLL

DIMENSION VLAP(8),ATRAC(16)

N(X,Y)=(PI/(X+Y))**{(3D0/2D0)}

TH(X,Y)=Q*DSQRT(X+Y)

Q=(2D0/DSQRT(PI))

I=1

J=1

IF(ISTATE.NE.0)GO TO 1000

C
C
C
COMPUTE S-S ELEMENTS

A=XP1(I)

B=XP1(J)

NN=N(A,B)

VLAP(1)=NN

THETA=TH(A,B)

ATRAC(1)=THETA*NN

T=(A+B)*R**2

CALL FT

ATRAC(2)=ATRAC(1)*FT0

TEST=A*B*R**2/(A+B)

IF(TEST.GE.25D0)GO TO 11

W=NN*DEXP(-TEST)

VLAP(2)=W

T=(B*R)**2/(A+B)

CALL FT

ATRAC(4)=THETA*W*FT0

T=(A*R)**2/(A+B)

CALL FT

DTRAC=THETA*W*FT0

GO TO 12

11 VLAP(2)=0D0

ATRAC(4)=0D0

DTRAC=0D0

12 CONTINUE

HC(I,J)=4D0*(VLAP(1)*(ATRAC(1)+ATRAC(2))+VLAP(2)*(ATRAC(4)+DTRAC))

HC(J,I)=HC(I,J)

IF(LLL.EQ.1)GO TO 2000

C
C
C
COMPUTE S-PZ ELEMENTS

JJ=J+8

A=XP1(I)

LEVEL 1, MOD 3

HCMTRX

DATE = 69133

15/33/50

```

C=XP2(J)
TEST=A*C*R**2/(A+C)
IF(TEST.GE.25D0)GO TO 21
NN=N(A,C)
THETA=TH(A,C)
W=NN*DEXP(-TEST)
VLAP(6)=-(A/(A+C))*R*W
T=(A*R)**2/(A+C)
CALL FT
ATRAC(13)=THETA*W*(A*R/(A+C))*(FT0-FT1)
T=(C*R)**2/(A+C)
CALL FT
ATRAC(15)=THETA*W*R/(A+C)*(A*FT0+C*FT1)
GO TO 22
21 VLAP(6)=0D0
   ATRAC(13)=0D0
   ATRAC(15)=0D0
22 CONTINUE
   HC(I,JJ)=+ 4D0*VLAP(6)*(ATRAC(13)+ATRAC(15))
   HC(JJ,I)=HC(I,JJ)

C
C
C   COMPUTE S-PX ELEMENTS

   HC(1,12)=0D0
   HC(12,1)=0D0
   HC(9,12)=0D0
   HC(12,9)=0D0
C
C   COMPUTE PZ/PZ ELEMENTS

   JJ=J+8
   II=I+8
   C=XP2(I)
   D=XP2(J)
   NN=N(C,D)
   VLAP(3)=NN*(1D0/(2D0*(C+D)))
   THETA=TH(C,D)
   THN=THETA*NN
   ATRAC(6)=THN*(1D0/(3D0*(C+D)))
   T=(C+D)*R**2
   CALL FT
   ATRAC(7)=THN*(FT2*R**2-1D0/(2D0*(C+D))*FT1+1D0/(2D0*(C+D))*FT0)
   TEST=C*D*R**2/(C+D)
   IF(TEST.GE.25D0)GO TO 41
   W=NN*DEXP(-TEST)
   T=(D*R)**2/(C+D)
   CALL FT
   ATRAC(8)=THETA*W/(C+D)*(((D*R)**2/(C+D))*FT2-FT1/2D0+(1D0/2D0-C*D
1     *R**2/(C+D))*FT0)
   VLAP(7)=W*(1D0/(2D0*(C+D))-C*D*R**2/((C+D)**2))
   GO TO 42
41 ATRAC(8)=0D0
   VLAP(7)=0D0

```

LEVEL 1, MOD 3

HCMTRX

DATE = 69133

15/33/50

42 CONTINUE

HC(II,JJ)=4D0*(VLAP(3)*(ATRAC(6)+ATRAC(7)) + VLAP(7)*2D0*ATRAC(8))
 HC(JJ,II)=HC(II,JJ)

IF(LLL.EQ.2)GO TO 2001

COMPUTE PX-PX ELEMENTS

JJ=J+11

II=I+11

E=XP3(I)

F=XP3(J)

NN=N(E,F)

THETA=TH(E,F)

THN=THETA*NN

VLAP(4)=NN*(1D0/(2D0*(E+F)))

ATRAC(6)=THN*(1D0/(3D0*(E+F)))

T=(E+F)*R**2

CALL FT

ATRAC(10)=THN/(2D0*(E+F))*(FT0-FT1)

TEST=E*F*R**2/(E+F)

IF(TEST.GE.25D0) GO TO 51

W=NN*DEXP(-TEST)

VLAP(8)=W*(1D0/(2D0*(E+F)))

T=(F*R)**2/(E+F)

CALL FT

ATRAC(9)=THETA*W/(2D0*(E+F))*(FT0-FT1)

GO TO 52

51 VLAP(8)=0D0

ATRAC(9)=0D0

52 CONTINUE

HC(II,JJ)=8D0*(VLAP(4)*(ATRAC(6)+ATRAC(10))+VLAP(8)*2D0*ATRAC(9))

HC(JJ,II)=HC(II,JJ)

MULTIPLY MATRIX BY -Z(NUCLEAR CHARGE)

RETURN AFTER GROUND STATE CALCULATION

GO TO 2003

EXCITED STATE COMPUTATION - ELEMENTS COMPUTED IN SAME ORDER AS ABOVE

1000 CONTINUE

A=XP1(I)

B=XP1(J)

NN=N(A,B)

VLAP(1)=NN

THETA=TH(A,B)

ATRAC(1)=THETA*NN

T=(A+B)*R**2

CALL FT

LEVEL 1, MOD 3

HCMTRX

DATE = 69133

15/33/50

```

ATRAC(2)=ATRAC(1)*FTO
TEST=A*B*R**2/(A+B)
IF(TEST.GE.25D0)GO TO 61
W=NN*DEXP(-TEST)
VLAP(2)=W
T=(B*R)**2/(A+B)
CALL FT
ATRAC(4)=THETA*W*FTO
T=(A*R)**2/(A+B)
CALL FT
DTRAC=THETA*W*FTO
GO TO 62
61 VLAP(2)=0D0
   ATRAC(4)=0D0
   DTRAC=0D0
62 CONTINUE
   HC(I,J)=4D0*(VLAP(1)*(ATRAC(1)+ATRAC(2))-VLAP(2)*(ATRAC(4)+DTRAC))
   HC(J,I)=HC(I,J)
C
   JJ=J+8
   A=XP1(I)
   C=XP2(J)
   TEST=A*C*R**2/(A+C)
   IF(TEST.GE.25D0)GO TO 71
   NN=N(A,C)
   THETA=TH(A,C)
   W=NN*DEXP(-TEST)
   VLAP(6)=- (A/(A+C))*R*W
   T=(A*R)**2/(A+C)
   CALL FT
   ATRAC(13)=THETA*W*(A*R/(A+C))*(FTO-FT1)
   T=(C*R)**2/(A+C)
   CALL FT
   ATRAC(15)=THETA*W*R/(A+C)*(A*FTO+C*FT1)
   GO TO 72
71 VLAP(6)=0D0
   ATRAC(13)=0D0
   ATRAC(15)=0D0
72 CONTINUE
   HC(I,JJ)=- 4D0*VLAP(6)*(ATRAC(13)+ATRAC(15))
   HC(JJ,I)=HC(I,JJ)
C
101 HC(1,12)=0D0
102 HC(12,1)=0D0
   HC(9,12)=0D0
   HC(12,9)=0D0
C
2000 JJ=J+8
   II=I+8
   C=XP2(I)
   D=XP2(J)
2001 NN=N(C,D)

```


G LEVEL 1, MOD 3

HCMTRX

DATE = 69133

15/33/50

```

VLAP(3)=NN*(1D0/(2D0*(C+D)))
THETA=TH(C,D)
THN=THETA*NN
ATRAC(6)=THN*(1D0/(3D0*(C+D)))
T=(C+D)*R**2
CALL FT
ATRAC(7)=THN*(FT2*R**2-1D0/(2D0*(C+D))*FT1+1D0/(2D0*(C+D))*FT0)
TEST=C*D*R**2/(C+D)
IF(TEST.GE.25D0)GO TO 91
W=NN*DEXP(-TEST)
T=(D*R)**2/(C+D)
CALL FT
ATRAC(8)=THETA*W/(C+D)*(((D*R)**2/(C+D))*FT2-FT1/2D0+(1D0/2D0-C*D
1      *R**2/(C+D))*FT0)
VLAP(7)=W*(1D0/(2D0*(C+D))-C*D*R**2/((C+D)**2))
GO TO 92
91 ATRAC(8)=0D0
VLAP(7)=0D0
92 CONTINUE
HC(II,JJ)=4D0*(VLAP(3)*(ATRAC(6)+ATRAC(7)) - VLAP(7)*2D0*ATRAC(8))
HC(JJ,II)=HC(II,JJ)

C
JJ=J+11
II=I+11
E=XP3(I)
F=XP3(J)
NN=N(E,F)
THETA=TH(E,F)
THN=THETA*NN
VLAP(4)=NN*(1D0/(2D0*(E+F)))
ATRAC(6)=THN*(1D0/(3D0*(E+F)))
T=(E+F)*R**2
CALL FT
ATRAC(10)=THN/(2D0*(E+F))*(FT0-FT1)
TEST=E*F*R**2/(E+F)
IF(TEST.GE.25D0)GO TO 101
W=NN*DEXP(-TEST)
VLAP(8)=W*(1D0/(2D0*(E+F)))
T=(F*R)**2/(E+F)
CALL FT
ATRAC(9)=THETA*W/(2D0*(E+F))*(FT0-FT1)
GO TO 102
101 VLAP(8)=0D0
ATRAC(9)=0D0
102 CONTINUE
HC(II,JJ)=8D0*(VLAP(4)*(ATRAC(6)+ATRAC(10))-VLAP(8)*2D0*ATRAC(9))
HC(JJ,II)=HC(II,JJ)

C
2000 HC(1,9)=0D0
HC(9,1)=0D0
HC(9,9)=0D0
2001 HC(9,12)=0D0

```

LEVEL 1, MOD 3

HCMTRX

DATE = 69133

15/33/50

HC(12,9)=0D0

HC(1,12)=0D0

HC(12,1)=0D0

HC(12,12)=0D0

2003

HC(1,1)=-Z*HC(1,1)

HC(9,9)=-Z*HC(9,9)

HC(12,12)=-Z*HC(12,12)

HC(1,9)=-Z*HC(1,9)

HC(9,1)=-Z*HC(9,1)

RETURN

END

PROGRAM TO READ PUNCHED
CARD OUTPUT OF ENERGY
MINIMIZATION AND PRODUCE
THE TABLE FOUND IN THIS
THESIS

LEVEL 1, MOD 3

MAIN

DATE = 69135

10/39/36

```

      IMPLICIT REAL*8(A-H,O-Z)
      DIMENSION CARD1(80),Z(200),NK(200),X(200),VIRIAL(200),BINDEN(200),
1EXPT(200),EXPV(200),EXPR12(200),DEDR(200),C1(200),C2(200),C3(200),
2EXPRA(200),CHISQ(200),R(200)
99  READ(5,1,END=999)NOTBL,OPTION
      NOTBL=NOTBL/5
      READ(5,2)(CARD1(I),I=1,80)
1   FORMAT(I5,F10.0)
2   FORMAT(80A1)
      DO 100 K=1,NOTBL
      READ(5,3)Z(K),R(K),NK(K),X(K),VIRIAL(K),BINDEN(K),EXPT(K),EXPV(K),
1EXPR12(K),DEDR(K),C1(K),C2(K),C3(K),EXPRA(K),CHISQ(K)
3   FORMAT(F10.5,F15.10,5X,I5,D25.16,/3D25.16,/3D25.16,/3D20.10,D15.8,
1/D25.16)
100 CONTINUE
      N=NK(1)-1
      LL=1
98  L=1
      WRITE(6,10)(CARD1(MM),MM=1,80)
      IF(N.EQ.0)WRITE(6,4)
      IF(N.EQ.1)WRITE(6,6)
      IF(N.EQ.2)WRITE(6,7)
97  IF(N.EQ.0)WRITE(6,5)R(LL),CHISQ(LL),X(LL)
      IF(N.EQ.1)WRITE(6,5)R(LL),CHISQ(LL),X(LL),C2(LL)
      IF(N.EQ.2)WRITE(6,5)R(LL),CHISQ(LL),X(LL),C2(LL),C3(LL)
      LL=LL+1
      IF(LL.EQ.( NOTBL+1))GO TO 101
      IF(L.EQ.50)GO TO 98
      L=L+1
      GO TO 97
101 CONTINUE
4   FORMAT(/10X,' R (BOHR) ',5X,' ENERGY (HARTREES) ', ' ZETA ',/)
6   FORMAT(/10X,' R (BOHR) ',5X,' ENERGY (HARTREES) ', ' ZETA ',
19X,' ALPHA ',/)
7   FORMAT(/10X,' R (BOHR) ',5X,' ENERGY (HARTREES) ',2X,' ZETA ',
17X,' BETA ',9X,' GAMMA',/)
5   FORMAT(10X,F10.5,5X,F15.10,3X,F10.5,2(3X,F12.8))
10  FORMAT('1', ///10X,80A1)
      L2=1
102 L1=1
      WRITE(6,10)(CARD1(MM),MM=1,80)
      WRITE(6,12)
      PI=3.1415926535
103 IF(Z(L2).GT.1D0)BINDEN(L2)=CHISQ(L2)+(8D0*Z(L2)**2)/(3D0*PI)
      WRITE(6,13)R(L2),BINDEN(L2),EXPV(L2),VIRIAL(L2),DEDR(L2)
      L2=L2+1
      IF(L2.EQ.( NOTBL+1))GO TO 104
      IF(L1.EQ.50)GO TO 102
      L1=L1+1
      GO TO 103
104 CONTINUE
12  FORMAT(/12X,' R (BOHR) ',1X,' BINDING ENERGY ',5X,' (V) ',5X, '

```

LEVEL 1, MOD 3

MAIN

DATE = 69135

10/39/36

```

1 -V/2T ', 5X,' DE/DR ',/)
13 FORMAT(10X,F10.5,4F15.10)
   IF(N.EQ.0)GO TO 108
   L4=1
105 L3=1
   WRITE(6,10)(CARD1(MM),MM=1,80)
   IF(N.EQ.1)WRITE(6,20)
   IF(N.EQ.2)WRITE(6,21)
106 ZR=Z(1)*R(L4)
   XZET=X(L4)/Z(1)**2
   IF(N.GE.1)ALPZ=C2(L4)/Z(1)**2
   IF(N.EQ.2)GAMZ=C3(L4)/Z(1)
   IF(N.EQ.1)WRITE(6,107)ZR,XZET,ALPZ
177 FORMAT(10X,F10.5,10X,F10.5,2(5X,F15.10))
107 FORMAT(10X,F10.5,2(10X,F15.10))
   IF(N.EQ.2)WRITE(6,177)ZR,XZET,ALPZ,GAMZ
   L4=L4+1
   IF(L4.EQ.(NOTBL +1))GO TO 108
   IF(L3.EQ.50)GO TO 105
   L3=L3+1
   GO TO 106
108 CONTINUE
20 FORMAT(/14X,'   ZR   ', 7X,'   ZETA/Z**2   ',13X,'   ALPHA/Z**2',/)
21 FORMAT(/14X,'   ZR   ', 7X,'   ZETA/Z**2',10X,'   BETA/Z' ,10X,
1'   GAMMA/Z',/)
   L6=1
110 L5=1
   WRITE(6,10)(CARD1(MM),MM=1,80)
   WRITE(6,113)
111 WRITE(6,112)R(L6),EXPR12(L6),EXPRA(L6)
   L6=L6+1
   IF(L6.EQ.( NOTBL+1))GO TO 115
   IF(L5.EQ.50)GO TO 110
   L5=L5+1
   GO TO 111
115 CONTINUE
113 FORMAT(/10X,'   R (BOHR) ',11X,'(1/R12) ',11X,'(1/RA)',/)
112 FORMAT(10X,F10.5,2(5X,F15.10))
   IF(Z(1).GT.1D0)GO TO 99
   L8=1
117 L7=1
   WRITE(6,10)(CARD1(MM),MM=1,80)
   WRITE(6,30)
30 FORMAT(/10X,'   SCALED R', 7X,'   SCALED ENERGY', 7X,'   SCALED DE/DR'/)
118 IF(N.EQ.0.OR.N.EQ.1)R(L8)=R(L8)*(1.401D0/1.55D0 )
   IF(N.EQ.2)R(L8)=R(L8)*(1.401D0/1.53D0)
   IF(N.EQ.0)BINDEN(L8)=BINDEN(L8)*(.1744746/.1380708)
   IF(N.EQ.1)BINDEN(L8)=BINDEN(L8)*(.1744746/.1457276)
   IF(N.EQ.2)BINDEN(L8)=BINDEN(L8)*(.1744746/.1541438)
   IF(N.EQ.0)DEDR(L8)=DEDR(L8)*(.1744746/.1380708)*(1.55/1.401)
   IF(N.EQ.1)DEDR(L8)=DEDR(L8)*(.1744746/.1457276)*(1.55/1.401)
   IF(N.EQ.2)DEDR(L8)=DEDR(L8)*(.1744746/.1541438)*(1.53/1.401)

```

G LEVEL 1, MOD 3

MAIN

DATE = 69135

10/39/36

```
WRITE(6,119)R(L8),BINDEN(L8),DEDR(L8)
119 FORMAT(10X,F10.5,5X,F15.10,5X,F15.10)
L8=L8+1
IF(L8.EQ.(NOTBL+1))GO TO 99
IF(L7.EQ.50)GO TO 117
L7=L7+1
GO TO 118
999 STOP
END
```


MODIFIED Q.C.P.E.
SUBROUTINES

LEVEL 1, MOD 3

DSIMPX

DATE = 69132

14/44/18

SUBROUTINE DSIMPX(FUNK)

DOUBLE PRECISION VERSION OF SIMPLX

SIMPLEX-MINIMUM OF A FUNCTION OF SEVERAL CONSTRAINED VARIABLES

FUNCTION MINIMIZATION BY THE SIMPLEX METHOD. J.P. CHANDLER BIN 27SMPLX

(NELDER AND MEAD, THE COMPUTER JOURNAL, JANUARY 1965) SMPLX

AT PRESENT MATRIX AND ERR ARE INOPERATIVE. SMPLX

THIS PROGRAM IS STILL IN EXPERIMENTAL FORM. NOTHING IS GUARANTEED. SMPLX

COMMANDMENT 1 THOU SHALT NOT OMIT THINE 'EXTERNAL' CARD. SMPLX

IMPLICIT REAL*8(A-H,O-Z)

INTEGER SWITCH

COMMON/S1/CHISQ,X(20)

COMMON/S2/XMAX(20),XMIN(20),DELTAX(20),DELMIN(20),

\$ NV,NTRACE,MASK(20)

DIMENSION CHI(21),Z(21,20),ZBAR(20),ZSTAR(20) SMPLX

MATRIX=0

SWITCH=65535

KW=6

30 HUGE=1.0D75

SIGNIF=1.0D17

ALPHA=1.0D0

BETA=0.7D0

GAMMA=2.0D0

IF(NV)890,890,40 SMPLX

40 DO 120 J=1,NV SMPLX

IF(MASK(J))120,50,120 SMPLX

50 IF(SIGNIF*DABS(DELTAX(J))-DABS(X(J))) 60,60,90

60 IF(X(J))80,70,80 SMPLX

70 DELTAX(J)=0.01D0

GO TO 90 SMPLX

80 DELTAX(J)=0.01D0*X(J)

90 IF(XMAX(J)-XMIN(J))100,100,110 SMPLX

100 XMAX(J)=HUGE SMPLX

XMIN(J)=-HUGE SMPLX

110 X(J)=DMAX1(XMIN(J),DMIN1(XMAX(J),X(J)))

120 CONTINUE SMPLX

C CALCULATE INITIAL P(I) AND Y(I). SMPLX

NVA=0 SMPLX

NF=0 SMPLX

DO 160 J=1,NV SMPLX

IF(MASK(J))160,130,160 SMPLX

130 NVA=NVA+1 SMPLX

DO 140 K=1,NV SMPLX

140 Z(NVA,K)=X(K) SMPLX

Z(NVA,J)=Z(NVA,J)+DELTAX(J) SMPLX

XS=X(J) SMPLX

LEVEL 1, MOD 3

DSIMPX

DATE = 69132

14/44/18

```

      X(J)=Z(NVA,J)
      NGO=1
      GO TO 210
150  X(J)=XS
      CHI(NVA)=CHISQ
160  CONTINUE
      IF(NVA)170,170,190
170  DO 180 J=1,NV
180  MASK(J)=0
      GO TO 40
190  NVP=NVA+1
      DO 200 J=1,NV
200  Z(NVP,J)=X(J)
      NGO=2
C
210  DO 240 JF=1,NV
      IF(MASK(JF))240,220,240
220  IF(X(JF)-XMAX(JF))230,230,250
230  IF(X(JF)-XMIN(JF))250,240,240
240  CONTINUE
      CALL FUNK
      NF=NF+1
      GO TO 260
250  CHISQ=HUGE
260  GO TO (150,270,400,460,590,720 ),NGO
C
270  CHI(NVP)=CHISQ
      WRITE          (KW,81)
81  FORMAT(94H1SIMPLEX MINIMIZATION....   CODED BY J. P. CHANDLER, I. USMPLX
X. PHYSICS DEPT., BLOOMINGTON, INDIANA.///19H INITIAL VALUES....//)SMPLX
      WRITE          (KW,82)(MASK(J),J=1,NV)
82  FORMAT(/10H MASK      = 5(I12,12X)/(10X5I24))
      WRITE          (KW,83)(X(J),J=1,NV)
83  FORMAT(/10H X        = 4D25.16/(10X4D25.16))
      WRITE          (KW,84)(XMAX(J),J=1,NV)
84  FORMAT(/10H XMAX     = 4D25.16/(10X4D25.16))
      WRITE          (KW,85)(XMIN(J),J=1,NV)
85  FORMAT(/10H XMIN     = 4D25.16/(10X4D25.16))
      WRITE          (KW,86)(DELTAX(J),J=1,NV)
86  FORMAT(/10H DELTAX   = 4D25.16/(10X4D25.16))
      WRITE          (KW,87)(DELMIN(J),J=1,NV)
87  FOKMAT(/10H DELMIN   = 4D25.16/(10X4D25.16))
      WRITE          (KW,88)NV,NVA,MATRIX,ALPHA,BETA,GAMMA,CHISQ
88  FORMAT(//20XI3,11H VARIABLES,I3,8H ACTIVE.10X9HMATRIX = I3//20X7HASMPLX
$LPHA =F4.1,10X6HBETA =F5.2,10X7HGAMMA =F4.1//30X8HCHISQ = D25.16/)
      IF(NTRACE)280,290,280
280  WRITE          (KW,92)
92  FORMAT(/60(1X1H*)//10X37HTRACE MAP OF THE MINIMIZATION PROCESS///)SMPLX
C
C  DETERMINE H AND L.
C
290  JH=1

```

SMPLX10

14/44/18

```

JL=1
DO 330 J=2,NVP
  IF(CHI(J)-CHI(JH))310,310,300
300 JH=J
310 IF(CHI(J)-CHI(JL))320,330,330
320 JL=J
330 CONTINUE

C
C CALCULATE PBAR.
C
  DO 370 J=1,NV
  IF(MASK(J))370,340,370
340 ZBAR(J)=0.000
  DO 360 K=1,NVP
  IF(K-JH)350,360,350
350 ZBAR(J)=ZBAR(J)+Z(K,J)
360 CONTINUE
  ZBAR(J)=ZBAR(J)/DFLOAT(NVA)
370 CONTINUE

C
C ATTEMPT A REFLECTION.
C FORM P* .
C
  DO 390 J=1,NV
  IF(MASK(J))390,380,390
380 X(J)=(1.000+ALPHA)*ZBAR(J)-ALPHA*Z(JH,J)
390 ZSTAR(J)=X(J)
  NG0=3
  GO TO 210
400 CHISTR=CHISQ
  IF(CHISQ-CHISTR)410,470,470

C
C THE REFLECTION SUCCEEDED. ATTEMPT AN EXPANSION.
C FORM P** .
C
410 IF(NTRACE)420,430,420
420 WRITE (KW,43)CHISQ
43 FORMAT(10X8HCHISQ = D25.16,10X20HREFLECTION SUCCEEDED )
  WRITE (KW,44)(X(J),J=1,NV)
44 FORMAT(5X8HX(I)...../(5(1XD24.15)))
  WRITE (KW,155)
155 FORMAT(1H )
430 DO 450 J=1,NV
  IF(MASK(J))450,440,450
440 X(J)=GAMMA*X(J)+(1.000-GAMMA)*ZBAR(J)
450 CONTINUE
  NG0=4
  GO TO 210
460 IF(CHISQ-CHISTR)760,500,500

C
C THE REFLECTION FAILED.
C

```

14/44/18

SMPL X
SMPL X
SMPL X
SMPL X
SMPL X
SMPL X
SMPL X

SMPL X1

SMPL X1
SMPL X1
SMPL X1
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SMPLX1

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SMPL X1

SMPL X1
SMPL X1

SMPL X1

SAMPL X1

SMPLX2

SMPL X2

SMPL X2

SMPL X2

SMPL X2

SMPL X2

LEVEL 1, MOD 3

DSIMPX

DATE = 69132

14/44/18

680 X(K)=0.5D0*(Z(J,K)+Z(JL,K))
 IF(X(K)-Z(J,K))700,690,700

690 X(K)=Z(JL,K)

700 Z(J,K)=X(K)

710 CONTINUE

NGO=6

GO TO 210

720 IF(CHISQ-CHI(JS))730,740,740

730 JS=J

740 CHI(J)=CHISQ

750 CONTINUE

JL=JS

GO TO 800

SMPLX2

SMPLX2

SMPLX2

SMPLX2

SMPLX2

SMPLX2

SMPLX2

SMPLX2

SMPLX2

SMPLX2

SMPLX2

SMPLX2

C

760 IF(NTRACE)770,780,770

770 WRITE (KW,52)CHISQ

52 FORMAT(10X8HCHISQ = D25.16,10X19HEXPANSION SUCCEEDED)

WRITE

(KW,44)(X(J),J=1,NV)

WRITE

(KW,155)

SMPLX2

C

C

C

REPLACE P(JH) BY P* OR P** .

SMPLX2

780 DO 790 J=1,NV

790 Z(JH,J)=X(J)

CHI(JH)=CHISQ

SMPLX2

SMPLX2

SMPLX2

C

C

C

TEST FOR CONVERGENCE.

SMPLX2

800 DO 840 J=1,NV

IF(MASK(J))840,810,840

810 ZMAX=-HUGE

ZMIN=HUGE

DO 820 K=1,NVP

ZMAX=DMAX1(ZMAX,Z(K,J))

820 ZMIN=DMIN1(ZMIN,Z(K,J))

IF(SIGNIF*(ZMAX-ZMIN)-DMIN1(DABS(ZMAX),DABS(ZMIN)))840,840,830

830 IF(ZMAX-ZMIN-DABS(DELMIN(J)))840,840,900

840 CONTINUE

SMPLX2

SMPLX2

SMPLX2

SMPLX2

SMPLX2

SMPLX2

C

850 IF(CHI(JH)-CHI(JL))860,870,870

860 JL=JH

870 CHISQ=CHI(JL)

WRITE (KW,61)NF

61 FORMAT(///10X15,23H FUNCTION COMPUTATIONS.)

WRITE (KW,15)CHISQ

15 FORMAT(///10X23HFINAL VALUE OF CHISQ = D25.16)

DO 880 J=1,NV

880 X(J)=Z(JL,J)

890 WRITE (KW,21)(X(J),J=1,NV)

21 FORMAT(///10X24HFINAL VALUES OF X(I).../(5(1XD24.15)))

RETURN

900 IF(SWITCH)910,910,290

SMPLX2

SMPLX2

SMPLX2

SMPLX2

SMPLX2

SMPLX2

SMPLX2

SMPLX2

V G LEVEL 1, MOD 3

DSIMPX

DATE = 69132

14/44/18

```
910 WRITE          (KW,39)
 39 FORMAT(///24H TERMINATED BY OPERATOR. )
   DO 920 J=1,NVP
   WRITE           (KW,532)J,CHI(J)
532 FORMAT(/10X13HSIMPLEX POINTI3,15H ... CHISO = D25.16)
920 WRITE          (KW,44)(Z(J,K),K=1,NV)
   GO TO 850
   END
```

SMPLX2

SMPLX2

5

SMPLX2

SMPLX2

SUBROUTINE CEIG (N,N1,NN,HMAT,SMAT,E,COET,VEC,KP)
IMPLICIT REAL*8(A-H,O-Z)

```
CCEIG
C
C SUBROUTINE SOLVES SECULAR EQUATIONS OF FORM %H-LS<X#0, WHERE L
C IS A SCALAR. THIS ROUTINE BEGINS BY TRIANGULARIZATION OF S
C FOLLOWED BY A SINGLE DIAGONALIZATION. CMAT %WHICH CAN OCCUPY THE
C SAME LOCATION AS THE ORIGINAL OVERLAP MATRIX, SMAT< * CMAT TRANS-
C POSE # SMAT. THE TRANSFORMED HMAT IS STORED BACK OVER THE ORIGINAL
C HMAT BEFORE THE DIAGONALIZATION ROUTINE GIVENS IS CALLED AND THUS
C DESTROYS THE ORIGINAL HAMILTONIAN MATRIX. THE PARAMETERS ARE...
C N SIZE OF MATRIX BEING DIAGONALIZED
C N1 NUMBER OF ROOTS WANTED.
C NN FORTRAN DIMENSION OF THE MATRIX IN THE CALLING PROGRAM.
C HMAT HAMILTONIAN MATRIX - INPUT
C SMAT OVERLAP MATRIX - INPUT
C E EIGENVALUE - OUTPUT
C COET EIGENVECTOR - OUTPUT
C VEC TEMPORARY STORAGE
C KP TEMPORARY STORAGE
C
C DIMENSION E(1), HMAT(1), SMAT(1), VEC(NN,5), COET(NN,NN), KP(1)
C DO 30 I=1,N
30 KP(I) = (I*(I-1))/2
C COET(1,1) =DSQRT(SMAT(1))
C CMAT%1< # 1.0/ COET%1,1<
C SMAT(1) = 1.0/ COET(1,1)
C CMAT HAS BEEN REPLACED HERE BY SMAT BECAUSE FORTRAN RULES SPECIFY
C THAT A VARIABLE APPEARING IN THE CALLING SEQUENCE CANNOT BE EQUI-
C VALENCED TO ANOTHER VARIABLE. ALL ORIGINAL STATEMENTS USING CMAT
C ARE SAVED ON COMMENT CARDS SO THAT THE USER CAN FOLLOW THE LOGIC
C MORE READILY.
C IF(N-1) 2,2,3
3 DO 10 J = 2,N
C III = KP(J) +1
10 COET(1,J) = SMAT(III)/COET(1,1)
C DO 11 I = 2,N
C SUM = 0.0
C III=KP(I)+I
C IM1 = I-1
C IP1 = I+1
C DO 12 K = 1,IM1
12 SUM = SUM + COET(K,I)**2
C WWW=SMAT(III)-SUM
C IF(WWW.LE.0D0)GO TO 100
C COET(I,I)=DSQRT(WWW)
C GO TO 101
100 WWW=0D0
C COET(I,I)=1D-30
101 CONTINUE
C CMAT%III< # 1.0/ COET%I,I<
C SMAT(III) = 1.0/ COET(I,I)
C IF(IP1-N) 6,6,4
```

70CE004
70CE038
70CE039
70CE048
70CE043
70CE04
70CE04
70CE04
70CE043
70CE043
70CE04
70CE04
70CE05
70CE05
70CE05
70CE05

17/11/31

```

6      DO 13 J = 1, N
      SUM = 0.0
      DO 14 K = 1, IM1
14     SUM = SUM + COET(K, I) * COET(K, J)
      III = KP(J) + I
13     COET(I, J) = (SMAT(III) - SUM) / COET(I, I)
4      II = I - 1
      DO 16 I1 = 1, IM1
      IJW = II + KP(I)
      SUM = 0.0
      IIP = II + 1
      DO 15 K = IIP, I
      KJW = K + KP(I)
C 15     SUM # SUM & COET%II, K < * CMAT%KJW<
15     SUM = SUM + COET(II, K) * SMAT(KJW)
C      CMAT%IJW< # - SUM / COET%II, II<
      SMAT(IJW) = - SUM / COET(II, II)
16     II = II - 1
11     CONTINUE
2      DO 40 J1 = 1, N
      DO 40 L = 1, J1
      COET(L, J1) = 0.0
      DO 41 K = 1, J1
      KJ1 = K + KP(J1)
      IF(L - K) 42, 42, 43
43     III = K + KP(L)
      GO TO 41
42     III = L + KP(K)
C 41     COET%L, J1< # COET%L, J1< & HMAT%III< * CMAT%KJ1<
41     COET(L, J1) = COET(L, J1) + HMAT(III) * SMAT(KJ1)
40     CONTINUE
      DO 44 J1 = 1, N
      DO 44 I1 = 1, J1
      KKK = I1 + KP(J1)
C      W%KKK< # 0.0
      HMAT(KKK) = 0.0
C      HMAT REPLACES W FOR THE SAME REASON THAT SMAT REPLACES CMAT.
      DO 44 L = 1, I1
      LI1 = L + KP(I1)
C 44     W%KKK< # W%KKK< & CMAT%LI1< * COET%L, J1<
44     HMAT(KKK) = HMAT(KKK) + SMAT(LI1) * COET(L, J1)
C      IF ONLY ONE EIGENVALUE IS WANTED, DELETE THE LAST CARD AND USE
C      THE FOLLOWING CALL.
      CALL NESBET (N, N1, NN, HMAT, VEC, E, COET)
      N1ABS = IABS(N1)
63     DO 61 J = 1, N1ABS
      DO 60 I = 1, N
      VEC(I, 1) = 0.
      DO 60 JJ = I, N
      IJJ = I + KP(JJ)
C 60     VEC%I, 1< # VEC%I, 1< & CMAT%IJJ< * COET%JJ, J<
60     VEC(I, 1) = VEC(I, 1) + SMAT(IJJ) * COET(JJ, J)

```


G LEVEL 1, MOD 3

CEIG

DATE = 69131

17/11/31

DO 50 I = 1,N

50 COET(I,J) = VEC(I,1)

61 CONTINUE

RETURN

END

70CE106

LEVEL 1, MOD 3

NESBET

DATE = 69131

17/11/31

SUBROUTINE NESBET(N,NROOTX,NN,H,KP, E,C)
 IMPLICIT REAL*8(A-H,O-Z)

C
 C NESBET METHOD FOR LOWEST EIGENVALUE, CALLING SEQUENCE IS
 C COMPATIBLE WITH PROSSER,S GIVENS. THE PARAMETERS ARE...
 C N#SIZE OF THE MATRIX BEING DIAGONILIZED.
 C NROOTX#1 ONLY FOR THIS PROGRAM, I.E. ONLY ONE EIGENVALUE IS GIVEN.
 C NN#FORTRAN DIMENSION OF THE MATRIX IN THE CALLING PROGRAM.
 C H#THE MATRIX BEING DIAGONILIZED.
 C KP #TEMPORARY STORAGE TO BE COMPATIBLE WITH PROSSER,S GIVENS,
 C USED HERE FOR UPPER TRIANGLE INDEXING.
 C E#EIGENVALUE. ONLY 1 IS RETURNED FROM THIS VERSION.
 C C#EIGENVECTOR MATRIX. ONLY 1 VECTOR IS RETURNED FROM THIS VERSION.
 C DIMENSION H(1),KP(1),E(1),C(NN,NN)
 C TOL=1D-12
 C DO 30 I = 1,N
 30 KP(I) = (I*(I-1))/2
 C NROOTX = 1
 C CA=2.0
 C CTEST=0.0999
 C DO 5 I =1,N
 5 C(I,1) = 0.0
 48 E(1) =10.0
 C DO 50 J=1,N
 C JJJ = J+ KP(J)
 C IF(E(1) -H(JJJ)) 50,50,52
 52 E(1) = H(JJJ)
 C JS=J
 50 CONTINUE
 C JJS=JS+KP(JS)
 C C(JS,1)=1.0
 C IF(N-1)43,43,55
 55 JS2=0
 C DO 70 J=1,N
 C IF(J.EQ.JS) GO TO 70
 C JJJ=J+KP(J)
 C IF (E(1).LT.H(JJJ)) GO TO 70
 71 J12=JS+KP(J)
 C IF (H(J12).EQ.0.) GO TO 70
 C JS2=J
 C GO TO 72
 70 CONTINUE
 72 IF (JS2.EQ.0) GO TO 73
 C H12=H(J12)
 C E(1)=H(JJS)-DABS(H12)
 C C(JS2,1)=DSIGN(1D0,-H12)
 73 CONTINUE
 8 CMAX = 0.0
 C DO 3 J = 1,N
 C IF(J-JS) 9,3,9
 9 SIG = -E(1)*C(J,1)
 C JJJ = J + KP(J)

MLEW00

MLEW01

MLEW01

MLEW01

MLEW01

MLEW01

MLEW02

MLEW02

G LEVEL 1, MOD 3

NESBET

DATE = 69131

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DO 4 I =1,N
IF (I-J) 1,1,2
2 IJJ=J+KP(I)
GO TO 4
1 IJJ = I +KP(J)
4 SIG = SIG +H(IJJ) *C(I,1)
21 DELC = SIG/(E(1)-H(JJJ))
7 DELD = (C(J,1) +C(J,1) +DELC)*DELC
D= 0.0
DO 6 K = 1,N
6 D = D + C(K,1)**2
22 DELE = SIG*DELC/(D+DELD)
24 C(J,1) = C(J,1) + DELC
CMAX= DMAX1(CMAX,DABS(DELC))
25 E(1) = E(1) + DELE
26 IF(DABS(DELC)-CA)3,3,8
3 CONTINUE
CA=CA/2.0
31 IF(CMAX-CTEST) 13,13,8
13 CTEST=.01*CTEST
E1=0.
D=0.
DO 36 KI=1,N
D=D+C(KI,1)**2
DO 36 KJ=KI,N
KKK=KI+KP(KJ)
TERM=C(KI,1)*C(KJ,1)*H(KKK)
IF(KI-KJ) 35,34,35
34 E1=E1+TERM
GO TO 36
35 E1=E1+TERM+TERM
36 CONTINUE
E(1) = E1/D
IF(CMAX-TOL)59,59,8
59 BRAFN=H(JJS)-E(1)
DO 60 I=1,N
IF(I-JS)61,60,62
61 KI=I+KP(JS)
GO TO 63
62 KI=JS+KP(I)
63 BRAFN=BRAFN+H(KI)*C(I,1)
60 CONTINUE
E(1)=E(1)+BRAFN/D
D=DSQRT(D)
DO 16 I =1,N
16 C(I,1)=C(I,1)/D
43 RETURN
END

```

MLEW02

MLEW02

MLEW02

MLEW02

MLEW03

MLEW03

MLEW03

MLEW03

MLEW03

MLEW04C

MLEW041

MLEW043

- A TABLES -

TABLE A-1

H2 MOLECULE:	WAVEFUNCTION PSI 0	
R (BOHR)	ENERGY (HARTREES)	ZETA
0.10000	7.7054839291	0.76152
0.20000	2.7243912607	0.74571
0.30000	1.0876692697	0.72128
0.40000	0.2933240449	0.69055
0.50000	-0.1608738961	0.65597
0.60000	-0.4437500122	0.61970
0.70000	-0.6286246878	0.58345
0.80000	-0.7527509940	0.54839
0.90000	-0.8371500953	0.51529
1.00000	-0.8945869450	0.48453
1.05000	-0.9158700384	0.47009
1.10000	-0.9332348148	0.45629
1.15000	-0.9472891541	0.44312
1.20000	-0.9585373526	0.43057
1.25000	-0.9674003363	0.41863
1.30000	-0.9742313741	0.40729
1.35000	-0.9793284251	0.39652
1.40000	-0.9829439334	0.38630
1.45000	-0.9852926645	0.37662
1.50000	-0.9865580251	0.36745
1.51000	-0.9866953362	0.36568
1.52000	-0.9867968143	0.36393
1.53000	-0.9868635702	0.36218
1.54000	-0.9868966817	0.36048
1.55000	-0.9868971951	0.35878
1.60000	-0.9864453216	0.35058
1.65000	-0.9853189674	0.34283
1.70000	-0.9836189607	0.33551
1.75000	-0.9814327630	0.32862
1.80000	-0.9788364449	0.32212
1.85000	-0.9758963418	0.31601
1.90000	-0.9726704470	0.31027
1.95000	-0.9692095885	0.30489
2.00000	-0.9655584255	0.29984
2.05000	-0.9617562952	0.29513
2.10000	-0.9578379349	0.29074
2.15000	-0.9538340970	0.28666
2.20000	-0.9497720763	0.28289
2.25000	-0.9456761597	0.27940
2.30000	-0.9415680115	0.27620
2.35000	-0.9374670016	0.27328
2.40000	-0.9333904846	0.27063
2.45000	-0.9293540358	0.26824
2.50000	-0.9253716481	0.26611
2.55000	-0.9214558945	0.26424
2.60000	-0.9176180600	0.26260
2.65000	-0.9138682446	0.26120
2.70000	-0.9102154413	0.26004
2.75000	-0.9066675928	0.25909
2.80000	-0.9032316277	0.25835

H2 MOLECULE: WAVEFUNCTION PSI 0

R (BOHR)	ENERGY (HARTREES)	ZETA
2.85000	-0.8999134838	0.25782
2.90000	-0.8967181183	0.25747
2.95000	-0.8936495139	0.25729
3.00000	-0.8907106828	0.25728
3.05000	-0.8879036749	0.25742
3.10000	-0.8852295944	0.25768
3.15000	-0.8826886281	0.25806
3.20000	-0.8802800885	0.25854
3.25000	-0.8780024705	0.25910
3.30000	-0.8758535231	0.25973
3.35000	-0.8738303323	0.26042
3.40000	-0.8719294116	0.26115
3.45000	-0.8701467982	0.26191
3.50000	-0.8684781483	0.26270
3.55000	-0.8669188311	0.26349
3.60000	-0.8654640148	0.26430
3.65000	-0.8641087466	0.26510
3.70000	-0.8628480220	0.26590
3.75000	-0.8616768444	0.26668
3.80000	-0.8605902750	0.26746
3.85000	-0.8595834727	0.26822
3.90000	-0.8586517253	0.26896
3.95000	-0.8577904735	0.26969
4.00000	-0.8569953272	0.27039
4.10000	-0.8555867011	0.27174
4.20000	-0.8543944308	0.27301
4.30000	-0.8533901193	0.27418
4.40000	-0.8525482984	0.27527
4.50000	-0.8518462630	0.27627
4.60000	-0.8512638731	0.27718
4.70000	-0.8507833491	0.27800
4.80000	-0.8503890730	0.27874
4.90000	-0.8500673991	0.27939
5.00000	-0.8498064740	0.27996
5.10000	-0.8495960658	0.28046
5.20000	-0.8494274013	0.28089
5.30000	-0.8492930099	0.28126
5.40000	-0.8491865756	0.28157
5.50000	-0.8491027972	0.28184
5.60000	-0.8490372579	0.28206
5.70000	-0.8489863049	0.28224
5.80000	-0.8489469393	0.28238
5.90000	-0.8489167169	0.28250
6.00000	-0.8488936610	0.28260
6.10000	-0.8488761841	0.28268
6.20000	-0.8488630209	0.28274
6.30000	-0.8488531703	0.28279
6.40000	-0.8488458463	0.28282
6.50000	-0.8488404360	0.28285
6.60000	-0.8488364653	0.28288

H2 MOLECULE:	WAVEFUNCTION PSI 0	
R (BOHR)	ENERGY (HARTREES)	ZETA
6.70000	-0.8488335701	0.28289
6.80000	-0.8488314727	0.28291
6.90000	-0.8488299633	0.28292
7.00000	-0.8488288841	0.28292
7.20000	-0.8488275764	0.28293
7.40000	-0.8488269327	0.28294
7.60000	-0.8488266240	0.28294
7.80000	-0.8488264797	0.28294
8.00000	-0.8488264140	0.28294
8.20000	-0.8488263848	0.28294
8.40000	-0.8488263721	0.28294
8.60000	-0.8488263668	0.28294
8.80000	-0.8488263646	0.28294
9.00000	-0.8488263637	0.28294
9.20000	-0.8488263634	0.28294
9.40000	-0.8488263632	0.28294
9.60000	-0.8488263632	0.28294
9.80000	-0.8488263632	0.28294
10.00000	-0.8488263632	0.28294
18.00000	-0.8488263632	0.28294

TABLE A-2

H2 MOLECULE:	WAVEFUNCTION PSI 1		
R (BOHR)	ENERGY (HARTREES)	ZETA	ALPHA
0.10000	7.6976759700	0.76230	-0.15139238
0.20000	2.7181927048	0.74483	-0.13550278
0.30000	1.0835622664	0.71867	-0.11115652
0.40000	0.2912020375	0.68709	-0.08077986
0.50000	-0.1615659263	0.65307	-0.04676497
0.60000	-0.4437885952	0.61881	-0.01121116
0.70000	-0.6287969273	0.58570	0.02404200
0.80000	-0.7537047297	0.55434	0.05725002
0.90000	-0.8393098772	0.52481	0.08665005
1.00000	-0.8981282356	0.49692	0.11060236
1.05000	-0.9200956992	0.48352	0.12015613
1.10000	-0.9381090232	0.47044	0.12799782
1.15000	-0.9527583404	0.45769	0.13413597
1.20000	-0.9645353456	0.44528	0.13864199
1.25000	-0.9738533144	0.43322	0.14163554
1.30000	-0.9810622630	0.42154	0.14326888
1.35000	-0.9864605164	0.41027	0.14371763
1.40000	-0.9903036407	0.39941	0.14315715
1.45000	-0.9928114462	0.38900	0.14175945
1.50000	-0.9941735753	0.37903	0.13968421
1.51000	-0.9943233595	0.37709	0.13920452
1.52000	-0.9944351475	0.37517	0.13869318
1.53000	-0.9945101059	0.37326	0.13817064
1.54000	-0.9945493688	0.37138	0.13762925
1.55000	-0.9945540383	0.36952	0.13707322
1.60000	-0.9940949536	0.36047	0.13404884
1.65000	-0.9929196709	0.35187	0.13071786
1.70000	-0.9911354048	0.34372	0.12716848
1.75000	-0.9888354715	0.33601	0.12347440
1.80000	-0.9861011986	0.32873	0.11969473
1.85000	-0.9830035596	0.32187	0.11587798
1.90000	-0.9796045785	0.31542	0.11206231
1.95000	-0.9759585366	0.30935	0.10827848
2.00000	-0.9721130127	0.30367	0.10454935
2.05000	-0.9681097787	0.29835	0.10089207
2.10000	-0.9639855728	0.29338	0.09731959
2.15000	-0.9597727661	0.28876	0.09384075
2.20000	-0.9554999384	0.28447	0.09046124
2.25000	-0.9511923749	0.28050	0.08718415
2.30000	-0.9468724949	0.27684	0.08401045
2.35000	-0.9425602204	0.27348	0.08093945
2.40000	-0.9382732938	0.27041	0.07796925
2.45000	-0.9340275489	0.26763	0.07509663
2.50000	-0.9298371421	0.26513	0.07231771
2.55000	-0.9257147474	0.26290	0.06962797
2.60000	-0.9216717182	0.26093	0.06702250
2.65000	-0.9177182207	0.25922	0.06449606
2.70000	-0.9138633395	0.25777	0.06204338
2.75000	-0.9101151591	0.25655	0.05965924
2.80000	-0.9064808231	0.25557	0.05733842

H2 MOLECULE:

WAVEFUNCTION PSI 1

R (BOHR)	ENERGY (HARTREES)	ZETA	ALPHA
2.85000	-0.9029665736	0.25482	0.05507640
2.90000	-0.8995777741	0.25428	0.05286875
2.95000	-0.8963189182	0.25395	0.05071178
3.00000	-0.8931936288	0.25382	0.04860270
3.05000	-0.8902046517	0.25386	0.04653930
3.10000	-0.8873538488	0.25408	0.04452039
3.15000	-0.8846421953	0.25444	0.04254565
3.20000	-0.8820697857	0.25494	0.04061561
3.25000	-0.8796358526	0.25556	0.03873184
3.30000	-0.8773388013	0.25628	0.03689657
3.35000	-0.8751762604	0.25708	0.03511245
3.40000	-0.8731451482	0.25795	0.03338276
3.45000	-0.8712417540	0.25886	0.03171126
3.50000	-0.8694618289	0.25982	0.03010155
3.55000	-0.8678006834	0.26080	0.02855681
3.60000	-0.8662532868	0.26179	0.02708064
3.65000	-0.8648143648	0.26278	0.02567547
3.70000	-0.8634784911	0.26376	0.02434385
3.75000	-0.8622401705	0.26473	0.02308733
3.80000	-0.8610939120	0.26568	0.02190706
3.85000	-0.8600342905	0.26661	0.02080319
3.90000	-0.8590559978	0.26751	0.01977545
3.95000	-0.8581538818	0.26838	0.01882296
4.00000	-0.8573229769	0.26922	0.01794410
4.10000	-0.8558559875	0.27081	0.01639821
4.20000	-0.8546196483	0.27227	0.01511486
4.30000	-0.8535822262	0.27360	0.01406532
4.40000	-0.8527155478	0.27481	0.01321668
4.50000	-0.8519947709	0.27591	0.01253482
4.60000	-0.8513980986	0.27689	0.01198587
4.70000	-0.8509064849	0.27777	0.01153837
4.80000	-0.8505033557	0.27855	0.01116443
4.90000	-0.8501743539	0.27923	0.01084047
5.00000	-0.8499071077	0.27983	0.01054752
5.10000	-0.8496910188	0.28034	0.01027120
5.20000	-0.8495170656	0.28078	0.01000124
5.30000	-0.8493776201	0.28116	0.00973089
5.40000	-0.8492662767	0.28148	0.00945628
5.50000	-0.8491776929	0.28175	0.00917573
5.60000	-0.8491074436	0.28197	0.00888914
5.70000	-0.8490518873	0.28215	0.00859753
5.80000	-0.8490080471	0.28230	0.00830257
5.90000	-0.8489735049	0.28242	0.00800624
6.00000	-0.8489463086	0.28252	0.00771063
6.10000	-0.8489248917	0.28260	0.00741776
6.20000	-0.8489080045	0.28267	0.00712945
6.30000	-0.8488946562	0.28272	0.00684728
6.40000	-0.8488840649	0.28276	0.00657257
6.50000	-0.8488756174	0.28280	0.00630634
6.60000	-0.8488688350	0.28282	0.00604934

H2 MOLECULE:

WAVEFUNCTION PSI 1

R (BOHR)	ENERGY (HARTREES)	ZETA	ALPHA
6.70000	-0.8488633459	0.28284	0.00580210
6.80000	-0.8488588623	0.28286	0.00556492
6.90000	-0.8488551627	0.28287	0.00533792
7.00000	-0.8488520765	0.28288	0.00512107
7.20000	-0.8488472529	0.28290	0.00471717
7.40000	-0.8488436721	0.28291	0.00435106
7.60000	-0.8488409107	0.28291	0.00401983
7.80000	-0.8488387155	0.28292	0.00372026
8.00000	-0.8488369305	0.28292	0.00344911
8.20000	-0.8488354556	0.28292	0.00320337
8.40000	-0.8488342231	0.28293	0.00298026
8.60000	-0.8488331846	0.28293	0.00277732
8.80000	-0.8488323043	0.28293	0.00259235
9.00000	-0.8488315544	0.28293	0.00242343
9.20000	-0.8488309129	0.28293	0.00226885
9.40000	-0.8488303621	0.28294	0.00212714
9.60000	-0.8488298876	0.28294	0.00199699
9.80000	-0.8488294775	0.28294	0.00187724
10.00000	-0.8488291220	0.28294	0.00176687
18.00000	-0.8488264443	0.28294	0.00030301

H2 MOLECULE:

WAVEFUNCTION PSI 2

R (BOHR)	ENERGY (HARTREES)	ZETA	BETA	GAMMA
0.10000	7.6817573413	0.76521	-0.14641889	-0.15111877
0.20000	2.7024372622	0.74763	-0.13045100	-0.14861926
0.30000	1.0680671837	0.72131	-0.10600794	-0.14476609
0.40000	0.2760512151	0.68951	-0.07556118	-0.13991382
0.50000	-0.1763013556	0.65521	-0.04155918	-0.13440265
0.60000	-0.4580476226	0.62063	-0.00616637	-0.12850282
0.70000	-0.6425256528	0.58712	0.02871251	-0.12239859
0.80000	-0.7668546634	0.55531	0.06128164	-0.11619933
0.90000	-0.8518388538	0.52529	0.08977713	-0.10996825
1.00000	-0.9100040826	0.49689	0.11263627	-0.10375902
1.05000	-0.9316373163	0.48323	0.12161523	-0.10068386
1.10000	-0.9493140639	0.46992	0.12889237	-0.09764293
1.15000	-0.9636265780	0.45695	0.13449468	-0.09464829
1.20000	-0.9750685431	0.44434	0.13850460	-0.09171176
1.25000	-0.9840549828	0.43211	0.14105123	-0.08884448
1.30000	-0.9909373514	0.42028	0.14229431	-0.08605610
1.35000	-0.9960150777	0.40887	0.14240721	-0.08335410
1.40000	-0.9995445099	0.39790	0.14156588	-0.08074384
1.45000	-1.0017459540	0.38738	0.13993557	-0.07822823
1.50000	-1.0028093082	0.37733	0.13766103	-0.07580739
1.51000	-1.0029002564	0.37537	0.13714484	-0.07533506
1.52000	-1.0029535146	0.37344	0.13661477	-0.07486718
1.53000	-1.0029702490	0.37151	0.13605449	-0.07440153
1.54000	-1.0029515930	0.36962	0.13548926	-0.07394122
1.55000	-1.0028986476	0.36773	0.13489729	-0.07348331
1.60000	-1.0021560097	0.35861	0.13175454	-0.07125330
1.65000	-1.0007045566	0.34995	0.12833326	-0.06911471
1.70000	-0.9986512415	0.34175	0.12471941	-0.06706441
1.75000	-0.9960890709	0.33400	0.12098478	-0.06509891
1.80000	-0.9930990338	0.32666	0.11717527	-0.06321242
1.85000	-0.9897517525	0.31975	0.11334931	-0.06140251
1.90000	-0.9861088971	0.31326	0.10953748	-0.05966391
1.95000	-0.9822244026	0.30715	0.10577345	-0.05799314
2.00000	-0.9781455138	0.30143	0.10206711	-0.05638373
2.05000	-0.9739136871	0.29607	0.09844770	-0.05483380
2.10000	-0.9695653663	0.29106	0.09491860	-0.05333762
2.15000	-0.9651326531	0.28640	0.09149056	-0.05189172
2.20000	-0.9606438850	0.28207	0.08816757	-0.05049201
2.25000	-0.9561241342	0.27805	0.08495192	-0.04913469
2.30000	-0.9515956387	0.27436	0.08184597	-0.04781668
2.35000	-0.9470781732	0.27096	0.07884853	-0.04653461
2.40000	-0.9425893688	0.26786	0.07595381	-0.04528423
2.45000	-0.9381449867	0.26505	0.07316154	-0.04406341
2.50000	-0.9337591515	0.26252	0.07046569	-0.04286864
2.55000	-0.9294445486	0.26025	0.06786164	-0.04169722
2.60000	-0.9252125886	0.25827	0.06534402	-0.04054650
2.65000	-0.9210735414	0.25655	0.06290715	-0.03941408
2.70000	-0.9170366438	0.25507	0.06054513	-0.03829769
2.75000	-0.9131101803	0.25385	0.05825265	-0.03719539
2.80000	-0.9093015407	0.25288	0.05602262	-0.03610531

H2 MOLECULE:

WAVEFUNCTION PSI 2

R (BOHR)	ENERGY (HARTREES)	ZETA	BETA	GAMMA
2.85000	-0.9056172562	0.25214	0.05385103	-0.03502620
2.90000	-0.9020630158	0.25162	0.05173307	-0.03395709
2.95000	-0.8986436674	0.25131	0.04966208	-0.03289680
3.00000	-0.8953632047	0.25123	0.04763798	-0.03184589
3.05000	-0.8922247482	0.25132	0.04565380	-0.03080356
3.10000	-0.8892305223	0.25160	0.04371113	-0.02977124
3.15000	-0.8863818361	0.25204	0.04180795	-0.02874972
3.20000	-0.8836790734	0.25262	0.03994547	-0.02774067
3.25000	-0.8811216971	0.25332	0.03812271	-0.02674526
3.30000	-0.8787082716	0.25413	0.03634258	-0.02576568
3.35000	-0.8764365059	0.25504	0.03460735	-0.02480387
3.40000	-0.8743033174	0.25601	0.03292394	-0.02386299
3.45000	-0.8723049140	0.25704	0.03129129	-0.02294374
3.50000	-0.8704368909	0.25810	0.02971803	-0.02204941
3.55000	-0.8686943370	0.25919	0.02820359	-0.02118042
3.60000	-0.8670719459	0.26029	0.02675502	-0.02033923
3.65000	-0.8655641257	0.26138	0.02537592	-0.01952709
3.70000	-0.8641651025	0.26246	0.02406451	-0.01874349
3.75000	-0.8628690158	0.26353	0.02282902	-0.01799083
3.80000	-0.8616700015	0.26456	0.02166584	-0.01726778
3.85000	-0.8605622626	0.26557	0.02057785	-0.01657500
3.90000	-0.8595401268	0.26656	0.01956368	-0.01591178
3.95000	-0.8585980915	0.26750	0.01862578	-0.01527869
4.00000	-0.8577308573	0.26840	0.01775809	-0.01467353
4.10000	-0.8562007436	0.27011	0.01623567	-0.01354746
4.20000	-0.8549121444	0.27167	0.01497237	-0.01252555
4.30000	-0.8538314043	0.27309	0.01394089	-0.01160000
4.40000	-0.8529287425	0.27439	0.01310808	-0.01076200
4.50000	-0.8521779891	0.27554	0.01244099	-0.01000377
4.60000	-0.8515562589	0.27657	0.01190549	-0.00931715
4.70000	-0.8510436176	0.27749	0.01146936	-0.00869404
4.80000	-0.8506227691	0.27832	0.01110566	-0.00812826
4.90000	-0.8502787697	0.27902	0.01079067	-0.00761350
5.00000	-0.8499987720	0.27964	0.01050523	-0.00714363
5.10000	-0.8497717912	0.28019	0.01023551	-0.00671439
5.20000	-0.8495884922	0.28064	0.00997105	-0.00632080
5.30000	-0.8494409917	0.28104	0.00970534	-0.00595921
5.40000	-0.8493226757	0.28137	0.00943457	-0.00562611
5.50000	-0.8492280316	0.28165	0.00915736	-0.00531890
5.60000	-0.8491524939	0.28189	0.00887346	-0.00503447
5.70000	-0.8490923060	0.28207	0.00858421	-0.00477096
5.80000	-0.8490443954	0.28224	0.00829110	-0.00452603
5.90000	-0.8490062645	0.28237	0.00799637	-0.00429817
6.00000	-0.8489758944	0.28247	0.00770209	-0.00408573
6.10000	-0.8489516629	0.28256	0.00741036	-0.00388739
6.20000	-0.8489322733	0.28263	0.00712301	-0.00370191
6.30000	-0.8489166944	0.28268	0.00684177	-0.00352829
6.40000	-0.8489041105	0.28273	0.00656765	-0.00336535
6.50000	-0.8488938791	0.28277	0.00630201	-0.00321245
6.60000	-0.8488854966	0.28279	0.00604551	-0.00306872

H2 MOLECULE:

WAVEFUNCTION PSI 2

R (BOHR)	ENERGY (HARTREES)	ZETA	BETA	GAMMA
6.70000	-0.8488785693	0.28281	0.00579871	-0.00293350
6.80000	-0.8488727909	0.28283	0.00556191	-0.00280613
6.90000	-0.8488679235	0.28285	0.00533539	-0.00268613
7.00000	-0.8488637824	0.28287	0.00511870	-0.00257275
7.20000	-0.8488571397	0.28287	0.00471537	-0.00236462
7.40000	-0.8488520614	0.28289	0.00434952	-0.00217825
7.60000	-0.8488480607	0.28290	0.00401860	-0.00201101
7.80000	-0.8488448344	0.28290	0.00371923	-0.00186043
8.00000	-0.8488421878	0.28291	0.00344835	-0.00172455
8.20000	-0.8488399895	0.28291	0.00320275	-0.00160154
8.40000	-0.8488381470	0.28292	0.00297975	-0.00148995
8.60000	-0.8488365922	0.28293	0.00277684	-0.00138845
8.80000	-0.8488352730	0.28292	0.00259194	-0.00129598
9.00000	-0.8488341488	0.28292	0.00242314	-0.00121158
9.20000	-0.8488331869	0.28293	0.00226856	-0.00113428
9.40000	-0.8488323609	0.28293	0.00212690	-0.00106345
9.60000	-0.8488316493	0.28293	0.00199682	-0.00099841
9.80000	-0.8488310342	0.28294	0.00187706	-0.00093853
10.00000	-0.8488305011	0.28294	0.00176672	-0.00088336
18.00000	-0.8488264848	0.28295	0.00030300	-0.00015150

TABLE A-4

HE2+2 MOLECULAR ION: WAVEFUNCTION PSI 2

R (BOHR)	ENERGY (HARTREES)	ZETA	BETA	GAMMA
0.05000	68.7264608494	3.73389	-0.31776931	-0.34948823
0.10000	28.8376705409	3.64183	-0.22079096	-0.34309171
0.15000	15.6769256611	3.50547	-0.07348199	-0.33323108
0.20000	9.2294227057	3.34264	0.10746578	-0.32076930
0.25000	5.4804583311	3.16824	0.30422522	-0.30647203
0.30000	3.0843676906	2.99165	0.49838211	-0.29088237
0.35000	1.4605640203	2.81686	0.67059711	-0.27435403
0.40000	0.3170582347	2.64450	0.80245596	-0.25720178
0.45000	-0.5091700249	2.47496	0.88202751	-0.23985947
0.50000	-1.1166178276	2.31037	0.90887128	-0.22288080
0.55000	-1.5686503277	2.15413	0.89269880	-0.20677986
0.60000	-1.9079920476	2.00927	0.84723207	-0.19189042
0.65000	-2.1643847653	1.87755	0.78494509	-0.17834266
0.70000	-2.3589780668	1.75936	0.71507315	-0.16612154
0.75000	-2.5070480791	1.65424	0.64365239	-0.15512946
0.80000	-2.6197734193	1.56122	0.57434002	-0.14523681
0.85000	-2.7054322679	1.47917	0.50914120	-0.13630377
0.90000	-2.7702247143	1.40693	0.44904918	-0.12819919
0.95000	-2.8188454623	1.34341	0.39441165	-0.12080225
1.00000	-2.8548873795	1.28767	0.34520562	-0.11400750
1.05000	-2.8811289841	1.23888	0.30118678	-0.10772257
1.10000	-2.8997413917	1.19631	0.26199351	-0.10186722
1.15000	-2.9124387483	1.15939	0.22720673	-0.09637274
1.20000	-2.9205885440	1.12762	0.19638860	-0.09117965
1.25000	-2.9252930893	1.10061	0.16910547	-0.08623680
1.30000	-2.9274499582	1.07801	0.14494453	-0.08150027
1.35000	-2.9277968182	1.05958	0.12352203	-0.07693312
1.40000	-2.9269444177	1.04504	0.10448953	-0.07250531
1.45000	-2.9254003768	1.03419	0.08754238	-0.06819424
1.50000	-2.9235857110	1.02676	0.07241642	-0.06398525
1.55000	-2.9218456577	1.02250	0.05890933	-0.05987348
1.60000	-2.9204563114	1.02108	0.04686002	-0.05586272
1.65000	-2.9196287087	1.02214	0.03617271	-0.05196689
1.70000	-2.9195121284	1.02526	0.02679261	-0.04820644
1.75000	-2.9201982337	1.03002	0.01870335	-0.04460601
1.80000	-2.9217271066	1.03595	0.01190812	-0.04119030
1.85000	-2.9240953432	1.04270	0.00640764	-0.03797991
1.90000	-2.9272655212	1.04991	0.00218754	-0.03498949
1.95000	-2.9311758980	1.05730	-0.00079378	-0.03222693
2.00000	-2.9357492462	1.06467	-0.00261806	-0.02969231
2.05000	-2.9409001370	1.07186	-0.00340352	-0.02737957
2.10000	-2.9465404631	1.07874	-0.00329793	-0.02527839
2.15000	-2.9525833553	1.08524	-0.00247137	-0.02337513
2.20000	-2.9589458308	1.09128	-0.00110339	-0.02165462
2.25000	-2.9655505233	1.09685	0.00062833	-0.02010039
2.30000	-2.9723267785	1.10188	0.00256044	-0.01869622
2.35000	-2.9792112976	1.10640	0.00455173	-0.01742655
2.40000	-2.9861484345	1.11041	0.00648840	-0.01627666
2.45000	-2.9930902058	1.11390	0.00828510	-0.01523330
2.50000	-2.9999960593	1.11694	0.00988470	-0.01428415

HE2+2 MOLECULAR ION: WAVEFUNCTION PSI 2

R (BOHR)	ENERGY (HARTREES)	ZETA	BETA	GAMMA
2.55000	-3.0068324455	1.11955	0.01125391	-0.01341845
2.60000	-3.0135722464	1.12176	0.01237892	-0.01262685
2.65000	-3.0201941125	1.12362	0.01326187	-0.01190089
2.70000	-3.0266817594	1.12518	0.01391540	-0.01123331
2.75000	-3.0330232646	1.12647	0.01435899	-0.01061793
2.80000	-3.0392103953	1.12753	0.01461644	-0.01004926
2.85000	-3.0452379865	1.12839	0.01471337	-0.00952245
2.90000	-3.0511033839	1.12910	0.01467509	-0.00903337
2.95000	-3.0568059521	1.12966	0.01452574	-0.00857852
3.00000	-3.0623466518	1.13012	0.01428766	-0.00815459
3.05000	-3.0677276794	1.13047	0.01398069	-0.00775892
3.10000	-3.0729521661	1.13076	0.01362220	-0.00738895
3.15000	-3.0780239280	1.13099	0.01322700	-0.00704255
3.20000	-3.0829472633	1.13116	0.01280749	-0.00671775
3.25000	-3.0877267877	1.13130	0.01237381	-0.00641281
3.30000	-3.0923673039	1.13140	0.01193422	-0.00612623
3.35000	-3.0968736993	1.13148	0.01149518	-0.00585661
3.40000	-3.1012508670	1.13154	0.01106153	-0.00560259
3.45000	-3.1055036465	1.13159	0.01063709	-0.00536313
3.50000	-3.1096367792	1.13163	0.01022450	-0.00513715
3.60000	-3.1175624019	1.13167	0.00944155	-0.00472195
3.70000	-3.1250627497	1.13171	0.00872014	-0.00435030
3.80000	-3.1321701268	1.13172	0.00806120	-0.00401663
3.90000	-3.1389140710	1.13173	0.00746206	-0.00371620
4.00000	-3.1453214654	1.13174	0.00691822	-0.00344495
4.10000	-3.1514167303	1.13175	0.00642469	-0.00319946
4.20000	-3.1572220446	1.13175	0.00597638	-0.00297672
4.30000	-3.1627575681	1.13175	0.00556855	-0.00277417
4.40000	-3.1680416516	1.13176	0.00519689	-0.00258958
4.50000	-3.1730910274	1.13175	0.00485750	-0.00242098
4.60000	-3.1779209805	1.13175	0.00454704	-0.00226670
4.70000	-3.1825454996	1.13176	0.00426249	-0.00212525
4.80000	-3.1869774108	1.13176	0.00400121	-0.00199531
4.90000	-3.1912284955	1.13176	0.00376085	-0.00187575
5.00000	-3.1953095942	1.13176	0.00353939	-0.00176555
9.00000	-3.2841944632	1.13176	0.00060617	-0.00030297

TABLE A-5

LI2+4 MOLECULAR ION:

WAVEFUNCTION PSI 2

R (BOHR)	ENERGY (HARTREES)	ZETA	BETA	GAMMA
0.10000	63.7067904528	8.38735	0.16323396	-0.52169692
0.20000	20.5279063621	7.13323	1.59285179	-0.45219481
0.30000	7.6281333345	5.83273	2.36919228	-0.36736834
0.40000	2.1643846640	4.67078	2.06874188	-0.29054141
0.50000	-0.5346586579	3.81674	1.47422340	-0.23384018
0.60000	-2.0132300942	3.23354	0.96716646	-0.19295349
0.70000	-2.8892402203	2.83922	0.60019465	-0.16200232
0.80000	-3.4434439552	2.57593	0.34912743	-0.13701197
0.90000	-3.8177449292	2.41016	0.18095786	-0.11553836
1.00000	-4.0908390084	2.32306	0.06874473	-0.09613472
1.10000	-4.3093952182	2.30021	-0.00518287	-0.07821685
1.20000	-4.5008262525	2.32285	-0.04896545	-0.06211471
1.30000	-4.6787827651	2.36825	-0.06506048	-0.04861144
1.40000	-4.8477192783	2.41808	-0.05790661	-0.03807599
1.50000	-5.0075886387	2.46189	-0.03746918	-0.03021908
1.60000	-5.1570424753	2.49509	-0.01503462	-0.02443487
1.70000	-5.2949954009	2.51740	0.00239136	-0.02012697
1.80000	-5.4211507200	2.53102	0.01305749	-0.01684254
1.90000	-5.5359320722	2.53871	0.01815015	-0.01427501
2.00000	-5.6402027173	2.54277	0.01959999	-0.01222404
2.10000	-5.7350072843	2.54479	0.01904685	-0.01055717
2.20000	-5.8214045225	2.54573	0.01758700	-0.00918395
2.30000	-5.9003801603	2.54615	0.01584644	-0.00804035
2.40000	-5.9728120326	2.54633	0.01413375	-0.00707940
2.60000	-6.1009952478	2.54643	0.01120102	-0.00557197
2.80000	-6.2108777240	2.54645	0.00897280	-0.00446355
3.00000	-6.3061117383	2.54646	0.00729192	-0.00363042
3.20000	-6.3894425619	2.54647	0.00600565	-0.00299224
6.00000	-6.9727707234	2.54648	0.00090935	-0.00045443

TABLE A-6

BE2+6 MOLECULAR ION: WAVEFUNCTION PSI 2

R (BOHR)	ENERGY (HARTREES)	ZETA	BETA	GAMMA
0.10000	112.8256278529	14.63481	1.47666318	-0.68192331
0.20000	37.8037231151	11.40870	4.40428466	-0.53432272
0.30000	16.2439166320	8.43008	3.80429756	-0.38891868
0.40000	7.2419416098	6.46571	2.28013033	-0.29224928
0.40000	7.2419416098	6.46571	2.28013033	-0.29224928
0.50000	2.6580919616	5.30028	1.19134939	-0.22896547
0.60000	-0.0110858084	4.61295	0.53456899	-0.18283002
0.70000	-1.7373015833	4.23715	0.15794463	-0.14526636
0.80000	-2.9691340122	4.09462	-0.05296347	-0.11218769
0.90000	-3.9377969255	4.12100	-0.15595847	-0.08305819
1.00000	-4.7586884989	4.22936	-0.16914968	-0.05987160
1.10000	-5.4786376266	4.34544	-0.11873334	-0.04350511
1.20000	-6.1133123711	4.43233	-0.05350698	-0.03259570
1.30000	-6.6700760300	4.48365	-0.00715890	-0.02524664
1.40000	-7.1567572513	4.50921	0.01587611	-0.02008168
1.50000	-7.5825443459	4.52041	0.02363743	-0.01629365
1.60000	-7.9566319246	4.52480	0.02400995	-0.01342316
1.70000	-8.2872363607	4.52635	0.02167862	-0.01119589
1.80000	-8.5812727358	4.52685	0.01879168	-0.00943687
1.90000	-8.8444057294	4.52700	0.01612185	-0.00802795
2.00000	-9.0812384995	4.52703	0.01385295	-0.00688590
2.10000	-9.2955194800	4.52705	0.01196887	-0.00595037
2.20000	-9.4903216702	4.52706	0.01040650	-0.00517676
2.30000	-9.6681851712	4.52706	0.00910401	-0.00453154
2.40000	-9.8312271051	4.52707	0.00801007	-0.00398916
2.50000	-9.9812259540	4.52706	0.00708475	-0.00352994
4.50000	-11.5812219322	4.52708	0.00121252	-0.00060589

- B TABLES -

TABLE B-1

H2 MOLECULE: WAVEFUNCTION PSI 0

R (BOHR)	BINDING ENERGY	(V)	-V/2T	DE/DR
0.10000	8.5543102922	5.4238225587	-1.1885686959	-99.8714529941
0.20000	3.5732176239	0.4982250816	-0.1119020418	-24.7527871994
0.30000	1.9364956329	-1.0535055569	0.2460111019	-10.7628136541
0.40000	1.1421504080	-1.7422757024	0.4279514440	-5.8223094806
0.50000	0.6879524671	-2.0793882159	0.5419266863	-3.5152808476
0.60000	0.4050763510	-2.2414092653	0.6234243952	-2.2565154016
0.70000	0.2202016753	-2.3074117402	0.6872258566	-1.5002319494
0.80000	0.0960753692	-2.3184155129	0.7403934511	-1.0161419061
0.90000	0.0116762679	-2.2975987392	0.7866071665	-0.6925539430
1.00000	-0.0457605819	-2.2586889519	0.8279032435	-0.4695150619
1.05000	-0.0670436752	-2.2352079941	0.8470945539	-0.3842551594
1.10000	-0.0844084516	-2.2100584130	0.8654517414	-0.3123534395
1.15000	-0.0984627909	-2.1837969877	0.8830502033	-0.2514945040
1.20000	-0.1097109895	-2.1568726116	0.8999454015	-0.1998315886
1.25000	-0.1185739731	-2.1296275432	0.9161838281	-0.1558614965
1.30000	-0.1254050109	-2.1023435126	0.9317972216	-0.1183698188
1.35000	-0.1305020620	-2.0752306246	0.9468137876	-0.0863509440
1.40000	-0.1341175703	-2.0484626386	0.9612513739	-0.0589819798
1.45000	-0.1364663013	-2.0221703397	0.9751248330	-0.0355758695
1.50000	-0.1377316619	-1.9964578538	0.9884435055	-0.0155612024
1.51000	-0.1378689730	-1.9913990187	0.9910379813	-0.0119260572
1.52000	-0.1379704512	-1.9863374679	0.9936251521	-0.0083841048
1.53000	-0.1380372071	-1.9813303403	0.9961772479	-0.0049694117
1.54000	-0.1380703186	-1.9763652005	0.9987003947	-0.0016700241
1.55000	-0.1380708319	-1.9713994746	1.0012163078	0.0015451069
1.60000	-0.1376189585	-1.9470630849	1.0134432026	0.0161422240
1.65000	-0.1364926042	-1.9234886659	1.0251283264	0.0285753145
1.70000	-0.1347925975	-1.9007101231	1.0362710933	0.0391339990
1.75000	-0.1326063998	-1.8787571289	1.0468662171	0.0480619412
1.80000	-0.1300100818	-1.8576450945	1.0569110212	0.0555709974
1.85000	-0.1270699786	-1.8373887438	1.0663986934	0.0618399674
1.90000	-0.1238440839	-1.8179906061	1.0753266597	0.0670264673
1.95000	-0.1203832254	-1.7994637055	1.0836824947	0.0712592162
2.00000	-0.1167320623	-1.7818042439	1.0914630150	0.0746563035
2.05000	-0.1129299321	-1.7650207607	1.0986548245	0.0773130877
2.10000	-0.1090115717	-1.7491062639	1.1052548167	0.0793188599
2.15000	-0.1050077338	-1.7340669302	1.1112496529	0.0807447739
2.20000	-0.1009457131	-1.7199006241	1.1166321707	0.0816561493
2.25000	-0.0968497965	-1.7066080892	1.1213934014	0.0821085468
2.30000	-0.0927416484	-1.6941859239	1.1255285690	0.0821522170
2.35000	-0.0886406384	-1.6826325621	1.1290326951	0.0818304005
2.40000	-0.0845641215	-1.6719511670	1.1318983036	0.0811790843
2.45000	-0.0805276727	-1.6621391308	1.1341245491	0.0802322208
2.50000	-0.0765452849	-1.6531917454	1.1357145477	0.0790206203
2.55000	-0.0726295313	-1.6451053619	1.1366728202	0.0775711479
2.60000	-0.0687916969	-1.6378737656	1.1370085324	0.0759085978
2.65000	-0.0650418814	-1.6314916521	1.1367324665	0.0740546555
2.70000	-0.0613890782	-1.6259474006	1.1358633491	0.0720309193
2.75000	-0.0578412296	-1.6212225127	1.1344282066	0.0698591538
2.80000	-0.0544052646	-1.6172960172	1.1324581096	0.0675597280

H2 MOLECULE: WAVEFUNCTION PSI 0

R (BOHR)	BINDING ENERGY	(V)	-V/2T	DE/DR
2.85000	-0.0510871206	-1.6141503261	1.1299825425	0.0651496987
2.90000	-0.0478917551	-1.6117482870	1.1270491494	0.0626510171
2.95000	-0.0448231507	-1.6100538499	1.1237047076	0.0600831111
3.00000	-0.0418843196	-1.6090317760	1.1199947984	0.0574631965
3.05000	-0.0390773117	-1.6086264755	1.1159813969	0.0548134014
3.10000	-0.0364032312	-1.6087965717	1.1117122686	0.0521492313
3.15000	-0.0338622650	-1.6094806619	1.1072497958	0.0494909823
3.20000	-0.0314537253	-1.6106243209	1.1026473883	0.0468549550
3.25000	-0.0291761073	-1.6121709587	1.0979570661	0.0442566099
3.30000	-0.0270271600	-1.6140632509	1.0932281100	0.0417102410
3.35000	-0.0250039691	-1.6162438800	1.0885064564	0.0392288909
3.40000	-0.0231030485	-1.6186645598	1.0838277559	0.0368218422
3.45000	-0.0213204350	-1.6212758848	1.0792258705	0.0344978874
3.50000	-0.0196517852	-1.6240338887	1.0747280459	0.0322635451
3.55000	-0.0180924679	-1.6268929848	1.0703607332	0.0301252612
3.60000	-0.0166376516	-1.6298261376	1.0661348129	0.0280838589
3.65000	-0.0152823835	-1.6327935484	1.0620696186	0.0261435465
3.70000	-0.0140216589	-1.6357756436	1.0581687068	0.0243028109
3.75000	-0.0128504813	-1.6387501509	1.0544372953	0.0225609435
3.80000	-0.0117639119	-1.6416940062	1.0508809142	0.0209175116
3.85000	-0.0107571095	-1.6445933834	1.0474984844	0.0193697564
3.90000	-0.0098253621	-1.6474332246	1.0442899752	0.0179154426
3.95000	-0.0089641103	-1.6502085038	1.0412487100	0.0165499856
4.00000	-0.0081689641	-1.6529088451	1.0383721397	0.0152704523
4.10000	-0.0067603380	-1.6580602344	1.0330934079	0.0129544312
4.20000	-0.0055680677	-1.6628497653	1.0284116477	0.0109378801
4.30000	-0.0045637561	-1.6672615878	1.0242781890	0.0091903839
4.40000	-0.0037219352	-1.6712871302	1.0206472841	0.0076839697
4.50000	-0.0030198999	-1.6749357470	1.0174688048	0.0063903953
4.60000	-0.0024375099	-1.6782092165	1.0147038313	0.0052866369
4.70000	-0.0019569859	-1.6811240530	1.0123097934	0.0043494990
4.80000	-0.0015627098	-1.6836961343	1.0102495302	0.0035587524
4.90000	-0.0012410359	-1.6859501566	1.0084848273	0.0028948248
5.00000	-0.0009801108	-1.6879096926	1.0069819893	0.0023406511
5.10000	-0.0007697027	-1.6895957659	1.0057121245	0.0018816404
5.20000	-0.0006010382	-1.6910336520	1.0046465617	0.0015040674
5.30000	-0.0004666468	-1.6922543136	1.0037556328	0.0011946616
5.40000	-0.0003602124	-1.6932815959	1.0030159846	0.0009428806
5.50000	-0.0002764340	-1.6941372301	1.0024072180	0.0007397026
5.60000	-0.0002108948	-1.6948444131	1.0019094795	0.0005768041
5.70000	-0.0001599418	-1.6954228502	1.0015061730	0.0004473263
5.80000	-0.0001205761	-1.6958981078	1.0011782088	0.0003440984
5.90000	-0.0000903538	-1.6962783754	1.0009175884	0.0002635692
6.00000	-0.0000672979	-1.6965845555	1.0007094370	0.0002004611
6.10000	-0.0000498209	-1.6968303516	1.0005436712	0.0001511503
6.20000	-0.0000366577	-1.6970226516	1.0004146567	0.0001134500
6.30000	-0.0000268071	-1.6971716685	1.0003151364	0.0000848686
6.40000	-0.0000194831	-1.6972891852	1.0002372034	0.0000628918
6.50000	-0.0000140728	-1.6973793579	1.0001776666	0.0000463868
6.60000	-0.0000101021	-1.6974488178	1.0001320466	0.0000339565

H2 MOLECULE: WAVEFUNCTION PSI 0

R (BOHR)	BINDING ENERGY	(V)	-V/2T	DE/DR
6.70000	-0.0000072069	-1.6975034245	1.0000964542	0.0000244352
6.80000	-0.0000051096	-1.6975432799	1.0000704984	0.0000175979
6.90000	-0.0000036002	-1.6975712714	1.0000522275	0.0000128486
7.00000	-0.0000025209	-1.6975934518	1.0000378882	0.0000091881
7.20000	-0.0000012132	-1.6976238599	1.0000184336	0.0000043462
7.40000	-0.0000005695	-1.6976364644	1.0000102502	0.0000023515
7.60000	-0.0000002608	-1.6976441452	1.0000053620	0.0000011977
7.80000	-0.0000001165	-1.6976479024	1.0000029789	0.0000006483
8.00000	-0.0000000508	-1.6976500133	1.0000016580	0.0000003518
8.20000	-0.0000000216	-1.6976509118	1.0000010943	0.0000002266
8.40000	-0.0000000090	-1.6976537178	0.9999994265	-0.0000001159
8.60000	-0.0000000036	-1.6976537197	0.9999994191	-0.0000001147
8.80000	-0.0000000014	-1.6976537205	0.9999994161	-0.0000001126
9.00000	-0.0000000006	-1.6976537208	0.9999994149	-0.0000001104
9.20000	-0.0000000002	-1.6976537209	0.9999994144	-0.0000001081
9.40000	-0.0000000001	-1.6976537209	0.9999994142	-0.0000001058
9.60000	-0.0000000000	-1.6976537209	0.9999994142	-0.0000001036
9.80000	-0.0000000000	-1.6976537209	0.9999994141	-0.0000001015
10.00000	-0.0000000000	-1.6976537209	0.9999994141	-0.0000000995
18.00000	0.0000000000	-1.6976537209	0.9999994141	-0.0000000553

TABLE B2

H2 MOLECULE: WAVEFUNCTION PSI 1

R (BOHR)	BINDING ENERGY	(V)	-V/2T	DE/DR
0.10000	8.5465023331	5.4093842040	-1.1819699490	-99.8596773597
0.20000	3.5670190679	0.4897305009	-0.1098808183	-24.7332745431
0.30000	1.9323886295	-1.0553284878	0.2466999508	-10.7415100685
0.40000	1.1400284007	-1.7394629683	0.4282988487	-5.8046676083
0.50000	0.6872604369	-2.0754754150	0.5422083508	-3.5046871249
0.60000	0.4050377680	-2.2400075052	0.6235341062	-2.2540505247
0.70000	0.2200294358	-2.3111829135	0.6868765350	-1.5051272269
0.80000	0.0951216335	-2.3286045561	0.7392865619	-1.0264938709
0.90000	0.0095164859	-2.3139312428	0.7845848761	-0.7059016538
1.00000	-0.0493018724	-2.2796737652	0.8250447475	-0.4834172940
1.05000	-0.0712693361	-2.2577276055	0.8439270905	-0.3976535305
1.10000	-0.0892826600	-2.2335413206	0.8620833852	-0.3248393402
1.15000	-0.1039319772	-2.2076969702	0.8796035590	-0.2627654691
1.20000	-0.1157089824	-2.1806934177	0.8965501556	-0.2096856055
1.25000	-0.1250269512	-2.1529519223	0.9129651701	-0.1641962348
1.30000	-0.1322358999	-2.1248241038	0.9288752378	-0.1251535214
1.35000	-0.1376341533	-2.0966167886	0.9442890344	-0.0916264857
1.40000	-0.1414772775	-2.0685703233	0.9592109061	-0.0628307442
1.45000	-0.1439850830	-2.0408852234	0.9736362400	-0.0381119524
1.50000	-0.1453472121	-2.0137231165	0.9875553051	-0.0169173107
1.51000	-0.1454969963	-2.0083782964	0.9902709524	-0.0130672698
1.52000	-0.1456087843	-2.0030207359	0.9929850073	-0.0093095007
1.53000	-0.1456837428	-1.9977189628	0.9956645364	-0.0056854582
1.54000	-0.1457230056	-1.9924436356	0.9983240218	-0.0021720117
1.55000	-0.1457276751	-1.9872073138	1.0009574152	0.0012262985
1.60000	-0.1452685905	-1.9614270489	1.0138333353	0.0167267865
1.65000	-0.1440933078	-1.9364567569	1.0261688627	0.0299288394
1.70000	-0.1423090416	-1.9123455160	1.0379529560	0.0411325256
1.75000	-0.1400091084	-1.8891304895	1.0491730221	0.0505945449
1.80000	-0.1372748354	-1.8668313857	1.0598202565	0.0585394508
1.85000	-0.1341771965	-1.8454631328	1.0698838474	0.0651589116
1.90000	-0.1307782153	-1.8250311258	1.0793552270	0.0706200164
1.95000	-0.1271321735	-1.8055416158	1.0882223017	0.0750643372
2.00000	-0.1232866495	-1.7869911436	1.0964775442	0.0786174409
2.05000	-0.1192834155	-1.7693725865	1.1041150103	0.0813887663
2.10000	-0.1151592096	-1.7526821331	1.1111257620	0.0834709583
2.15000	-0.1109464029	-1.7369127253	1.1175031632	0.0849454916
2.20000	-0.1066735752	-1.7220577544	1.1232406209	0.0858827829
2.25000	-0.1023660117	-1.7081099642	1.1283328518	0.0863443491
2.30000	-0.0980461317	-1.6950622219	1.1327756588	0.0863838121
2.35000	-0.0937338572	-1.6829072576	1.1365664837	0.0860481630
2.40000	-0.0894469306	-1.6716436071	1.1396995329	0.0853762418
2.45000	-0.0852011857	-1.6612608912	1.1421787167	0.0844057986
2.50000	-0.0810107790	-1.6517553438	1.1440045007	0.0831675762
2.55000	-0.0768883842	-1.6431189995	1.1451834825	0.0816903903
2.60000	-0.0728453550	-1.6353512617	1.1457181844	0.0799969903
2.65000	-0.0688918576	-1.6284400632	1.1456240443	0.0781118408
2.70000	-0.0650369764	-1.6223767089	1.1449160871	0.0760555445
2.75000	-0.0612887960	-1.6171485961	1.1436153593	0.0738478990
2.80000	-0.0576544599	-1.6127480464	1.1417406848	0.0715048571

H2 MOLECULE: WAVEFUNCTION PSI 1

R (BOHR)	BINDING ENERGY	(V)	-V/2T	DE/DR
2.85000	-0.0541402104	-1.6091480371	1.1393304132	0.0690474071
2.90000	-0.0507514109	-1.6063330814	1.1364138796	0.0664905058
2.95000	-0.0474925550	-1.6042751730	1.1330326995	0.0638517503
3.00000	-0.0443672656	-1.6029372072	1.1292368511	0.0611500168
3.05000	-0.0413782885	-1.6022829535	1.1250749738	0.0584020819
3.10000	-0.0385274857	-1.6022674438	1.1206021644	0.0556258883
3.15000	-0.0358158322	-1.6028408471	1.1158757004	0.0528392202
3.20000	-0.0332434225	-1.6039506835	1.1109524358	0.0500590275
3.25000	-0.0308094895	-1.6055370921	1.1058922377	0.0473029579
3.30000	-0.0285124382	-1.6075399155	1.1007514808	0.0445871779
3.35000	-0.0263498972	-1.6099022385	1.0955800437	0.0419254574
3.40000	-0.0243187850	-1.6125635051	1.0904270161	0.0393314092
3.45000	-0.0224153909	-1.6154617921	1.0853388174	0.0368178887
3.50000	-0.0206354658	-1.6185421990	1.0803528324	0.0343947025
3.55000	-0.0189743202	-1.6217601693	1.0754955668	0.0320679429
3.60000	-0.0174269236	-1.6250626956	1.0707976711	0.0298455216
3.65000	-0.0159880017	-1.6284162836	1.0662730433	0.0277294373
3.70000	-0.0146521280	-1.6317804988	1.0619394994	0.0257233739
3.75000	-0.0134138074	-1.6351280086	1.0578042040	0.0238272887
3.80000	-0.0122675488	-1.6384312107	1.0538740476	0.0220412140
3.85000	-0.0112079274	-1.6416746476	1.0501470611	0.0203620606
3.90000	-0.0102296346	-1.6448411188	1.0466227183	0.0187874043
3.95000	-0.0093275186	-1.6479164504	1.0432986545	0.0173142565
4.00000	-0.0084966138	-1.6508926800	1.0401686668	0.0159383185
4.10000	-0.0070296244	-1.6565218669	1.0344651306	0.0134610020
4.20000	-0.0057932851	-1.6617008152	1.0294508677	0.0113186860
4.30000	-0.0047558630	-1.6664151542	1.0250662201	0.0094765810
4.40000	-0.0038891847	-1.6706786159	1.0212433062	0.0078982909
4.50000	-0.0031684078	-1.6744982539	1.0179277588	0.0065536196
4.60000	-0.0025717355	-1.6779004316	1.0150609168	0.0054121230
4.70000	-0.0020801218	-1.6809084196	1.0125930732	0.0044477766
4.80000	-0.0016769925	-1.6835430626	1.0104818826	0.0036382602
4.90000	-0.0013479907	-1.6858327701	1.0086853296	0.0029624362
5.00000	-0.0010807445	-1.6878114163	1.0071623925	0.0024005598
5.10000	-0.0008646557	-1.6895071988	1.0058791668	0.0019362429
5.20000	-0.0006907025	-1.6909470326	1.0048055685	0.0015552113
5.30000	-0.0005512570	-1.6921622562	1.0039114287	0.0012439593
5.40000	-0.0004399135	-1.6931790967	1.0031718067	0.0009913809
5.50000	-0.0003513298	-1.6940228982	1.0025640719	0.0007877250
5.60000	-0.0002810804	-1.6947243033	1.0020639276	0.0006233186
5.70000	-0.0002255241	-1.6952975217	1.0016580604	0.0004923250
5.80000	-0.0001816839	-1.6957647296	1.0013294046	0.0003881663
5.90000	-0.0001471418	-1.6961435795	1.0010643850	0.0003056662
6.00000	-0.0001199454	-1.6964491404	1.0008516059	0.0002405795
6.10000	-0.0000985285	-1.6966919043	1.0006828993	0.0001898162
6.20000	-0.0000816414	-1.6968870741	1.0005477346	0.0001498282
6.30000	-0.0000682930	-1.6970434249	1.0004397150	0.0001183948
6.40000	-0.0000577017	-1.6971654670	1.0003552257	0.0000941660
6.50000	-0.0000492542	-1.6972600473	1.0002894840	0.0000755673
6.60000	-0.0000424718	-1.6973355597	1.0002369629	0.0000609258

H2 MOLECULE: WAVEFUNCTION PSI 1

R (BOHR)	BINDING ENERGY		(V)	-V/2T	DE/DR
6.70000	-0.0000369827	-1.6973962227	1.0001947296	0.0000493237	
6.80000	-0.0000324992	-1.6974425497	1.0001621378	0.0000404669	
6.90000	-0.0000287995	-1.6974787951	1.0001364152	0.0000335551	
7.00000	-0.0000257133	-1.6975070452	1.0001161295	0.0000281583	
7.20000	-0.0000208897	-1.6975457395	1.0000876437	0.0000206620	
7.40000	-0.0000173090	-1.6975728881	1.0000674280	0.0000154670	
7.60000	-0.0000145476	-1.6975898640	1.0000541724	0.0000120997	
7.80000	-0.0000123523	-1.6975996323	1.0000458307	0.0000099742	
8.00000	-0.0000105674	-1.6976084903	1.0000385090	0.0000081713	
8.20000	-0.0000090925	-1.6976148496	1.0000330249	0.0000068368	
8.40000	-0.0000078599	-1.6976219148	1.0000274105	0.0000055395	
8.60000	-0.0000068215	-1.6976262912	1.0000236088	0.0000046602	
8.80000	-0.0000059412	-1.6976277169	1.0000217318	0.0000041922	
9.00000	-0.0000051912	-1.6976330898	1.0000176832	0.0000033354	
9.20000	-0.0000045497	-1.6976357928	1.0000153351	0.0000028297	
9.40000	-0.0000039989	-1.6976376645	1.0000135836	0.0000024532	
9.60000	-0.0000035244	-1.6976397605	1.0000117898	0.0000020849	
9.80000	-0.0000031143	-1.6976414884	1.0000102888	0.0000017823	
10.00000	-0.0000027588	-1.6976427657	1.0000091176	0.0000015478	
18.00000	-0.0000000811	-1.6976510413	1.0000010881	0.0000001026	

TABLE B-3

H2 MOLECULE: WAVEFUNCTION PSI 2

R (BOHR)	BINDING ENERGY (V)		-V/2T	DE/DR
0.10000	8.5305837044	5.3776559295	-1.1669746614	-99.8585875303
0.20000	3.5512636254	0.4586456976	-0.1022032761	-24.7311441343
0.30000	1.9168935469	-1.0854068554	0.2520129882	-10.7384707429
0.40000	1.1248775782	-1.7682376347	0.4324823361	-5.8008501621
0.50000	0.6725250075	-2.1027112653	0.5457590450	-3.5002171081
0.60000	0.3907787406	-2.2654977300	0.6267110004	-2.2490041414
0.70000	0.2063007103	-2.3347528823	0.6898461512	-1.4995736809
0.80000	0.0819716997	-2.3500947779	0.7421788889	-1.0204818139
0.90000	-0.0030124907	-2.3332370569	0.7875117751	-0.6995103880
1.00000	-0.0611777194	-2.2967800693	0.8281006057	-0.4767719042
1.05000	-0.0828109531	-2.2737581746	0.8470765358	-0.3909367067
1.10000	-0.1004877007	-2.2485348310	0.8653397821	-0.3180970029
1.15000	-0.1148002148	-2.2217020035	0.8829764728	-0.2560424761
1.20000	-0.1262421799	-2.1937560316	0.9000486393	-0.2030157879
1.25000	-0.1352286197	-2.1651213210	0.9165959824	-0.1576090843
1.30000	-0.1421109882	-2.1361574559	0.9326405673	-0.1186790408
1.35000	-0.1471887145	-2.1071610550	0.9481927209	-0.0852821478
1.40000	-0.1507181467	-2.0783772272	0.9632527795	-0.0566344339
1.45000	-0.1529195908	-2.0499942676	0.9778190153	-0.0320705929
1.50000	-0.1539829451	-2.0221343398	0.9918986963	-0.0110104823
1.51000	-0.1540738933	-2.0166484854	0.9946495726	-0.0071840878
1.52000	-0.1541271515	-2.0112082975	0.9973710671	-0.0034876765
1.53000	-0.1541438858	-2.0057527183	1.0000936294	0.0001227319
1.54000	-0.1541252298	-2.0003696274	1.0027739415	0.0035932198
1.55000	-0.1540722845	-1.9949772803	1.0054532043	0.0069806548
1.60000	-0.1533296465	-1.9685850598	1.0184840054	0.0223293498
1.65000	-0.1518781934	-1.9430215977	1.0309808233	0.0353863730
1.70000	-0.1498248784	-1.9183402730	1.0429287549	0.0464483589
1.75000	-0.1472627077	-1.8945848086	1.0543092911	0.0557676189
1.80000	-0.1442726707	-1.8717188586	1.0651471807	0.0635995606
1.85000	-0.1409253893	-1.8498203776	1.0753911511	0.0700989878
1.90000	-0.1372825340	-1.8288640703	1.0850506342	0.0754493283
1.95000	-0.1333980394	-1.8088899111	1.0940881726	0.0797737918
2.00000	-0.1293191506	-1.7898049500	1.1025590723	0.0832430388
2.05000	-0.1250873239	-1.7717101545	1.1103772873	0.0859108389
2.10000	-0.1207390032	-1.7545273606	1.1175874586	0.0879063677
2.15000	-0.1163062900	-1.7382756666	1.1241617891	0.0892975068
2.20000	-0.1118175219	-1.7229357534	1.1301024089	0.0901600076
2.25000	-0.1072977710	-1.7084934883	1.1354087450	0.0905576800
2.30000	-0.1027692755	-1.6949764247	1.1400458934	0.0905281968
2.35000	-0.0982518100	-1.6823946631	1.1439935634	0.0901113545
2.40000	-0.0937630057	-1.6706534992	1.1473257845	0.0893855160
2.45000	-0.0893186236	-1.6598487407	1.1499515774	0.0883433603
2.50000	-0.0849327884	-1.6499194716	1.1519204746	0.0870395326
2.55000	-0.0806181855	-1.6408751815	1.1532221876	0.0854956532
2.60000	-0.0763862254	-1.6327045923	1.1538678768	0.0837386865
2.65000	-0.0722471782	-1.6254191482	1.1538505617	0.0817841262
2.70000	-0.0682102806	-1.6190078815	1.1531867650	0.0796538541
2.75000	-0.0642838171	-1.6134284788	1.1519251191	0.0773788661
2.80000	-0.0604751775	-1.6087571357	1.1500066245	0.0749449806

H2 MOLECULE: WAVEFUNCTION PSI 2

R (BOHR)	BINDING ENERGY	(V)	-V/2T	DE/DR
2.85000	-0.0567908930	-1.6048966183	1.1475360958	0.0723992610
2.90000	-0.0532366527	-1.6018344555	1.1445411778	0.0697557159
2.95000	-0.0498173042	-1.5996229221	1.1409916280	0.0670048856
3.00000	-0.0465368415	-1.5981166373	1.1370393676	0.0642032573
3.05000	-0.0433983850	-1.5974002261	1.1326260456	0.0613276296
3.10000	-0.0404041591	-1.5973347437	1.1278952274	0.0584278390
3.15000	-0.0375554729	-1.5979030220	1.1228780348	0.0555113175
3.20000	-0.0348527102	-1.5990272182	1.1176566471	0.0526034151
3.25000	-0.0322953339	-1.6006952367	1.1122527084	0.0497071253
3.30000	-0.0298819084	-1.6028241379	1.1067456276	0.0468461834
3.35000	-0.0276101427	-1.6053602876	1.1011852870	0.0440336490
3.40000	-0.0254769543	-1.6081686792	1.0956837337	0.0413052811
3.45000	-0.0234785509	-1.6112838799	1.0902095691	0.0386452024
3.50000	-0.0216105277	-1.6145532868	1.0848795267	0.0360915700
3.55000	-0.0198679738	-1.6180100458	1.0796584315	0.0336277826
3.60000	-0.0182455828	-1.6215372751	1.0746267671	0.0312796158
3.65000	-0.0167377625	-1.6250824769	1.0698111995	0.0290536368
3.70000	-0.0153387393	-1.6286990967	1.0651580629	0.0269273265
3.75000	-0.0140426526	-1.6322275389	1.0607717272	0.0249361314
3.80000	-0.0128436383	-1.6357457324	1.0565799101	0.0230511238
3.85000	-0.0117358995	-1.6391852880	1.0526180414	0.0212829188
3.90000	-0.0107137637	-1.6425602503	1.0488620924	0.0196205137
3.95000	-0.0097717284	-1.6457807747	1.0453613944	0.0180798502
4.00000	-0.0089044941	-1.6489531773	1.0420289820	0.0166271343
4.10000	-0.0073743804	-1.6548503546	1.0360302765	0.0140368616
4.20000	-0.0060857813	-1.6602806891	1.0307583405	0.0117960952
4.30000	-0.0050050411	-1.6652081862	1.0261620885	0.0098731680
4.40000	-0.0041023793	-1.6696760044	1.0221497409	0.0082230638
4.50000	-0.0033516260	-1.6736458440	1.0186922313	0.0068244743
4.60000	-0.0027298957	-1.6771510702	1.0157228747	0.0056437929
4.70000	-0.0022172545	-1.6802909007	1.0131422405	0.0046375180
4.80000	-0.0017964059	-1.6830141538	1.0109512092	0.0037982051
4.90000	-0.0014524066	-1.6853561429	1.0091017893	0.0031023258
5.00000	-0.0011724088	-1.6874224528	1.0075082013	0.0025150182
5.10000	-0.0009454281	-1.6891394126	1.0061976240	0.0020400333
5.20000	-0.0007621291	-1.6906267317	1.0050831534	0.0016442794
5.30000	-0.0006146286	-1.6918824922	1.0041542892	0.0013206587
5.40000	-0.0004963126	-1.6929574005	1.0033710981	0.0010533242
5.50000	-0.0004016684	-1.6938017202	1.0027554392	0.0008462442
5.60000	-0.0003261308	-1.6945457666	1.0022233565	0.0006712895
5.70000	-0.0002659429	-1.6951201929	1.0018110627	0.0005376174
5.80000	-0.0002180323	-1.6956240553	1.0014557021	0.0004249544
5.90000	-0.0001799013	-1.6960190971	1.0011767424	0.0003378698
6.00000	-0.0001495312	-1.6963439760	1.0009487098	0.0002679688
6.10000	-0.0001252998	-1.6965983330	1.0007697741	0.0002139333
6.20000	-0.0001059101	-1.6968042126	1.0006252914	0.0001710216
6.30000	-0.0000903313	-1.6969434865	1.0005246900	0.0001412543
6.40000	-0.0000777473	-1.6970972297	1.0004191211	0.0001110924
6.50000	-0.0000675160	-1.6971997520	1.0003465768	0.0000904625
6.60000	-0.0000591334	-1.6972863588	1.0002856163	0.0000734294

H2 MOLECULE: WAVEFUNCTION PSI 2

R (BOHR)	BINDING ENERGY	(V)	-V/2T	DE/DR
6.70000	-0.0000522061	-1.6973503150	1.0002397390	0.0000607199
6.80000	-0.0000464277	-1.6974016913	1.0002026392	0.0000505721
6.90000	-0.0000415603	-1.6974099069	1.0001920588	0.0000472377
7.00000	-0.0000374192	-1.6974733798	1.0001497656	0.0000363121
7.20000	-0.0000307765	-1.6974934679	1.0001300978	0.0000306683
7.40000	-0.0000256983	-1.6975546983	1.0000880311	0.0000201925
7.60000	-0.0000216975	-1.6975712419	1.0000735690	0.0000164315
7.80000	-0.0000184713	-1.6975913750	1.0000579053	0.0000126018
8.00000	-0.0000158246	-1.6975754920	1.0000641447	0.0000136104
8.20000	-0.0000136263	-1.6975843560	1.0000563320	0.0000116613
8.40000	-0.0000117838	-1.6975923871	1.0000494294	0.0000099889
8.60000	-0.0000102290	-1.6976240799	1.0000289262	0.0000057098
8.80000	-0.0000089099	-1.6976333170	1.0000219304	0.0000042306
9.00000	-0.0000077856	-1.6976083895	1.0000352909	0.0000066565
9.20000	-0.0000068237	-1.6976409626	1.0000149687	0.0000027621
9.40000	-0.0000059977	-1.6976397242	1.0000147251	0.0000026593
9.60000	-0.0000052861	-1.6976222360	1.0000241889	0.0000042774
9.80000	-0.0000046711	-1.6976452751	1.0000098923	0.0000017136
10.00000	-0.0000041379	-1.6976451816	1.0000093192	0.0000015821
18.00000	-0.0000001217	-1.6976630224	0.9999940785	-0.0000005585

TABLE B-4

HE2+2 MOLECULAR ION: WAVEFUNCTION PSI 2

R (BOHR)	BINDING ENERGY	(V)	-V/2T	DE/DR
0.05000	72.1217663022	57.5291928976	-2.5688941778*****	
0.10000	32.2329759936	17.9637775995	-0.8260048952-397.1156348234	
0.15000	19.0722311139	5.2825067371	-0.2541030324-173.8089639014	
0.20000	12.6247281584	-0.5915365774	0.0301160284	-95.2519099439
0.25000	8.8757637839	-3.7260828452	0.2023606246	-58.7479980299
0.30000	6.4796731434	-5.5024310120	0.3204006058	-38.9038879777
0.35000	4.8558694731	-6.5204528408	0.4084976234	-26.9759453755
0.40000	3.7123636874	-7.0812812669	0.4785723381	-19.2884943406
0.45000	2.8861354278	-7.3543443175	0.5371918963	-14.0800094837
0.50000	2.2786876251	-7.4455719748	0.5882150354	-10.4246726390
0.55000	1.8266551250	-7.4254519074	0.6339169772	-7.7966386401
0.60000	1.4873134051	-7.3408273528	0.6755981859	-5.8747387627
0.65000	1.2309206874	-7.2216391147	0.7139881263	-4.4505685909
0.70000	1.0363273859	-7.0864132450	0.7494987216	-3.3835101592
0.75000	0.8882573737	-6.9462138836	0.7823782879	-2.5761569673
0.80000	0.7755320334	-6.8076846390	0.8127780511	-1.9601722505
0.85000	0.6898731848	-6.6745265252	0.8408122978	-1.4866611641
0.90000	0.6250807384	-6.5489470577	0.8665557380	-1.1205529211
0.95000	0.5764599905	-6.4320440891	0.8900761837	-0.8361612259
1.00000	0.5404180733	-6.3244685690	0.9114167134	-0.6146938101
1.05000	0.5141764687	-6.2265238210	0.9306112020	-0.4421579551
1.10000	0.4955640610	-6.1383154450	0.9476879861	-0.3080296923
1.15000	0.4828667044	-6.0599459536	0.9626579954	-0.2044073539
1.20000	0.4747169087	-5.9914765720	0.9755283353	-0.1252495700
1.25000	0.4700123634	-5.9329925049	0.9863007710	-0.0659250610
1.30000	0.4678554945	-5.8845676690	0.9949836707	-0.0228213481
1.35000	0.4675086345	-5.8462820216	1.0015952822	0.0068974924
1.40000	0.4683610350	-5.8181935089	1.0061729940	0.0254966618
1.45000	0.4699050759	-5.8002394204	1.0087937677	0.0348698850
1.50000	0.4717197418	-5.7923116365	1.0095616986	0.0365731903
1.55000	0.4734597951	-5.7939147485	1.0086656284	0.0321139141
1.60000	0.4748491413	-5.8044991643	1.0063129191	0.0227584116
1.65000	0.4756767441	-5.8230371637	1.0027933124	0.0098304567
1.70000	0.4757933243	-5.8483581902	0.9984065510	-0.0054905490
1.75000	0.4751072190	-5.8790739864	0.9934641529	-0.0221014394
1.80000	0.4735783461	-5.9137221617	0.9882573421	-0.0390377492
1.85000	0.4712101095	-5.9509515703	0.9830251462	-0.0555464238
1.90000	0.4680399315	-5.9895250776	0.9779584270	-0.0710494922
1.95000	0.4641295547	-6.0283298433	0.9732047470	-0.0851169473
2.00000	0.4595562066	-6.0665554283	0.9688487686	-0.0975284680
2.05000	0.4544053157	-6.1036100211	0.9649335925	-0.1081998766
2.10000	0.4487649897	-6.1390172236	0.9614818970	-0.1171125226
2.15000	0.4427220974	-6.1724675516	0.9584921655	-0.1243259725
2.20000	0.4363596219	-6.2037053644	0.9559576450	-0.1299153195
2.25000	0.4297549294	-6.2326622816	0.9538489563	-0.1340272155
2.30000	0.4229786742	-6.2592995421	0.9521374213	-0.1368026022
2.35000	0.4160941551	-6.2836300310	0.9507920360	-0.1383861429
2.40000	0.4091570183	-6.3057531839	0.9497746961	-0.1389401312
2.45000	0.4022152469	-6.3257395542	0.9490556751	-0.1385955684
2.50000	0.3953093934	-6.3437912796	0.9485914749	-0.1375196644

HE2+2 MOLECULAR ION:

WAVEFUNCTION PSI 2

R (BOHR)	BINDING ENERGY	(V)	-V/2T	DE/DR
2.55000	0.3884730072	-6.3600733845	0.9483472110	-0.1358464680
2.60000	0.3817332063	-6.3747032828	0.9482973460	-0.1336764576
2.65000	0.3751113403	-6.3879044963	0.9484046679	-0.1311382156
2.70000	0.3686236934	-6.3998531307	0.9486403782	-0.1283294859
2.75000	0.3622821881	-6.4106557683	0.9489865699	-0.1253124506
2.80000	0.3560950575	-6.4204561714	0.9494216919	-0.1221554932
2.85000	0.3500674662	-6.4294325900	0.9499206375	-0.1189321463
2.90000	0.3442020688	-6.4376866032	0.9504692763	-0.1156827018
2.95000	0.3384995006	-6.4452645436	0.9510614295	-0.1124246235
3.00000	0.3329588009	-6.4523288384	0.9516759209	-0.1092118449
3.05000	0.3275777733	-6.4588771238	0.9523138437	-0.1060399229
3.10000	0.3223532867	-6.4650366699	0.9529592589	-0.1029459154
3.15000	0.3172815247	-6.4708337748	0.9536098495	-0.0999320377
3.20000	0.3123581894	-6.4763229965	0.9542596379	-0.0970088968
3.25000	0.3075786650	-6.4815627154	0.9549021894	-0.0941874277
3.30000	0.3029381488	-6.4865395415	0.9555407162	-0.0914560405
3.35000	0.2984317535	-6.4912804359	0.9561730428	-0.0888158321
3.40000	0.2940545857	-6.4958761618	0.9567883931	-0.0862865964
3.45000	0.2898018062	-6.5002768667	0.9573948604	-0.0838462532
3.50000	0.2856686736	-6.5045210347	0.9579886301	-0.0814992790
3.60000	0.2777430508	-6.5125810055	0.9591377494	-0.0770711671
3.70000	0.2702427030	-6.5201665315	0.9602308133	-0.0729840627
3.80000	0.2631353260	-6.5273286694	0.9612700832	-0.0692074779
3.90000	0.2563913818	-6.5341000820	0.9622595140	-0.0657107539
4.00000	0.2499839873	-6.5405479157	0.9631975969	-0.0624762462
4.10000	0.2438887224	-6.5466600192	0.9640929180	-0.0594698923
4.20000	0.2380834081	-6.5524745284	0.9649465776	-0.0566739141
4.30000	0.2325478846	-6.5580192642	0.9657604997	-0.0540707275
4.40000	0.2272638012	-6.5632891054	0.9665406122	-0.0516376823
4.50000	0.2222144253	-6.5683705664	0.9672797911	-0.0493752248
4.60000	0.2173844722	-6.5732039738	0.9679905897	-0.0472526115
4.70000	0.2127599531	-6.5778293510	0.9686714924	-0.0452634791
4.80000	0.2083280419	-6.5822637422	0.9693238066	-0.0433976918
4.90000	0.2040769572	-6.5865196598	0.9699491650	-0.0416454426
5.00000	0.1999958585	-6.5906034914	0.9705497802	-0.0399968606
9.00000	0.1111109895	-6.6795114475	0.9836359136	-0.0123469468

TABLE B-5

LI2+4 MOLECULAR ION:

WAVEFUNCTION PSI 2

R (BOHR)	BINDING ENERGY		(V)	-V/2T	DE/DR
0.10000	71.3462277215	38.8796798734	-0.7830085533	-885.3390103223	
0.20000	28.1673436307	0.1431922168	-0.0035122449	-204.5631025366	
0.30000	15.2675706031	-8.4220888470	0.2623667371	-78.9278517200	
0.40000	9.8038219326	-10.4284120425	0.4140625901	-36.8929534260	
0.50000	7.1047786107	-10.7678139969	0.5261238416	-19.3969933622	
0.60000	5.6262071744	-10.7009340700	0.6158666375	-11.1241231360	
0.70000	4.7501970483	-10.5635257171	0.6882416429	-6.8357789664	
0.80000	4.1959933134	-10.4658286512	0.7451762545	-4.4736759260	
0.90000	3.8216923395	-10.4604190131	0.7873650642	-3.1388101719	
1.00000	3.5485982602	-10.5806351989	0.8151746903	-2.3989571820	
1.10000	3.3300420504	-10.8375949849	0.8300599991	-2.0170950440	
1.20000	3.1386110161	-11.2018687949	0.8358302998	-1.8335135749	
1.30000	2.9606545036	-11.6094195763	0.8375434965	-1.7321954201	
1.40000	2.7917179903	-11.9997430715	0.8389054216	-1.6459317963	
1.50000	2.6318486300	-12.3386004991	0.8415346158	-1.5489488145	
1.60000	2.4823947933	-12.6152437369	0.8457296401	-1.4382242414	
1.70000	2.3444418678	-12.8346052625	0.8511451851	-1.3203614475	
1.80000	2.2182865487	-13.0086341736	0.8572430011	-1.2035181854	
1.90000	2.1035051964	-13.1497113998	0.8635469216	-1.0936038186	
2.00000	1.9992345514	-13.2675806341	0.8697340540	-0.9935875998	
2.10000	1.9044299844	-13.3690276012	0.8756216938	-0.9042919203	
2.20000	1.8180327461	-13.4584923477	0.8811272474	-0.8253105921	
2.30000	1.7390571083	-13.5388124395	0.8862297880	-0.7556748343	
2.40000	1.6666252360	-13.6117893735	0.8909431699	-0.6942355451	
2.60000	1.5384420208	-13.7403196542	0.8993151045	-0.5916650610	
2.80000	1.4285595446	-13.8502452010	0.9065047102	-0.5101749117	
3.00000	1.3333255303	-13.9455233519	0.9127354342	-0.4444332918	
3.20000	1.2499947067	-14.0288455833	0.9181899125	-0.3906126436	
6.00000	0.6666665452	-14.6122218196	0.9563659506	-0.1111133954	

TABLE B-6

BE2+6 MOLECULAR ION:

WAVEFUNCTION PSI 2

R (BOHR)	BINDING ENERGY	(V)	-V/2T	DE/DR
0.10000	126.4068496637	69.9870561970	-0.8168696281*****	
0.20000	51.3849449260	6.1337485235	-0.0968385451-347.3684885335	
0.30000	29.8251384429	-6.4575959132	0.1422283185-129.8180972570	
0.40000	20.8231634207	-10.0944687330	0.2911349159 -61.4458798814	
0.40000	20.8231634207	-10.0944687330	0.2911349159 -61.4458798814	
0.50000	16.2393137725	-11.6424694086	0.4070633700 -33.9173066638	
0.60000	13.5701360025	-12.5941403452	0.5004405055 -20.9532812139	
0.70000	11.8439202276	-13.4677983925	0.5740506396 -14.2759931800	
0.80000	10.6120877987	-14.5239891056	0.6284799328 -10.7321513516	
0.90000	9.6434248854	-15.8194684108	0.6657088790 -8.8265272888	
1.00000	8.8225333120	-17.1800155050	0.6915531447 -7.6626385072	
1.10000	8.1025841843	-18.3919483546	0.7121314101 -6.7587937286	
1.20000	7.4679094398	-19.3614424905	0.7307235933 -5.9456814569	
1.30000	6.9111457809	-20.1035934123	0.7482624558 -5.2026471941	
1.40000	6.4244645596	-20.6787183517	0.7646345895 -4.5465741778	
1.50000	5.9986774650	-21.1420952435	0.7796016034 -3.9846710344	
1.60000	5.6245898863	-21.5305764479	0.7930847371 -3.5108203742	
1.70000	5.2939854502	-21.8661777034	0.8051503115 -3.1127676365	
1.80000	4.9999490751	-22.1618048957	0.8159402236 -2.7773663468	
1.90000	4.7368160815	-22.4253974440	0.8256170799 -2.4929399922	
2.00000	4.4999833114	-22.6623424640	0.8343335904 -2.2499327325	
2.10000	4.2857023309	-22.8766702560	0.8422213490 -2.0407768077	
2.20000	4.0909001407	-23.0715069363	0.8493922469 -1.8594834526	
2.30000	3.9130366397	-23.2493655064	0.8559405343 -1.7013022452	
2.40000	3.7499947058	-23.4124298161	0.8619424330 -1.5624898358	
2.50000	3.5999958569	-23.5624167403	0.8674650519 -1.4399859329	
4.50000	1.9999998787	-25.1624537290	0.9263686132 -0.4444466366	

- C TABLES -

TABLE C-1

H2 MOLECULE:

WAVEFUNCTION PSI 0

R (BOHR)	(1/R12)	(1/RA)
0.10000	0.9834275282	-1.3899012000
0.20000	0.9695317535	-1.3678267000
0.30000	0.9478098714	-1.3336622000
0.40000	0.9200425659	-1.2905796000
0.50000	0.8881514070	-1.2418849000
0.60000	0.8539072949	-1.1904958000
0.70000	0.8187634833	-1.1386867000
0.80000	0.7838046748	-1.0880550000
0.90000	0.7497789055	-1.0396222000
1.00000	0.7171527209	-0.9939604200
1.05000	0.7014523018	-0.9722603100
1.10000	0.6861867808	-0.9513340300
1.15000	0.6713650664	-0.9311818200
1.20000	0.6569923479	-0.9117995700
1.25000	0.6430662105	-0.8931734400
1.30000	0.6295832902	-0.8752893900
1.35000	0.6165345944	-0.8581264900
1.40000	0.6039109999	-0.8416648400
1.45000	0.5917005099	-0.8258815100
1.50000	0.5798904752	-0.8107537500
1.51000	0.5775765820	-0.8078068100
1.52000	0.5752725250	-0.8048761800
1.53000	0.5729887300	-0.8019784600
1.54000	0.5707226321	-0.7991096200
1.55000	0.5684662153	-0.7962567500
1.60000	0.5574147724	-0.7823694600
1.65000	0.5467204615	-0.7690674300
1.70000	0.5363685184	-0.7563284800
1.75000	0.5263449859	-0.7441326700
1.80000	0.5166348056	-0.7324588600
1.85000	0.5072238858	-0.7212882900
1.90000	0.4980971834	-0.7106008900
1.95000	0.4892419451	-0.7003815400
2.00000	0.4806436454	-0.6906119700
2.05000	0.4722899834	-0.6812789100
2.10000	0.4641671312	-0.6723659700
2.15000	0.4562633250	-0.6638616300
2.20000	0.4485661687	-0.6557530600
2.25000	0.4410639640	-0.6480291200
2.30000	0.4337449847	-0.6406783800
2.35000	0.4265981203	-0.6336906500
2.40000	0.4196130527	-0.6270577200
2.45000	0.4127794193	-0.6207704500
2.50000	0.4060872801	-0.6148197600
2.55000	0.3995274093	-0.6091974100
2.60000	0.3930911369	-0.6038950700
2.65000	0.3867706243	-0.5989051900
2.70000	0.3805586207	-0.5942191000
2.75000	0.3744486675	-0.5898268900
2.80000	0.3684354045	-0.5857185700

H2 MOLECULE: WAVEFUNCTION PSI 0

R (BOHR)	(1/R12)	(1/RA)
2.85000	0.3625147217	-0.5818855600
2.90000	0.3566833037	-0.5783147900
2.95000	0.3509392140	-0.5749940300
3.00000	0.3452817284	-0.5719117100
3.05000	0.3397111302	-0.5690516100
3.10000	0.3342288295	-0.5664015100
3.15000	0.3288370662	-0.5639445100
3.20000	0.3235387798	-0.5616657800
3.25000	0.3183373597	-0.5595501600
3.30000	0.3132364310	-0.5575825000
3.35000	0.3082396464	-0.5557477500
3.40000	0.3033503769	-0.5540331500
3.45000	0.2985716699	-0.5524256600
3.50000	0.2939060499	-0.5509135600
3.55000	0.2893555428	-0.5494846700
3.60000	0.2849213051	-0.5481313100
3.65000	0.2806041087	-0.5468425600
3.70000	0.2764038188	-0.5456124300
3.75000	0.2723198001	-0.5444341500
3.80000	0.2683509296	-0.5433007100
3.85000	0.2644954905	-0.5422072800
3.90000	0.2607513981	-0.5411487200
3.95000	0.2571160950	-0.5401222900
4.00000	0.2535868393	-0.5391239200
4.10000	0.2468342651	-0.5371992300
4.20000	0.2404678309	-0.5353532100
4.30000	0.2344603377	-0.5335700200
4.40000	0.2287845457	-0.5318361000
4.50000	0.2234139316	-0.5301429800
4.60000	0.2183234633	-0.5284810000
4.70000	0.2134897869	-0.5268449500
4.80000	0.2088915160	-0.5252302500
4.90000	0.2045092346	-0.5236352600
5.00000	0.2003254934	-0.5220588000
5.10000	0.1963246906	-0.5204997200
5.20000	0.1924929045	-0.5189585600
5.30000	0.1888177339	-0.5174378200
5.40000	0.1852881462	-0.5159387300
5.50000	0.1818942989	-0.5144624300
5.60000	0.1786273861	-0.5130108100
5.70000	0.1754795052	-0.5115852400
5.80000	0.1724435320	-0.5101888600
5.90000	0.1695130246	-0.5088207300
6.00000	0.1666821217	-0.5074833400
6.10000	0.1639454736	-0.5061775600
6.20000	0.1612981749	-0.5049027900
6.30000	0.1587357085	-0.5036593800
6.40000	0.1562538999	-0.5024482700
6.50000	0.1538488788	-0.5012686000
6.60000	0.1515170445	-0.5001202500

H2 MOLECULE: WAVEFUNCTION PSI 0

R (BOHR)	(1/R ¹²)	(1/R ⁴)
6.70000	0.1492550388	-0.4990030500
6.80000	0.1470597213	-0.4979154600
6.90000	0.1449281492	-0.4968567400
7.00000	0.1428575589	-0.4958270400
7.20000	0.1388890773	-0.4938504600
7.40000	0.1351352185	-0.4919767000
7.60000	0.1315789834	-0.4902005200
7.80000	0.1282051434	-0.4885145400
8.00000	0.1250000063	-0.4869125000
8.20000	0.1219512220	-0.4853883400
8.40000	0.1190476200	-0.4839372400
8.60000	0.1162790702	-0.4825529600
8.80000	0.1136363638	-0.4812316100
9.00000	0.1111111112	-0.4799689900
9.20000	0.1086956522	-0.4787612600
9.40000	0.1063829787	-0.4776049200
9.60000	0.1041666667	-0.4764967600
9.80000	0.1020408163	-0.4754338400
10.00000	0.1000000000	-0.4744134300
18.00000	0.0555555556	-0.4521912100

TABLE C-2

H2 MOLECULE:	WAVEFUNCTION PSI 1	
R (BOHR)	(1/R12)	(1/RA)
0.10000	0.9673465872	-1.3894906000
0.20000	0.9542951538	-1.3661412000
0.30000	0.9343469237	-1.3307522000
0.40000	0.9095151572	-1.2872445000
0.50000	0.8816837961	-1.2392898000
0.60000	0.8522967777	-1.1897427000
0.70000	0.8222647130	-1.1405048000
0.80000	0.7920334182	-1.0926595000
0.90000	0.7617269480	-1.0466923000
1.00000	0.7313615837	-1.0027588000
1.05000	0.7161840283	-0.9815731500
1.10000	0.7010463516	-0.9609196500
1.15000	0.6859912469	-0.9408133600
1.20000	0.6710703520	-0.9212742800
1.25000	0.6563375443	-0.9023223700
1.30000	0.6418442742	-0.8839747900
1.35000	0.6276396223	-0.8662492900
1.40000	0.6137623504	-0.8491546000
1.45000	0.6002440399	-0.8326961100
1.50000	0.5871078961	-0.8168744200
1.51000	0.5845301717	-0.8137900300
1.52000	0.5819618593	-0.8107193300
1.53000	0.5794142739	-0.8076820000
1.54000	0.5768824755	-0.8046691900
1.55000	0.5743684206	-0.8016842600
1.60000	0.5620323116	-0.7871148400
1.65000	0.5501018231	-0.7731548000
1.70000	0.5385734592	-0.7597885700
1.75000	0.5274404738	-0.7469998800
1.80000	0.5166925465	-0.7347698700
1.85000	0.5063178982	-0.7230803900
1.90000	0.4963029799	-0.7119124700
1.95000	0.4866339670	-0.7012490200
2.00000	0.4772957613	-0.6910717300
2.05000	0.4682729399	-0.6813626000
2.10000	0.4595505671	-0.6721057900
2.15000	0.4511136197	-0.6632856600
2.20000	0.4429474353	-0.6548876600
2.25000	0.4350376762	-0.6468980200
2.30000	0.4273704517	-0.6393038200
2.35000	0.4199323439	-0.6320928800
2.40000	0.4127108132	-0.6252552700
2.45000	0.4056932758	-0.6187793600
2.50000	0.3988681460	-0.6126558700
2.55000	0.3922242075	-0.6068750200
2.60000	0.3857512333	-0.6014294700
2.65000	0.3794391219	-0.5963094200
2.70000	0.3732786753	-0.5915064400
2.75000	0.3672613160	-0.5870115700
2.80000	0.3613794101	-0.5828175800

H2 MOLECULE:

WAVEFUNCTION PSI 1

R (BOHR)	(1/R12)	(1/RA)
2.85000	0.3556255935	-0.5789127100
2.90000	0.3499937284	-0.5752886000
2.95000	0.3444782536	-0.5719341200
3.00000	0.3390743852	-0.5688362300
3.05000	0.3337782908	-0.5659825200
3.10000	0.3285868954	-0.5633587500
3.15000	0.3234979108	-0.5609497700
3.20000	0.3185097757	-0.5587401100
3.25000	0.3136215366	-0.5567127300
3.30000	0.3088327827	-0.5548507500
3.35000	0.3041435022	-0.5531383000
3.40000	0.2995539427	-0.5515587700
3.45000	0.2950645116	-0.5500953400
3.50000	0.2906756409	-0.5487330300
3.55000	0.2863876486	-0.5474594900
3.60000	0.2822007476	-0.5462603100
3.65000	0.2781148517	-0.5451259300
3.70000	0.2741296765	-0.5440451100
3.75000	0.2702446015	-0.5430098200
3.80000	0.2664587480	-0.5420119600
3.85000	0.2627708979	-0.5410464500
3.90000	0.2591796076	-0.5401077500
3.95000	0.2556831960	-0.5391910500
4.00000	0.2522797450	-0.5382931100
4.10000	0.2457432126	-0.5365418800
4.20000	0.2395515913	-0.5348369100
4.30000	0.2336849638	-0.5331645600
4.40000	0.2281225681	-0.5315184800
4.50000	0.2228436244	-0.5298910300
4.60000	0.2178277118	-0.5282798600
4.70000	0.2130552772	-0.5266824100
4.80000	0.2085078996	-0.5250960700
4.90000	0.2041684439	-0.5235207100
5.00000	0.2000211709	-0.5219581500
5.10000	0.1960517695	-0.5204093500
5.20000	0.1922472987	-0.5188755100
5.30000	0.1885961001	-0.5173594000
5.40000	0.1850877001	-0.5158630000
5.50000	0.1817126879	-0.5143884400
5.60000	0.1784625976	-0.5129395800
5.70000	0.1753297981	-0.5115164800
5.80000	0.1723073867	-0.5101214800
5.90000	0.1693890983	-0.5087560500
6.00000	0.1665692247	-0.5074212600
6.10000	0.1638425435	-0.5061172200
6.20000	0.1612042601	-0.5048454100
6.30000	0.1586499540	-0.5036058800
6.40000	0.1561755355	-0.5023977500
6.50000	0.1537772096	-0.5012208500
6.60000	0.1514514443	-0.5000755400

H2 MOLECULE: WAVEFUNCTION PSI 1

R (BOHR)	(1/R12)	(1/RA)
6.70000	0.1491949421	-0.4989612200
6.80000	0.1470046171	-0.4978765000
6.90000	0.1448775763	-0.4968209800
7.00000	0.1428111009	-0.4957938200
7.20000	0.1388497585	-0.4938211000
7.40000	0.1351018119	-0.4919524600
7.60000	0.1315504886	-0.4901798200
7.80000	0.1281807441	-0.4884963800
8.00000	0.1249790353	-0.4868968800
8.20000	0.1219331321	-0.4853748000
8.40000	0.1190319607	-0.4839253700
8.60000	0.1162654693	-0.4825427100
8.80000	0.1136245126	-0.4812221500
9.00000	0.1111007530	-0.4799612400
9.20000	0.1086865722	-0.4787545000
9.40000	0.1063749967	-0.4775989100
9.60000	0.1041596309	-0.4764915100
9.80000	0.1020345985	-0.4754292300
10.00000	0.0999944913	-0.4744093100
18.00000	0.0555553934	-0.4521905000

TABLE C-3

H2 MOLECULE:

WAVEFUNCTION PSI 2

R (BOHR)	(1/R12)	(1/RA)
0.10000	0.9375253495	-1.3899674000
0.20000	0.9247261164	-1.3665201000
0.30000	0.9051763208	-1.3309791000
0.40000	0.8808620819	-1.2872749000
0.50000	0.8536409616	-1.2390881000
0.60000	0.8249315766	-1.1892740000
0.70000	0.7956320638	-1.1397391000
0.80000	0.7661834634	-1.0915696000
0.90000	0.7367225862	-1.0452677000
1.00000	0.7072866466	-1.0010167000
1.05000	0.6926095188	-0.9796871600
1.10000	0.6779979747	-0.9589059300
1.15000	0.6634931615	-0.9386901000
1.20000	0.6491417361	-0.9190577800
1.25000	0.6349936937	-0.9000287500
1.30000	0.6210976441	-0.8816214700
1.35000	0.6074964660	-0.8638495700
1.40000	0.5942263413	-0.8467223200
1.45000	0.5813136430	-0.8302407700
1.50000	0.5687724951	-0.8143933800
1.51000	0.5663122855	-0.8113031100
1.52000	0.5638708427	-0.8082434700
1.53000	0.5614374584	-0.8051962400
1.54000	0.5590273145	-0.8021869000
1.55000	0.5566262425	-0.7991912000
1.60000	0.5448755615	-0.7846151600
1.65000	0.5335204945	-0.7706506700
1.70000	0.5225580460	-0.7572834000
1.75000	0.5119824229	-0.7444989500
1.80000	0.5017755122	-0.7322624800
1.85000	0.4919349851	-0.7205739800
1.90000	0.4824434012	-0.7094058200
1.95000	0.4732916637	-0.6987505200
2.00000	0.4644542960	-0.6885648100
2.05000	0.4559292335	-0.6788610700
2.10000	0.4476934076	-0.6696028100
2.15000	0.4397352149	-0.6607817900
2.20000	0.4320391217	-0.6523800800
2.25000	0.4245906236	-0.6443821400
2.30000	0.4173792805	-0.6367845800
2.35000	0.4103929677	-0.6295798900
2.40000	0.4036116899	-0.6227329600
2.45000	0.3970311942	-0.6162608000
2.50000	0.3906353274	-0.6101387000
2.55000	0.3844138596	-0.6043614800
2.60000	0.3783556289	-0.5989189000
2.65000	0.3724513667	-0.5938072500
2.70000	0.3666910170	-0.5890173200
2.75000	0.3610638562	-0.5845321700
2.80000	0.3555652623	-0.5803663100

H2 MOLECULE: WAVEFUNCTION PSI 2

R (BOHR)	(1/R12)	(1/RA)
2.85000	0.3501836016	-0.5764893500
2.90000	0.3449121851	-0.5728935600
2.95000	0.3397469899	-0.5695882400
3.00000	0.3346787756	-0.5665321900
3.05000	0.3297060156	-0.5637437700
3.10000	0.3248223139	-0.5611844300
3.15000	0.3200254386	-0.5588471900
3.20000	0.3153128947	-0.5567100300
3.25000	0.3106840011	-0.5547678900
3.30000	0.3061377638	-0.5529980500
3.35000	0.3016742129	-0.5513854900
3.40000	0.2972934172	-0.5498949400
3.45000	0.2929967741	-0.5485339300
3.50000	0.2887849585	-0.5472631300
3.55000	0.2846592684	-0.5460898600
3.60000	0.2806206345	-0.5449839200
3.65000	0.2766700102	-0.5439312700
3.70000	0.2728078605	-0.5429443100
3.75000	0.2690348010	-0.5419822500
3.80000	0.2653505875	-0.5410635500
3.85000	0.2617550588	-0.5401701500
3.90000	0.2582474821	-0.5393045000
3.95000	0.2548272804	-0.5384431500
4.00000	0.2514927712	-0.5376114900
4.10000	0.2450761683	-0.5359572400
4.20000	0.2389836829	-0.5343399000
4.30000	0.2331993365	-0.5327414200
4.40000	0.2277054113	-0.5311635400
4.50000	0.2224838151	-0.5295879700
4.60000	0.2175161221	-0.5280146200
4.70000	0.2127842475	-0.5264602800
4.80000	0.2082712693	-0.5249046900
4.90000	0.2039610904	-0.5233497200
5.00000	0.1998387750	-0.5218153100
5.10000	0.1958908143	-0.5202771600
5.20000	0.1921047831	-0.5187598000
5.30000	0.1884695265	-0.5172578200
5.40000	0.1849749635	-0.5157793900
5.50000	0.1816119993	-0.5143079800
5.60000	0.1783724485	-0.5128724100
5.70000	0.1752488829	-0.5114519200
5.80000	0.1722346065	-0.5100681100
5.90000	0.1693234923	-0.5087085300
6.00000	0.1665099694	-0.5073801500
6.10000	0.1637889208	-0.5060804200
6.20000	0.1611556479	-0.5048125500
6.30000	0.1586058003	-0.5035698600
6.40000	0.1561353812	-0.5023706500
6.50000	0.1537406293	-0.5011966300
6.60000	0.1514180715	-0.5000549000

H2 MOLECULE:

WAVEFUNCTION PSI 2

R (BOHR)	(1/R12)	(1/RA)
6.70000	0.1491644504	-0.4989421200
6.80000	0.1469767199	-0.4978593100
6.90000	0.1448520113	-0.4967973600
7.00000	0.1427876570	-0.4957795400
7.20000	0.1388299545	-0.4938030800
7.40000	0.1350850134	-0.4919437100
7.60000	0.1315361722	-0.4901715900
7.80000	0.1281684937	-0.4884912500
8.00000	0.1249685079	-0.4868860000
8.20000	0.1219240538	-0.4853649100
8.40000	0.1190241041	-0.4839160300
8.60000	0.1162586486	-0.4825404500
8.80000	0.1136185710	-0.4812220600
9.00000	0.1110955592	-0.4799537600
9.20000	0.1086820213	-0.4787546600
9.40000	0.1063709965	-0.4775984200
9.60000	0.1041561046	-0.4764862500
9.80000	0.1020314832	-0.4754293900
10.00000	0.0999917316	-0.4744092300
18.00000	0.0555553122	-0.4521934700

TABLE C-4

C4-1

158

HE2+2 MOLECULAR ION: WAVEFUNCTION PSI 2

R (BOHR)	(1/R12)	(1/RA)
0.05000	2.1275473357	-6.1495886000
0.10000	2.0960449915	-6.0330668000
0.15000	2.0481421149	-5.8580755000
0.20000	1.9886682930	-5.6450512000
0.25000	1.9216999894	-5.4119457000
0.30000	1.8498075233	-5.1713930000
0.35000	1.7741694329	-4.9307984000
0.40000	1.6953729174	-4.6941635000
0.45000	1.6144600132	-4.4644233000
0.50000	1.5333519185	-4.2447310000
0.55000	1.4543190189	-4.0381245000
0.60000	1.3792100582	-3.8466760000
0.65000	1.3091033140	-3.6711471000
0.70000	1.2444016506	-3.5112752000
0.75000	1.1850470284	-3.3661486000
0.80000	1.1307388932	-3.2346059000
0.85000	1.0810464301	-3.1153638000
0.90000	1.0355123344	-3.0072260000
0.95000	0.9936771615	-2.9090619000
1.00000	0.9551162494	-2.8198962000
1.05000	0.9194396436	-2.7388718000
1.10000	0.8862951532	-2.6652436000
1.15000	0.8553720006	-2.5983947000
1.20000	0.8263937325	-2.5378009000
1.25000	0.7991166607	-2.4830273000
1.30000	0.7733253760	-2.4337040000
1.35000	0.7488313443	-2.3895191000
1.40000	0.7254711254	-2.3502019000
1.45000	0.7031048744	-2.3154912000
1.50000	0.6816188700	-2.2851493000
1.55000	0.6609231956	-2.2588708000
1.60000	0.6409570244	-2.2363640000
1.65000	0.6216850279	-2.2172412000
1.70000	0.6030969288	-2.2010991000
1.75000	0.5852012453	-2.1874974000
1.80000	0.5680179263	-2.1759906000
1.85000	0.5515697214	-2.1661709000
1.90000	0.5358752224	-2.1576659000
1.95000	0.5209442321	-2.1501390000
2.00000	0.5067744199	-2.1433325000
2.05000	0.4933514096	-2.1370452000
2.10000	0.4806504796	-2.1311074000
2.15000	0.4686382716	-2.1253927000
2.20000	0.4572756299	-2.1197907000
2.25000	0.4465194558	-2.1142399000
2.30000	0.4363255271	-2.1086889000
2.35000	0.4266501436	-2.1031020000
2.40000	0.4174514018	-2.0974678000
2.45000	0.4086903136	-2.0917707000
2.50000	0.4003310198	-2.0860306000

HE2+2 MOLECULAR ION: WAVEFUNCTION PSI 2

R (BOHR)	(1/R12)	(1/RA)
2.55000	0.3923412348	-2.0802605000
2.60000	0.3846920996	-2.0744642000
2.65000	0.3773578504	-2.0686741000
2.70000	0.3703156516	-2.0629126000
2.75000	0.3635452353	-2.0571866000
2.80000	0.3570285394	-2.0515140000
2.85000	0.3507494326	-2.0459227000
2.90000	0.3446934589	-2.0404226000
2.95000	0.3388475885	-2.0350111000
3.00000	0.3332000202	-2.0297155000
3.05000	0.3277400149	-2.0245231000
3.10000	0.3224577563	-2.0194543000
3.15000	0.3173442267	-2.0145048000
3.20000	0.3123911110	-2.0096785000
3.25000	0.3075907123	-2.0049807000
3.30000	0.3029358769	-2.0003992000
3.35000	0.2984199415	-1.9959326000
3.40000	0.2940366844	-1.9915959000
3.45000	0.2897802699	-1.9873694000
3.50000	0.2856452256	-1.9832559000
3.60000	0.2777189531	-1.9753528000
3.70000	0.2702201212	-1.9678669000
3.80000	0.2631150480	-1.9607688000
3.90000	0.2563735414	-1.9540287000
4.00000	0.2499684369	-1.9476291000
4.10000	0.2438752125	-1.9415362000
4.20000	0.2380716726	-1.9357318000
4.30000	0.2325376752	-1.9301974000
4.40000	0.2272548988	-1.9249087000
4.50000	0.2222066428	-1.9198665000
4.60000	0.2173776497	-1.9150367000
4.70000	0.2127539558	-1.9104118000
4.80000	0.2083227559	-1.9059800000
4.90000	0.2040722862	-1.9017296000
5.00000	0.1999917206	-1.8976488000
9.00000	0.1111108677	-1.8087667000

TABLE C-5

LI2+4 MOLECULAR ION: WAVEFUNCTION PSI 2

R (BOHR)	(1/R12)	(1/RA)
0.10000	3.1930833321	-13.5783510000
0.20000	2.8727055980	-11.9323780000
0.30000	2.4823961686	-10.2261210000
0.40000	2.1011643258	-8.7573941000
0.50000	1.7973793658	-7.6412983000
0.60000	1.5675210039	-6.8171138000
0.70000	1.3904505854	-6.2027798000
0.80000	1.2488675363	-5.7411740000
0.90000	1.1308907662	-5.3978274000
1.00000	1.0286676088	-5.1523257000
1.10000	0.9375120243	-4.9892313000
1.20000	0.8557680025	-4.8894092000
1.30000	0.7839292023	-4.8291064000
1.40000	0.7224823402	-4.7876992000
1.50000	0.6706279105	-4.7523071000
1.60000	0.6266595655	-4.7167258000
1.70000	0.5888022365	-4.6793813000
1.80000	0.5556606178	-4.6410737000
1.90000	0.5262519100	-4.6032014000
2.00000	0.4998910612	-4.5668679000
2.10000	0.4760832077	-4.5327063000
2.20000	0.4544540255	-4.5009639000
2.30000	0.4347087422	-4.4716412000
2.40000	0.4166080956	-4.4445994000
2.60000	0.3845786613	-4.3966092000
2.80000	0.3571192748	-4.3554125000
3.00000	0.3333177441	-4.3197103000
3.20000	0.3124894171	-4.2884588000
6.00000	0.1666664233	-4.0697221000

TABLE C-6

BE2+6 MOLECULAR ION: WAVEFUNCTION PSI 2

R (BOHR)	(1/R12)	(1/RA)
0.10000	4.2069305699	-23.5549690000
0.20000	3.5359699704	-19.3505550000
0.30000	2.8215555676	-15.6531210000
0.40000	2.2959086583	-13.0975940000
0.40000	2.2959086583	-13.0975940000
0.50000	1.9343031946	-11.3941930000
0.60000	1.6712825173	-10.2330220000
0.70000	1.4652517255	-9.4475482000
0.80000	1.2927695141	-8.9541897000
0.90000	1.1436231351	-8.6852173000
1.00000	1.0179112073	-8.5494817000
1.10000	0.9166421321	-8.4635113000
1.20000	0.8358760626	-8.3826630000
1.30000	0.7698844137	-8.2952925000
1.40000	0.7143463832	-8.2054090000
1.50000	0.6665823734	-8.1188361000
1.60000	0.6249036454	-8.0388700000
1.70000	0.5881571904	-7.9665249000
1.80000	0.5554972767	-7.9015478000
1.90000	0.5262730030	-7.8431808000
2.00000	0.4999684163	-7.7905777000
2.10000	0.4761668865	-7.7429712000
2.20000	0.4545276089	-7.6996905000
2.30000	0.4347689420	-7.6601640000
2.40000	0.4166560811	-7.6239381000
2.50000	0.3999917149	-7.5906021000
4.50000	0.2222219788	-7.2350578000

- D TABLES -

TABLE D-1

H2 MOLECULE:	WAVEFUNCTION PSI 0	
SCALED R	SCALED ENERGY	SCALED DE/DR
0.09039	10.8097434300	-139.6255903214
0.18077	4.5153337223	-34.6057098520
0.27116	2.4470729059	-15.0469845479
0.36155	1.4432902768	-8.1398975772
0.45194	0.8693383110	-4.9145491407
0.54232	0.5118789562	-3.1547282588
0.63271	0.2782601439	-2.0974038654
0.72310	0.1214066424	-1.4206202998
0.81348	0.0147548377	-0.9682271582
0.90387	-0.0578258366	-0.6564069683
0.94906	-0.0847204395	-0.5372091009
0.99426	-0.1066636203	-0.4366866814
1.03945	-0.1244235328	-0.3516026605
1.08465	-0.1386374362	-0.2793751637
1.12984	-0.1498372380	-0.2179026419
1.17503	-0.1584693501	-0.1654872872
1.22023	-0.1649102919	-0.1207232013
1.26542	-0.1694790666	-0.0824599373
1.31061	-0.1724470651	-0.0497369531
1.35581	-0.1740460513	-0.0217553866
1.36485	-0.1742195659	-0.0166732608
1.37388	-0.1743477998	-0.0117214234
1.38292	-0.1744321566	-0.0069475012
1.39196	-0.1744739983	-0.0023347823
1.40100	-0.1744746470	0.0021601414
1.44619	-0.1739036324	0.0225676857
1.49139	-0.1724803031	0.0399498058
1.53658	-0.1703320718	0.0547114070
1.58177	-0.1675694604	0.0671931439
1.62697	-0.1642885959	0.0776912029
1.67216	-0.1605733039	0.0864555556
1.71735	-0.1564968684	0.0937065576
1.76255	-0.1521235184	0.0996241651
1.80774	-0.1475096882	0.1043734735
1.85294	-0.1427050866	0.1080877987
1.89813	-0.1377536097	0.1108919747
1.94332	-0.1326941182	0.1128854780
1.98852	-0.1275611033	0.1141596293
2.03371	-0.1223852556	0.1147921050
2.07890	-0.1171939513	0.1148531582
2.12410	-0.1120116674	0.1144032416
2.16929	-0.1068603342	0.1134926671
2.21448	-0.1017596335	0.1121689016
2.25968	-0.0967272477	0.1104750199
2.30487	-0.0917790649	0.1084485805
2.35006	-0.0869293453	0.1061242474
2.39526	-0.0821908519	0.1035323376
2.44045	-0.0775749490	0.1007030470
2.48565	-0.0730916731	0.0976668036
2.53084	-0.0687497801	0.0944520843

H2 MOLECULE: WAVEFUNCTION PSI 0

SCALED R	SCALED ENERGY	SCALED DE/DR
2.57603	-0.0645567728	0.0910827356
2.62123	-0.0605189159	0.0875894460
2.66642	-0.0566412419	0.0839993773
2.71161	-0.0529275574	0.0803365977
2.75681	-0.0493804526	0.0766320435
2.80200	-0.0460013229	0.0729073923
2.84719	-0.0427904044	0.0691910192
2.89239	-0.0397468281	0.0655057132
2.93758	-0.0368686924	0.0618730889
2.98277	-0.0341531526	0.0583131300
3.02797	-0.0315965264	0.0548440709
3.07316	-0.0291944082	0.0514788891
3.11835	-0.0269417901	0.0482298770
3.16355	-0.0248331833	0.0451061480
3.20874	-0.0228627358	0.0421167136
3.25394	-0.0210243420	0.0392627248
3.29913	-0.0193117433	0.0365500652
3.34432	-0.0177186155	0.0339766191
3.38952	-0.0162386447	0.0315413960
3.43471	-0.0148655900	0.0292437910
3.47990	-0.0135933336	0.0270799471
3.52510	-0.0124159213	0.0250467393
3.57029	-0.0113275915	0.0231377580
3.61548	-0.0103227967	0.0213489026
3.70587	-0.0085427716	0.0181109821
3.79626	-0.0070361468	0.0152917367
3.88665	-0.0057670380	0.0128486443
3.97703	-0.0047032623	0.0107425973
4.06742	-0.0038161280	0.0089341118
4.15781	-0.0030801848	0.0073909989
4.24819	-0.0024729656	0.0060808303
4.33858	-0.0019747346	0.0049753247
4.42897	-0.0015682480	0.0040471187
4.51935	-0.0012385273	0.0032723544
4.60974	-0.0009726428	0.0026306330
4.70013	-0.0007595082	0.0021027661
4.79052	-0.0005896831	0.0016702003
4.88090	-0.0004551862	0.0013181971
4.97129	-0.0003493187	0.0010341435
5.06168	-0.0002664994	0.0008064027
5.15206	-0.0002021121	0.0006253858
5.24245	-0.0001523672	0.0004810678
5.33284	-0.0001141765	0.0003684838
5.42323	-0.0000850417	0.0002802552
5.51361	-0.0000629567	0.0002113161
5.60400	-0.0000463229	0.0001586091
5.69439	-0.0000338751	0.0001186508
5.78477	-0.0000246200	0.0000879260
5.87516	-0.0000177833	0.0000648512
5.96555	-0.0000127656	0.0000474730

H2 MOLECULE: WAVEFUNCTION PSI 0

SCALED R	SCALED ENERGY	SCALED DE/DR
6.05594	-0.0000091071	0.0000341617
6.14632	-0.0000064568	0.0000246028
6.23671	-0.0000045494	0.0000179630
6.32710	-0.0000031856	0.0000128454
6.50787	-0.0000015331	0.0000060762
6.68865	-0.0000007197	0.0000032875
6.86942	-0.0000003296	0.0000016745
7.05019	-0.0000001473	0.0000009064
7.23097	-0.0000000642	0.0000004919
7.41174	-0.0000000273	0.0000003167
7.59252	-0.0000000113	-0.0000001620
7.77329	-0.0000000046	-0.0000001603
7.95406	-0.0000000018	-0.0000001575
8.13484	-0.0000000007	-0.0000001543
8.31561	-0.0000000003	-0.0000001511
8.49639	-0.0000000001	-0.0000001479
8.67716	-0.0000000000	-0.0000001448
8.85794	-0.0000000000	-0.0000001419
9.03871	-0.0000000000	-0.0000001391
16.26968	0.0000000000	-0.0000000773

TABLE D-2

H2 MOLECULE:	WAVEFUNCTION PSI 1	
SCALED R	SCALED ENERGY	SCALED DE/DR
0.09039	10.2324253069	-132.2737278893
0.18077	4.2706659120	-32.7615962040
0.27116	2.3135806374	-14.2281611306
0.36155	1.3649157285	-7.6888394196
0.45194	0.8228326411	-4.6422945012
0.54232	0.4849374102	-2.9857062794
0.63271	0.2634334702	-1.9936854846
0.72310	0.1138857712	-1.3596896620
0.81348	0.0113937524	-0.9350344978
0.90387	-0.0590273901	-0.6403326077
0.94906	-0.0853282582	-0.5267302707
0.99426	-0.1068949746	-0.4302808865
1.03945	-0.1244340845	-0.3480580859
1.08465	-0.1385342768	-0.2777487116
1.12984	-0.1496903517	-0.2174936737
1.17503	-0.1583213712	-0.1657778522
1.22023	-0.1647845093	-0.1213680753
1.26542	-0.1693857462	-0.0832253516
1.31061	-0.1723882531	-0.0504829393
1.35581	-0.1740190821	-0.0224086018
1.36485	-0.1741984135	-0.0173088532
1.37388	-0.1743322533	-0.0123313272
1.38292	-0.1744219984	-0.0075309351
1.39196	-0.1744690064	-0.0028770380
1.40100	-0.1744745971	0.0016243501
1.44619	-0.1739249512	0.0221562343
1.49139	-0.1725178268	0.0396436205
1.53658	-0.1703815879	0.0544839784
1.58177	-0.1676279591	0.0670173311
1.62697	-0.1643543107	0.0775411216
1.67216	-0.1606456170	0.0863092328
1.71735	-0.1565761370	0.0935429903
1.76255	-0.1522108599	0.0994299198
1.80774	-0.1476067499	0.1041363467
1.85294	-0.1428138193	0.1078072332
1.89813	-0.1378760533	0.1105652964
1.94332	-0.1328322086	0.1125184572
1.98852	-0.1277165030	0.1137599896
2.03371	-0.1225592094	0.1143713784
2.07890	-0.1173871696	0.1144236508
2.12410	-0.1122242358	0.1139790515
2.16929	-0.1070916500	0.1130890273
2.21448	-0.1020083696	0.1118035821
2.25968	-0.0969913437	0.1101634376
2.30487	-0.0920557461	0.1082067632
2.35006	-0.0872151701	0.1059636923
2.39526	-0.0824817872	0.1034666309
2.44045	-0.0778664742	0.1007428691
2.48565	-0.0733789102	0.0978186306
2.53084	-0.0690276480	0.0947150467

H2 MOLECULE: WAVEFUNCTION PSI 1

SCALED R	SCALED ENERGY	SCALED DE/DR
2.57603	-0.0648201613	0.0914599183
2.62123	-0.0607628713	0.0880730572
2.66642	-0.0568611583	0.0845777722
2.71161	-0.0531193597	0.0809990668
2.75681	-0.0495407630	0.0773591634
2.80200	-0.0461275975	0.0736818285
2.84719	-0.0428810305	0.0699906190
2.89239	-0.0398011753	0.0663079869
2.93758	-0.0368871133	0.0626573082
2.98277	-0.0341369349	0.0590599969
3.02797	-0.0315478010	0.0555342926
3.07316	-0.0291160222	0.0520982268
3.11835	-0.0268371556	0.0487688276
3.16355	-0.0247061141	0.0455590849
3.20874	-0.0227172833	0.0424770685
3.25394	-0.0208646400	0.0395332582
3.29913	-0.0191418696	0.0367303013
3.34432	-0.0175424752	0.0340730779
3.38952	-0.0160598777	0.0315615309
3.43471	-0.0146875028	0.0291957036
3.47990	-0.0134188555	0.0269715038
3.52510	-0.0122475801	0.0248857203
3.57029	-0.0111675085	0.0229343947
3.61548	-0.0101726955	0.0211118327
3.70587	-0.0084163209	0.0178303892
3.79626	-0.0069360956	0.0149926861
3.88665	-0.0056940268	0.0125526411
3.97703	-0.0046563834	0.0104620444
4.06742	-0.0037934227	0.0086808982
4.15781	-0.0030790480	0.0071688764
4.24819	-0.0024904563	0.0058915071
4.33858	-0.0020078039	0.0048192248
4.42897	-0.0016139016	0.0039240312
4.51935	-0.0012939373	0.0031797719
4.60974	-0.0010352217	0.0025647396
4.70013	-0.0008269537	0.0020600266
4.79052	-0.0006600005	0.0016477434
4.88090	-0.0005266929	0.0013131791
4.97129	-0.0004206347	0.0010434174
5.06168	-0.0003365277	0.0008256453
5.15206	-0.0002700120	0.0006521318
5.24245	-0.0002175237	0.0005141635
5.33284	-0.0001761676	0.0004048842
5.42323	-0.0001436064	0.0003186706
5.51361	-0.0001179647	0.0002514298
5.60400	-0.0000977463	0.0001984619
5.69439	-0.0000817648	0.0001568253
5.78477	-0.0000690842	0.0001247320
5.87516	-0.0000589703	0.0001000961
5.96555	-0.0000508500	0.0000807021

H2 MOLECULE: WAVEFUNCTION PSI 1

SCALED R	SCALED ENERGY	SCALED DE/DR
6.05594	-0.0000442781	0.0000653340
6.14632	-0.0000389101	0.0000536023
6.23671	-0.0000344806	0.0000444470
6.32710	-0.0000307857	0.0000372983
6.50787	-0.0000250105	0.0000273688
6.68865	-0.0000207234	0.0000204876
6.86942	-0.0000174173	0.0000160272
7.05019	-0.0000147890	0.0000132118
7.23097	-0.0000126519	0.0000108237
7.41174	-0.0000108861	0.0000090560
7.59252	-0.0000094104	0.0000073375
7.77329	-0.0000081671	0.0000061729
7.95406	-0.0000071131	0.0000055530
8.13484	-0.0000062153	0.0000044181
8.31561	-0.0000054472	0.0000037482
8.49639	-0.0000047878	0.0000032494
8.67716	-0.0000042197	0.0000027616
8.85794	-0.0000037287	0.0000023608
9.03871	-0.0000033031	0.0000020502
16.26968	-0.0000000971	0.0000001359

TABLE D-3

H2 MOLECULE:	WAVEFUNCTION PSI 2	
SCALED R	SCALED ENERGY	SCALED DE/DR
0.09157	9.6557255992	-123.4368832776
0.18314	4.0196577732	-30.5705841363
0.27471	2.1697223465	-13.2740046946
0.36627	1.2732433799	-7.1705286653
0.45784	0.7612277373	-4.3266773675
0.54941	0.4423205281	-2.7800319288
0.64098	0.2335107560	-1.8536483040
0.73255	0.0927833624	-1.2614347715
0.82412	-0.0034098233	-0.8646765817
0.91569	-0.0692467587	-0.5893457873
0.96147	-0.0937333092	-0.4832434528
1.00725	-0.1137415326	-0.3932050672
1.05304	-0.1299417967	-0.3164984206
1.09882	-0.1428929005	-0.2509512375
1.14461	-0.1530646073	-0.1948232458
1.19039	-0.1608547263	-0.1467011629
1.23618	-0.1666021797	-0.1054187004
1.28196	-0.1705971265	-0.0700067784
1.32775	-0.1730889303	-0.0396430005
1.37353	-0.1742925357	-0.0136102427
1.38269	-0.1743954795	-0.0088803720
1.39184	-0.1744557622	-0.0043111757
1.40100	-0.1744747037	0.0001517109
1.41016	-0.1744535870	0.0044416396
1.41931	-0.1743936585	0.0086289051
1.46510	-0.1735530703	0.0276016856
1.51088	-0.1719101777	0.0437416922
1.55667	-0.1695860405	0.0574155993
1.60245	-0.1666859322	0.0689352938
1.64824	-0.1633015240	0.0786164889
1.69402	-0.1595127527	0.0866505404
1.73980	-0.1553894228	0.0932641866
1.78559	-0.1509925825	0.0986097287
1.83137	-0.1463757085	0.1028981234
1.87716	-0.1415857247	0.1061958361
1.92294	-0.1366638819	0.1086625428
1.96873	-0.1316465157	0.1103821534
2.01451	-0.1265657012	0.1114483051
2.06029	-0.1214498176	0.1119398748
2.10608	-0.1163240358	0.1119034300
2.15186	-0.1112107389	0.1113881643
2.19765	-0.1061298834	0.1104909430
2.24343	-0.1010993092	0.1092027168
2.28922	-0.0961350040	0.1075910334
2.33500	-0.0912513263	0.1056826181
2.38078	-0.0864611916	0.1035108019
2.42657	-0.0817762245	0.1010947370
2.47235	-0.0772068801	0.0984614717
2.51814	-0.0727625354	0.0956493207
2.56392	-0.0684515550	0.0926407538

H2 MOLECULE:

WAVEFUNCTION PSI 2

SCALED R	SCALED ENERGY	SCALED DE/DR
2.60971	-0.0642813316	0.0894939470
2.65549	-0.0602583045	0.0862262162
2.70127	-0.0563879608	0.0828258686
2.74706	-0.0526748213	0.0793627286
2.79284	-0.0491224179	0.0758081167
2.83863	-0.0457332683	0.0722236366
2.88441	-0.0425088545	0.0686184753
2.93020	-0.0394496107	0.0650239681
2.97598	-0.0365549291	0.0614438155
3.02176	-0.0338231847	0.0579073569
3.06755	-0.0312517843	0.0544307358
3.11333	-0.0288372388	0.0510581542
3.15912	-0.0265752559	0.0477699861
3.20490	-0.0244608497	0.0446133980
3.25069	-0.0224884615	0.0415678689
3.29647	-0.0206520851	0.0386652603
3.34225	-0.0189453908	0.0359136902
3.38804	-0.0173618433	0.0332853222
3.43382	-0.0158948092	0.0308239723
3.47961	-0.0145376508	0.0284938827
3.52539	-0.0132838067	0.0263081746
3.57118	-0.0121268562	0.0242532477
3.61696	-0.0110605711	0.0223488076
3.66275	-0.0100789530	0.0205530810
3.75431	-0.0083470248	0.0173512012
3.84588	-0.0068884658	0.0145813521
3.93745	-0.0056651814	0.0122043894
4.02902	-0.0046434629	0.0101646677
4.12059	-0.0037936889	0.0084358477
4.21216	-0.0030899555	0.0069763876
4.30373	-0.0025096994	0.0057325142
4.39529	-0.0020333430	0.0046950253
4.48686	-0.0016439718	0.0038348373
4.57843	-0.0013270437	0.0031088564
4.67000	-0.0010701254	0.0025217196
4.76157	-0.0008626502	0.0020325215
4.85314	-0.0006956950	0.0016324885
4.94471	-0.0005617738	0.0013020319
5.03627	-0.0004546465	0.0010460567
5.12784	-0.0003691458	0.0008297923
5.21941	-0.0003010194	0.0006645579
5.31098	-0.0002467897	0.0005252933
5.40255	-0.0002036294	0.0004176465
5.49412	-0.0001692537	0.0003312407
5.58569	-0.0001418262	0.0002644465
5.67725	-0.0001198791	0.0002114027
5.76882	-0.0001022455	0.0001746069
5.86039	-0.0000880018	0.0001373232
5.95196	-0.0000764210	0.0001118222
6.04353	-0.0000669328	0.0000907674

H2 MOLECULE: WAVEFUNCTION PSI 2

SCALED R	SCALED ENERGY	SCALED DE/DR
6.13510	-0.0000590918	0.0000750569
6.22667	-0.0000525513	0.0000625131
6.31824	-0.0000470419	0.0000583913
6.40980	-0.0000423547	0.0000448861
6.59294	-0.0000348358	0.0000379096
6.77608	-0.0000290878	0.0000249603
6.95922	-0.0000245593	0.0000203113
7.14235	-0.0000209075	0.0000155773
7.32549	-0.0000179118	0.0000168241
7.50863	-0.0000154235	0.0000144148
7.69176	-0.0000133380	0.0000123475
7.87490	-0.0000115782	0.0000070580
8.05804	-0.0000100850	0.0000052295
8.24118	-0.0000088125	0.0000082282
8.42431	-0.0000077237	0.0000034142
8.60745	-0.0000067888	0.0000032872
8.79059	-0.0000059833	0.0000052873
8.97373	-0.0000052872	0.0000021182
9.15686	-0.0000046837	0.0000019556
16.48235	-0.0000001377	-0.0000006904

- E TABLES -

TABLE E-1

HE2+2 MOLECULAR ION:

WAVEFUNCTION PSI 2

ZR	ZETA/Z**2	BETA/Z	GAMMA/Z
0.10000	0.93347	-0.0794423280	-0.1747441154
0.20000	0.91046	-0.0551977403	-0.1715458562
0.30000	0.87637	-0.0183704975	-0.1666155376
0.40000	0.83566	0.0268664444	-0.1603846494
0.50000	0.79206	0.0760563058	-0.1532360168
0.60000	0.74791	0.1245955284	-0.1454411833
0.70000	0.70422	0.1676492786	-0.1371770144
0.80000	0.66112	0.2006139909	-0.1286008905
0.90000	0.61874	0.2205068786	-0.1199297364
1.00000	0.57759	0.2272178189	-0.1114403978
1.10000	0.53853	0.2231747003	-0.1033899302
1.20000	0.50232	0.2118080172	-0.0959452102
1.30000	0.46939	0.1962362736	-0.0891713299
1.40000	0.43984	0.1787682869	-0.0830607686
1.50000	0.41356	0.1609130967	-0.0775647310
1.60000	0.39031	0.1435850046	-0.0726184038
1.70000	0.36979	0.1272853000	-0.0681518830
1.80000	0.35173	0.1122622942	-0.0640995951
1.90000	0.33585	0.0986029133	-0.0604011253
2.00000	0.32192	0.0863014044	-0.0570037494
2.10000	0.30972	0.0752966961	-0.0538612839
2.20000	0.29908	0.0654983779	-0.0509336100
2.30000	0.28985	0.0568016828	-0.0481863692
2.40000	0.28190	0.0490971494	-0.0455898262
2.50000	0.27515	0.0422763665	-0.0431183984
2.60000	0.26950	0.0362361319	-0.0407501345
2.70000	0.26489	0.0308805066	-0.0384665613
2.80000	0.26126	0.0261223824	-0.0362526540
2.90000	0.25855	0.0218855955	-0.0340971200
3.00000	0.25669	0.0181041055	-0.0319926258
3.10000	0.25563	0.0147273313	-0.0299367377
3.20000	0.25527	0.0117150058	-0.0279313577
3.30000	0.25553	0.0090431783	-0.0259834434
3.40000	0.25632	0.0066981526	-0.0241032215
3.50000	0.25750	0.0046758369	-0.0223030059
3.60000	0.25899	0.0029770297	-0.0205951506
3.70000	0.26068	0.0016019088	-0.0189899555
3.80000	0.26248	0.0005468852	-0.0174947443
3.90000	0.26433	-0.0001984440	-0.0161134634
4.00000	0.26617	-0.0006545157	-0.0148461567
4.10000	0.26796	-0.0008508804	-0.0136897849
4.20000	0.26968	-0.0008244814	-0.0126391935
4.30000	0.27131	-0.0006178413	-0.0116875635
4.40000	0.27282	-0.0002758464	-0.0108273120
4.50000	0.27421	0.0001570837	-0.0100501936
4.60000	0.27547	0.0006401111	-0.0093481083
4.70000	0.27660	0.0011379332	-0.0087132757
4.80000	0.27760	0.0016221012	-0.0081383315
4.90000	0.27848	0.0020712760	-0.0076166515
5.00000	0.27924	0.0024711745	-0.0071420763

HE2+2 MOLECULAR ION: WAVEFUNCTION PSI 2

ZR	ZETA/Z**2	BETA/Z	GAMMA/Z
5.10000	0.27989	0.0028134786	-0.0067092227
5.20000	0.28044	0.0030947308	-0.0063134250
5.30000	0.28091	0.0033154672	-0.0059504460
5.40000	0.28129	0.0034788508	-0.0056166540
5.50000	0.28162	0.0035897463	-0.0053089633
5.60000	0.28188	0.0036541094	-0.0050246315
5.70000	0.28210	0.0036783418	-0.0047612236
5.80000	0.28227	0.0036687733	-0.0045166858
5.90000	0.28242	0.0036314359	-0.0042892624
6.00000	0.28253	0.0035719151	-0.0040772954
6.10000	0.28262	0.0034951733	-0.0038794624
6.20000	0.28269	0.0034055503	-0.0036944771
6.30000	0.28275	0.0033067506	-0.0035212740
6.40000	0.28279	0.0032018729	-0.0033588764
6.50000	0.28282	0.0030934530	-0.0032064043
6.60000	0.28285	0.0029835557	-0.0030631135
6.70000	0.28287	0.0028737958	-0.0029283026
6.80000	0.28289	0.0027653819	-0.0028012961
6.90000	0.28290	0.0026592723	-0.0026815660
7.00000	0.28291	0.0025561249	-0.0025685774
7.20000	0.28292	0.0023603879	-0.0023609754
7.40000	0.28293	0.0021800338	-0.0021751511
7.60000	0.28293	0.0020152992	-0.0020083137
7.80000	0.28293	0.0018655140	-0.0018580993
8.00000	0.28293	0.0017295546	-0.0017224755
8.20000	0.28294	0.0016061721	-0.0015997280
8.40000	0.28294	0.0014940959	-0.0014883612
8.60000	0.28294	0.0013921366	-0.0013870857
8.80000	0.28294	0.0012992234	-0.0012947919
9.00000	0.28294	0.0012143744	-0.0012104887
9.20000	0.28294	0.0011367601	-0.0011333490
9.40000	0.28294	0.0010656229	-0.0010626226
9.60000	0.28294	0.0010003016	-0.0009976565
9.80000	0.28294	0.0009402137	-0.0009378762
10.00000	0.28294	0.0008848465	-0.0008827758
18.00000	0.28294	0.0001515435	-0.0001514826

TABLE E-2

LI2+4 MOLECULAR ION:

WAVEFUNCTION PSI 2

ZR	ZETA/Z**2	BETA/Z	GAMMA/Z
0.30000	0.93193	0.0181371071	-0.1738989747
0.60000	0.79258	0.1769835321	-0.1507316038
0.90000	0.64808	0.2632435867	-0.1224561132
1.20000	0.51898	0.2298602094	-0.0968471361
1.50000	0.42408	0.1638026001	-0.0779467278
1.80000	0.35928	0.1074629395	-0.0643178315
2.10000	0.31547	0.0666882940	-0.0540007732
2.40000	0.28621	0.0387919370	-0.0456706567
2.70000	0.26780	0.0201064284	-0.0385127870
3.00000	0.25812	0.0076383030	-0.0320449058
3.30000	0.25558	-0.0005758748	-0.0260722827
3.60000	0.25809	-0.0054406058	-0.0207049046
3.90000	0.26314	-0.0072289418	-0.0162038117
4.20000	0.26868	-0.0064340675	-0.0126919967
4.50000	0.27354	-0.0041632421	-0.0100730268
4.80000	0.27723	-0.0016705132	-0.0081449573
5.10000	0.27971	0.0002657067	-0.0067089911
5.40000	0.28122	0.0014508324	-0.0056141797
5.70000	0.28208	0.0020166833	-0.0047583378
6.00000	0.28253	0.0021777765	-0.0040746816
6.30000	0.28275	0.0021163171	-0.0035190552
6.60000	0.28286	0.0019541109	-0.0030613175
6.90000	0.28291	0.0017607155	-0.0026801153
7.20000	0.28293	0.0015704163	-0.0023598008
7.80000	0.28294	0.0012445577	-0.0018573228
8.40000	0.28294	0.0009969778	-0.0014878500
9.00000	0.28294	0.0008102130	-0.0012101387
9.60000	0.28294	0.0006672941	-0.0009974135
18.00000	0.28294	0.0001010383	-0.0001514764

TABLE E-3

BE2+6 MOLECULAR ION:

WAVEFUNCTION PSI 2

ZR	ZETA/Z**2	BETA/Z	GAMMA/Z
0.40000	0.91468	0.0922914487	-0.1704808276
0.80000	0.71304	0.2752677912	-0.1335806811
1.20000	0.52688	0.2377685977	-0.0972296691
1.60000	0.40411	0.1425081456	-0.0730623192
1.60000	0.40411	0.1425081456	-0.0730623192
2.00000	0.33127	0.0744593372	-0.0572413675
2.40000	0.28831	0.0334105617	-0.0457075049
2.80000	0.26482	0.0098715395	-0.0363165895
3.20000	0.25591	-0.0033102169	-0.0280469237
3.60000	0.25756	-0.0097474045	-0.0207645473
4.00000	0.26434	-0.0105718548	-0.0149678995
4.40000	0.27159	-0.0074208335	-0.0108762777
4.80000	0.27702	-0.0033441862	-0.0081489249
5.20000	0.28023	-0.0004474311	-0.0063116603
5.60000	0.28183	0.0009922569	-0.0050204206
6.00000	0.28253	0.0014773395	-0.0040734125
6.40000	0.28280	0.0015006221	-0.0033557911
6.80000	0.28290	0.0013549136	-0.0027989728
7.20000	0.28293	0.0011744801	-0.0023592186
7.60000	0.28294	0.0010076159	-0.0020069885
8.00000	0.28294	0.0008658095	-0.0017214751
8.40000	0.28294	0.0007480542	-0.0014875937
8.80000	0.28294	0.0006504060	-0.0012941909
9.20000	0.28294	0.0005690006	-0.0011328860
9.60000	0.28294	0.0005006296	-0.0009972901
10.00000	0.28294	0.0004427967	-0.0008824860
18.00000	0.28294	0.0000757823	-0.0001514733

