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ABSTRACT

In the new partitioning perturbation formalism for electron exchange problems, the exchange function W plays an important role. For H_2 and H_2^+ the W is determined variationally in terms of a 14 term Slater orbital basis set. Tables are given for expressing W at 14 values of the internuclear separation ranging from $R = 1a_o$ to $20a_o$.

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The Interaction of Ground State Hydrogen Atoms.

Consider the interaction of two ground state hydrogen atoms, a and b, separated by a distance R. There are two molecular states which arise from this separated-atom state: $({}^{g}E, {}^{g}\Psi)$, the ${}^{1}\Sigma_{g}^{+}$ ground state; and $({}^{u}E, {}^{u}\Psi)$, the ${}^{3}\Sigma_{u}^{+}$ repulsive excited state. The exact spatial wavefunctions for these states satisfy

$$(H - {}^{i}E)\,{}^{i}\Psi = 0,$$

and

$$A_{i}\,{}^{i}\Psi = {}^{i}\Psi \quad , \quad i = g \text{ or } u.$$

The hamiltonian H is defined by

$$H = -\tfrac{1}{2}(\nabla_1^2 + \nabla_2^2) - \frac{1}{r_{a1}} - \frac{1}{r_{a2}} - \frac{1}{r_{b1}} - \frac{1}{r_{b2}} + \frac{1}{r_{12}} + \frac{1}{R},$$

and A_{i} is a symmetry projector defined by

$$A_{\substack{g\\u}} = \left(\frac{1 \pm P_{12}}{2}\right)\left(\frac{1 \pm P_{ab}}{2}\right)\left(\frac{1+\sigma}{2}\right)\mathcal{O}_{\Sigma}.$$

The upper sign is for g symmetry; the lower, for u. P_{12} permutes the electron labels, P_{ab} permutes the nuclei labels, σ reflects the electronic coordinates across any plane which includes the internuclear axis, and $\mathcal{O}_{\Sigma}$ is the projection operator for the $M=0$ eigenfunction of the total azimuthal orbital angular momentum $\mathcal{L}_{z}$:

$$\mathcal{O}_{\Sigma} = \prod_{M>0}^{\infty} \frac{M - \mathcal{L}_{z}}{M}.$$

A_{i} is seen to be a compound projector for the symmetry group of H. The first factor in A_{i} projects onto the space of either singlet (upper sign) or triplet (lower sign) functions; the second,

onto either gerade or ungerade functions; the third, onto + functions; and the last factor projects onto the space of Σ functions.

Zeroth Order Primitive Functions. When the atoms are infinitely separated $(R \to \infty)$, an exact wavefunction for the system is

$$\phi_1^{(0)} = a_0(1)\, b_0(2),$$

where a_0 is a 1s orbital centered about nucleus a, and b_0 is a 1s orbital centered about nucleus b. The subscript "1" indicates the arbitrary assignment of electron 1 to atom a and electron 2 to atom b. Because of the physical indistinguishability of electrons, $\phi_1^{(0)}$ is degenerate with the configuration "2",

$$\phi_2^{(0)} = P_{12}\, \phi_1^{(0)} = b_0(1)\, a_0(2)$$

in the sense that

$$\langle \phi_1^{(0)} | H | \phi_1^{(0)} \rangle = \langle \phi_2^{(0)} | H | \phi_2^{(0)} \rangle .$$

This is a different type of degeneracy from that discussed in I in that $\phi_1^{(0)}$, $\phi_2^{(0)}$ are not degenerate eigenfunctions of the same unperturbed hamiltonian. In particular,

$$(H_1^{(0)} - \epsilon^{(0)})\, \phi_1^{(0)} = 0, \qquad (7)$$

where

$$H_1^{(0)} = h_a(1) + h_b(2) \quad ; \quad \epsilon^{(0)} = 2e_0 ; \qquad (8)$$

and

$$h_a = -\tfrac{1}{2}\nabla^2 - \frac{1}{r_a} \,, \qquad (9)$$

and ϵ_0 is the energy of a ground state hydrogen atom ($= -\frac{1}{2}$ Hartree), but

$$(H_2^{(0)} - \epsilon^{(0)})\,\phi_2^{(0)} = 0 \,,$$

where

$$H_2^{(0)} = P_{12} H_1^{(0)} P_{12} = h_b(1) + h_a(2) \,. \qquad (10)$$

Eq. (8) and (10) give $H_1^{(0)} - H_2^{(0)} = \left(\frac{1}{r_{b1}} + \frac{1}{r_{a2}} - \frac{1}{r_{a1}} - \frac{1}{r_{b2}}\right)$.

In group theoretic language, $\phi_1^{(0)}$ and $\phi_2^{(0)}$ are "primitive functions", i.e., they are a basis for <u>reducible</u> representation of the symmetry group of H. Since $\phi_1^{(0)}$ and $\phi_2^{(0)}$ do not have pure symmetry, there is no Rayleigh-Schrödinger expansion of ${}^g\Psi$, ${}^u\Psi$ which starts from $\phi_1^{(0)}$, $\phi_2^{(0)}$ as the unperturbed states and produces a wavefunction that has the symmetry of the exact functions, <u>order by order</u>.

<u>Heitler-London Wavefunctions</u>.[32] The projectors A_g, A_u allow the construction of zeroth order functions which do have the symmetry of the exact wavefunction. Putting

$${}^g\Psi^{(0)} = \frac{A_g \phi_1^{(0)}}{\langle A_g \phi_1^{(0)} | A_g \phi_1^{(0)} \rangle^{1/2}} = \frac{a_0(1) b_0(2) + b_0(1) a_0(2)}{\sqrt{2}\,\langle \phi_1^{(0)} | 1 + P_{12} | \phi_1^{(0)} \rangle^{1/2}} \,,$$

and

(11)

$$ {}^{u}\Psi^{(0)} = \frac{A_u \phi_1^{(0)}}{\langle A_u \phi_1^{(0)} | A_u \phi_1^{(0)} \rangle^{1/2}} = \frac{a_0(1) b_0(2) \mp b_0(1) a_0(2)}{\sqrt{2} \langle \phi_1^{(0)} | 1 - P_{12} | \phi_1^{(0)} \rangle^{1/2}} , $$

yields the Heitler-London approximation to the wavefunctions. In perturbation theory, the energy through first order is simply the expectation value of H computed with the zeroth order wavefunction. Thus

$$ {}^{i}E^{(0)} + {}^{i}E^{(1)} = \langle {}^{i}\Psi^{(0)} | H | {}^{i}\Psi^{(0)} \rangle . $$

Eq. (7), (9), and (11) yield

$$ {}^{g}E^{(0)} = {}^{u}E^{(0)} = \epsilon^{(0)} , $$

and

$$ {}^{g}_{u}E^{(1)} = \frac{\langle \phi_1^{(0)} | (H - H_1^{(0)})(1 \pm P_{12}) | \phi_1^{(0)} \rangle}{\langle \phi_1^{(0)} | 1 \pm P_{12} | \phi_1^{(0)} \rangle} $$

(12)

$$ = \frac{V_{aa} \pm V'_{aa}}{1 \pm S_{ab}^2} , $$

where

$$V_{oo} = \iint [a_0(1)\, b_0(2)]^2 \left[\frac{1}{r_{12}} - \frac{1}{r_{a2}} - \frac{1}{r_{b1}} + \frac{1}{R}\right] d\tau_1 d\tau_2 ,$$

$$V'_{oo} = \iint a_0(1)\, b_0(1)\, a_0(2)\, b_0(2) \left[\frac{1}{r_{12}} - \frac{1}{r_{a2}} - \frac{1}{r_{b1}} + \frac{1}{R}\right] d\tau_1 d\tau_2 ,$$

$$S_{oo} = \int a_0(1)\, b_0(1)\, d\tau_1 . \qquad (13)$$

The integrals in Eq. (13) are all well known.[32,33]

It is not possible to proceed in a straightforward manner to higher order, however, since ${}^{g}\Psi^{(0)}$, ${}^{u}\Psi^{(0)}$ are not eigenfunctions of $H_1^{(0)}$ or $H_2^{(0)}$.

Exact Primitive Functions. On the other hand, given the exact spatial wavefunctions ${}^{g}\Psi$ and ${}^{u}\Psi$, it is possible to construct two exact primitive functions Φ_1 and Φ_2 which have precisely the same transformation properties as $\phi_1^{(0)}$ and $\phi_2^{(0)}$. That is,

$$\Phi_2 = P_{12}\, \Phi_1 , \qquad (14)$$

where

$$\Phi = \Psi\, C , \qquad (15)$$

and

$$\Phi = (\Phi_1, \Phi_2),$$

$$\Psi = ({}^{g}\Psi, {}^{u}\Psi).$$

Eq. (14) and the requirement that Φ_1 and Φ_2 be normalized implies

$$C = \begin{pmatrix} \cos\theta & \cos\theta \\ \sin\theta & -\sin\theta \end{pmatrix}.$$

As R increases without limit, θ approaches $\theta_0 = \arctan[(1+S_{ab}^2)/(1-S_{ab}^2)]^{1/2}$ and Φ_1 approaches $\phi_1^{(0)}$.

Exact primitive functions have been discussed previously by Herring,[16] Hirschfelder and Silbey,[15] and Musher.[34] Intuitively one expects Φ_1 to have electron 1 localized about atom a and electron 2 about atom b. Herring, who calls Φ_1 the "home base" function, enforces this intuition by asserting a set of auxiliary conditions that Φ_1 must satisfy, such as the requirement that Φ_1 approach $\phi_1^{(0)}$ when $r_{a1} = 0$ or $r_{b2} = 0$. (It is not obvious that this condition can be satisfied.) By contrast, Hirschfelder and Silbey enforce their intuition only in zeroth order by setting up a perturbation sequence for Φ_1 which starts from $\phi_1^{(0)}$. This is the approach followed here.

The set of coupled equations satisfied by Φ is

$$H\Phi = \Phi\mathcal{E}, \qquad (16)$$

where

$$\mathbb{G} = \mathbb{C}^{-1}\,\mathbb{E}\,\mathbb{C}$$

and

$$\mathbb{E} = \begin{pmatrix} {}^{g}E & 0 \\ 0 & {}^{u}E \end{pmatrix}.$$

It is convenient to define two energies, the Coulomb energy

$$E(coul) = \tfrac{1}{2}\left({}^{g}E + {}^{u}E\right),$$

and the exchange energy

$$E(exch) = \tfrac{1}{2}\left({}^{g}E - {}^{u}E\right).$$

Then,

$$\mathbb{G} = \begin{pmatrix} E(coul) & E(exch) \\ E(exch) & E(coul) \end{pmatrix}.$$

Given Φ_1, Φ_2; the exact wavefunctions ${}^{g}\Psi$, ${}^{u}\Psi$ are obtained by projection

$${}^{i}\Psi = \frac{A_i\,\Phi_1}{\langle A_i\Phi_1 | A_i\Phi_1\rangle^{1/2}}.$$

The energies are given by

$${}^{i}E = \langle {}^{i}\Psi | H | {}^{i}\Psi \rangle.$$

Perturbation Expansion. The formalism developed in I suggests itself as a means of solving Eq. (16). It must be extended somewhat, however, since the previous analysis assumed that all of the unperturbed functions are eigenfunctions of the same hamiltonian. This assumption is no longer valid in exchange perturbation problems.

The zeroth order equations corresponding to Eq. (16) are defined to be

$$(H_1^{(0)} - \epsilon^{(0)})\phi_1^{(0)} = 0,$$

and (17)

$$(H_2^{(0)} - \epsilon^{(0)})\phi_2^{(0)} = 0.$$

Corresponding to $\phi_1^{(0)}$ and $\phi_2^{(0)}$ are the perturbations

$$H_1^{(1)} = H - H_1^{(0)},$$

and

$$H_2^{(1)} = H - H_2^{(0)},$$

respectively. The superscripts are used in a loose sense to denote the order of perturbation. As discussed previously, , "order" is not a well defined concept, however, since

$$[H_1^{(1)}, P_{12}] = [P_{12}, H_1^{(0)}] = \left(\frac{1}{r_{a1}} + \frac{1}{r_{b2}} - \frac{1}{r_{a2}} - \frac{1}{r_{b1}}\right)P_{12}. \quad (18)$$

Eq. (18) states that a "zeroth order" quantity is equal to a "first order" quantity, so that the apparent order of terms can be arbitrarily shifted.

Nevertheless, Eq. (16) can be expanded into different orders in a consistent, though arbitrary, manner by defining

$$\mathcal{E} = \epsilon^{(0)} 1 + \sum_{n=1}^{\infty} \lambda^n \mathcal{E}^{(n)},$$

and (19)

$$\Phi = \phi^{(0)} + \sum_{n=1}^{\infty} \lambda^n \phi_1^{(n)},$$

where λ is a formal ordering parameter whose physical value is unity. The hamiltonian can be resolved in two ways, either as $H_1 = H_1^{(0)} + \lambda H_1^{(1)}$ or as $H_2 = H_2^{(0)} + \lambda H_2^{(1)}$. Only for $\lambda = 1$ does $H_1 = H_2 = H$. The convention adopted here is that when H acts on Φ_k, it is replaced by H_k, $k = 1$ or 2.

Substituting the expansions (19) into Eq. (16) and equating the coefficient of each power of λ to zero yields, in addition to Eq. (17), for $k = 1$ and 2,

$$(H_k^{(0)} - \epsilon^{(0)})\phi_k^{(1)} + H_k^{(1)}\Phi_k^{(0)} = \sum_{l=1}^{2} \Phi_l^{(0)} \epsilon_{lk}^{(1)};$$

(20)

$$(H_k^{(0)} - \epsilon^{(0)})\phi_k^{(n)} + H_k^{(1)}\phi_k^{(n-1)} = \sum_{m=1}^{n} \sum_{l=1}^{2} \phi_l^{(n-m)} \epsilon_{lk}^{(m)}; \quad n \geq 1.$$

Given the solution of the first N perturbation equations (20) the energy is given by

$$\mathcal{E} = \frac{\langle A_i \Phi_1^{(N)} | H | A_i \Phi_1^{(N)} \rangle}{\langle A_i \Phi_1^{(N)} | A_i \Phi_1^{(N)} \rangle},$$

where

$$\Phi_1(N) = \sum_{n=0}^{N} \phi_1^{(n)}.$$

The justification for this procedure has been developed in I.

If χ is any wavefunction which is orthogonal to $\Phi_1(N)$ and $\Phi_2(N)$ then the hamiltonian matrix elements $\langle A_i \Phi_1(N) | H | A_i \chi \rangle$ vanish through $O(\lambda^{N+1})$. Hence the addition of χ to the basis $\Phi(N)$ affects the energy only by $O(\lambda^{2N+2})$ terms.

Equivalence to Hirschfelder-Silbey Perturbation Theory.[15] It is easily verified that Eq. (16) is identical to the equation solved in the Hirschfelder-Silbey exchange perturbation theory for the interaction of ground state hydrogen atoms. Nevertheless, the solution of first order Eq. (20) is discussed in detail below in order (1) to demonstrate that, in analogy with almost degenerate perturbation theory, the off-diagonal elements of $\mathcal{E}$ are not completely fixed by the formalism; and (2) to develop a method of solving Eq. (20) which reduces the corresponding equation for many-electron systems to one and two electron equations.

Solution of the First Order Equation. Eq. (14) implies that $\phi_2^{(1)} = P_{12}\phi_1^{(1)}$, so that it is sufficient to consider only $k=1$ in Eq. (20), which may be written

$$(H_1^{(0)} - \epsilon^{(0)})\phi_1^{(1)} + H_1^{(1)}\phi_1^{(0)} = E^{(1)}(\text{coul})\phi_1^{(0)} + E^{(1)}(\text{exch})\phi_2^{(0)}. \qquad (21)$$

Multiplying Eq. (21) from the left by $\phi_1^{(0)*}$ and integrating yields

$$V_{oo} = E^{(1)}(Coul) + S_{oo}^2 E^{(1)}(exch), \qquad (22)$$

where V_{oo} is defined by Eq. (13). Thus, in analog, with almost degenerate perturbation theory, the requirement of mathematical consistency gives only one equation to determine the two unknown first-order energies.

In the Hirschfelder-Silbey procedure,[15] a further relation between $E^{(1)}(Coul)$ and $E^{(1)}(exch)$ is obtained by arbitrarily imposing the requirement that the energy through first order agree with the Heitler-London result, Eq. (12). This yields

$$E^{(1)}(Coul) = \frac{V_{oo} - S_{oo}^2 V_{oo}'}{1 - S_{oo}^4}, \qquad (23)$$

and

$$E^{(1)}(exch) = \frac{V_{oo}' - S_{oo}^2 V_{oo}}{1 - S_{oo}^4},$$

which clearly satisfy Eq. (22).

Another way to fix the unknown constants is by a variational method analogous to that introduced in the almost degenerate perturbation theory [1]. It was shown there that such a procedure can be expected to have a small effect upon the energy in a rapidly converging perturbation expansion. Thus, the question of applying the variational procedure to the present case cannot be answered without testing the convergence properties of the formalism with numerical examples. For the present, it is assumed that $E^{(1)}(Coul)$ and $E^{(1)}(exch)$ are fixed by Eq. (23).

With the constants in Eq. (21) fixed, the $\phi_i^{(1)}$ can be obtained. To this end, it is convenient to separate Eq. (21) into a polarization equation

$$(H_1^{(0)} - \epsilon^{(0)})\hat{\phi}_i^{(1)} + (H_1^{(1)} - V_{ee})\phi_i^{(0)} = D, \quad (24)$$

and an exchange equation

$$(H_1^{(0)} - \epsilon^{(0)})\omega_i^{(1)} = \phi_2^{(0)} - S_{ee}^2\,\phi_i^{(0)}, \quad (25)$$

where

$$\phi_i^{(1)} = \hat{\phi}_i^{(1)} + \omega_i^{(1)}\,E^{(1)}(exch).$$

The polarization equation is the first order equation in the unsymmetrical polarization expansion[35] of ${}^{1}\Psi$ or ${}^{3}\Psi$. For the case of H_2, it has been solved to high accuracy by variational methods by Hirschfelder and Löwdin[36] and by Kolos.[37] The primary effect of $\hat{\phi}_i^{(1)}$ is to introduce correlations between the electrons which give rise to van der Waals interactions. The solution of Eq. (24) will not be considered further.

The solution of the exchange equation will be considered in detail. In terms of the orbitals a_e and b_e, Eq. (25) may be written

$$(h_a(1) - e_e + h_b(2) - e_e)\omega_i^{(1)}(1,2) = b_e(1)a_e(2) - S_{ee}^2\,a_e(1)b_e(2) \quad (26)$$

Thus, Eq. (26) is a coupled, two electron, two center equation. Introducing the complete set of eigenfunctions of h_a and h_b,

$$(h_a - e_k)a_k = 0 \quad , \quad (h_b - e_k)b_k = 0 ,$$

the solution of Eq. (26) is

$$\omega_1^{(1)}(1,2) = \sum_{k\neq 0}\sum_{l\neq 0} \frac{\langle a_k | b_0\rangle a_k(1)\,\langle b_l | b_0\rangle b_l(2)}{e_k' + e_l'} \qquad (27)$$

$$+ S_{ab}\left[\sum_{k\neq 0}\frac{\langle a_k|b_0\rangle a_k(1)}{e_k'} b_0(2) + \sum_{l\neq 0} a_0(1)\frac{\langle b_l|a_0\rangle b_l(2)}{e_l'}\right],$$

where $e_k' = e_k - e_0$; $e_l' = e_l - e_0$.

The infinite sums in Eq. (27) may be evaluated by a technique which[38] has been used successfully for the calculation of atomic polarizabilities, van der Waals C_6 coefficients, etc. The first sum in Eq. (27) is analogous to dispersion energies in the polarization equation and the last two sums are analogous to induction energies. The sums for $\alpha > 0$ and $\beta > 0$ may be evaluated using the identity,

$$\frac{1}{\alpha+\beta} = \frac{1}{2\pi}\int_0^\infty \left[\frac{1}{\alpha+iu} + \frac{1}{\alpha-iu}\right]\left[\frac{1}{\beta+iu} + \frac{1}{\beta-iu}\right] du \qquad (28)$$

which can be shown to be an application of the residue theorem. Putting $\alpha = e_k'$, $\beta = e_l'$, substituting Eq. (28) into

Eq. (27) and interchanging the order of summation and integration yields

$$\omega_1^{(1)} = \frac{1}{\pi}\int_0^\infty \Big[\sum_{k\neq 0}\frac{\langle a_k|b_0\rangle}{e_k'+iu}a_k(1) + \sum_{k\neq 0}\frac{\langle a_k|b_0\rangle}{e_k'-iu}a_k(1)\Big]$$

$$\times\Big[\sum_{\ell\neq 0}\frac{\langle b_\ell|a_0\rangle}{e_\ell'+iu}b_\ell(2) + \sum_{\ell\neq 0}\frac{\langle b_\ell|a_0\rangle}{e_\ell'-iu}b_\ell(2)\Big]du$$

$$+ S_{00}\Big[\sum_{k\neq 0}\frac{\langle a_k|b_0\rangle}{e_k'}a_k(1)b_0(2) + \sum_{\ell\neq 0}\frac{\langle b_\ell|a_0\rangle}{e_\ell'}a_0(1)b_\ell(2)\Big],$$

or

$$\omega_1^{(1)} = \frac{1}{\pi}\int_0^\infty \big[\xi_+^a(1)+\xi_-^a(1)\big]\big[\xi_+^b(2)+\xi_-^b(2)\big]du \qquad (29)$$

$$+\Big(S_{00}\big[\xi_0^a(1)b_0(2) + a_0(1)\xi_0^b(2)\big],$$

where

$$(h_0 - e_0 + iu)\xi_+^a = b_0 - S_{00}a_0, \qquad (30)$$

and

$$(h_0 - e_0 + iu)\xi_+^b = a_0 - S_{00}b_0,$$

and $\xi_-^a = (\xi_+^a)^*$, $\xi_-^b = (\xi_-^b)^*$. The ξ_0^a and ξ_0^b are the solutions of Eq. (30) for $u=0$. In the application[29] of the Hirschfelder-Silbey formalism to H_2^+, the first order exchange function $\omega_1^{(1)}$ is simply ξ_0^a defined by Eq. (30).

Thus it has been shown that $\omega_1^{(1)}$ can be obtained by solving the one electron, two center Eq. (30) and performing the quadrature, Eq. (29)..

Variational Approach. Eq. (30) is still a coupled two-dimensional partial differential equation, and an exact closed form solution does not appear possible. Variational approximations to the exact solution may be obtained by finding the extreme points of the functional[39]

$$J[\tilde{\xi}^a] = \langle \tilde{\xi}^a_- | h_0 - e_0 + \nu u \,|\, \tilde{\xi}^a_+ \rangle - \langle \tilde{\xi}^a_- \,|\, b_0 - S_{00}\, a_0 \rangle - \langle b_0 - S_{00}\, a_0 \,|\, \tilde{\xi}^a_+ \rangle , \qquad (31)$$

where $\tilde{\xi}^a_+$, $\tilde{\xi}^a_- = (\tilde{\xi}^a_+)^*$ are trial functions.

The functional J is analogous to the Hylleraas functional for second order energies. For $u = 0$, $J[\tilde{\xi}^a_+]$ provides an upper bound to $J[\xi^a_0]$; where ξ^a_0 is the exact $(u = 0)$ solution of Eq. (30). If $\tilde{\xi}^a_0$ is a linear variational function, increasing the size of the basis set necessarily yields a better bound to $J[\xi^a_0]$. If $\hat{\xi}^a_0$ denotes the value of $\tilde{\xi}^a_0$ which minimizes J , then

$$J[\hat{\xi}^a_+] = -\langle b_0 - S_{00}\, a_0 \,|\, \hat{\xi}^a_0 \rangle \geq J[\xi^a_0].$$

We have chosen the trial function $\tilde{\xi}^a_+$ to have the form

$$\tilde{\xi}^a_+ = \sum_{k=1}^{N} c_k \chi^a_k , \qquad (32)$$

where the χ_k^a are linear combinations of Slater-type orbitals, centered on nucleus a and b, which diagonalize the hydrogen atom hamiltonian h_a; i.e.

$$\langle \chi_k^a | h_a | \chi_l^a \rangle = \tilde{e}_k \delta_{kl} \quad ; \quad \langle \chi_k^a | \chi_l^a \rangle = \delta_{kl} \tag{33}$$

The values of the variational parameters c_k which minimize J are given by

$$c_k = \frac{\langle \chi_k^a | b_0 - \xi_0 a_0 \rangle}{\tilde{e}_k - e_0 + i\nu} \, . \tag{34}$$

We have computed the χ_k^a and c_k for values of R ranging from $1a_0$ to $20a_0$ with various size basis sets.

Here

$$\chi_k^a = \sum_j D_{kj} \theta_j \, ,$$

where the D_{kj} are the coefficients of the Slater orbitals θ_j. Half of the Slater orbitals are centered on a and the others

are centered on b. They have the form

$$ns_a = (2^{2n-1} / (2n)! \pi)^{1/2} r_a^{n-1} \exp(-r_a) \quad ,$$

$$np_a = (2^{2n-1} 3 / (2n)! \pi)^{1/2} r_a^{n-1} \cos\theta_a \exp(-r_a).$$

The ns_b , np_b are the reflection of ns_a , np_a through the midpoint of the internuclear axis. The following tables give $\tilde{e}(k)$ which the computer output calls E(k); $\langle \chi_k^a | h_0 - a_0 S_{00} \rangle$ designated (B-SA,X(K)); the coefficients D_{kj} ; and the minimum value of the functional J.

Substituting Eq. (32) into (29) and integrating yields an expression for $\omega_1^{(1)}$ which has the same form as Eq. (27), with χ_k^a replacing a_k, $\tilde{e}_k' = \tilde{e}_k - e_0$ replacing e_k' and (the reflection of χ_k^a through the midpoint of the internuclear axis) replacing b_k . Because χ_k^a involves Slater functions centered on a and on b , it is seen that $\omega_1^{(1)}$ contains the polarized ionic states (e.g. $2p_{0a}(1)\, 2p_{0a}(2)$) which have been shown[23] to be necessary to obtain good exchange energies.

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VARIATIONAL APPROXIMATION TO THE EXCHANGE FUNCTION ZETA

(H(A)-E(0)+IU)ZETA = B-SA

H(A) = HYDROGEN ATOM HAMILTONIAN E(0) = -0.5

ZETA = S((B-SA,X(K))/(E(K)-E(0)+IU))X(K)

INTERNUCLEAR DISTANCE R = 1.0000

FUNCTIONS X(K) WHICH DIAGONALIZE H(A)

E(K)	-0.4999999996	-0.1204360864	-0.1145222367	0.0077123659	0.0824532319	0.1558005626	0.1917956985
(B-SA,X(K))	0.0000000001	-0.2905395081	-0.0055123483	0.0075649599	-0.2963095990	0.0177955714	0.0093666058

STO EXPANSION COEFFICIENTS OF SLATER-TYPE ORBITALS

(EXPONENTS=1)							
1SA	0.9999986297	0.0180401482	0.5505855953	-5.3999527735	5.2882956261	74.6797177084	0.1958909152
1SB	0.0000013693	0.0739598980	-0.0571450496	5.7654634442	-5.2889357577	-74.6585807726	-0.5141492876
2SA	-0.0000023988	0.0369778439	-0.2056296419	-10.0108193427	8.3059776968	130.8147765473	-0.3723628404
3SA	-0.0000026818	-0.5330812770	0.8606919470	-9.4165513639	11.6522361659	145.9056045748	6.1327169322
4SA	-0.0000032457	0.1757497589	-1.0770714073	-11.9491831970	8.8791720576	163.7106480002	-0.5147734141
2PA	-0.0000000966	-0.2343945212	0.1172674418	-0.9521068270	0.3241286665	5.5677095962	0.2019857673
3PA	-0.0000001048	-0.0049956327	-0.1908503976	-0.4913526387	-0.7524522816	8.6437250157	-1.7377342847
4PA	-0.0000008983	-0.7120647525	0.4267067138	-6.4819592260	4.7668537243	44.5931609208	2.1357263041
2SB	0.0000023994	-0.1565035610	-0.3329620349	9.8324237824	-7.9000766230	**********	-1.9582415423
3SB	0.0000026839	0.7871636709	0.2464500844	11.7137872137	-13.3242108740	**********	0.5061842621
4SB	0.0000032441	-0.5727291682	-0.6642162888	10.2522812830	-7.6618469284	**********	-3.7828148224
2PB	0.0000000964	0.0408416010	0.0306939489	-0.0086808517	-0.4792831919	-5.6360871429	0.1351200658
3PB	0.0000001067	-0.1540301100	-0.1010984366	1.4812442948	0.2754273616	-8.3667885514	-0.7061898337
4PB	0.0000008931	0.2773406980	0.0567185648	-0.8158998775	-3.4393333457	-45.4362539016	0.0397345533

FUNCTIONS X(K) WHICH DIAGONALIZE H(A)

E(K)	0.4573760379	0.7978861430	1.0710492814	1.7963005423	3.3325046275	4.9806209044	8.6513550607
(B-SA,X(K))	0.0102778936	-0.2697521216	0.0399089551	-0.0137940575	-0.0135399599	-0.1213504447	0.0300973435

STO EXPANSION COEFFICIENTS OF SLATER-TYPE ORBITALS

(EXPONENTS=1)							
1SA	2.5972867903	-1.9568651436	-18.8150831307	2.6263045126	3.5613285266	6.7562417471	17.5286187399
1SB	-2.1172047332	2.2375657147	18.7634847257	-0.0290574162	1.7168443989	-9.4721582565	-16.8217744571
2SA	6.4192433421	-2.7432786212	-37.5213387590	-4.0284323463	-12.5581610845	9.8832483306	62.7046738463
3SA	0.1612121288	-11.7066196830	-39.3461581534	5.5820915570	12.1310847369	-10.8569142714	-64.6453038901
4SA	19.4233367634	-33.1184249306	**********	5.4732136221	-9.6623617497	57.0152100902	223.1659473740
2PA	-0.2486145076	-0.3952142272	4.1150817592	3.3428051967	-3.3571543994	7.5342711338	19.3198955171
3PA	-6.8986969673	8.6535333490	32.1879248526	-7.8798446818	8.3974857708	-20.7697724444	-58.2801253553
4PA	10.5603598163	-12.3395664750	-62.0170965856	5.9635988586	-6.6705467668	19.2434615344	60.0860413788
2SB	-3.0313010335	0.3737485647	38.1859496683	-3.7723233888	-1.2575939336	-3.0015327153	-64.4704014938
3SB	-7.1635996622	15.3829866620	38.2951779384	3.5547857973	2.4227360618	3.6649592593	66.4719203152
4SB	-16.0339622288	31.3876011632	229.2099168897	-9.4638589262	4.1275534502	-54.2390821157	**********
2PB	0.3726807996	-0.0836780540	-3.8842617276	1.8522867876	-4.2388163614	-5.5196126204	-20.0655592363
3PB	-3.8098196237	-6.5735450877	-33.5742636304	-2.8960457241	8.8884345649	15.9730611998	59.9782429272
4PB	1.7804525168	10.3935890407	63.3186167916	0.7800408450	-5.2320372299	-15.8093858708	-61.2679122128

J(MINIMUM) = -0.4340430412

VARIATIONAL APPROXIMATION TO THE EXCHANGE FUNCTION ZETA

(H(A)-E(0)+IU)ZETA = B-SA

H(A) = HYDROGEN ATOM HAMILTONIAN E(0) = -0.5

ZETA = S((B-SA+X(K))/(E(K)-E(0)+IU))X(K)

INTERNUCLEAR DISTANCE R = 1.5000

FUNCTIONS X(K) WHICH DIAGONALIZE H(A)

E(K)	-0.4999999994	-0.1209387132	-0.1147617313	0.0039917255	0.0713076908	0.1490852534	0.1845057124
(B-SA+X(K))	0.0000000001	0.4072927093	-0.0193843700	-0.0111817522	-0.3986802828	-0.0417212097	0.0319369384

STO (EXPONENTS=1) — EXPANSION COEFFICIENTS OF SLATER-TYPE ORBITALS

1SA	0.9999998533	-0.0908956006	0.5221039306	2.0864237140	2.8988642121	-21.6405837494	0.0062512161
1SB	0.0000001461	-0.0234469425	-0.0413139173	-2.4414004109	-2.9222063562	21.6155765303	-0.2983583363
2SA	-0.0000002663	-0.0723500957	-0.2488290016	4.2881044575	4.4204093225	-38.7266435632	-0.7091857938
3SA	-0.0000002505	0.2672482694	0.8340522080	-2.9478596702	-5.8563922138	39.6477073329	5.3822034932
4SA	-0.0000004693	-0.1310346618	-1.1435414527	6.1790877886	5.0865508885	-54.3273194646	-1.0701453480
2PA	-0.0000000153	0.2344078463	0.1421549138	0.7050504588	0.3256492526	-2.5974838374	0.2478750110
3PA	0.0000000122	-0.0042487419	-0.2209935123	0.0490183883	-0.9092462778	-2.9894192948	-2.0950627017
4PA	-0.0000001835	0.6657225810	0.5032009970	-4.3427340770	-4.2166365545	20.7117683729	2.4537821159
2SB	0.0000002670	0.2249994345	-0.2790010810	-4.2043485480	-3.9254852303	38.8268203130	-1.4611567546
3SB	0.0000002508	-0.5965506685	0.2625249624	-4.9330285051	-8.0440601970	39.1118049305	0.9154695484
4SB	0.0000004689	0.6456294509	-0.5838660494	-4.7086296576	-3.4667659078	54.6924121985	-3.0579478850
2PB	0.0000000166	-0.0356538732	0.0270228933	0.1046974581	-0.4150653523	2.6946857868	0.1457117309
3PB	-0.0000000156	0.1350949756	-0.0891088249	-1.2251299940	0.3371727064	2.5608658707	-0.7146803403
4PB	0.0000001856	-0.2189623824	0.0374199484	0.8196494252	-2.8150891160	21.6959644244	0.0474938934

FUNCTIONS X(K) WHICH DIAGONALIZE H(Ā)

E(K)	0.4243342089	0.7045158304	0.9994316172	1.5675811372	2.8576081232	4.0449147541	7.0196026305
(B-SA+X(K))	-0.0082126486	0.3404023019	-0.0791799084	-0.0438532010	0.0437526701	-0.1284786814	-0.0589453470

STO (EXPONENTS=1) — EXPANSION COEFFICIENTS OF SLATER-TYPE ORBITALS

1SA	-1.4189178999	0.8925831669	5.8985603446	1.8346612685	-4.2136523983	0.9118676142	-2.2304514308
1SB	0.8434855254	-1.1003375712	-5.8369137947	-0.1204122210	0.0930522648	-5.3298377052	0.7977506452
2SA	-4.1810493448	2.0689597926	13.9957460456	-2.3168422210	9.7857258499	11.1956877266	-25.7877927362
3SA	3.7157924697	3.5461421359	1.3655134679	3.1247799963	-9.7313658949	-13.7701854340	30.9741024654
4SA	-9.9541656408	17.1784278629	74.5468610283	4.8573895989	-0.1317675978	30.4466021601	-67.8524054047
2PA	-0.0745058073	0.6804446375	-1.4543653664	3.6191794789	-0.2166332273	5.7835279135	-8.3563462351
3PA	4.4720419499	-7.4802944219	-15.3159380232	-8.5408107301	0.4289245875	-15.6523038459	24.7057654345
4PA	-6.5885334720	9.7897857439	27.9739791146	6.4949637160	-0.3686597964	14.1108448147	-24.9056688957
2SB	1.2399976553	0.9957239428	-15.0747975917	-3.1032901743	1.2823415544	0.1949280029	29.3838829333
3SB	2.7431538380	-8.6207770174	0.3785046954	3.4666745065	-2.1133313372	1.7592609168	-34.7099982062
4SB	6.7674135072	-14.7407791540	-75.3401190974	-7.8685620724	4.7105249666	-25.7739812909	69.2876205575
2PB	-0.5003895740	-0.0948263059	0.9708782739	1.9922800269	3.7622737383	-4.0755379366	9.1153616970
3PB	3.3636270057	5.1029344946	17.2308838936	-2.8670356986	-8.4546629461	11.4183590044	-26.4610592425
4PB	-1.8399122363	-7.5935899249	-29.6024044319	0.4985273627	5.8783744614	-10.9904893166	26.1447343328

J(MINIMUM) = -0.8272841415

VARIATIONAL APPROXIMATION TO THE EXCHANGE FUNCTION ZETA

(H(A)-E(0)+IU)ZETA = B-SA

H(A) = HYDROGEN ATOM HAMILTONIAN E(0) = -0.5

ZETA = S((B-SA,X(K))/(E(K)-E(0)+IU))X(K)

INTERNUCLEAR DISTANCE R = 2.0000

FUNCTIONS X(K) WHICH DIAGONALIZE H(A)

E(K)	-0.4999999998	-0.1213250856	-0.1149050283	0.0000368644	0.0627550249	0.1425962567	0.1790571656
(B-SA,X(K))	-0.0000000002	0.4960677428	-0.0393086679	0.0182888188	0.4648492962	0.0685057208	-0.0651106028

STO EXPANSION COEFFICIENTS OF SLATER-TYPE ORBITALS

(EXPONENTS=1)							
1SA	-0.9999999777	-0.1261158382	0.4995037604	-0.9373408414	-1.8131461069	8.7796443801	0.0719958500
1SB	-0.0000000210	-0.0035414690	-0.0289158393	1.2983739280	1.8743129255	-8.7450141544	0.2061711568
2SA	0.0000000410	-0.0700304907	-0.2820697462	-2.3494415238	-2.7574096610	16.3339586719	0.8205473628
3SA	0.0000000255	0.1286243056	0.8164264564	-0.7783872931	-3.0979510857	14.4125307556	-4.9055739341
4SA	0.0000000870	-0.0695471078	-1.2018378926	-4.1333995872	-3.5653850571	25.9962308449	1.3014055495
2PA	0.0000000053	0.2390686463	0.1528506896	-0.5913861910	-0.3555871965	1.5528287248	-0.2735488191
3PA	-0.0000000120	-0.0211999417	-0.2263367016	0.1791828224	1.0843090602	1.1743053340	2.2729799309
4PA	0.0000000455	0.6378554412	0.5326989856	-3.2363735452	-3.8438706227	12.0807032690	-2.6226373515
2SB	-0.0000000424	0.2492255579	-0.2373602815	2.3054560400	2.1887532313	-16.4773654058	1.2159233461
3SB	-0.0000000265	-0.5149547998	0.2749679170	2.4845316777	5.6856489517	-13.6603415385	-1.1096762513
4SB	-0.0000000860	0.6682715023	-0.5168282479	2.8929139943	1.6327066604	-26.5076325932	2.6842021426
2PB	-0.0000000044	-0.0258941101	0.0170161666	-0.1657423220	0.3475344357	-1.6971446614	-0.1249317330
3PB	0.0000000090	0.1036737203	-0.0610392437	1.1230122211	-0.2990262830	-0.5494890234	0.6567402173
4PB	-0.0000000422	-0.1586639910	0.0123871006	-0.8386280663	2.3160120952	-13.2316970425	-0.0010279466

FUNCTIONS X(K) WHICH DIAGONALIZE H(A)

E(K)	0.3912857336	0.6470527845	0.9369275918	1.4103369245	2.4430131767	3.5354313936	6.0763183541
(B-SA,X(K))	-0.0103291194	-0.3711867986	0.1190338930	-0.0839267821	0.0466452227	-0.1175599946	0.0883574545

STO EXPANSION COEFFICIENTS OF SLATER-TYPE ORBITALS

(EXPONENTS=1)							
1SA	-0.9731613421	-0.5704509831	-2.6779608951	1.2587564221	-3.5529694344	-1.5925217140	-0.5976608723
1SB	0.4042686007	0.7048902986	2.5837595738	-0.2166080635	0.4475343425	-3.3463905703	2.7504669366
2SA	-3.3057998341	-2.3570372608	-7.5826449479	-0.8100058838	7.5957738917	12.4606593228	14.7559436755
3SA	4.9117775066	0.4144709186	5.1407843657	0.8860624851	-7.4255205572	-15.4784318043	-18.9633589080
4SA	-6.6878207708	-11.7733687342	-34.8003313662	4.8439126671	-1.7349373235	20.3758790679	29.5798830586
2PA	-0.2075589678	-0.9200724939	0.7593684711	3.8043628684	-1.6148845593	4.1545908231	4.4313241300
3PA	3.0645020290	6.9244751468	8.6863351385	-8.9704521822	3.7595738592	-11.3413610528	-12.8933886809
4PA	-4.4125059043	-8.4729377034	-15.5215374827	6.8320380433	-2.8975146234	10.2563929886	12.7801695059
2SB	0.7510047404	-1.3048871994	9.2100178646	-2.7134322510	0.9773192318	0.4231621593	-20.1797669656
3SB	0.8984903299	5.9078903456	-7.7689017325	3.6152140464	-1.8875663327	1.7981844179	24.6150354343
4SB	3.7917490107	8.6952340056	35.9937690645	-7.0335533585	5.3746978129	-15.0069445912	-31.7656274149
2PB	-0.5918098444	-0.1219300978	0.1464446483	2.0161780828	3.6657353002	-3.5485655949	-4.9960751878
3PB	3.2404354046	-4.2267803876	-11.4284277104	-2.6616856399	-8.3125520458	9.4420244333	14.2708784346
4PB	-1.9513243329	6.1120659405	17.6396746687	0.1837898393	5.9898488249	-8.6455691881	-13.7981138004

J(MINIMUM) = -1.1912576019

VARIATIONAL APPROXIMATION TO THE EXCHANGE FUNCTION ZETA

(H(A)-E(0)+IU)ZETA = B-SA

H(A) = HYDROGEN ATOM HAMILTONIAN E(0) = -0.5

ZETA = S((B-SA•X(K))/(E(K)-E(0)+IU))X(K)

INTERNUCLEAR DISTANCE R = 3.0000

FUNCTIONS X(K) WHICH DIAGONALIZE H(A)

E(K)	-0.4999999995	-0.1217371854	-0.1150518796	-0.0073526723	0.0538525179	0.1323156078	0.1701388904
(B-SA•X(K))	0.0000000000	-0.5859000937	-0.0850976123	0.0560363005	-0.5118654796	-0.1126092602	-0.1495547990

STO (EXPONENTS=1) — EXPANSION COEFFICIENTS OF SLATER-TYPE ORBITALS

1SA	0.9999999980	0.1550367917	0.4739849748	-0.1460748451	0.8468032531	-2.2434945255	0.0706176768
1SB	0.0000000010	-0.0071583604	-0.0112898999	0.5070658678	-1.0118103097	2.1669929905	0.1582085634
2SA	0.0000000032	0.0466113865	-0.3291752304	-1.0127185516	1.4521740055	-4.8675014586	0.7512458663
3SA	-0.0000000061	-0.0079632775	0.8082940881	0.4727329088	0.6106690390	-2.1679590186	-4.2788273633
4SA	0.0000000013	-0.0290543631	-1.2924733242	-2.5359964556	2.5285583318	-9.8091728280	1.1262649035
2PA	-0.0000000002	-0.2428568365	0.1581548775	-0.4161062478	0.3934018010	-0.7884426884	-0.2970483888
3PA	0.0000000001	0.0372517239	-0.2208898080	0.2383057511	-1.2986833308	-0.2357858562	2.4134159405
4PA	-0.0000000014	-0.6006174168	0.5441765114	-1.9755548442	3.3477768947	-5.3820905330	-2.9429394828
2SB	-0.0000000014	-0.2509687645	-0.1852977360	1.1059674761	-0.8168893636	4.9938787136	1.1335807808
3SB	0.0000000045	0.4362457899	0.2785236494	0.5130253066	-3.6388014152	1.2469116599	-1.3676772823
4SB	-0.0000000006	-0.6517102659	-0.4191765204	1.8621408636	-0.2214699251	10.4537767069	2.6705479593
2PB	0.0000000000	0.0105613954	-0.0005736688	-0.1714858390	-0.2655118990	0.9853590790	-0.0226641088
3PB	0.0000000005	-0.0479501496	-0.0157973844	0.8922498705	0.1829578221	-0.7918843984	0.4955382673
4PB	-0.0000000008	0.0637032102	-0.0152316854	-0.7515376775	-1.6929188727	6.8973713932	0.2961385457

FUNCTIONS X(K) WHICH DIAGONALIZE H(A)

E(K)	0.3338711924	0.6072696874	0.8773583024	1.3484359015	2.0442873170	2.9270025555	5.2026455777
(B-SA•X(K))	-0.5595382147	-0.3628999128	-0.2413520385	-0.0994430595	-0.0238859298	0.0870079505	-0.1276910518

STO (EXPONENTS=1) — EXPANSION COEFFICIENTS OF SLATER-TYPE ORBITALS

1SA	0.6165198326	-0.4338729687	0.9504372249	0.7261912166	2.3131536971	3.3532974563	1.1500150268
1SB	-0.1031458974	0.4394544488	-0.7281682958	-0.2790307241	-0.3650313884	1.5292723006	-4.2019639375
2SA	2.3267534219	-3.0384053314	2.9608405357	0.4927309966	-4.8328407215	-13.0991990196	-7.1291162120
3SA	-5.1100205448	4.4497311288	-4.8210933912	-1.5550349350	4.5651737123	16.1143466672	9.6016549692
4SA	4.4992050565	-8.6468309858	11.4736929194	4.2181828386	1.5128175346	-12.4202838116	-9.9683778782
2PA	0.0392376033	-0.7891474644	-0.5504458088	4.6144767626	1.6671714227	-2.1515845404	-1.7775665145
3PA	-1.1604495718	5.4080571395	-2.8373192341	-10.2527662534	-4.0478437593	6.1512234778	5.0533422666
4PA	2.0218690148	-6.5801736218	5.6227578437	7.3265757605	3.2145610030	-5.7341677444	-4.8988225266
2SB	-0.7018676063	-0.8473488077	-6.3678470460	-1.6976545702	-1.0079408491	0.0062122276	14.9350885632
3SB	0.9538322761	2.6995058573	10.4010366125	3.0012170826	2.0652941334	-1.9716018372	-17.8269610903
4SB	-2.3570087804	5.0341091427	-14.0837585926	-5.0686356849	-4.1274128427	6.7843666326	13.1840760014
2PB	0.4791272020	0.4325575336	-0.7564526754	1.5500789561	-4.2129402219	2.7776048391	1.9959784822
3PB	-2.6459744414	-4.3151135843	6.2191987564	-1.6963877169	9.1103778223	-6.8085621259	-5.7409123525
4PB	1.7123641155	5.5061616552	-8.0849024993	-0.2993899457	-6.3450569959	5.7372861638	5.5054878405

J(MINIMUM) = -1.6353152377

VARIATIONAL APPROXIMATION TO THE EXCHANGE FUNCTION ZETA

(H(A)-E(0)+IU)ZETA = B-SA

H(A) = HYDROGEN ATOM HAMILTONIAN E(0) = -0.5

ZETA = S((B-SA*X(K))/(E(K)-E(0)+IU))X(K)

INTERNUCLEAR DISTANCE R = 4.0000

FUNCTIONS X(K) WHICH DIAGONALIZE H(A)

E(K)	-0.4999999996	-0.1218733661	-0.1150666488	-0.0150641890	0.0526401570	0.1217811993	0.1632930544
(B-SA*X(K))	-0.0000000001	-0.5786397662	0.12187343$_{66}$	0.1458746519	-0.4916126572	-0.1115210401	0.2507681386

STO EXPANSION COEFFICIENTS OF SLATER-TYPE ORBITALS

(EXPONENTS=1)							
1SA	-0.9999999987	0.1573413263	-0.4636285051	0.0751277710	-0.4165074911	-0.7041619973	-0.0684621392
1SB	-0.0000000003	-0.0076459678	0.0025894936	0.2435516636	0.6428551175	0.6104527551	-0.0737439343
2SA	-0.0000000025	0.0278111147	0.3537974792	-0.5798359397	-0.9397522902	-2.0618955346	-0.6082791995
3SA	0.0000000029	0.0304022408	-0.8119380043	0.6865925508	0.4677824431	0.2609812126	3.5114065211
4SA	-0.0000000010	-0.1020796157	1.3541947817	-1.8509795822	-2.1995761494	-4.8951252346	-0.6636085656
2PA	0.0000000005	-0.2401285043	-0.1599162519	-0.3043862468	-0.3747482638	-0.4520710403	0.3245365044
3PA	-0.0000000013	0.0526062402	0.2153039422	0.2420395491	1.4781117591	-0.5044356007	-2.4958118712
4PA	0.0000000012	-0.6065206618	-0.5319535109	-1.3689078735	-3.0308674617	-2.3235197410	3.2046435059
2SB	0.0000000003	-0.2268400812	0.1483580781	0.7801346592	0.2864562293	2.0635606687	-1.1108220114
3SB	-0.0000000002	0.3869572342	-0.2516825431	-0.2349099023	2.7164164289	-1.0744738816	1.7897366217
4SB	-0.0000000006	-0.5957808848	0.3499019124	1.6274819800	-0.2610069871	5.4745319568	-2.9779725868
2PB	0.0000000000	0.0022603090	0.0047211506	-0.1417863332	0.2275868202	0.6698983386	-0.0577147163
3PB	0.0000000000	0.0002445770	-0.0029840256	0.7124976397	-0.0861147349	-1.2045519873	-0.3461149748
4PB	-0.0000000004	-0.0113444848	0.0259131491	-0.6520477161	1.3484672191	4.4663158077	-0.6525775959

FUNCTIONS X(K) WHICH DIAGONALIZE H(A)

E(K)	0.2815268277	0.5531135891	0.8762609229	1.4209118529	2.0746961019	2.7133536518	4.9355636038
(B-SA*X(K))	-0.1770109786	0.2988844263	-0.3581859820	0.0496996728	-0.0220869996	-0.0616470213	0.1431735968

STO EXPANSION COEFFICIENTS OF SLATER-TYPE ORBITALS

(EXPONENTS=1)							
1SA	-0.5156931360	0.3750916209	0.4444419898	-0.8120892307	1.4872844004	-3.9232859145	-0.8529608035
1SB	-0.0110730041	-0.2153445329	-0.2468323440	0.2051699871	-0.2752233483	-0.8456142943	4.4411347274
2SA	-1.9838206042	2.4165648700	1.3660442842	0.1287730342	-3.1221883646	13.3843120008	4.2448707365
3SA	5.1558288586	-4.6600042266	-3.0222393671	1.1405049055	2.8097886193	-16.3369696541	-5.8959583319
4SA	-4.2238347580	5.9669948085	4.8492682161	-3.1008786519	0.9087627506	9.8131596029	5.1176666269
2PA	0.0396254176	0.2398267848	-0.4063298170	-5.1035911650	0.4879900715	1.6484300262	0.9304360265
3PA	0.5437990651	-3.0338428398	-0.9963634535	10.6670010916	-1.7653997360	-4.4811128235	-2.7057607248
4PA	-1.3030699830	4.0905387580	2.3597866754	-7.1560942852	1.7825427147	4.0282060718	2.6273834331
2SB	0.7264242790	0.3707039470	-5.4916255455	1.3464852447	-0.9578428517	-0.1966559595	-13.5897673520
3SB	-1.5638021536	-0.9622820260	10.0048391204	-2.6919677447	2.0799092822	1.8232719452	15.8640412951
4SB	2.2940017412	-2.9587317164	-8.2234908564	3.8906766487	-2.8281661225	-3.9719888812	-9.0451267699
2PB	-0.3115536833	-0.7016890605	-0.3554332864	-0.3621316267	-4.8822503440	-1.9610169270	-1.2904001960
3PB	2.0167743950	4.3702541473	2.8540696600	-0.6638483931	9.7355618242	4.7447356315	3.5269486957
4PB	-1.2025759525	-4.8585008361	-3.7114121339	1.6047876531	-6.2511160830	-3.9074845547	-3.2451533845

J(MINIMUM) = -1.7446506090

VARIATIONAL APPROXIMATION TO THE EXCHANGE FUNCTION ZETA

(H(A)-E(0)+IU)ZETA = B-SA

H(A) = HYDROGEN ATOM HAMILTONIAN E(0) = -0.5

ZETA = S((B-SA*X(K))/(E(K)-E(0)+IU))X(K)

INTERNUCLEAR DISTANCE R = 5.0000

FUNCTIONS X(K) WHICH DIAGONALIZE H(A)

E(K)	-0.4999999996	-0.1218807605	-0.1150479859	-0.0210544810	0.0580842419	0.1092538955	0.1591018383
(B-SA*X(K))	0.0000000000	-0.5132468839	0.1364351098	0.2558288706	0.4477936730	-0.1253818168	-0.3239741983

STO (EXPONENTS=1)	EXPANSION COEFFICIENTS OF SLATER-TYPE ORBITALS						
1SA	0.9999999990	0.1527743961	-0.4592246568	0.1431238433	-0.1991048301	-0.1957805476	0.1255806810
1SB	0.0000000002	-0.0063158409	-0.0006307746	0.1332528760	0.4591920419	0.0860265897	-0.0515917039
2SA	0.0000000009	-0.0010893030	0.3729021170	-0.4240317780	-0.8313673067	-0.8965705650	0.6000140725
3SA	-0.0000000007	0.0721590112	-0.8295468394	0.6992889948	1.1557029686	0.3594911649	-2.8421943405
4SA	-0.0000000011	-0.1742227480	1.4019697484	-1.4659752334	-2.2736046025	-2.4262361785	0.5544573926
2PA	-0.0000000005	-0.2473633092	-0.1561156955	-0.2555403220	-0.4088146048	-0.1807230107	-0.3201916718
3PA	0.0000000014	0.0932271814	0.1972562140	0.2327045922	1.6700721748	-1.1647039587	2.5272394030
4PA	-0.0000000019	-0.6470375827	-0.5062195336	-1.0215464196	-2.9064385422	-0.3419853091	-3.1520341340
2SB	0.0000000008	-0.2089900466	0.1245982485	0.6497573787	0.0440889020	1.0609514545	0.9511502737
3SB	-0.0000000017	0.3617890833	-0.2271164019	-0.5578658973	2.1958808810	-1.7856976358	-2.1569611634
4SB	0.0000000026	-0.5384928865	0.3041153239	1.5598517271	-0.2846296796	3.3825921396	2.9536676639
2PB	0.0000000004	-0.0109787275	0.0080917791	-0.1257205033	0.2127057054	0.5151331729	0.0741062735
3PB	-0.0000000012	0.0537206945	-0.0256661086	0.5720043411	-0.1171112233	-1.4906349425	0.1386733431
4PB	0.0000000018	-0.0763364130	0.0464841253	-0.5289453120	1.4001530464	3.2727797417	0.8018238258

FUNCTIONS X(K) WHICH DIAGONALIZE H(A)

E(K)	0.2504712744	0.4811032371	0.8585702781	1.4034408791	2.1080396202	2.6693191214	4.8731633610
(B-SA*X(K))	0.2711254889	0.2036783283	0.4243028467	-0.0449616440	-0.0274346342	-0.0474145133	-0.1481192928

STO (EXPONENTS=1)	EXPANSION COEFFICIENTS OF SLATER-TYPE ORBITALS						
1SA	0.4471513359	0.3406431518	-0.2627066845	0.6941458580	1.2770896356	-4.0956980234	0.6341463175
1SB	0.0799677394	-0.0978030737	0.1016713546	-0.1088559259	-0.2367135700	-0.5512402200	-4.5151268104
2SA	1.9706619837	1.7297131862	-0.6716016098	-0.5729612741	-2.6641263888	13.1428425871	-2.9298788400
3SA	-5.5046810069	-3.9626466670	1.8651187034	-0.3660080529	2.2566275066	-15.8699594182	4.1908630300
4SA	4.3004104764	4.1799613223	-2.4122942566	1.7048690376	0.4196373212	8.4050882026	-3.2459360122
2PA	0.0224623181	-0.0454487130	0.5325400480	4.9221468646	0.6500175544	1.4910559898	-0.6983171550
3PA	-0.5068921666	-1.5958698281	-0.0527470195	-9.7133890593	-1.9571574549	-3.6537900461	1.9749425730
4PA	1.1229552515	2.4782384112	-0.8910460527	6.0816782801	1.7334205852	3.0461483444	-1.8230122129
2SB	-0.6154428144	0.2059400045	4.9311209978	-1.3243429973	-0.5881178529	-0.2624420640	12.9932789868
3SB	1.6904046582	-0.3459212454	-9.1901641532	2.6909916696	1.5088102650	1.6727305653	-14.8977966695
4SB	-2.2151267399	-1.7406940532	6.0013768023	-2.8520888249	-1.8635238130	-2.6780833494	7.4673992653
2PB	-0.2566218663	-0.6949192525	0.0979292263	0.2646462118	-4.8044997745	-1.7300326967	1.0312977603
3PB	-1.6567440047	4.0765626221	-1.1731484078	0.6322369168	9.0740158788	4.0275238409	-2.5667711879
4PB	0.8758279347	-4.1744693745	1.6906529372	-1.2913223462	-5.4792010509	-3.1238610750	2.2152400418

J(MINIMUM) = -1.7049133532

VARIATIONAL APPROXIMATION TO THE EXCHANGE FUNCTION ZETA

(H(A)-E(0)+IU)ZETA = B-SA

H(A) = HYDROGEN ATOM HAMILTONIAN E(0) = -0.5

ZETA = S((B-SA,X(K))/(E(K)-E(0)+IU))X(K)

INTERNUCLEAR DISTANCE R = 6.0000

FUNCTIONS X(K) WHICH DIAGONALIZE H(A)

E(K)	-0.4999999998	-0.1216898665	-0.1149962595	-0.0255287200	0.0651615211	0.1112941695	0.1568263409
(B-SA,X(K))	-0.0000000000	-0.4232754742	0.1368141147	-0.3558877320	0.3527663330	0.2816128311	0.3603883042

STO EXPANSION COEFFICIENTS OF SLATER-TYPE ORBITALS

(EXPONENTS=1)							
1SA	0.9999999984	0.1429556847	-0.4589202661	-0.1621800104	-0.0544919776	0.0257399144	-0.1677213815
1SB	-0.0000000001	-0.0051192170	-0.0016129239	-0.0794111819	0.2936747047	0.2031875388	0.1411257089
2SA	0.0000000045	-0.0280541107	0.3911807968	0.3361391132	-0.7889242158	0.1194621261	-0.6301742049
3SA	-0.0000000060	0.0982886753	-0.8502573883	-0.6054484636	1.3404452417	0.3415438660	2.4615271997
4SA	0.0000000031	-0.2179728246	1.4418562719	1.1850139324	-2.2818182980	0.5166905555	-0.6168735061
2PA	0.0000000001	-0.2597127125	-0.1470271332	0.2172331700	-0.4011538404	-0.1319228581	0.3003450637
3PA	-0.0000000002	0.1255067872	0.1800303258	-0.1525223058	1.2032662291	2.1836824113	-2.5177969764
4PA	0.0000000001	-0.6872507793	-0.4764650011	0.7563375050	-2.2934652937	-1.5486189973	2.9935503217
2SB	0.0000000002	-0.1931054018	0.1129415879	-0.6072296609	0.0544469548	-0.7859488777	-0.8536784360
3SB	-0.0000000006	0.3314108040	-0.2112398763	0.7642833014	1.2436272186	2.6035963638	2.4543245779
4SB	0.0000000004	-0.4751231352	0.2738317245	-1.5656021416	0.2509128704	-2.5223574206	-2.8668213299
2PB	0.0000000001	-0.0225501827	0.0132955199	0.0956030437	0.3297143713	-0.3675434012	-0.1016880790
3PB	-0.0000000002	0.0840417781	-0.0471018488	-0.3891972467	-0.7459986983	1.4026154634	0.1773597520
4PB	0.0000000003	-0.1119674860	0.0659472849	0.3465193779	2.1605028643	-1.9950400438	-0.9401240824

FUNCTIONS X(K) WHICH DIAGONALIZE H(A)

E(K)	0.2394979262	0.4268379169	0.8402436356	1.3393946858	2.0690165200	2.6172462181	4.8186963389
(B-SA,X(K))	0.2989869000	0.1015538858	0.4595723323	-0.0595039144	-0.0198327523	-0.0418345344	-0.1517193513

STO EXPANSION COEFFICIENTS OF SLATER-TYPE ORBITALS

(EXPONENTS=1)							
1SA	0.4044963984	0.2997176196	-0.2067220560	0.4514712559	1.3589707871	-4.1118152997	0.5514854781
1SB	0.1030789414	-0.0464842798	0.0432624553	-0.0862439984	-0.1477268602	-0.4205340998	-4.5246580926
2SA	2.0874987284	1.2094609709	-0.2972264794	-0.5010254433	-3.1179600552	12.6285550010	-2.3220587014
3SA	-6.0084380483	-3.1329518599	1.1398986860	-0.1195285674	2.9098385158	-15.0123302646	3.2981183553
4SA	4.4935438731	3.0280378783	-1.3649973852	0.9349854668	-0.3747260320	7.3364190307	-2.2763969530
2PA	0.1017389294	-0.1434268942	0.6403565431	4.7096930973	0.9191346683	1.1564652998	-0.6237240805
3PA	-0.7779850168	-0.7923488159	-0.6272495278	-8.9393925716	-2.1698943696	-2.6697371245	1.6025567278
4PA	1.2435572524	1.5092058507	-0.1854094448	5.2889967996	1.6068027542	2.1353434246	-1.3567169609
2SB	-0.4726964711	0.0598667951	4.6713139542	-1.2081628846	-0.3078846413	-0.1418452943	12.5165271044
3SB	1.5762140918	0.0294127209	-8.7256789964	2.4711930808	0.9112157966	1.2723291456	-14.0978923400
4SB	-2.0189843996	-1.1609779162	5.1134333102	-2.1327849159	-1.0928195014	-1.7768729477	6.5392134999
2PB	0.2334512742	-0.7267786527	0.0515317541	0.4528323577	-4.5500709262	-1.8144157783	0.7406742711
3PB	-1.3515258674	4.1437792944	-0.5430444940	-0.0222879202	8.2813582632	3.8634908660	-1.7475684477
4PB	0.6234781478	-3.9378026924	0.8615127830	-0.6380195438	-4.7459523305	-2.7056684437	1.4653905566

J(MINIMUM) = -1.6333759902

VARIATIONAL APPROXIMATION TO THE EXCHANGE FUNCTION ZETA

(H(A)-E(0)+IU)ZETA = B-SA

H(A) = HYDROGEN ATOM HAMILTONIAN E(0) = -0.5

ZETA = S((B-SA*X(K))/(E(K)-E(0)+IU))X(K)

INTERNUCLEAR DISTANCE R = 8.0000

FUNCTIONS X(K) WHICH DIAGONALIZE H(A)

E(K)	-0.4999999997	-0.1212296377	-0.1148042813	-0.0313043114	0.0549878004	0.1435089286	0.1657296158
(B-SA*X(K))	0.0000000000	0.2452588697	0.1071217723	-0.4840354735	0.1320523786	-0.2840738563	-0.5489359636

STO (EXPONENTS=1) — EXPANSION COEFFICIENTS OF SLATER-TYPE ORBITALS

1SA	1.0000000001	-0.1186132638	-0.4630476132	-0.1555799357	0.0832648846	-0.1150895719	0.1751197495
1SB	0.0000000001	0.0027959789	-0.0016213098	-0.0368728243	0.0707724185	-0.1860732841	-0.3386603649
2SA	-0.0000000010	0.0492048301	0.4168471249	0.2076267860	-0.3369121489	-0.2756042274	0.6129230187
3SA	0.0000000018	-0.1011486285	-0.8803229650	-0.3934749401	0.6579442247	0.8569717721	-1.9683064652
4SA	-0.0000000010	0.2487312177	1.5114767373	0.7881427289	-1.0869556069	-0.3559787010	0.7662463976
2PA	0.0000000000	0.2781357747	-0.1274204388	-0.1528137469	-0.1917780714	0.3250074420	-0.1689738651
3PA	-0.0000000002	-0.1530987383	0.1621226181	-0.0180507427	0.0484200515	-3.2559656672	1.3018305648
4PA	0.0000000003	0.7665753351	-0.4085125523	-0.4326011755	-0.5910273268	3.1475216705	-1.5664820598
2SB	0.0000000002	0.1414937549	0.0897125243	-0.6007531135	-0.0121955922	0.3033077438	1.0384021419
3SB	-0.0000000007	-0.2407833857	-0.1663444583	0.9548721774	0.2951289898	-1.4455000112	-3.7370704135
4SB	0.0000000006	0.3408310081	0.2115172979	-1.5483676170	0.1140038058	0.8357329793	3.3094093247
2PB	0.0000000002	0.0264153937	0.0172241096	0.0242064040	0.3869579346	-0.0276413841	0.1480881408
3PB	-0.0000000003	-0.0804519524	-0.0555748382	-0.0924829683	-1.2231950880	0.0443995702	-0.5445054263
4PB	0.0000000002	-0.1266956453	0.0775260846	0.0406891491	2.1400629446	-0.2994776824	0.9000958020

FUNCTIONS X(K) WHICH DIAGONALIZE H(A)

E(K)	0.2453104020	0.4156285645	0.8478599047	1.2712695124	2.0298350037	2.4984895051	4.7266287699
(B-SA*X(K))	-0.1799636165	0.0190613120	-0.4835288357	-0.0489530343	-0.0090658675	-0.0257224711	-0.1575501264

STO (EXPONENTS=1) — EXPANSION COEFFICIENTS OF SLATER-TYPE ORBITALS

1SA	-0.4087032816	0.1137128356	0.1355018793	0.1935744829	0.9394775361	-4.2409654626	0.3531780931
1SB	-0.6789214635	0.0058761322	0.0002332495	-0.0631613922	-0.0511315166	-0.2197195367	-4.5072871653
2SA	-2.3360385615	0.3733423665	0.0048149657	-0.2229049093	-2.3360909374	12.3981931200	-1.3206109796
3SA	6.8049767629	-1.0837464908	-0.3980271567	-0.2024435560	2.3684304733	-14.3807952756	1.8176000255
4SA	-4.8927032870	1.1696866965	0.5682236286	0.5020001029	-0.6048192498	6.4155496083	-1.1276902634
2PA	-0.1466969461	-0.0464496614	-0.4454515546	4.7102302526	0.5375515590	0.5475315791	-0.3359594594
3PA	1.3576790965	-0.1434793109	0.6366884483	-8.7856302299	-1.0933720102	-1.2556535954	0.7783649636
4PA	-1.6398943171	0.5347596063	-0.0950706541	4.9333186725	0.7961175678	1.0029609631	-0.6389934795
2SB	0.3382878691	-0.0437251310	-4.6312011613	-0.6724550582	-0.1403219308	0.0053686629	11.9896388913
3SB	-1.2208386158	0.2823999475	0.0453176490	1.4023721872	0.5108546105	0.5668107006	-13.2090293330
4SB	1.5294934656	-0.5947817714	-4.7226491929	-1.1356584103	-0.5340865826	-0.7593176199	5.6719697072
2PB	-0.1945716071	-0.8197859579	-0.0701383691	0.2069768833	-4.5639507333	-1.2298738689	0.3492185027
3PB	0.1814952717	4.5211123737	0.4259942336	-0.2598733203	8.1340781604	2.4057538789	-0.8348281980
4PB	0.3243176335	-3.8276142272	-0.5349279780	-0.1679335783	-4.4199658774	-1.5561346226	0.6974863006

J(MINIMUM) = -1.0215979601

VARIATIONAL APPROXIMATION TO THE EXCHANGE FUNCTION ZETA

(H(A)-E(0)+IU)ZETA = B-SA

H(A) = HYDROGEN ATOM HAMILTONIAN E(0) = -0.5

ZETA = S((B-SA•X(K))/(E(K)-E(0)+IU))X(K)

INTERNUCLEAR DISTANCE R = 10.0000

FUNCTIONS X(K) WHICH DIAGONALIZE H(A)

E(K)	-0.4999999998	-0.1207814376	-0.1146109069	-0.0323132743	0.0435277055	0.1417379172	0.1795831125
(B-SA•X(K))	-0.0000000001	0.1220693197	0.0651343421	0.5082164989	-0.0325762872	0.2711246079	-0.5872515713

STO (EXPONENTS=1) EXPANSION COEFFICIENTS OF SLATER-TYPE ORBITALS

1SA	0.9999999992	-0.1011196222	-0.4705685073	0.1304695657	0.0945254595	0.1096011700	0.2033595688
1SB	-0.0000000001	-0.0020529123	-0.0026161942	0.0202208523	0.0135276044	0.1382897407	-0.3560245296
2SA	0.0000000007	0.0642227747	0.4402109762	-0.1061154840	-0.0797789840	0.3767441063	0.7873613311
3SA	0.0000000002	-0.1309495775	-0.9276671776	0.1873436879	0.1085700244	-1.1087170036	-2.3623121479
4SA	-0.0000000003	0.2768662674	1.5837350510	-0.4739563092	-0.3783659591	0.5848888305	1.3093968413
2PA	-0.0000000000	0.3019518631	-0.1032860092	-0.0940021252	-0.0582350629	-0.2736320303	-0.1246257034
3PA	0.0000000003	-0.2159231938	0.1217283236	-0.1132085993	-0.4539895408	3.0975350052	1.0468411475
4PA	-0.0000000004	0.8754099931	-0.3164961765	-0.1749806727	0.1571750375	-2.9381502926	-1.1209321627
2SB	0.0000000004	0.1044503636	0.0686780644	0.5943504576	-0.1112709963	-0.2334811363	0.9521225386
3SB	-0.0000000009	-0.1988176891	-0.1342062391	-1.0089220175	0.2392637266	1.1011928213	-3.6073825000
4SB	0.0000000005	0.2580097623	0.1642296378	1.5076975544	-0.2041280135	-0.6814194936	2.9555668237
2PB	0.0000000001	0.0301257104	0.0190116468	0.0230172926	0.3495575936	0.1023177083	0.0550267958
3PB	-0.0000000003	-0.0987957505	-0.0627372564	-0.0682318487	-1.1383318500	-0.3000683218	-0.2171026473
4PB	0.0000000003	0.1475905112	0.0881133436	0.1581666604	1.8126980656	0.5808863512	0.3337454031

FUNCTIONS X(K) WHICH DIAGONALIZE H(A)

E(K)	0.2442516716	0.4345422738	0.8684646349	1.2625554252	2.0477609002	2.4609737436	4.7111056198
(B-SA•X(K))	-0.1923549513	0.0253192727	0.4889712594	-0.0265019337	-0.0093756134	-0.0139761089	0.1594189146

STO (EXPONENTS=1) EXPANSION COEFFICIENTS OF SLATER-TYPE ORBITALS

1SA	-0.4042735563	0.0436630935	-0.0642482169	0.1569570621	0.5050173655	-4.3136034500	-0.1968755595
1SB	-0.1283348397	0.0132913519	-0.0007411764	-0.0166283316	-0.0459486817	-0.1044209346	4.4977382972
2SA	-2.1974102085	0.3280363807	-0.0279717925	-0.2139903684	-1.2568997637	12.4566955771	0.7174972607
3SA	6.5693679199	-0.9984074518	0.3240506459	-0.1182564772	1.1766962575	-14.3267354444	-1.0273221771
4SA	-4.4842864921	0.9292704234	-0.3964413818	0.3087315998	-0.2179173700	6.1909360832	0.6421505871
2PA	-0.0866178266	0.0411868069	0.2099116733	4.7141055011	0.2640294162	0.3801957871	0.1826846748
3PA	1.1608156656	-0.4361544054	-0.2176634160	-8.7291014125	-0.6178253430	-0.8847725710	-0.4555174912
4PA	-1.2975476196	0.6530492558	-0.0890611239	4.7675257286	0.5444282968	0.6615186182	0.4030907860
2SB	0.4142994373	0.0127174956	4.6111272122	-0.4147878923	-0.1003527086	-0.0223647346	-11.8433455871
3SB	-1.5236904223	0.1660289790	-8.5672237431	0.9389729616	0.4153510508	0.3901033190	12.9381140769
4SB	1.5015355487	-0.3399017622	4.5690666656	-0.7692050458	-0.3766888880	-0.4617809166	-5.4055639205
2PB	0.0419234224	-0.7838727534	0.0306145446	0.0655053114	-4.6290337446	-0.6936990941	-0.2450781930
3PB	-0.0594296827	4.3775517260	-0.3052556502	0.1116513537	8.1923304719	1.3932176630	0.5886012558
4PB	0.4206324368	-3.5339504746	0.3540455259	-0.3499654059	-4.3323276044	-0.9363192535	-0.4532266643

J(MINIMUM) = -1.4570168136

VARIATIONAL APPROXIMATION TO THE EXCHANGE FUNCTION ZETA

(H(A)-E(0)+IU)ZETA = G-SA

H(A) = HYDROGEN ATOM HAMILTONIAN E(0) = -0.5

ZETA = S((G-SA*X(K))/(E(K)-E(0)+IU))X(K)

INTERNUCLEAR DISTANCE R = 12.0000

FUNCTIONS X(K) WHICH DIAGONALIZE H(A)

E(K)	-0.4999999999	-0.1199603453	-0.1142736793	-0.0286827460	0.0407314928	0.1318076472	0.1861068826
(B-SA*X(K))	-0.0000000000	-0.0522496783	0.0356426416	0.4914594503	-0.1268522756	0.2164881601	-0.5950964905

STO (EXPONENTS=1) — EXPANSION COEFFICIENTS OF SLATER-TYPE ORBITALS

1SA	-0.9999999990	0.0672054009	-0.4835381774	0.0911951349	0.0742194074	0.0604975467	0.2105928709
1SB	0.0000000001	0.0054790934	-0.0042946216	0.0072831026	-0.0107201725	0.1057478655	-0.3504078977
2SA	-0.0000000025	-0.0555554128	0.4658256700	-0.0157382131	0.0549668293	0.2421992378	0.9426349095
3SA	0.0000000030	0.1168024247	-0.9840984601	-0.0063427567	-0.1970651918	-0.6919180799	-2.7763312938
4SA	-0.0000000014	-0.2134503594	1.6578336334	-0.2070883605	-0.0377357649	0.3848141302	1.6906211295
2PA	-0.0000000001	-0.3290892948	-0.0625627466	-0.0335371676	0.0207574151	-0.2566126413	-0.0733537656
3PA	0.0000000001	0.2799263571	0.0642794319	-0.2268449637	-0.6607211527	3.0753251580	0.8373004360
4PA	-0.0000000001	-0.9733424292	-0.1856585631	0.0348539685	0.4545742758	-2.8520616019	-0.8520830152
2SB	0.0000000000	-0.0776028302	0.0576186665	0.6119357722	-0.1235642810	-0.2213292615	0.9069822580
3SB	-0.0000000006	0.1628286169	-0.1209050753	-1.0939204179	0.1625054651	0.9083604839	-3.4675215302
4SB	0.0000000007	-0.1832256405	0.1339705146	1.5362138568	-0.2691123094	-0.5862281027	2.7560939076
2PB	0.0000000000	-0.0312884664	0.0221667855	0.0612126823	0.3502210085	0.0828136296	0.0184557199
3PB	-0.0000000000	0.1071011137	-0.0756473526	-0.2015685030	-1.1626615099	-0.2200165208	-0.1039470660
4PB	0.0000000000	-0.1370366621	0.0955085903	0.3194798095	1.7438454600	0.5169744058	0.0949826727

FUNCTIONS X(K) WHICH DIAGONALIZE H(A)

E(K)	0.2331356666	0.4366538460	0.8757009176	1.2431777562	2.0405286099	2.4420530412	4.7004956142
(B-SA*X(K))	-0.2594391191	-0.0114323811	0.4928614776	-0.0328968865	0.0058555547	-0.0115446240	-0.1605209861

STO (EXPONENTS=1) — EXPANSION COEFFICIENTS OF SLATER-TYPE ORBITALS

1SA	-0.4106552651	-0.0595574251	-0.0545710220	0.1046586256	-0.5422578070	-4.2946127139	0.1625511607
1SB	-0.1644096526	-0.0042534569	0.0012478644	-0.0102855466	0.0302349925	-0.0733590349	-4.4812995418
2SA	-2.0920927968	-0.3017676196	-0.0119272780	-0.1596554174	1.3827928896	12.3349136559	-0.5758580707
3SA	6.2676390272	1.0111553193	0.2697193962	-0.0328595980	-1.3005673988	-14.0696153019	0.8319177045
4SA	-4.1461313444	-0.8174742353	-0.2862949643	0.1468080532	0.3397973823	5.9914866877	-0.4864569308
2PA	-0.0321769685	0.0344458992	0.2774772409	4.6334009970	-0.3942759446	0.2651810055	-0.1814960694
3PA	0.6966389484	0.3676852601	-0.3232643471	-8.4688857163	0.9014298051	-0.6035302603	0.4553316997
4PA	-0.7484650092	-0.5346831025	0.0107070379	4.5088803580	-0.6505002680	0.4218737864	-0.3622223778
2SB	0.4312254654	-0.0322120469	4.5527500066	-0.4716812700	0.0473891176	-0.0222178456	11.7323273979
3SB	-1.7029691910	-0.0341486318	-3.3861083786	1.0678564663	-0.2239402536	0.3309948153	-12.7219122529
4SB	1.4993749684	0.1243920974	4.3915143962	-0.7489640501	0.1937913906	-0.3378203142	5.2334756770
2PB	-0.0042552651	0.7501798052	0.0115779626	0.1152750214	4.5505651030	-0.7408083468	0.1536720900
3PB	0.1003670618	-4.1953042840	-0.1355810920	0.1098147717	-7.9462914189	1.4759800240	-0.3595972520
4PB	-0.1612963577	3.2631248154	0.1495662424	-0.3178420199	4.0994009748	-0.9233825449	0.2581836875

J(MINIMUM) = -1.4171925583

VARIATIONAL APPROXIMATION TO THE EXCHANGE FUNCTION ZETA

(H(A)-E(0)+IU)ZETA = B-SA

H(A) = HYDROGEN ATOM HAMILTONIAN E(0) = -0.5

ZETA = S((B-SA+X(K))/(E(K)-E(0)+IU))X(K)

INTERNUCLEAR DISTANCE R = 14.0000

FUNCTIONS X(K) WHICH DIAGONALIZE H(A)

E(K)	-0.4999999999	-0.1192744919	-0.1138774996	-0.0205679420	0.0465379758	0.1229059147	0.1921915414
(B-SA+X(K))	-0.0000000000	-0.0191110077	-0.0162426036	-0.4852132357	-0.1375695995	-0.1352892695	-0.6088895405

STO (EXPONENTS=1) — EXPANSION COEFFICIENTS OF SLATER-TYPE ORBITALS

1SA	-0.9999999991	0.0272538401	0.4927592656	-0.0488198230	0.0487443878	-0.0235014111	0.2005573632
1SB	-0.0000000001	0.0049749065	0.0043190391	0.0000713253	-0.0180073740	-0.0668735716	-0.3553573059
2SA	-0.0000000028	-0.0256508982	-0.4807823953	-0.0307045940	0.1018216173	-0.1047237718	0.9735075271
3SA	0.0000000039	0.0545737477	1.0163562052	0.0987506756	-0.2906089983	0.2929916976	-2.8507230784
4SA	-0.0000000020	-0.0925073839	-1.7009795902	0.0412252241	0.0978619838	-0.1657396192	1.7872181964
2PA	-0.0000000002	-0.3431001738	0.0232875495	-0.0038213756	0.0536642646	0.2667547110	-0.0333996802
3PA	0.0000000003	0.3060325869	-0.0204195188	0.2314544997	-0.6630749270	-3.1703240651	0.5574789959
4PA	-0.0000000001	-1.0170979876	0.0677967817	-0.1190564162	0.5141362335	2.8968687568	-0.5633980375
2SB	0.0000000002	-0.0476273300	-0.0414536131	-0.6409629606	-0.0934573009	0.1622927652	0.9229688624
3SB	-0.0000000005	0.1036656005	0.0899734719	1.1738096109	0.0837091442	-0.5982791021	-3.5037528989
4SB	0.0000000003	-0.1043514112	-0.0904925216	-1.5917007813	-0.2195790363	0.3830918227	2.7509178861
2PB	-0.0000000000	-0.0226075996	-0.0190607128	-0.0755490779	0.3691985215	-0.0581954072	0.0150476237
3PB	0.0000000000	0.0772989143	0.0650710750	0.2531151661	-1.2326555060	0.1530143404	-0.1004895214
4PB	0.0000000000	-0.0890096309	-0.0748353971	-0.3654067131	1.7955023771	-0.4029640690	0.0337788153

FUNCTIONS X(K) WHICH DIAGONALIZE H(A)

E(K)	0.2232176136	0.4370991269	0.8796669188	1.2207911361	2.0269045905	2.4213616883	4.6865276109
(B-SA+X(K))	0.2664625971	-0.0096916699	-0.4964551148	-0.0339838542	-0.0016286106	0.0091431215	0.1615556685

STO (EXPONENTS=1) — EXPANSION COEFFICIENTS OF SLATER-TYPE ORBITALS

1SA	0.4186726270	0.0579694533	0.0495242726	0.0470926832	0.5052047715	4.2650925600	-0.1310478281
1SB	0.1719532514	-0.0060468161	-0.0009795742	-0.0136395996	-0.0117635461	0.0620130743	4.4656395580
2SA	2.0630494460	0.1960652240	-0.0178471236	-0.0771383018	-1.3141277166	-12.2520829914	0.4508240901
3SA	-6.3176971970	-0.7191246625	-0.1641295405	0.0016264461	1.2859173696	13.9059656360	-0.6334986734
4SA	4.0524833798	0.5531589312	0.1760910857	0.0478379915	-0.4103455047	-5.8461726082	0.3452530830
2PA	0.0092716242	-0.0694668391	-0.2907627677	4.5733318998	0.3951084645	-0.1348761787	0.1534433802
3PA	-0.3376037338	-0.1893610553	0.3887687377	-8.2617844797	-0.8616706774	0.2992044190	-0.3699590366
4PA	0.3563599941	0.3127249872	-0.1013060669	4.3163126426	0.5693628592	-0.1988849588	0.2689852638
2SB	-0.4270834038	0.0193255943	-4.5259564007	-0.4269153832	-0.0094200518	-0.0002197706	-11.6395212533
3SB	1.7117586473	-0.0401333922	0.2855015425	0.9457668733	0.0673063968	-0.2117736426	12.5465784678
4SB	-1.4305561144	0.0058644915	-4.2904694330	-0.6075076344	-0.0600440595	0.2056171206	-5.1119392919
2PB	0.1171568465	-0.7467139407	-0.0101232170	0.1382857522	-4.4972271513	0.6722258473	-0.0666404887
3PB	-0.1042768211	4.1020177596	0.0341762022	0.0196636969	7.7647847354	-1.3017809990	0.1524961012
4PB	-0.0494067446	-3.1162695304	-0.0318063696	-0.1886994179	-3.9372744993	0.7653853071	-0.1046385515

J(MINIMUM) = -1.3902769151

VARIATIONAL APPROXIMATION TO THE EXCHANGE FUNCTION ZETA

(H(A)-E(0)+IU)ZETA = 6-SA

H(A) = HYDROGEN ATOM HAMILTONIAN E(0) = -0.5

ZETA = S((6-SA+X(K))/(E(K)-E(0)+IU))X(K)

INTERNUCLEAR DISTANCE R = 16.0000

FUNCTIONS X(K) WHICH DIAGONALIZE H(A)

E(K)	-0.5000000001	-0.1159940907	-0.1136632993	-0.0114670371	0.0555827841	0.1183460241	0.1997822281
(B-SA+X(K))	0.0000000001	-0.0063243655	-0.0059769508	0.4898051543	0.1099618872	0.0696467376	0.6234578157

STO EXPANSION COEFFICIENTS OF SLATER-TYPE ORBITALS

(EXPONENTS=1)							
1SA	-0.9999999993	0.0046232375	0.4954747868	0.0205013564	-0.0258720133	0.0063253293	-0.1875968589
1SB	-0.0000000001	0.0029599700	0.0027545561	-0.0014776072	0.0157687158	0.0354227409	0.3639027717
2SA	-0.0000000010	-0.0066809843	-0.4842813502	0.0304169302	-0.0840164556	0.0309888163	-0.9417938261
3SA	0.0000000003	0.0147013926	1.0235402560	-0.0634779681	0.2282352509	-0.0654052840	2.7612767387
4SA	-0.0000000006	-0.0239120322	-1.7117943577	0.0114486530	-0.1045965257	0.0489262515	-1.7560112109
2PA	-0.0000000001	-0.3462119307	0.0054344333	0.0113525506	-0.0485251030	-0.2799008940	0.0101313541
3PA	0.0000000002	0.3097466605	-0.0040302697	-0.1477801844	0.4855045070	3.2685891260	-0.2927997454
4PA	-0.0000000002	-1.0255592351	0.0136573006	0.0945355023	-0.3942710220	-2.9658448806	0.2987401736
2SB	0.0000000005	-0.0238902009	-0.0224462404	0.6554272109	0.0657603551	-0.0947173750	-0.9496391380
3SB	-0.0000000004	0.0524016663	0.0491350117	-1.2037779778	-0.0465848270	0.3242466300	3.5894510865
4SB	0.0000000001	-0.0469365857	-0.0460494160	1.6209075407	0.1584968581	-0.2052241645	-2.8108718146
2PB	0.0000000000	-0.0122436304	-0.0112541635	0.0669284469	-0.3832606923	0.0348918434	-0.0163202944
3PB	-0.0000000000	0.0413851910	0.0380272394	-0.2246250679	1.2703761113	-0.0951411408	0.1002484549
4PB	-0.0000000000	-0.0445910142	-0.0410593475	0.3165439555	-1.8576245584	0.2542946640	-0.0280240947

FUNCTIONS X(K) WHICH DIAGONALIZE H(A)

E(K)	0.2170054138	0.4369916168	0.8854305986	1.2078097366	2.0220123540	2.4070570742	4.6803696108
(B-SA+X(K))	-0.2799246424	-0.3164673213	-0.4987423667	0.0244212471	0.0006341131	-0.0057771914	-0.1621735666

STO EXPANSION COEFFICIENTS OF SLATER-TYPE ORBITALS

(EXPONENTS=1)							
1SA	-0.4255265529	0.0390540407	0.0343764865	-0.0141282085	0.3455289279	-4.2940210757	0.0839633480
1SB	-0.1643447750	-0.0094942637	-0.0082453895	0.0115279203	-0.0013522682	-0.0397940473	-4.4573689061
2SA	-2.1101967040	0.1003706439	-0.0247423851	0.0243722175	-0.9092076552	12.2454278115	-0.2833729962
3SA	6.2776704120	-0.3965975044	0.0702194756	-0.0043129562	0.9116336482	-13.6476970000	0.3888805887
4SA	-4.3656240021	0.3000716305	0.0694711586	-0.0105997907	-0.3144787964	5.7919350326	-0.2029830205
2PA	-0.0017502760	-0.0571522568	-0.2101921025	-4.5560903131	0.2683961640	0.0458653307	-0.0975923456
3PA	0.1394372913	-0.0727659368	0.2999297247	8.1666590912	-0.5700922975	-0.0993194281	0.2283468703
4PA	-0.1463342980	0.1456076725	-0.1021647081	-4.2441647269	0.3596224621	0.0638365590	-0.1577594730
2SB	0.4101604385	0.0040875523	-4.5272900381	0.2835483357	0.0052744607	0.0093707182	11.5914305539
3SB	-1.6209352154	-0.0542931364	0.2696103854	-0.6194182497	-0.0023040533	0.1067431828	-12.4578239170
4SB	1.3155447383	0.0510573206	-4.2703325985	0.3816113726	-0.0030334992	-0.1050491713	5.0544792949
2PB	-0.0120461739	-0.7431111041	-0.0109456364	-0.1017066687	-4.4931204967	-0.4513448429	0.0176755656
3PB	0.0564450387	4.0810250574	0.0033991147	0.0182384254	7.7164380677	0.8577361939	-0.0403427673
4PB	0.0161345774	-3.0616117996	0.0033876384	0.0091062939	-3.8841399962	-0.4678409509	0.0272356907

J(MINIMUM) = -1.3708512463

VARIATIONAL APPROXIMATION TO THE EXCHANGE FUNCTION ZETA

(H(A)-E(0)+IU)ZETA = B-SA

H(A) = HYDROGEN ATOM HAMILTONIAN E(0) = -0.5

ZETA = S((B-SA*X(K))/(E(K)-E(0)+IU))X(K)

INTERNUCLEAR DISTANCE R = 18.0000

FUNCTIONS X(K) WHICH DIAGONALIZE H(A)

E(K)	-0.5000000014	-0.1159233566	-0.1136026429	-0.0036968669	0.0634156108	0.1169196921	0.2072024246
(B-SA*X(K))	-0.0000030000	-0.0019559263	-0.0019116594	0.4939574344	-0.0840863672	-0.0299853822	0.6263407990

STO EXPANSION COEFFICIENTS OF SLATER-TYPE ORBITALS

(EXPONENTS=1)							
1SA	-0.9999999989	0.0011919993	0.4959647630	0.0073354325	0.0111031951	-0.0011960374	-0.1883104322
1SB	-0.0000000001	0.0013835044	0.0013105963	-0.0010714574	-0.0119764755	-0.0156762878	0.3657963974
2SA	-0.0000000073	-0.0012572412	-0.4845964770	0.0167098433	0.0462037824	-0.0063509010	-0.9488428247
3SA	0.0000000128	0.0026961744	1.0240758330	-0.0437418145	-0.1230243998	0.0173221205	2.7954283315
4SA	-0.0000000100	-0.0042570508	-1.7132231601	0.0132606928	0.0622710927	-0.0100288146	-1.7929757871
2PA	0.0000000000	-0.3465712914	0.0008984470	0.0073038284	0.0263134223	0.2862923955	0.0013143888
3PA	0.0000000000	0.3095534491	-0.0005675869	-0.0700071543	-0.2633139999	-3.3164805011	-0.1211416010
4PA	-0.0000000001	-1.0262796375	0.0025766000	0.0486237322	0.2107289333	3.0029333223	0.1254411301
2SB	0.0000000005	-0.0102102903	-0.0097676631	0.6590562537	-0.0507618544	0.0445120094	-0.9543300851
3SB	-0.0000000010	0.0223433454	0.0213512920	-1.2062025681	0.0366517648	-0.1451879024	3.6087913532
4SB	0.0000000005	-0.0198300437	-0.0190435084	1.6290664607	-0.1215657570	0.0909669568	-2.8284667791
2PB	0.0000000001	-0.0054423635	-0.0051230419	0.0538904465	0.3861282475	-0.0170739135	-0.0143070287
3PB	-0.0000000003	0.0181724254	0.0171150140	-0.1807575848	-1.2928777570	0.0483145607	0.0838683647
4PB	0.0000000003	-0.0187349179	-0.0177021503	0.2540325769	1.8864262708	-0.1272275051	-0.0271025458

FUNCTIONS X(K) WHICH DIAGONALIZE H(A)

E(K)	0.2155365063	0.4440480292	0.8917615965	1.2034438978	2.0248031655	2.4013197828	4.6820355515
(B-SA*X(K))	-0.2813466749	0.0185329130	-0.4996624531	0.0130812734	0.0011905110	0.0029592895	-0.1623941337

STO EXPANSION COEFFICIENTS OF SLATER-TYPE ORBITALS

(EXPONENTS=1)							
1SA	-0.4255650007	-0.0200243668	0.0182514539	-0.0029135993	0.1840653036	4.3019807179	0.0430065364
1SB	-0.1641408081	0.0088630758	-0.0000507649	0.0068379834	0.0018891486	0.0207235627	-4.4547218567
2SA	-2.1131226604	-0.0414201378	-0.0171156430	0.0052311078	-0.4863123734	-12.2566222260	-0.1433908770
3SA	6.2753835901	0.1765765754	-0.0301406714	-0.0015069093	0.4976865996	13.8427593017	0.1936366832
4SA	-4.0547631534	-0.1331559123	0.0377773125	-0.0016315627	-0.1785762688	-5.7797823724	-0.0984948155
2PA	0.0000516653	0.0325400254	-0.1136613702	-4.5567695037	0.1378526611	-0.0104634056	-0.0491356646
3PA	0.0542669375	0.0207766768	0.1660894130	8.1736464133	-0.2863871868	0.0224272674	0.1126892840
4PA	-0.0569972588	-0.0587904984	-0.0635802555	-4.2276548625	0.1775056117	-0.0141059088	-0.0755375744
2SB	0.4172359051	0.0023046193	-4.5321566951	0.1448527909	0.0074913549	-0.0082229562	11.5759770984
3SB	-1.6170906422	0.0467790141	8.2751433125	-0.3142503511	-0.0165043781	-0.0469806800	-12.4296936912
4SB	1.2886778072	-0.0517931374	-4.2792362430	0.1695541594	0.0106496436	0.0460469036	5.0369164253
2PB	-0.0045035210	0.7450661536	-0.0098752373	-0.0552594185	-4.5002481015	0.2370397760	0.0011438515
3PB	0.0147374594	-4.0803901915	-0.0013216156	0.0197246401	7.7173414438	-0.4454748610	-0.0033381487
4PB	-0.0089769368	3.0531015569	0.0079450722	-0.0346678076	-3.8771914163	0.2488302838	0.0026629855

J(MINIMUM) = -1.3561622100

VARIATIONAL APPROXIMATION TO THE EXCHANGE FUNCTION ZETA

(H(A)-E(0)+IU)ZETA = B-SA

H(A) = HYDROGEN ATOM HAMILTONIAN E(0) = -0.5

ZETA = S((B-SA,X(K))/(E(K)-E(0)+IU))X(K)

INTERNUCLEAR DISTANCE R = 20.0000

FUNCTIONS X(K) WHICH DIAGONALIZE H(A)

E(K)	-0.4999999979	-0.1189107988	-0.1135914966	0.0020531926	0.0694074316	0.1166262702	0.2127744564
(B-SA,X(K))	-0.0000000001	0.0005657325	-0.0005604646	0.4961710292	0.0672539230	-0.0110973531	0.4933879876

STO (EXPONENTS=1) — EXPANSION COEFFICIENTS OF SLATER-TYPE ORBITALS

1SA	-0.9999999927	-0.0001588100	0.4960344746	0.0023584705	-0.0040672692	-0.0001705924	-0.3231985443
1SB	-0.0000000001	-0.0005457595	0.0005184683	-0.0006872230	0.0095885646	-0.0059253473	0.2881922988
2SA	-0.0000000018	0.0001730039	-0.4845838383	0.0070375221	-0.0198157083	-0.0009659598	-1.6145334152
3SA	-0.0000000038	-0.0003702985	1.0240194867	-0.0180044722	0.0521955922	0.0026150416	4.7812566104
4SA	-0.0000000030	0.0005743671	-1.7133414343	0.0068120785	-0.0276795217	-0.0015256639	-3.0821720188
2PA	-0.0000000000	0.3465901607	0.0001140525	0.0032748045	-0.0127170461	0.2880000904	-0.0003343744
3PA	-0.0000000000	-0.3093876838	-0.0000623828	-0.0274664370	0.1148337570	-3.3294747753	-0.0335478094
4PA	0.0000000001	1.0262657688	0.0003283093	0.0198725342	-0.0966372955	3.0134012498	0.0352366239
2SB	0.0000000002	0.0038176621	-0.0036595557	0.6600203663	0.0406153113	0.0174690462	-0.7520803354
3SB	-0.0000000005	-0.0083089380	0.0079615291	-1.2082510513	-0.0294303876	-0.0551414657	2.8432320960
4SB	0.0000000003	0.0071123050	-0.0068518304	1.6314846512	0.0972821257	0.0341984978	-2.2283233561
2PB	-0.0000000001	0.0020797148	-0.0019693296	0.0438337445	-0.3891632950	-0.0071326568	-0.0104779558
3PB	0.0000000002	-0.0068691912	0.0065096274	-0.1469174084	1.2955022503	0.0208419453	0.0587801901
4PB	-0.0000000001	0.0068647101	-0.0065294634	0.2063205123	-1.8950257588	-0.0533110348	-0.0194658398

FUNCTIONS X(K) WHICH DIAGONALIZE H(A)

E(K)	0.2152083919	0.4494693647	0.8972909135	1.2024975164	2.0297593480	2.3998665081	4.6864377696
(B-SA,X(K))	0.4787064161	0.0161111886	0.4998936349	0.0056464251	0.0011628307	0.0012630682	-0.1624427676

STO (EXPONENTS=1) — EXPANSION COEFFICIENTS OF SLATER-TYPE ORBITALS

1SA	0.3349537492	-0.0083803326	-0.0078589050	-0.0004387633	0.0802179383	4.3048005371	0.0182677221
1SB	0.2792983888	0.0074025693	0.0000802718	0.0031614543	0.0024726235	0.0089708426	-4.4541655008
2SA	1.6629354445	-0.0145018436	0.0084913418	0.0008116000	-0.2140210382	-12.2619690292	-0.0604082117
3SA	-4.9374713564	0.0664706901	0.0098090056	-0.0002971454	0.2205179154	13.8447880773	0.0806774585
4SA	3.1892009193	-0.0502018968	-0.0136717991	-0.0001857707	-0.0809770435	-5.7784494243	-0.0403645919
2PA	-0.0004488803	0.0145402130	0.0494611072	-4.5599711423	0.0576900309	-0.0017152843	-0.0205201263
3PA	-0.0323241553	0.0041426779	-0.0747818779	8.1729761024	-0.1195197789	0.0036398334	0.0464158558
4PA	0.0341036437	-0.0200255065	0.0298691811	-4.2254494572	0.0724819159	-0.0022562760	-0.0305149621
2SB	-0.7226044672	0.0043745990	4.5338602001	0.0605856296	0.0064945848	-0.0045728661	11.5727232904
3SB	2.7537833401	0.0370251264	-8.2700928263	-0.1309698927	-0.0186916274	-0.0174766311	-12.4238205221
4SB	-2.1688630638	-0.0437659256	4.2806402952	0.0780480753	0.0115623554	0.0175096700	5.0333208076
2PB	-0.0040434516	0.7453269377	0.0085683403	-0.0241141684	-4.5036451797	0.1021789250	-0.0024644190
3PB	0.0291594481	-4.0810074405	0.0015032915	0.0112859703	7.7214610046	-0.1906874030	0.0046546090
4PB	-0.0157434954	3.0527406384	-0.0073322613	0.0115639822	-3.8781544382	0.1053685651	-0.0025396689

J(MINIMUM) = -1.3446622049