

ROOTHAAN-HARTREE-FOCK ATOMIC WAVEFUNCTIONS  
Basis Functions and Their Coefficients for Ground and Certain  
Excited States of Neutral and Ionized Atoms,  $Z \leq 54$

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Tables are presented of the exponents of the basis functions and the coefficients to be used in analytic wavefunctions expanded in the Roothaan-Hartree-Fock method according to which  $\phi_{i\lambda\alpha} = \sum x_{p\lambda\alpha} C_{i\lambda p}$ , where the  $x$ 's are functions of the form  $Nr^{n-1}e^{-\zeta r}Y(\theta, \phi)$ . Values of  $C$  and  $\zeta$  are tabulated for  $Z \leq 54$  for configurations indicated in the Contents.

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## INTRODUCTION

### Preface

Why compute Hartree-Fock functions, an approximation over 40 years old, when most of contemporary physics pays relatively minor attention to atomic physics? The simple answer is that there are several unsettled problems and gaps in our knowledge of the electronic structure of the periodic system and that the Hartree-Fock method (in the Roothaan form) is presently the most efficient technique available for solving them. In the present literature on atomic functions there is no systematic atomic wavefunction collection comparable to the one presented in these tables. In a previous tabulation one of us (E.C.) presented some results similar to those given here, but only for atoms or ions with  $Z \leq 36$ . That earlier tabulation has now been recomputed and improved. The revised data are included in the present tables.

The functions here tabulated have been obtained with the Roothaan-Hartree-Fock expansion technique. The work was stimulated by the realization that a by-product of a systematic study of the Hartree-Fock total energies would be a systematic body of data on the atomic correlation energy. This has been proven to be most useful in predicting the correlation correction in molecules or in stable negative ions.

The expansion method offers the interesting possibility of providing an excellent starting basis set for molecular and for solid-state computations. This was constantly in our minds during the preparation of the tables. For this reason we have added the two tables of functions involving either a single zeta or a double zeta basis set. For definitions, see Notes for Tables 37, 42, and 43 on page 184 immediately preceding Table 1.

Irrespective of the usefulness of the atomic functions in fields other than atomic physics, they are an aid to fundamental studies of the behavior of atoms and to the description of that behavior by means of computations.

These tables are dedicated to Professor C. C. J. Roothaan, to Professor R. S. Mulliken, and to the present and past members of the Laboratory of Molecular Structure and Spectra in the Department of Physics of the University of Chicago.

### The Roothaan-Hartree-Fock Method

The method has been described by Roothaan for closed shells,<sup>1</sup> by Roothaan for a single open shell,<sup>2</sup> by Huzinaga for two open shells,<sup>3</sup> and by Roothaan and Bagus for many open shells.<sup>4</sup> A number of additional references are given in our previous tabulation of atomic functions.<sup>5</sup>

In what follows we shall adhere, as closely as possible, to the presentation and the choice of symbols adopted by Roothaan. The physical model embodied in the Hartree-Fock method has been analyzed in many places, and therefore, we shall not repeat the analysis here. We refer instead to the expositions of Hartree<sup>6</sup> or Slater.<sup>7</sup>

We are interested in the solution of the Roothaan-Hartree-Fock equations, Eqs. (27), (28), for those states that belong to configurations with many open shells of different symmetry in addition to closed shells. The problem is that of obtaining the total energy  $E$  for a wavefunction  $\Phi$  obtained in the self-consistent-field framework. In computing  $E$  the Hamiltonian is

$$H = \sum_a^n \left( -\frac{1}{2} \nabla_a^2 - \frac{Z}{r_a} \right) + \Sigma_{a>b} \frac{1}{r_{ab}}. \quad (1)$$

The total wavefunction  $\Phi$  is a Slater determinant

$$\Phi = \Omega(\phi_1^{(1)} \cdots \phi_n^{(n)}) \quad (2)$$

where  $\Omega$  is the antisymmetrizing factor,  $n$  is the total number of electrons, and  $\phi_1, \phi_2, \dots$ , are spin-orbitals (one-electron functions). Since Eq. (1) is spin independent, the spin-orbitals are simply a product of a spin function and an orbital function. The orbitals are assumed to be orthogonal to each other, thus the same holds for the spin-orbitals. The orbitals are obtained by solving the Roothaan-Hartree-Fock equations, not by attempting to find solution of the Hamiltonian (1). The expectation value for the energy is given by the usual relation

$$E = \langle \Phi | H | \Phi \rangle / \langle \Phi | \Phi \rangle. \quad (3)$$

The orbitals are characterized by an index  $\lambda$ , which indicates the symmetry species ( $\lambda$  corresponds to the quantum number  $I$ ), by an index  $\alpha$ , which indicates the subspecies (the subspecies label the individual members of the degenerate set that transform according to the representation  $\lambda$ ) and by an index  $i$ , which refers to the  $i^{\text{th}}$  orbital of symmetry  $\lambda$ . The orbital  $\phi_{i\lambda\alpha}$  is expanded in terms of basis functions according to

$$\phi_{i\lambda\alpha} = \sum_p \chi_{p\lambda\alpha} C_{i\lambda p}. \quad (4)$$

The subscript  $p$  refers to the  $p^{\text{th}}$  basis function of symmetry  $\lambda$ . The expansion coefficient depends on  $i, \lambda$ , and  $p$  but not on the subspecies  $\alpha$ . The basis functions  $\chi$  are Slater-type orbitals with integer quantum numbers, namely

$$\chi_{p\lambda\alpha}(r, \theta, \phi) = R_{\lambda p}(r) Y_{\lambda\alpha}(\theta, \phi), \quad (5)$$

where

$$R_{\lambda p} = [(2n_{\lambda p}!)]^{-1/2} (2\xi_{\lambda p})^{n_{\lambda p}+1/2} r^{n_{\lambda p}-1} e^{-\xi_{\lambda p} r} \quad (6)$$

and  $Y_{\lambda\alpha}(\theta, \phi)$  are normalized spherical harmonics in complex form. It is noted that  $n_{\lambda p} \geq \lambda + 1$  and that the exponent  $\xi_{\lambda p}$  is to be chosen so as to give the best energy found by a laborious process of optimization.

Having defined the basis set  $\chi$  we shall now give an expression for the total energy. It will turn out to be convenient to subdivide  $E$  into two components,  $E^{(1)}$  for the one electron operators of  $H$ , and  $E^{(2)}$  for  $1/r_{ab}$ :

$$\begin{aligned} E &= \langle \Phi | -\sum_a \left( \frac{1}{2} \nabla_a^2 + \frac{Z}{r_a} \right) | \Phi \rangle + \langle \Phi | \sum_a \frac{1}{r_{ab}} | \Phi \rangle \\ &= E^{(1)} + E^{(2)}. \end{aligned} \quad (7)$$

We shall start by introducing the overlap matrix element  $S_{\lambda pq}$  defined as

$$S_{\lambda pq} = \langle \chi_{\lambda p\alpha} | \chi_{\lambda q\alpha} \rangle. \quad (8)$$

Since the basis functions, Eqs. (5) and (6), are normalized,  $S_{\lambda pq} = \delta_{pq}$ . The matrix elements of a given  $\lambda$  can be collected in a square matrix  $S_\lambda$ ; the total collection of all the  $S_{\lambda pq}$  for every  $\lambda$  can be collected in a square matrix  $S$ .

Whenever we shall need to consider the matrix elements of a matrix as a one-dimensional array, we shall call such an array a *supervector*.

Let us collect the expansion coefficients  $C_{i\lambda p}$  in a  $p$  component column vector  $C_{i\lambda}$ . We shall assume that the vectors  $C_{i\lambda}$  form an orthonormal set in the following sense:

$$C_{i\lambda}^\dagger S C_{j\lambda} = \delta_{ij}. \quad (9)$$

Let us indicate with  $N_{i\lambda}$  the occupation number of a shell. If needed we shall indicate by  $N_{c\lambda}$  and  $N_{o\lambda}$  the occupation numbers of closed and open shells, respectively. We shall define as *shell*, *closed-shell*, *open-shell*, and *total-density matrices* the quantities

$$D_{i\lambda} = N_{i\lambda} C_{i\lambda} C_{i\lambda}^\dagger \quad (10a)$$

$$D_{c\lambda} = \Sigma_k D_{k\lambda} \quad (10b)$$

$$D_{o\lambda} = \Sigma_m D_{m\lambda} \quad (10c)$$

$$D_{T\lambda} = D_{c\lambda} + D_{o\lambda}, \quad (10d)$$

where  $k = i \subset$  closed and  $m = i \subset$  open, respectively. (It is noted that  $C^\dagger$  is a row vector and  $C$  is a column vector, hence  $CC^\dagger$  is a matrix).

We are finally in a position to compute  $E^{(1)}$ . Remembering Eqs. (1), (6), and (7), let us define the nuclear potential and the kinetic energy matrix elements as

$$U_{\lambda pq} = \langle \chi_{\lambda p\alpha} | \frac{1}{r} | \chi_{\lambda q\alpha} \rangle, \quad (11)$$

$$T_{\lambda pq} = -\langle \chi_{\lambda p\alpha} | \frac{1}{2} \nabla^2 | \chi_{\lambda q\alpha} \rangle. \quad (12)$$

We can now define the matrices  $T_\lambda$ ,  $U_\lambda$  and  $T$ ,  $U$  in the same way we have defined the matrices  $S_\lambda$  and  $S$ . In addition we can define the one-electron Hamiltonian  $h$ , sometimes referred to as the bare-nucleus Hamiltonian,

$$h = -ZU + T. \quad (13)$$

The one-electron Hamiltonian will give the energy  $E^{(1)}$  according to

$$\begin{aligned} E^{(1)} &= \langle \Phi | h | \Phi \rangle = \Sigma \langle \phi_i | h | \phi_i \rangle \\ &= \Sigma_\lambda (\Sigma_k N_{\lambda k} \Sigma_{pq} H_{\lambda pq} C_{\lambda kq} C_{\lambda kp} \\ &\quad + \Sigma_m N_{\lambda m} \Sigma_{pq} H_{\lambda pm} C_{\lambda mp} C_{\lambda mq}), \end{aligned} \quad (14)$$

or in matrix notation, the *scalar*  $E^{(1)}$  is given by

$$E^{(1)} = \Sigma_\lambda H_\lambda^\dagger D_{c\lambda} + \Sigma_\lambda H_\lambda^\dagger D_{o\lambda} = H^\dagger D_T \quad (15)$$

It is noted that  $E^{(1)}$  does not depend on the symmetry subspecies  $\alpha$ , but only on  $i\lambda$ .

For the two-electron Hamiltonian the situation will clearly be different since, for this case, the matrix elements will depend on the subspecies. Therefore, one can expect a more complex situation. Following Roothaan and Bagus, we shall place emphasis on the fact that each  $\phi$  contains a doubly occupied closed-shell core  $\phi_c$  and a partially occupied open shell chosen from a set  $\phi_o$ . The combined set of orbitals  $\phi$  can, therefore, be defined by

$$\phi = (\phi_c, \phi_o). \quad (16)$$

It might be convenient to digress briefly and to comment on the special case of closed-shell configurations. The two-electron energy for a closed shell  $E_c^{(2)}$ , is given by the relation

$$E_c^{(2)} = 2 \Sigma_{kl} (J_{kl} - \frac{1}{2} K_{kl}), \quad (17)$$

where  $J_{kl}$  and  $K_{kl}$  are the usual Coulombic and exchange interactions between the orbitals  $l$  and  $k$ . In order to obtain  $E^{(2)}$  one has to compute matrix elements of the form

$$\begin{aligned} \Sigma_{pq} \Sigma_{rs} C_{l\lambda p} C_{l\lambda q} C_{k\mu r} C_{k\mu s} & \left\{ \int \int \chi_{p\lambda a}^{*b} \chi_{r\mu b}^{*a} \frac{1}{r_{ab}} \chi_{q\lambda a}^b \chi_{s\mu b}^a dV^a dV^b \right. \\ & \left. - \frac{1}{2} \int \int \chi_{p\lambda a}^{*b} \chi_{r\mu b}^{*a} \frac{1}{r_{ab}} \chi_{q\lambda a}^b \chi_{s\mu b}^a dV^a dV^b \right\}. \end{aligned} \quad (18)$$

Let us indicate by  $P$  the supermatrix with elements  $P_{\lambda pq, rs}$  given by the expression inside the brackets in Eq. (18). One obtains

$$E_c^{(2)} = \frac{1}{4} \sum_{pq} \sum_{rs} (D_{k\lambda})_{pq} (D_{l\mu})_{rs} (P_{\lambda, \mu})_{pq, rs} \quad (19a)$$

or

$$E_c^{(2)} = \frac{1}{2} D_c^\dagger P D_c. \quad (19b)$$

We shall not comment further on the closed-shell problem.

Let us turn now to the computation of  $E^{(2)}$  for the case of open shells. From what we have shown for the closed-shell case, and keeping in mind the definition of  $\Phi$ , Eq. (2) and  $\phi$ , Eq. (16), one would expect that, for open-shell configuration, the energy  $E^{(2)}$  could be partitioned into closed-closed-shell, open-open-shell, and closed-open-shell interactions. The latter can be constructed in a way similar to the previous one as long as an additional term is included which has the function of subtracting those interactions that were fictitiously added in the  $P$ -term (as we would do if we were to compute closed-shell interactions). We shall call this subtractive term a "Q-type" term, for reasons which will appear clearer in the following discussion.

We are finally in a position to state explicitly an expression for the energy  $E^{(2)}$ . We shall make use of two supermatrices, one the  $P$  supermatrix, as for the case of the closed-shell configurations, and a  $Q$  supermatrix for the open-shell-open-shell interactions. These are defined as

$$P_{\lambda pq, \mu rs} = \mathcal{J}_{\lambda pq, \mu rs}^0 - \frac{1}{2} \sum_{\nu=|\lambda-\mu|}^{|\lambda+\mu|} A_{\lambda\mu\nu} \mathcal{K}_{\lambda pq, \mu rs}^\nu, \quad (20)$$

$$Q_{\lambda pq, \mu rs} = \sum_{\nu=0}^{2(\lambda, \mu)} J_{\lambda\mu\nu} \mathcal{J}_{\lambda pq, \mu rs}^\nu - \frac{1}{2} \sum_{\nu=|\lambda-\mu|}^{|\lambda+\mu|} K_{\lambda\mu\nu} \mathcal{K}_{\lambda pq, \mu rs}^\nu, \quad (21)$$

where  $J_{\lambda\mu\nu}$  and  $K_{\lambda\mu\nu}$  are the vector coupling coefficients which vary from state to state and configuration to configuration and  $\mathcal{J}$  and  $\mathcal{K}$  are the Coulomb and exchange integrals. Clearly, for closed shells  $J_{\lambda\mu\nu}$  and  $K_{\lambda\mu\nu}$  are zero. The expression for the energy  $E^{(2)}$  is, in supervector and supermatrix notation,

$$E^{(2)} = \frac{1}{2} D_T^\dagger P D_T - \frac{1}{2} D_o^\dagger Q D_o. \quad (22)$$

The whole preceding section can be summarized with the following statement. *Given a wavefunction of appropriate symmetry and spin properties of determinant form, its energy is expressed by Eq. (22).* We shall now explain how one obtains such functions, as defined above, in the Roothaan–Hartree–Fock method.

### The Self-Consistent-Field Technique

In order to obtain a Hartree–Fock function in the expansion method, one makes use of the variational method for the density matrices and of "good sense" in the choice of the basis set. Unfortunately "good sense" does not go too far and a process of trial and error in the choice of the basis set is needed; this process is generally referred to as *optimization of the orbital exponent* and, nowadays is carried out by the computer,

instructed to compromise between efficiency for a specific case and complete generality of the procedure.

We now ask for the best function that can be obtained for a given basis set, that is for that function which minimizes the energy expression, Eq. (22). Let us subject every orbital  $\phi_i$  to a variation by an infinitesimal amount  $\delta\phi_i$ ; since the basis set is fixed, this is tantamount to an infinitesimal variation of the expansion coefficients  $C_{\lambda i}$ . The orbital  $\phi_i$  always has to conform to the orthogonality condition. Therefore the variation  $\delta C_{i\lambda p}$  is restricted by those conditions which are obtained by subjecting Eq. (9) to an infinitesimal variation. Let us sum the constraints for all possible orbitals ( $\Sigma_{ij}$ ) and for all the possible symmetries ( $\Sigma_\lambda$ ), and let us multiply the resulting expression by  $\Theta_{\lambda ji}$  and  $\Theta_{\lambda ij}$ , the Lagrangian multipliers; we then obtain

$$2\sum_{\lambda i j p q} |\delta C_{\lambda p i}| S_{\lambda p q} C_{\lambda q j} \Theta_{\lambda j i} = 0.$$

The standard mathematical technique is to add to the  $\delta E$  the constraints which must be satisfied, multiplied by the Lagrangian multipliers. Let us call  $\delta E'$  the result of this addition. The problem is now that of finding the condition for  $\delta E' = 0$  for any choice of the  $\delta C$ , without restriction, while at the same time giving suitable values to the Lagrangian multipliers.

We shall have Lagrangian multipliers between orbitals of closed shells, between orbitals of open shells, and between orbitals of closed and open shells. The latter type of multiplier will be eliminated by introducing new operators  $R_c$  and  $R_o$  for closed and open shells. The introduction of  $R_c$  and  $R_o$  in order to eliminate the  $\Theta_{\lambda k m}$  is convenient because the  $R$  operators, called *coupling operators*, are expressed in terms of previously defined quantities such as  $P$  and  $Q$ . The operators  $R_c$  and  $R_o$  for closed and open shells are of the form

$$R_{c, \lambda pq} = [N_{c\lambda}/(N_{c\lambda} - N_{o\lambda})] \sum_l [\sum_{u\omega} S_{\lambda pu} C_{l\lambda u} Q_{\lambda uq} C_{l\lambda v} + \sum_{u\omega} Q_{\lambda pu} C_{l\lambda u} S_{\lambda uq} C_{l\lambda v}], \quad (23a)$$

$$R_{o, \lambda pq} = [N_{o\lambda}/(N_{c\lambda} - N_{o\lambda})] \sum_l [\sum_{u\omega} S_{\lambda pu} C_{n\lambda u} Q_{\lambda uq} C_{n\lambda v} + \sum_{u\omega} Q_{\lambda pu} C_{n\lambda u} S_{\lambda uq} C_{n\lambda v}], \quad (23b)$$

which are, by definition, Hermitian. In addition, let us designate by  $F_c$  and  $F_o$  the quantities  $F_{c, \lambda pq} = H_{\lambda pq} + P_{\lambda pq} + R_{o, \lambda pq}$  and  $F_{o, \lambda pq} = H_{\lambda pq} + P_{\lambda pq} - Q_{\lambda pq} + R_{c, \lambda pq}$ .

We can now write the basic equations of our problem in the form

$$F_{c, \lambda pq} C_{k\lambda q} = \sum_{lq} S_{\lambda pq} C_{\lambda ql} \Theta_{\lambda lk} \quad (24a)$$

and

$$F_{o, \lambda pq} C_{m\lambda q} = \sum_{mq} S_{\lambda pq} C_{\lambda qn} \Theta_{\lambda mn}. \quad (24b)$$

By making use of a unitary transformation on the closed and open shells separately, we can bring the  $\Theta$  matrices into diagonal form. By designating as  $\epsilon_{m\lambda}$ , the diagonal elements of the transformed  $\Theta$  matrices, we can finally write

$$\sum_q F_{c,\lambda pq} C_{k\lambda q} = \epsilon_{k\lambda} \sum_q S_{\lambda pq} C_{k\lambda q}, \quad (25)$$

$$\sum_q F_{o,\lambda pq} C_{m\lambda q} = \epsilon_{m\lambda} \sum_q S_{\lambda pq} C_{m\lambda q}, \quad (26)$$

or, in a more compact notation, we have

$$\mathbf{F}_c \mathbf{C} = \boldsymbol{\epsilon} \mathbf{S} \mathbf{C}, \quad (27)$$

$$\mathbf{F}_o \mathbf{C} = \boldsymbol{\epsilon} \mathbf{S} \mathbf{C}. \quad (28)$$

These are the Hartree-Fock equations for closed and open shells. They are pseudoeigenvalue equations, because the matrices  $\mathbf{F}_c$  and  $\mathbf{F}_o$  depend on the solution  $\mathbf{C}$ . Self-consistency is achieved when the same vectors,

from which these matrices are constructed according to Eqs. (24), are solutions of Eqs. (25) and (26).

We refer to the computer program description<sup>8</sup> for additional details. All the computations reported were performed in double precision (64 bits) on an IBM 360/195 computer, with an updated version of the computer program above mentioned. The values for the total energy of the wavefunctions given in Table 1 (neutral atoms), Table 2 (first position ions) and Table 42 (double zeta functions) have been recently reported elsewhere,<sup>9</sup> but are reprinted here for the sake of completeness.

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**TABLES. BASIS FUNCTIONS AND THEIR COEFFICIENTS****Explanation of Tables**

1s(2), etc.	Shell designation and electron occupation number
T.E.	Total energy in atomic units (hartrees)
P.E.	Potential energy in atomic units (hartrees)
K.E.	Kinetic energy in atomic units (hartrees)
V.T.	P.E./K.E. a test of the virial theorem, that predicts a value of $-2$
S,P,D,	$\lambda = 0,1,2$ , for the basis set given below in the table
BASIS	Basis set
1S,2S	The values 1,2, . . . , indicate the value of $n$
ORB E	Orbital energy in atomic units (hartrees)
Column 1	The numbers in the first column are the values of $\xi$ in the basis function $\chi = Nr^{n-1}e^{-\xi r}$ where $N$ is the normalization factor
Others columns	The numbers in the others columns are: First entry: orbital energy Following entries: values of the coefficients C for the atomic orbital $\phi(n,\lambda)$

**Notes for Tables 32, 42, and 43**

In Table 32, we present the iso-electronic series with 19 electrons, that is, the iso-electronic series for potassium. The configuration we have chosen, however, is not . . . 4s<sup>1</sup>, but . . . 4s<sup>0</sup>3d<sup>1</sup>, since for most of the 19-electron ions the latter configuration is the lowest one. For Ca<sup>+</sup>, in the configuration . . . 4s<sup>1</sup>, the Roothaan-Hartree-Fock function is given both in Tables 2 and 32.

In Table 42, we report “double zeta” functions. A double zeta function is an approximate Roothaan-Hartree-Fock function in which a given electron orbital is described by *two* Slater functions (apart from additional linear combinations due to the orthogonality

constraints). We note that in the example given for the boron atom, the functions are double zeta functions.

In Table 43, we report the “single zeta” functions. A single zeta function is that approximation to the Roothaan-Hartree-Fock function, in which a given electron orbital is described by *one* Slater function (apart from additional linear combinations due to the orthogonality constraints). Whereas a double zeta function is nearly as accurate as a Hartree-Fock function, the single zeta function is much more rudimentary. However, the orbital exponents of a single zeta function are of physical interest, since they provide a simple and quantitative description of the electron’s screening.

## Example

BORON	1S(2)2S(2)2P(1), 2P				
T.E. =	-0.24527920D + 02	P.E. =	-0.49056561D + 02		
K.E. =	0.24528640D + 02	V.T. =	-0.19999706D + 01		
S	1S	2S	P	2P	
BASIS/ORB E	-7.69443*	-0.49408*	BASIS/ORB E	-0.30989*	
1S 6.56657	0.19030	0.00754	2P 2.21734	0.21526	
1S 4.24927	0.82091	-0.25055	2P 1.00551	0.84052	
2S 1.41314	-0.00364	0.87099			
2S 0.87564	0.00251	0.18515			
$n, \lambda$	Orbital exponents	$\phi(1s)$ expansion coefficients	$\phi(2s)$ expansion coefficients	$n, \lambda$	Orbital exponents
$\zeta$				$\zeta$	$\phi(2p)$ expansion coefficient

Description of orbitals of *s* symmetry... of orbitals of *p* symmetry

\*Orbital energy

The orbitals (1s), (2s) are of the form

$$\begin{aligned}\phi(1s) &= 0.19030\chi_1 + 0.82091\chi_2 - 0.00364\chi_3 + 0.00251\chi_4 \\ \phi(2s) &= 0.00754\chi_1 - 0.25055\chi_2 + 0.87099\chi_3 + 0.18515\chi_4 \\ \phi(2p) &= 0.21526\chi_5 + 0.84052\chi_6\end{aligned}$$

where  $\chi_1, \chi_2$  are Slater functions of 1s type,  $\chi_3$  and  $\chi_4$  are Slater functions of 2s type, and  $\chi_5$  and  $\chi_6$  are Slater functions of 2p type.

$$\begin{aligned}\chi_1 &= N_1 r^0 \exp(-6.56657r) Y_{00}(\vartheta, \phi) \\ \chi_2 &= N_2 r^0 \exp(-4.24927r) Y_{00}(\vartheta, \phi) \\ \chi_3 &= N_3 r^1 \exp(-1.41314r) Y_{00}(\vartheta, \phi) \\ \chi_4 &= N_4 r^1 \exp(-0.87564r) Y_{00}(\vartheta, \phi) \\ \chi_5 &= N_5 r^1 \exp(-2.21734r) Y_{10}(\vartheta, \phi) \\ \chi_6 &= N_6 r^1 \exp(-1.00551r) Y_{10}(\vartheta, \phi)\end{aligned}$$

The normalization factors  $N_1, N_2, \dots, N_6$  are given by Eq. (6).

## ROOTHAAN-HARTREE-FOCK ATOMIC WAVEFUNCTIONS

TABLE 1 (1). HARTREE-FOCK FUNCTIONS FOR NEUTRAL ATOMS.

HELIUM 1S(2), 1S  
 T.E.= -0.28616799D+01  
 P.E.= -0.57233927D+01  
 K.E.= 0.28617128D+01  
 V.T.= -0.19999885D+01

S	1S
BASIS/ORB E	-0.91795
1S 1.41714	0.76838
1S 2.37682	0.22346
1S 4.39628	0.04082
1S 6.52699	-0.00994
1S 7.94252	0.00230

LITHIUM 1S(2)2S(1), 2S  
 T.E.= -0.74327257D+01 P.E.= -0.14865480D+02  
 K.E.= 0.74327544D+01 V.T.= -0.19999961D+01

S	1S	2S
BASIS/ORB E	-2.47773	-0.19632
1S 2.47673	0.89786	-0.14629
1S 4.69873	0.11131	-0.01516
2S 0.38350	-0.00008	0.00377
2S 0.66055	0.00112	0.98053
2S 1.07000	-0.00216	0.10571
2S 1.63200	0.00884	-0.11021

BERYLLIUM 1S(2)2S(2), 1S  
 T.E.= -0.14573021D+02 P.E.= -0.29146057D+02  
 K.E.= 0.14573036D+02 V.T.= -0.19999990D+01

S	1S	2S
BASIS/ORB E	-4.73267	-0.30527
1S 3.47116	0.91796	-0.17092
1S 6.36861	0.08724	-0.01455
2S 0.77820	0.00108	0.21186
2S 0.94067	-0.00199	0.62499
2S 1.48725	0.00176	0.26662
2S 2.71830	0.00628	-0.09919

BORON 1S(2)2S(2)2P(1), 2P  
 T.E.= -0.24529057D+02 P.E.= -0.49058014D+02  
 K.E.= 0.24528956D+02 V.T.= -0.20000041D+01

S	1S	2S	P	2P
BASIS/ORB E	-7.69533	-0.49469	BASIS/ORB E	-0.30986
1S 4.44561	0.92705	-0.19484	2P 0.87481	0.53622
1S 7.91796	0.07780	-0.01254	2P 1.36992	0.40340
2S 0.86709	0.00088	0.06541	2P 2.32262	0.11653
2S 1.21924	-0.00200	0.75234	2P 5.59481	0.00821
2S 2.07264	0.00433	0.31856		
2S 3.44332	0.00270	-0.12642		

CARBON 1S(2)2S(2)2P(2), 3P  
 T.E.= -0.37688612D+02 P.E.= -0.75376969D+02  
 K.E.= 0.37688357D+02 V.T.= -0.20000068D+01

S	1S	2S	P	2P
BASIS/ORB E	-11.32554	-0.70563	BASIS/ORB E	-0.43335
1S 5.43595	0.93262	-0.20814	2P 0.98073	0.28241
1S 9.48256	0.06931	-0.01071	2P 1.44361	0.54697
2S 1.05749	0.00083	0.08C99	2P 2.60051	0.23195
2S 1.52427	-0.00176	0.75045	2P 6.51003	0.01025
2S 2.68435	0.00559	0.33549		
2S 4.20096	0.00382	-0.14765		

CARBON 1S(2)2S(2)2P(2), 1D  
 T.E.= -0.37631325D+02 P.E.= -0.75262363D+02  
 K.E.= 0.37631038D+02 V.T.= -0.20000076D+01

S	1S	2S	P	2P
BASIS/ORB E	-11.35153	-0.71867	BASIS/ORB E	-0.38134
1S 5.40758	0.93342	-0.20766	2P 0.94020	0.32274
1S 9.41395	0.07297	-0.01230	2P 1.41693	0.49812
2S 1.17869	0.00155	0.21047	2P 2.56379	0.25008
2S 1.64602	-0.00343	0.6E533	2P 6.48484	0.01020
2S 2.83132	0.00956	0.27241		
2S 4.25928	-0.00441	-0.14909		

See page 183 for Explanation of Tables and Notes for Tables 32, 42, and 43

TABLE 1 (2). HARTREE-FOCK FUNCTIONS FOR NEUTRAL ATOMS.

CARBON	1S(2)2S(2)2P(2), 1S			
T.E.=	-0.37549582D+02	P.E.=	-0.75099105D+02	
K.E.=	0.37549523D+02	V.T.=	-0.20000016D+01	
S	1S	2S	P	2P
BASIS/ORB E	-11.39149	-0.73961	BASIS/ORB E	-0.31000
1S 5.41189	0.93414	-0.20593	2P 1.10539	0.63602
1S 9.43757	0.07195	-0.01375	2P 0.61830	0.07877
2S 1.18421	0.00168	0.19836	2P 2.26857	0.36369
2S 1.64350	-0.00376	0.68142	2P 5.23303	0.02063
2S 2.73028	0.00863	0.26711		
2S 4.42841	-0.00304	-0.13084		
NITROGEN	1S(2)2S(2)2P(3), 4S			
T.E.=	-0.54400924D+02	P.E.=	-0.10880145D+03	
K.E.=	0.54400522D+02	V.T.=	-0.20000074D+01	
S	1S	2S	P	2P
BASIS/ORB E	-15.62909	-0.94531	BASIS/ORB E	-0.56758
1S 6.45739	0.93780	-0.23677	2P 1.16068	0.26639
1S 11.17200	0.05849	-0.00846	2P 1.70472	0.52319
2S 1.36405	0.00093	0.17991	2P 3.03935	0.27353
2S 1.89734	-0.00170	0.67416	2P 7.17482	0.01292
2S 3.25291	0.00574	0.31297		
2S 5.08238	0.00957	-0.14497		
NITROGEN	1S(2)2S(2)2P(3), 2D			
T.E.=	-0.54296158D+02	P.E.=	-0.10859205D+03	
K.E.=	0.54295890D+02	V.T.=	-0.20000049D+01	
S	1S	2S	P	2P
BASIS/ORB E	-15.66638	-0.96365	BASIS/ORB E	-0.50864
1S 6.47679	0.93910	-0.21761	2P 1.07797	0.25030
1S 11.28370	0.05528	-0.00806	2P 1.65171	0.54143
2S 1.28558	0.00063	0.11411	2P 3.05395	0.28075
2S 1.85215	-0.00103	0.71861	2P 7.22635	0.01191
2S 3.20431	0.00433	0.33357		
2S 5.09120	0.01274	-0.14531		
NITROGEN	1S(2)2S(2)2P(3), 2P			
T.E.=	-0.54228089D+02	P.E.=	-0.10845579D+03	
K.E.=	0.54227699D+02	V.T.=	-0.20000072D+01	
S	1S	2S	P	2P
BASIS/ORB E	-15.69161	-0.97632	BASIS/ORB E	-0.47128
1S 6.44100	0.93704	-0.21914	2P 1.04491	0.26490
1S 11.09040	0.06111	-0.00873	2P 1.63553	0.52829
2S 1.30621	0.00106	0.11705	2P 3.05150	0.28543
2S 1.84672	-0.00212	0.69789	2P 7.24780	0.01160
2S 3.13942	0.00609	0.34613		
2S 5.09737	0.00724	-0.13874		
CXYGEN	1S(2)2S(2)2P(4), 3P			
T.E.=	-0.74809370D+02	P.E.=	-0.14961872D+03	
K.E.=	0.74809346D+02	V.T.=	-0.20000003D+01	
S	1S	2S	P	2P
EASIS/ORB E	-20.66866	-1.24433	BASIS/ORB E	-0.63192
1S 7.61413	0.94516	-0.22157	2P 1.14394	0.16922
1S 13.75740	0.03391	-0.00476	2P 1.81730	0.57974
2S 1.69824	-0.00034	0.34844	2P 3.44988	0.32352
2S 2.48022	0.00241	0.60807	2P 7.56484	0.01660
2S 4.31196	-0.00486	0.25365		
2S 5.86596	0.03681	-0.19183		
OXYGEN	1S(2)2S(2)2P(4), 1D			
T.E.=	-0.74729223D+02	P.E.=	-0.14945857D+03	
K.E.=	0.74729350D+02	V.T.=	-0.19999983D+01	
S	1S	2S	P	2P
BASIS/ORB E	-20.69317	-1.25649	BASIS/ORB E	-0.60072
1S 7.61607	0.94511	-0.22258	2P 1.07244	0.14587
1S 13.75420	0.03380	-0.00453	2P 1.74273	0.59472
2S 1.69089	-0.00046	0.33561	2P 3.42230	0.33561
2S 2.47070	0.00275	0.61655	2P 7.51459	0.01698
2S 4.28660	-0.00596	0.25974		
2S 5.84187	0.03782	-0.19342		

See page 183 for Explanation of Tables and Notes for Tables 32, 42, and 43

## ROOTHAAAN-HARTREE-FOCK ATOMIC WAVEFUNCTIONS

TABLE 1 (3). HARTREE-FOCK FUNCTIONS FOR NEUTRAL ATOMS.

OXYGEN 1S(2)2S(2)2P(4), 1S  
 T.E.= -0.74610978D+02 P.E.= -0.14922197D+03  
 K.E.= 0.74610996D+02 V.T.= -0.19999998D+01

S	1S	2S	P	2P
BASIS/ORB E	-20.73021	-1.27513	BASIS/ORB E	-0.55553
1S 7.54465	0.94404	-0.22468	2P 1.04568	0.15594
1S 13.24420	0.04200	-0.00561	2P 1.72278	0.57517
2S 1.63883	0.00003	0.26777	2P 3.36836	0.34804
2S 2.38982	0.00112	0.65854	2P 7.19356	0.01977
2S 4.16525	-0.00026	0.28C72		
2S 5.81621	0.02498	-0.18640		

FLUORINE 1S(2)2S(2)2P(5), 2P  
 T.E.= -0.99409300D+02 P.E.= -0.19881844D+03  
 K.E.= 0.99409140D+02 V.T.= -0.20000016D+01

S	1S	2S	P	2P
BASIS/ORB E	-26.38273	-1.57254	BASIS/ORB E	-0.73001
1S 8.55760	0.94710	-0.22694	2P 1.26570	0.17830
1S 14.97660	0.03718	-0.00530	2P 2.05803	0.56185
2S 1.82142	0.00013	0.23518	2P 3.92853	0.33658
2S 2.67295	0.00093	0.68552	2P 8.20412	0.01903
2S 4.90066	0.00068	0.31489		
2S 6.57362	0.02602	-0.21822		

NEON 1S(2)2S(2)2P(6), 1S  
 T.E.= -0.12854705D+03 P.E.= -0.25709386D+03  
 K.E.= 0.12854681D+03 V.T.= -0.20000018D+01

S	1S	2S	P	2P
BASIS/ORB E	-32.77248	-1.93043	BASIS/ORB E	-0.85044
1S 9.48486	0.93717	-0.23093	2P 1.45208	0.21799
1S 15.56590	0.04899	-0.00635	2P 2.38168	0.53338
2S 1.96184	0.00058	0.16620	2P 4.48489	0.32933
2S 2.86423	-0.00064	0.66899	2P 9.13464	0.01872
2S 4.82530	0.00551	0.30910		
2S 7.79242	0.01999	-0.13871		

SODIUM K(2)L(8)3S(1), 2S  
 T.E.= -0.16185890D+03 P.E.= -0.32371559D+03  
 K.E.= 0.161856680D+03 V.T.= -0.20000137D+01

S	1S	2S	3S	P	2P
BASIS/ORB E	-40.47850	-2.79702	-0.18210	BASIS/ORB E	-1.51814
1S 11.01230	0.96179	-0.23474	0.03527	2P 5.54977	0.46417
3S 12.66010	0.04052	-0.00606	0.00121	4P 8.66846	0.03622
3S 8.36156	0.01919	0.11154	-0.01889	4P 5.43460	0.29282
3S 5.73805	-0.00298	0.43179	-0.06808	4P 3.55503	0.31635
3S 3.61287	0.00191	0.517C1	-0.09232	4P 2.31671	0.07543
3S 2.25096	-0.00049	0.04747	0.00076		
3S 1.11597	0.00016	-0.00324	0.40764		
3S 0.71028	-0.00007	0.00124	0.64467		

MAGNESIUM K(2)L(8)3S(2), 1S  
 T.E.= -0.19961461D+03 P.E.= -0.39522486D+03  
 K.E.= 0.19961025D+03 V.T.= -0.20000218D+01

S	1S	2S	3S	P	2P
BASIS/ORB E	-49.03160	-3.76760	-0.25300	BASIS/ORB E	-2.28211
1S 12.01140	0.96430	-0.24357	0.04691	2P 5.92580	0.52391
3S 13.91620	0.03548	-0.0C4E5	0.00144	4P 7.98979	0.07012
3S 9.48612	0.02033	0.08002	-0.01850	4P 5.32964	0.31965
3S 6.72188	-0.00252	0.399C2	-0.07964	4P 3.71678	0.20860
3S 4.24466	0.00162	0.57358	-0.13478	4P 2.59986	0.03888
3S 2.53466	-0.00038	0.05156	-0.01906		
3S 1.46920	0.00015	-0.00703	0.48239		
3S 0.89084	-0.00004	0.00161	0.60221		

See page 183 for Explanation of Tables and Notes for Tables 32, 42, and 43

TABLE 1 (4). HARTREE-FOCK FUNCTIONS FOR NEUTRAL ATOMS.

ALUMINUM K(2)L(8)3S(2)3P(1), 2P T.E.= -0.24187668D+03 P.E.= -0.4E374889D+03 K.E.= 0.24187221D+03 V.T.= -0.20000185D+01						
S	1S	2S	3S	P	2P	3P
BASIS/ORB E	-58.50105	-4.91069	-0.39340	BASIS/ORB E	-3.21834	-0.21002
1S 13.01270	0.96628	-0.25110	0.05795	2P 6.51941	0.53767	-0.09633
3S 15.15090	0.03266	-0.00424	0.00149	4P 10.48190	0.01909	-0.00661
3S 10.19020	0.02155	0.09248	-0.02529	4P 8.08430	0.06545	-0.00128
3S 7.25565	-0.00439	0.40331	-0.09664	4P 5.85779	0.32423	-0.06987
3S 4.70291	0.00247	0.56148	-0.16426	4P 3.99863	0.19557	0.01653
3S 2.96182	-0.00081	0.039C2	-0.03278	4P 2.01453	0.00829	0.35563
3S 1.77250	0.00030	-0.00231	0.57610	4P 1.25016	-0.00235	0.45241
3S 1.09108	-0.00008	0.00037	0.52921	4P 0.87219	0.00101	0.29407
SILICON K(2)L(8)3S(2)3P(2), 3P T.E.= -0.28885431D+03 P.E.= -0.57770268D+03 K.E.= 0.28884837D+03 V.T.= -0.20000206D+01						
S	1S	2S	3S	P	2P	3P
BASIS/ORB E	-68.81239	-6.15647	-0.53978	BASIS/ORB E	-4.25598	-0.29703
1S 14.01420	0.96800	-0.25755	0.06595	2P 7.14360	0.54290	-0.11535
3S 16.39320	0.03033	-0.00446	0.00185	4P 16.25720	0.00234	-0.00189
3S 10.87950	0.02248	0.11153	-0.03461	4P 10.79720	0.04228	-0.00473
3S 7.72709	-0.00617	0.40339	-0.10378	4P 6.85724	0.32155	-0.07552
3S 5.16500	0.00326	0.55032	-0.19229	4P 4.66598	0.22474	0.01041
3S 2.97451	-0.00143	0.03381	-0.06561	4P 2.32046	0.00732	0.46075
3S 2.14316	0.00081	-0.00815	0.59732	4P 1.33470	-0.00105	0.57665
3S 1.31306	-0.00016	0.00126	0.55390	4P 0.79318	0.00041	0.06274
SILICON K(2)L(8)3S(2)3P(2), 1D T.E.= -0.28881506D+03 P.E.= -0.57762575D+03 K.E.= 0.28881070D+03 V.T.= -0.20000151D+01						
S	1S	2S	3S	P	2P	3P
BASIS/ORB E	-68.82634	-6.16545	-0.54736	BASIS/ORB E	-4.26879	-0.26076
1S 14.C0800	0.96857	-0.25771	0.06623	2P 7.32834	0.51174	-0.10724
3S 16.05050	0.03101	-0.00552	0.00233	4P 16.31050	0.00811	-0.00330
3S 11.56610	0.01619	0.06991	-0.02275	4P 10.44200	0.04948	-0.00409
3S 8.17827	0.00096	0.38620	-0.10158	4P 7.16580	0.30763	-0.07706
3S 5.32930	0.00007	0.59217	-0.19570	4P 4.81425	0.26083	0.00566
3S 3.31070	0.00032	0.04972	-0.06554	4P 2.29363	0.00905	0.48789
3S 2.14010	-0.00018	-0.00585	0.58716	4P 1.25019	-0.00109	0.58720
3S 1.31623	0.00005	0.00121	0.55151	4P 0.61614	0.00043	0.03952
SILICON K(2)L(8)3S(2)3P(2), 1S T.E.= -0.28875853D+03 P.E.= -0.57751493D+03 K.E.= 0.28875640D+03 V.T.= -0.20000074D+01						
S	1S	2S	3S	P	2P	3P
BASIS/ORB E	-68.84726	-6.18908	-0.55908	BASIS/ORB E	-4.28817	-0.21014
1S 14.00410	0.96892	-0.25783	0.06665	2P 7.14897	0.54225	-0.11059
3S 15.75280	0.03351	-0.00489	0.00158	4P 15.31540	-0.04270	-0.02101
3S 11.31740	0.01260	0.07928	-0.02322	4P 14.78660	0.05923	0.01967
3S 8.07180	0.00199	0.39318	-0.10867	4P 7.47598	0.28171	-0.06939
3S 5.25929	-0.00045	0.58876	-0.19103	4P 4.91827	0.29144	0.00172
3S 2.98288	0.00069	0.04130	-0.12772	4P 2.23193	0.00992	0.53378
3S 2.19750	-0.00047	-0.01113	0.65505	4P 1.12025	-0.00071	0.58561
3S 1.31309	0.00009	0.00143	0.54825			
PHOSPHORUS K(2)L(8)3S(2)3P(3), 4S T.E.= -0.34071869D+03 P.E.= -0.68143250D+03 K.E.= 0.34071381D+03 V.T.= -0.20000143D+01						
S	1S	2S	3S	P	2P	3P
BASIS/ORB E	-79.96965	-7.51102	-0.69636	BASIS/ORB E	-5.40088	-0.39161
1S 15.01120	0.96992	-0.26326	0.07230	2P 7.60940	0.57352	-0.13569
3S 17.31520	0.02944	-0.00434	0.00186	4P 13.97590	0.00664	-0.00813
3S 11.77300	0.01933	0.10333	-0.03447	4P 11.89390	0.02478	0.00586
3S 8.66300	-0.00403	0.34612	-0.09503	4P 7.55531	0.30460	-0.08424
3S 5.90778	0.00196	0.58778	-0.21241	4P 5.17707	0.21442	0.02002
3S 3.69253	-0.00051	0.06043	-0.09001	4P 2.62934	0.00552	0.51314
3S 2.47379	0.00016	-0.00901	0.60361	4P 1.50494	-0.00045	0.55176
3S 1.51103	-0.00004	0.00193	0.56185	4P 0.77783	0.00011	0.02781

See page 183 for Explanation of Tables and Notes for Tables 32, 42, and 43

## ROOTHAAN-HARTREE-FOCK ATOMIC WAVEFUNCTIONS

TABLE 1 (5). HARTREE-FOCK FUNCTIONS FOR NEUTRAL ATOMS.

PHOSPHORUS K(2)L(8)3S(2)3P(3), 2C  
 T.E.= -0.34064875D+03 P.E.= -0.68129342D+03 K.E.= 0.34064466D+03 V.T.= -0.20000120D+01

S	1S	2S	3S	P	2P	3P
BASIS/ORB E	-79.98907	-7.52876	-0.70632	BASIS/ORB E	-5.41843	-0.35047
1S 15.01170	0.96988	-0.26329	0.07256	2P 7.65091	0.56643	-0.13302
3S 17.44740	0.02791	-0.00390	0.00194	4P 14.09220	0.00940	-0.01205
3S 12.23970	0.01949	0.06975	-0.02499	4P 12.39180	0.01713	0.01142
3S 8.96102	-0.00204	0.36111	-0.09967	4P 7.76961	0.29132	-0.08327
3S 5.91161	0.00120	0.61276	-0.22197	4P 5.30032	0.23936	0.01403
3S 3.58805	-0.00024	0.05362	-0.09427	4P 2.64294	0.00764	0.50921
3S 2.47408	0.00007	-0.00878	0.61997	4P 1.48065	-0.00054	0.55351
3S 1.50947	-0.00002	0.00164	0.55326	4P 0.80637	0.00032	0.04231

PHOSPHORUS K(2)L(8)3S(2)3P(3), 2P  
 T.E.= -0.34060320D+03 P.E.= -0.68120146D+03 K.E.= 0.34059827D+03 V.T.= -0.20000145D+01

S	1S	2S	3S	P	2P	3P
BASIS/ORB E	-80.00205	-7.54068	-0.71320	BASIS/ORB E	-5.43023	-0.32414
1S 15.00960	0.97005	-0.26334	0.07274	2P 7.53364	0.58658	-0.13726
3S 17.31480	0.02854	-0.00499	0.00261	4P 12.91660	0.00571	-0.01045
3S 12.27830	0.01777	0.07826	-0.02881	4P 10.97300	0.03713	0.00893
3S 8.77598	-0.00084	0.38002	-0.10258	4P 7.20008	0.31948	-0.09466
3S 5.84869	0.00075	0.58731	-0.22144	4P 4.98461	0.17388	0.04700
3S 3.74015	-0.00003	0.04636	-0.06215	4P 2.56522	0.00463	0.52754
3S 2.42888	-0.00004	-0.00378	0.60769	4P 1.41660	0.00048	0.53639
3S 1.50720	0.00001	0.00099	0.53784	4P 0.71730	0.00012	0.03428

SULFUR K(2)L(8)3S(2)3P(4), 3P  
 T.E.= -0.39750485D+03 P.E.= -0.79500652D+03 K.E.= 0.39750167D+03 V.T.= -0.20000080D+01

S	1S	2S	3S	P	2P	3P
BASIS/ORB E	-92.00447	-9.00431	-0.87955	BASIS/ORB E	-6.68253	-0.43737
1S 16.01910	0.97077	-0.26808	0.07778	2P 8.00375	0.61294	-0.15586
3S 19.45290	0.02122	-0.00390	0.00244	4P 7.67346	-0.75360	*****
3S 13.77880	0.02511	0.04669	-0.02131	4P 12.09980	0.03668	-0.01199
3S 9.85150	-0.00287	0.36323	-0.10107	4P 7.67727	1.07415	18.39285
3S 6.48374	0.00194	0.62663	-0.25158	4P 5.32630	0.14538	0.09041
3S 4.05540	-0.00068	0.05414	-0.06277	4P 2.87350	0.00199	0.52697
3S 2.67399	0.00025	-0.00517	0.65107	4P 1.67242	0.00094	0.49465
3S 1.66032	-0.00007	0.00135	0.50175	4P 1.03092	-0.00014	0.05112

SULFUR K(2)L(8)3S(2)3P(4), 1D  
 T.E.= -0.39745221D+03 P.E.= -0.79489835D+03 K.E.= 0.39744614D+03 V.T.= -0.20000153D+01

S	1S	2S	3S	P	2P	3P
BASIS/ORB E	-92.01699	-9.01563	-0.88589	BASIS/ORB E	-6.69373	-0.41535
1S 16.01400	0.97114	-0.26821	0.07797	2P 8.06921	0.60189	-0.15258
3S 18.96800	0.02429	-0.00289	0.00157	4P 12.84920	0.03330	-0.02915
3S 13.07410	0.02358	0.06531	-0.02483	4P 11.58840	-0.00380	0.03506
3S 9.75154	-0.00533	0.34635	-0.10102	4P 7.95447	0.30971	-0.10730
3S 6.46979	0.00249	0.62960	-0.24289	4P 5.50966	0.17511	0.05645
3S 3.77961	-0.00109	0.05768	-0.16836	4P 2.87841	0.00376	0.55255
3S 2.86995	0.00060	-0.01492	0.67747	4P 1.60671	0.00097	0.50726
3S 1.71311	-0.00010	0.00199	0.57499	4P 0.86354	-0.00001	0.02856

SULFUR K(2)L(8)3S(2)3P(4), 1S  
 T.E.= -0.39737450D+03 P.E.= -0.79474786D+03 K.E.= 0.39737337D+03 V.T.= -0.20000028D+01

S	1S	2S	3S	P	2P	3P
BASIS/ORB E	-92.03594	-9.03282	-0.89552	BASIS/ORB E	-6.71076	-0.38344
1S 16.01660	0.97097	0.26815	0.07814	2P 8.04067	0.60718	-0.15369
3S 19.21610	0.02215	0.00383	0.00194	4P 14.99880	-0.00704	-0.00439
3S 13.74220	0.02356	-0.04249	-0.01739	4P 12.51390	0.04917	-0.00102
3S 10.19980	-0.00225	-0.31274	-0.09089	4P 7.53004	0.35062	-0.09937
3S 6.76267	0.00151	-0.63422	-0.23457	4P 5.08459	0.11775	0.07993
3S 4.56119	-0.00033	-0.10204	-0.09201	4P 2.80653	0.00142	0.55767
3S 2.66298	0.00004	0.00432	0.66985	4P 1.54755	0.00197	0.49661
3S 1.64345	-0.00002	-0.00166	0.48086	4P 0.72210	-0.00007	0.02406

See page 183 for Explanation of Tables and Notes for Tables 32, 42, and 43

TABLE 1 (6). HARTREE-FOCK FUNCTIONS FOR NEUTRAL ATOMS.

CHLORINE K(2)L(8)3S(2)3P(5), 2P  
 T.E.= -0.45948187D+03 P.E.= -0.91854563D+03 K.E.= 0.45946376D+03 V.T.= -0.20000394D+01

S	1S	2S	3S	P	2P	3P
BASIS/ORB E	-104.88469	-10.6C777	-1.07311	BASIS/ORB E	-8.07252	-0.50652
1S 17.00140	0.97335	-0.27278	0.08249	2P 8.50000	0.63254	-0.16954
3S 19.26490	0.02682	-0.00266	0.00237	4P 15.01240	0.00287	-0.00982
3S 13.45290	0.01612	0.09766	-0.04193	4P 12.32570	0.03393	0.01280
3S 10.04290	-0.00266	0.34603	-0.08968	4P 8.37240	0.27156	-0.10925
3S 6.93920	0.00129	0.55554	-0.27243	4P 6.10920	0.16389	0.07066
3S 4.43640	-0.00029	0.04578	-0.03736	4P 3.19310	0.00707	0.56909
3S 2.90570	0.00005	-0.00324	0.67062	4P 1.78630	-0.00034	0.49144
3S 1.81900	-0.00002	0.00121	0.47342	4P 0.92930	0.00036	0.02336

ARGON K(2)L(8)3S(2)3P(6), 1S  
 T.E.= -0.52681739D+03 P.E.= -0.10536312D+04 K.E.= 0.52681380D+03 V.T.= -0.20000068D+01

S	1S	2S	3S	P	2P	3P
BASIS/ORB E	-118.61039	-12.32219	-1.27735	BASIS/ORB E	-9.57150	-0.59102
1S 18.01640	0.97349	0.27635	0.08634	2P 9.05477	0.64116	-0.17850
3S 22.04650	0.01684	0.00289	0.00186	4P 15.54410	0.00865	-0.00812
3S 16.08250	0.02422	-0.03241	-0.01540	4P 12.39970	0.04186	0.00520
3S 11.63570	-0.00114	-0.33229	-0.10236	4P 8.56120	0.31735	-0.10986
3S 7.70365	0.00123	-0.65E28	-0.27614	4P 5.94658	0.09642	0.10994
3S 4.87338	-0.00039	-0.06834	-0.11879	4P 3.42459	0.00003	0.56149
3S 3.32987	0.00010	0.06623	0.68436	4P 1.96709	0.00055	0.46314
3S 2.02791	-0.00003	-0.00174	0.52050	4P 1.06717	-0.00013	0.02951

POTASSIUM K(2)L(8)3S(2)3P(6)4S(1), 2S  
 T.E.= -0.59916453D+03 P.E.= -0.11983287D+04 K.E.= 0.59916415D+03 V.T.= -0.20000006D+01

S	1S	2S	3S	4S	P	2P	3P
BASIS/ORB E	-133.53311	-14.49000	-1.74879	-0.14739	BASIS/ORB E	-11.51935	-0.95442
1S 19.13500	-0.93619	0.27612	0.09267	-0.01825	2P 8.64187	0.66743	-0.20797
1S 31.52500	-0.01385	0.00055	-0.00066	0.00031	2P 15.19360	0.04207	-0.01176
2S 16.49860	-0.06342	0.14725	0.04980	-0.00899	3P 6.91359	0.34752	-0.12744
2S 7.67410	-0.00014	-0.95199	-0.33547	0.06350	3P 3.26163	0.01398	0.56718
3S 6.68508	-0.00139	-0.19289	-0.21345	0.05015	3P 2.00984	-0.00944	0.45273
3S 4.04102	0.00189	-0.00C59	0.43855	-0.11346	3P 1.68876	0.00526	0.09340
3S 2.66919	-0.00212	-0.00704	0.65200	-0.11474			
4S 2.59794	0.00118	0.00327	0.09749	-0.03065			
4S 0.56203	-0.00005	-0.00016	0.00560	0.05190			
4S 1.29017	-0.00015	-0.00045	0.01932	0.33431			
4S 0.76641	0.00011	0.00033	-0.01161	0.70417			

CALCIUM K(2)L(8)3S(2)3P(6)4S(2), 1S  
 T.E.= -0.67675803D+03 P.E.= -0.13535143D+04 K.E.= 0.67675626D+03 V.T.= -0.20000026D+01

S	1S	2S	3S	4S	P	2P	3P
BASIS/ORB E	-149.36382	-16.82280	-2.24535	-0.19551	BASIS/ORB E	-13.62934	-1.34066
1S 19.97310	-0.94194	-0.28216	-0.09896	-0.02394	2P 9.12915	0.67837	-0.22553
1S 32.15000	-0.01803	-0.00C53	0.00053	0.00028	2P 15.99470	0.04233	-0.01276
2S 17.23940	-0.05072	-0.15034	-0.05334	-0.01223	3P 7.37779	0.33353	-0.13716
2S 8.40361	-0.00216	0.89604	0.32943	0.07777	3P 3.62974	0.01241	0.54465
3S 7.46907	0.00051	0.25659	0.22440	0.06258	3P 2.34862	-0.00454	0.52593
3S 3.95936	-0.00010	0.08978	-0.70524	-0.24085	3P 1.64038	0.00132	0.04492
3S 3.01657	0.00017	0.00C87	-0.12144	0.05280			
4S 3.09105	-0.00006	-0.00173	-0.35525	-0.15243			
4S 1.62884	-0.00000	0.00051	-0.01549	0.32699			
4S 1.01203	0.00000	-0.00029	0.00566	0.66264			
4S 0.66733	-0.00000	0.00010	-0.00179	0.13150			

See page 183 for Explanation of Tables and Notes for Tables 32, 42, and 43

## ROOTHAAN-HARTREE-FOCK ATOMIC WAVEFUNCTIONS

TABLE 1 (7). HARTREE-FOCK FUNCTIONS FOR NEUTRAL ATOMS.

SCANDIUM K(2)L(8)3S(2)3P(6)4S(1)3D(2), 4F  
 T.E.= -0.75969860D+03 P.E.= -0.15193962D+04 K.E.= C. 75965760D+03 V.T.= -0.20000013D+01

S	1S	2S	3S	4S
BASIS/ORB E	-165.75811	-18.91665	-2.41325	-0.19537
1S 33.43000	-0.02013	-0.00114	-0.00011	-0.00013
1S 20.88130	-0.94537	-0.28660	-0.10055	-0.02178
2S 18.18780	-0.04302	-0.14705	-0.05537	-0.01254
2S 8.42800	-0.00472	1.01171	0.38472	0.08561
3S 7.45380	0.00331	0.12731	0.21487	0.05105
3S 4.78240	-0.00239	0.01004	-0.39743	-0.09233
3S 3.24065	0.00177	-0.00016	-0.73852	-0.20685
4S 2.65023	-0.00078	0.00040	-0.08548	0.03083
4S 1.47432	0.00041	-0.00003	-0.00356	0.37107
4S 1.06625	-0.00034	0.00004	0.00277	0.35736
4S 0.79396	0.00012	0.00001	-0.00046	0.34952

P	2P	3P	D	3D
BASIS/ORB E	-15.50808	-1.43541	BASIS/ORB E	-0.21529
2P 16.63600	0.04468	-0.01420	3D 9.82074	0.01277
2P 9.58828	0.68927	-0.23164	3D 5.12071	0.08923
3P 7.84586	0.31591	-0.14293	3D 3.44801	0.23086
3P 4.19594	0.01334	0.39187	3D 1.96214	0.44607
3P 2.91102	-0.00350	0.51763	3D 0.97339	0.43395
3P 2.03524	0.00090	0.22030		

SCANDIUM K(2)L(8)3S(2)3P(6)4S(2)3D(1), 2D  
 T.E.= -0.75973552D+03 P.E.= -0.15194685D+04 K.E.= 0.75973299D+03 V.T.= -0.20300033D+01

S	1S	2S	3S	4S
BASIS/ORB E	-165.90002	-19.08071	-2.56738	-0.21014
1S 20.88130	-0.94540	0.28654	-0.10222	-0.02400
1S 33.43000	-0.02010	0.00116	0.00026	-0.00007
2S 18.18780	-0.04294	0.14707	-0.05463	-0.01351
2S 8.42800	-0.00497	-1.01154	0.38509	0.09325
3S 7.45380	0.00385	-0.12762	0.22889	0.05788
3S 4.78240	-0.00392	-0.00992	-0.45514	-0.10274
3S 3.24065	0.00457	0.00040	-0.63181	-0.23446
4S 3.29855	-0.00244	-0.00051	-0.13662	0.02272
4S 1.54276	0.00021	-0.00008	-0.01874	0.48631
4S 0.96985	-0.00020	0.00008	0.01435	0.50614
4S 0.76062	0.00010	-0.00004	-0.00712	0.10593

P	2P	3P	D	3D
BASIS/ORB E	-15.66834	-1.57459	BASIS/ORB E	-0.34357
2P 9.58828	0.68938	-0.23514	3D 3.60600	0.31357
2P 16.63600	0.04459	-0.01406	3D 8.63190	0.02663
3P 7.83942	0.31660	-0.14208	3D 4.92190	0.06141
3P 4.10068	0.01293	0.43727	3D 1.88940	0.56780
3P 2.86710	-0.00397	0.49413	3D 1.01000	0.20271
3P 2.08891	0.00096	0.19247		

TITANIUM K(2)L(8)3S(2)3P(6)4S(1)3D(3), 5F  
 T.E.= -0.84838600D+03 P.E.= -0.16567711D+04 K.E.= 0.84838508D+03 V.T.= -0.20000011D+01

S	1S	2S	3S	4S
BASIS/ORB E	-183.11076	-21.23849	-2.70022	-0.20513
1S 34.96880	-0.01974	0.00092	0.00039	-0.00002
1S 21.84800	-0.94889	0.29029	-0.10425	-0.02239
2S 18.92010	-0.03922	0.15367	-0.05676	-0.01272
2S 9.20495	-0.00452	-0.94644	0.35898	0.07908
3S 8.32964	0.00268	-0.20462	0.22790	0.05313
3S 4.88574	-0.00170	-0.01393	-0.41824	-0.09527
3S 3.41764	0.00140	0.00191	-0.70058	-0.20002
4S 2.76107	-0.00056	-0.00064	-0.08081	0.04299
4S 1.51883	0.00023	-0.00001	-0.00030	0.44641
4S 0.98469	-0.00019	-0.00003	0.00055	0.47936
4S 0.75129	0.00009	-0.00002	0.00011	0.15020

See page 183 for Explanation of Tables and Notes for Tables 32, 42, and 43

TABLE 1 (8). HARTREE-FOCK FUNCTIONS FOR NEUTRAL ATOMS.

P	2P	3P	D	3D
BASIS/ORB E	-17.61065	-1.63709	BASIS/ORB E	-0.27342
2P 16.98400	0.05092	-0.01662	3D 9.65902	0.02081
2P 10.00440	0.69833	-0.24001	3D 4.96238	0.14301
3P 8.29486	0.29789	-0.14359	3D 3.55660	0.23499
3P 4.42269	0.01255	0.47723	3D 2.05023	0.47628
3P 2.82341	-0.00265	0.59390	3D 1.05347	0.32923
3P 1.76950	0.00074	0.06603		

TITANIUM K(2)L(8)3S(2)3P(6)4S(2)3D(2), 1G  
 T.E.= -0.84833198D+03 P.E.= -0.16966674D+04 K.E.= 0.84833545D+03 V.T.= -0.19999959D+01

S	1S	2S	3S	4S
BASIS/ORB E	-183.29522	-21.44831	-2.89196	-0.22329
1S 22.02170	-0.95038	-0.29003	0.10528	-0.02450
1S 37.07550	-0.01224	0.00062	-0.00092	0.00011
2S 18.59580	-0.04878	-0.16727	0.06217	-0.01519
2S 9.38742	0.00047	0.93278	-0.35705	0.08562
3S 8.16643	-0.00129	0.24725	-0.26501	0.06550
3S 4.97992	0.00176	-0.02318	0.47015	-0.10021
3S 3.62435	-0.00177	0.03229	0.51976	-0.20315
4S 3.45183	0.00077	-0.01334	0.23271	-0.00620
4S 1.64946	-0.00009	0.00159	0.01520	0.47473
4S 1.02450	0.00007	-0.00123	-0.00911	0.53841
4S 0.74989	-0.00003	0.00056	0.00391	0.08845

P	2P	3P	D	3D
BASIS/ORB E	-17.81623	-1.81187	BASIS/ORB E	-0.36962
2P 9.88635	0.71465	-0.24806	3D 2.21884	0.51076
2P 16.94760	0.05235	-0.01778	3D 9.53594	0.02502
3P 8.17705	0.28072	-0.14631	3D 4.72184	0.20126
3P 4.49598	0.00864	0.47048	3D 3.66705	0.16253
3P 2.84463	-0.00057	0.63987	3D 1.20875	0.27371
3P 1.51290	0.00006	0.02563		

TITANIUM K(2)L(8)3S(2)3P(6)4S(2)3D(2), 3F  
 T.E.= -0.84840575D+03 P.E.= -0.16968141D+04 K.E.= 0.84840837D+03 V.T.= -0.19999969D+01

S	1S	2S	3S	4S
BASIS/ORB E	-183.27250	-21.42292	-2.87350	-0.22080
1S 22.02960	-0.95015	-0.28972	0.10510	-0.02387
1S 37.11330	-0.01209	0.00055	-0.00094	-0.00004
2S 18.60820	-0.04928	-0.16752	0.06192	-0.01572
2S 9.39745	0.00058	0.93056	-0.35502	0.08607
3S 8.17280	-0.00140	0.24986	-0.26666	0.05985
3S 4.98509	0.00187	-0.02361	0.47346	-0.07272
3S 3.62802	-0.00187	0.03254	0.50703	-0.24523
4S 3.45561	0.00080	-0.01329	0.24381	0.02662
4S 1.58708	-0.00009	0.00159	0.01578	0.50408
4S 1.00652	0.00008	-0.00137	-0.01098	0.48670
4S 0.75064	-0.00004	0.00064	0.00487	0.10196

P	2P	3P	D	3D
BASIS/ORB E	-17.79122	-1.79520	BASIS/ORB E	-0.44071
2P 9.74943	0.71614	-0.24806	3D 2.17900	0.52678
2P 16.39080	0.06307	-0.02143	3D 9.54575	0.02539
3P 8.15953	0.26624	-0.14149	3D 4.81759	0.17639
3P 4.50482	0.01033	0.46677	3D 3.67072	0.21326
3P 2.84111	-0.00126	0.64339	3D 1.23154	0.21819
3P 1.51430	0.00022	0.03031		

See page 183 for Explanation of Tables and Notes for Tables 32, 42, and 43

## ROOTHAAN-HARTREE-FOCK ATOMIC WAVEFUNCTIONS

TABLE 1 (9). HARTREE-FOCK FUNCTIONS FOR NEUTRAL ATOMS.

TITANIUM K(2)L(8)3S(2)3P(6)4S(2)3D(2), 1D  
 T.E.= -0.848358230+03 P.E.= -0.16567201D+04 K.E.= 0.84836182D+03 V.T.= -0.19999958D+01

S	1S	2S	3S	4S
BASIS/ORB E	-183.28688	-21.43911	-2.88523	-0.22231
1S 22.00640	-0.95075	-0.28923	0.10500	-0.02429
1S 37.02710	-0.01256	0.00009	-0.00076	0.00006
2S 18.60710	-0.04772	-0.16903	0.06286	-0.01540
2S 9.37455	-0.00007	0.94155	-0.36093	0.08649
3S 7.96918	-0.00089	0.25537	-0.29274	0.07101
3S 5.17127	0.00121	-0.05439	0.47884	-0.09572
3S 3.61964	-0.00114	0.05919	0.52896	-0.21085
4S 3.51899	0.00054	-0.02653	0.24555	-0.00454
4S 1.64738	-0.00005	0.00258	0.01841	0.47233
4S 1.02320	0.00004	-0.00203	-0.01146	0.53924
4S 0.74892	-0.00002	0.00092	0.00497	0.08998

P	2P	3P	D	3D
BASIS/ORB E	-17.80717	-1.80578	BASIS/ORB E	-0.39473
2P 9.76567	0.71628	-0.24839	3D 2.13341	0.50765
2P 16.45980	0.06161	-0.02098	3D 9.16334	0.02944
3P 8.15980	0.26787	-0.14246	3D 4.71575	0.17120
3P 4.50734	0.01002	0.46668	3D 3.66034	0.22374
3P 2.84626	-0.00114	0.64396	3D 1.20606	0.23589
3P 1.50810	0.00019	0.02999		

TITANIUM K(2)L(8)3S(2)3P(6)4S(2)3D(2), 3P  
 T.E.= -0.84834818D+03 P.E.= -0.16967003D+04 K.E.= 0.84835214D+03 V.T.= -0.19999953D+01

S	1S	2S	3S	4S
BASIS/ORB E	-183.28941	-21.44189	-2.88711	-0.22258
1S 22.00440	-0.95129	-0.29024	0.10586	-0.02451
1S 37.01780	-0.01236	0.00055	-0.00116	0.00015
2S 18.48150	-0.04789	-0.17233	0.06272	-0.01540
2S 9.52272	0.00098	0.91586	-0.34716	0.08332
3S 8.13700	-0.00176	0.28295	-0.29474	0.07133
3S 5.17000	0.00212	-0.04590	0.44947	-0.09182
3S 3.61874	-0.00211	0.05342	0.55715	-0.21952
4S 3.51806	0.00100	-0.02414	0.23158	0.00003
4S 1.64699	-0.00010	0.00240	0.01976	0.47308
4S 1.02295	0.00008	-0.00190	-0.01263	0.53923
4S 0.74873	-0.00004	0.00086	0.00552	0.08871

P	2P	3P	D	3D
BASIS/ORB E	-17.80992	-1.80748	BASIS/ORB E	-0.38497
2P 9.76721	0.71632	-0.24846	3D 2.17093	0.51054
2P 16.46720	0.06146	-0.02093	3D 9.52092	0.02525
3P 8.15978	0.26802	-0.14255	3D 4.80558	0.17623
3P 4.50729	0.00998	0.46682	3D 3.65944	0.20851
3P 2.84691	-0.00113	0.64387	3D 1.20577	0.24896
3P 1.50775	0.00019	0.02995		

TITANIUM K(2)L(8)3S(2)3P(6)4S(2)3D(2), 1S  
 T.E.= -0.84823057D+03 P.E.= -0.16564645D+04 K.E.= 0.84823393D+03 V.T.= -0.19999960D+01

S	1S	2S	3S	4S
BASIS/ORB E	-183.33177	-21.48933	-2.92298	-0.22831
1S 22.03610	-0.94898	-0.28536	-0.10546	-0.02498
1S 36.89780	-0.01254	0.00045	0.00094	0.00011
2S 18.72680	-0.04975	-0.16331	-0.06031	-0.01506
2S 9.34020	-0.00005	0.93164	0.35589	0.08706
3S 8.27889	-0.00087	0.23517	0.25304	0.06343
3S 4.85654	0.00147	-0.00388	-0.51587	-0.10518
3S 3.60509	-0.00163	0.01571	-0.43792	-0.20561
4S 3.50606	0.00072	-0.00690	-0.25778	-0.00070
4S 1.64184	-0.00006	0.00076	-0.01545	0.51182
4S 1.00073	0.00005	-0.00062	0.00968	0.53957
4S 0.74633	-0.00002	0.00030	-0.00448	0.04895

See page 183 for Explanation of Tables and Notes for Tables 32, 42, and 43

TABLE 1 (10). HARTREE-FOCK FUNCTIONS FOR NEUTRAL ATOMS.

P	2P	3P	D	3D
BASIS/ORB E	-17.85662	-1.84001	BASIS/ORB E	-0.27622
2P 9.88021	0.71537	-0.24550	3D 2.14139	0.49260
2P 16.95410	0.05243	-0.01774	3D 9.48973	0.02431
3P 8.17508	0.27986	-0.14534	3D 4.78750	0.17845
3P 4.46993	0.00873	0.48121	3D 3.64779	0.19235
3P 2.83950	-0.00076	0.63117	3D 1.09666	0.31005
3P 1.47530	0.00010	0.02665		

VANADIUM K(2)L(8)3S(2)3P(6)4S(1)3D(4), 6D  
T.E.= -0.942879510D+03 P.E.= -0.188576240D+04 K.E.= 0.942882880D+03 V.T.= -0.199999640D+01

S	1S	2S	3S	4S
BASIS/ORB E	-201.32257	-23.67206	-2.99279	-0.21441
1S 37.02920	-0.00964	0.00077	-0.02020	-0.00018
1S 23.39970	-0.93492	-0.28557	-0.10148	-0.02151
2S 20.08310	-0.07154	-0.16081	-0.06481	-0.01447
2S 9.11921	0.00552	1.08184	0.43135	0.09457
3S 8.11916	-0.00786	0.04244	0.19857	0.04533
3S 5.26809	0.01060	0.04079	-0.46495	-0.08789
3S 4.00791	-0.00895	-0.02404	-0.50834	-0.17766
4S 3.50140	0.00280	0.00733	-0.27469	-0.01527
4S 1.69909	-0.00049	-0.00101	-0.01050	0.40874
4S 1.05325	0.00039	0.00052	0.00556	0.53716
4S 0.77575	-0.00018	-0.00037	-0.00200	0.15436

P	2P	3P	D	3D
BASIS/ORB E	-19.82389	-1.84417	BASIS/ORB E	-0.32069
2P 17.14970	0.05986	-0.02038	3D 10.48020	0.02070
2P 10.52830	0.68454	-0.23838	3D 5.06949	0.23919
3F 8.88560	0.29872	-0.15054	3D 3.05112	0.31844
3P 4.79752	0.01687	0.45436	3D 2.00201	0.34569
3P 3.06851	-0.00408	0.60889	3D 1.14525	0.27369
3P 1.93057	0.00118	0.07858		

VANADIUM K(2)L(8)3S(2)3P(6)4S(2)3D(3), 2H  
T.E.= -0.94279882D+03 P.E.= -0.18855976D+04 K.E.= 0.94279874D+03 V.T.= -0.20000001D+01

S	1S	2S	3S	4S
BASIS/ORB E	-201.52397	-23.89835	-3.19997	-0.23255
1S 23.18520	-0.94297	-0.28495	-0.10281	-0.02321
1S 38.93820	-0.01135	-0.00144	-0.00069	-0.00032
2S 20.31320	-0.05652	-0.15426	-0.06171	-0.01491
2S 9.04491	-0.00302	1.09094	0.43534	0.10249
3S 8.20892	0.00216	0.02344	0.19943	0.04645
3S 5.54603	-0.00184	0.04010	-0.33072	-0.05608
3S 4.21422	0.00136	-0.01708	-0.63120	-0.21988
4S 3.58417	-0.00035	0.00442	-0.28882	-0.02889
4S 1.72299	0.00006	-0.00053	-0.00810	0.47892
4S 1.05382	-0.00004	0.00036	0.00359	0.55320
4S 0.73065	0.00002	-0.00015	-0.00133	0.07141

P	2P	3P	D	3D
BASIS/ORB E	-20.04588	-2.03449	BASIS/ORB E	-0.45848
2P 10.34500	0.71826	-0.25435	3D 3.14025	0.37195
2P 17.42970	0.05691	-0.01936	3D 10.03150	0.02494
3P 8.67089	0.26867	-0.14521	3D 5.15397	0.23640
3P 4.82721	0.01125	0.45526	3D 2.00669	0.35613
3P 3.08452	-0.00151	0.63455	3D 1.26616	0.17611
3P 1.84857	0.00036	0.04952		

See page 183 for Explanation of Tables and Notes for Tables 32, 42, and 43

## ROOTHAAN-HARTREE-FOCK ATOMIC WAVEFUNCTIONS

TABLE 1 (11). HARTREE-FOCK FUNCTIONS FOR NEUTRAL ATOMS.

VANADIUM K(2)L(8)3S(2)3P(6)4S(2)3D(3), 2G  
 T.E.= -0.94281991D+03 P.E.= -0.18856397D+04 K.E.= 0.94281982D+03 V.T.= -0.20000001D+01

S	1S	2S	3S	4S
BASIS/ORB E	-201.5188C	-23.89261	-3.19596	-0.23207
1S 23.18380	-0.94303	-0.28498	-0.10279	-0.02316
1S 38.94040	-0.01136	-0.00144	-0.00069	-0.00031
2S 20.31210	-0.05642	-0.15425	-0.06168	-0.01485
2S 9.04614	-0.00304	1.09065	0.43506	0.10217
3S 8.20940	0.00219	0.02384	0.19958	0.04656
3S 5.54634	-0.00187	0.03597	-0.33105	-0.05674
3S 4.21445	0.00138	-0.01699	-0.62998	-0.21816
4S 3.58440	-0.00036	0.00440	-0.28977	-0.02970
4S 1.72310	0.00006	-0.00052	-0.00817	0.47684
4S 1.05388	-0.00004	0.00035	0.00364	0.55442
4S 0.73069	0.00002	-0.00015	-0.00135	0.07243

P	2P	3P	D	3D
BASIS/ORB E	-20.04021	-2.03C85	BASIS/ORB E	-0.47111
2P 10.34560	0.71822	-0.25420	3D 3.14043	0.37224
2P 17.43010	0.05689	-0.01935	3D 10.03210	0.02505
3P 8.67099	0.26874	-0.14526	3D 5.14971	0.23751
3P 4.82909	0.01125	0.45856	3D 2.00681	0.36084
3P 3.08391	-0.00150	0.63517	3D 1.26624	0.16808
3P 1.84866	0.00036	0.04969		

VANADIUM K(2)L(8)3S(2)3P(6)4S(2)3D(3), 4F  
 T.E.= -0.94288420D+03 P.E.= -0.18857669D+04 K.E.= 0.94288273D+03 V.T.= -0.20000016D+01

S	1S	2S	3S	4S
BASIS/ORB E	-201.50269	-23.67459	-3.18323	-0.23059
1S 23.05740	-0.94977	-0.29138	0.10566	-0.02384
1S 39.01750	-0.01180	0.00046	-0.00031	-0.00001
2S 19.85370	-0.04848	-0.15630	0.06121	-0.01436
2S 9.24671	-0.00233	1.05201	-0.41455	0.09588
3S 8.54632	0.00137	0.07670	-0.19175	0.04743
3S 5.11726	-0.00169	0.05858	0.45614	-0.08873
3S 4.22281	0.00165	-0.04248	0.42379	-0.16412
4S 3.67054	-0.00038	0.00932	0.34028	-0.05043
4S 1.76174	0.00005	-0.00105	0.01151	0.44160
4S 1.07700	-0.00004	0.00069	-0.00529	0.57980
4S 0.73215	0.00001	-0.00028	0.00195	0.08713

P	2P	3P	D	3D
BASIS/ORB E	-20.02244	-2.01927	BASIS/ORB E	-0.50966
2P 10.33610	0.72031	-0.25528	3D 3.14686	0.37700
2P 17.45840	0.05657	-0.01900	3D 10.05350	0.02512
3P 8.65722	0.26705	-0.14260	3D 5.15213	0.23791
3P 4.79067	0.01107	0.47C76	3D 2.01131	0.37270
3P 3.05940	-0.00158	0.62323	3D 1.26881	0.14492
3P 1.85188	0.00038	0.04815		

VANADIUM K(2)L(8)3S(2)3P(6)4S(2)3D(3), 2F  
 T.E.= -0.94273633D+03 P.E.= -0.18854726D+04 K.E.= 0.94273624D+03 V.T.= -0.20000001D+01

S	1S	2S	3S	4S
BASIS/ORB E	-201.53984	-23.91595	-3.21241	-0.23415
1S 23.18270	-0.94290	-0.28504	-0.10286	-0.02335
1S 38.83960	-0.01149	-0.00143	-0.00072	-0.00034
2S 20.30820	-0.05645	-0.15422	-0.06191	-0.01507
2S 9.04432	-0.00296	1.09118	0.43631	0.10343
3S 8.20923	0.00207	0.02329	0.19743	0.04608
3S 5.52623	-0.00174	0.04055	-0.32972	-0.05495
3S 4.21237	0.00130	-0.01770	-0.63505	-0.22413
4S 3.57632	-0.00033	0.0452	-0.28441	-0.02673
4S 1.72306	0.00006	-0.00055	-0.00740	0.48593
4S 1.05286	-0.00004	0.00037	0.00313	0.54997
4S 0.73067	0.00002	-0.00015	-0.00115	0.06725

See page 183 for Explanation of Tables and Notes for Tables 32, 42, and 43

TABLE 1 (12). HARTREE-FOCK FUNCTIONS FOR NEUTRAL ATOMS.

P	2P	3P	D	3D
BASIS/ORB E	-20.06324	-2.04582	BASIS/ORB E	-0.42150
2P 10.34430	0.71850	-0.25487	3D 3.00887	0.39300
2P 17.43540	0.05683	-0.01932	3D 10.10590	0.02423
3P 8.66963	0.26855	-0.14504	3D 5.10343	0.25166
3P 4.81974	0.01119	0.46199	3D 1.92877	0.32577
3P 3.08637	-0.00154	0.63146	3D 1.21821	0.17753
3P 1.85663	0.00037	0.04955		

VANADIUM K(2)L(8)3S(2)3P(6)4S(2)3D(3), 2D  
T.E.= -0.94272261D+03 P.E.= -0.18854451D+04 K.E.= 0.94272249D+03 V.T.= -0.20000001D+01

S	1S	2S	3S	4S
BASIS/ORB E	-201.54382	-23.92041	-3.21570	-0.23455
1S 23.19540	-0.94251	-0.28474	-0.10281	-0.02336
1S 38.92120	-0.01128	-0.00146	-0.00071	-0.00034
2S 20.32440	-0.05719	-0.15430	-0.06186	-0.01513
2S 9.03689	-0.00287	1.09270	0.43677	0.10385
3S 8.20520	0.00196	0.02091	0.19840	0.04587
3S 5.54363	-0.00160	0.04089	-0.32969	-0.05346
3S 4.21238	0.00118	-0.01760	-0.63600	-0.22688
4S 3.58238	-0.00030	0.00454	-0.28480	-0.02550
4S 1.72219	0.00005	-0.00055	-0.00779	0.48761
4S 1.05335	-0.00004	0.00037	0.00339	0.54808
4S 0.73033	0.00001	-0.00015	-0.00125	0.06713

P	2P	3P	D	3D
BASIS/ORB E	-20.06764	-2.04882	BASIS/ORB E	-0.41364
2P 10.34450	0.71815	-0.23524	3D 3.07350	0.37283
2P 17.43040	0.05697	-0.01923	3D 10.13570	0.02394
3P 8.67308	0.26874	-0.14373	3D 5.13291	0.24429
3P 4.79194	0.01140	0.47(E3)	3D 2.00570	0.31969
3P 3.07265	-0.00177	0.62356	3D 1.26560	0.21222
3P 1.84786	0.00043	0.04744		

VANADIUM K(2)L(8)3S(2)3P(6)4S(2)3D(3), 4P  
T.E.= -0.94282008D+03 P.E. = -0.18856393D+04 K.E.= 0.94281925D+03 V.T.= -0.20000009D+01

S	1S	2S	3S	4S
BASIS/ORB E	-201.51798	-23.89162	-3.19502	-0.23194
1S 23.09660	-0.94661	-0.28704	0.10347	-0.02339
1S 38.94090	-0.01219	-0.00124	0.00064	-0.00026
2S 20.20970	-0.05083	-0.15356	0.06180	-0.01472
2S 9.07240	-0.00421	1.08711	-0.43508	0.10165
3S 8.04952	0.00401	0.03188	-0.22200	0.05383
3S 5.54641	-0.00443	0.03593	0.40003	-0.07990
3S 4.21451	0.00335	-0.01549	0.55109	-0.19115
4S 3.66246	-0.00094	0.00431	0.32124	-0.04466
4S 1.75712	0.00014	-0.00043	0.01132	0.45040
4S 1.07489	-0.00010	0.00028	-0.00511	0.57434
4S 0.73070	0.00004	-0.00011	0.00186	0.08307

P	2P	3P	D	3D
BASIS/ORB E	-20.03924	-2.02999	BASIS/ORB E	-0.47087
2P 10.34550	0.71823	-0.25417	3D 3.14048	0.37464
2P 17.43020	0.05689	-0.01936	3D 10.03220	0.02506
3P 8.67104	0.26872	-0.14527	3D 5.15276	0.23632
3P 4.82967	0.01126	0.45840	3D 2.00685	0.36081
3P 3.08381	-0.00150	0.63533	3D 1.26625	0.16623
3P 1.84868	0.00036	0.04972		

See page 183 for Explanation of Tables and Notes for Tables 32, 42, and 43

## ROOTHAAN-HARTREE-FOCK ATOMIC WAVEFUNCTIONS

TABLE 1 (13). HARTREE-FOCK FUNCTIONS FOR NEUTRAL ATOMS.

VANADIUM K(2)L(8)3S(2)3P(6)4S(2)3D(3), 2P  
 T.E.= -0.942798820+03 P.E.= -0.18855976D+04 K.E.= 0.94279874D+03 V.T.= -0.20000001D+01

	S	1S	2S	3S	4S
BASIS/ORB E	-201.52397	-23.89835	-3.19997	-0.23255	
1S	23.18520	-0.94297	-0.28495	-0.10281	-0.02321
1S	38.93820	-0.01135	-0.00144	-0.00069	-0.00032
2S	20.31320	-0.05652	-0.15426	-0.06171	-0.01491
2S	9.04491	-0.00302	1.09094	0.43534	0.10249
3S	8.20892	0.00216	0.02344	0.19943	0.04645
3S	5.54603	-0.00184	0.04010	-0.33072	-0.05608
3S	4.21422	0.00136	-0.01708	-0.63120	-0.21988
4S	3.58417	-0.00035	0.00442	-0.28882	-0.02889
4S	1.72299	0.00006	-0.00053	-0.00810	0.47892
4S	1.05382	-0.00004	0.00036	0.00359	0.55320
4S	0.73065	0.00002	-0.00015	-0.00133	0.07141
P		2P	3P	D	3D
BASIS/ORB E	-20.04588	-2.03449	BASIS/ORB E	-0.45848	
2P	10.34500	0.71826	-0.25435	3D 3.14025	0.37195
2P	17.42970	0.05691	-0.01936	3D 10.03150	0.02494
3P	8.67089	0.26867	-0.14521	3D 5.15397	0.23640
3P	4.82721	0.01125	0.45526	3D 2.00669	0.35613
3P	3.08452	-0.00151	0.63455	3D 1.26616	0.17611
3P	1.84857	0.00036	0.04552		

CHROMIUM K(2)L(8)3S(2)3P(6)4S(1)3D(5), 7S  
 T.E.= -0.10433552D+04 P.E.= -0.20867030D+04 K.E.= 0.10433478D+04 V.T.= -0.20000071D+01

	S	1S	2S	3S	4S
BASIS/ORB E	-220.38550	-26.20538	-3.28495	-0.22194	
1S	35.59110	-0.02722	-0.05777	-0.00127	-0.00018
1S	23.95440	-0.93357	-0.27707	-0.10429	-0.02218
2S	21.65020	-0.04720	-0.15417	-0.05407	-0.01125
2S	10.09060	-0.00604	0.93227	0.34969	0.07371
3S	9.65415	0.00363	0.19827	0.23940	0.05676
3S	5.940457	-0.00151	0.02629	-0.25716	-0.05977
3S	4.09494	0.00100	-0.00339	-0.82284	-0.21516
4S	3.12628	-0.00034	0.00078	-0.12469	0.01657
4S	1.76632	0.00014	0.00009	0.00348	0.40517
4S	1.07837	-0.00009	0.00005	-0.00196	0.57019
4S	0.75455	0.00004	0.00006	0.00086	0.12089

	P	2P	3P	D	3D
BASIS/ORB E	-22.13952	-2.05069	BASIS/ORB E	-0.37348	
2P	16.08310	0.11416	-0.04558	3D 9.76336	0.03088
2P	10.47530	0.67530	-0.22347	3D 5.47299	0.20871
3P	9.35810	0.24355	-0.16951	3D 3.45917	0.33792
3P	5.64044	0.01945	0.36285	3D 2.18964	0.35411
3P	3.41092	-0.00112	0.72269	3D 1.26443	0.25996
3P	1.98103	0.00034	0.08413		

CHROMIUM K(2)L(8)3S(2)3P(6)4S(2)3D(4), 11  
 T.E.= -0.10431793D+04 P.E.= -0.20863578D+04 K.E.= 0.10431785D+04 V.T.= -0.20000008D+01

	S	1S	2S	3S	4S
BASIS/ORB E	-220.62008	-26.47661	-3.52103	-0.24214	
1S	24.06860	-0.94208	-0.28644	-0.10825	-0.02411
1S	37.49210	-0.01736	-0.00316	0.00073	0.00007
2S	21.07880	-0.05073	-0.16164	-0.05677	-0.01309
2S	10.62100	-0.00176	0.84694	0.31787	0.07232
3S	9.78038	0.00022	0.30523	0.27859	0.06645
3S	5.98096	0.00026	0.02254	-0.19790	-0.04001
3S	4.31362	-0.00017	-0.00087	-0.81519	-0.23774
4S	3.52101	0.00008	-0.00013	-0.18275	-0.00983
4S	1.84469	-0.00002	0.00036	-0.00525	0.43581
4S	1.13444	0.00002	-0.00027	0.00250	0.56505
4S	0.77205	-0.00001	0.00011	-0.00096	0.10619

See page 183 for Explanation of Tables and Notes for Tables 32, 42, and 43

TABLE 1 (14). HARTREE-FOCK FUNCTIONS FOR NEUTRAL ATOMS.

P	2P	3P	D	3D
BASIS/ORB E	-22.39633	-2.26890	BASIS/ORB E	-0.51421
2P 9.58822	0.84627	-0.31282	3D 3.40042	0.37366
2P 16.49520	0.10705	-0.03504	3D 10.66500	0.02466
3P 7.41476	0.08839	-0.18012	3D 5.54922	0.23991
3P 5.66127	-0.00792	0.49407	3D 2.16683	0.35600
3P 3.38224	0.00241	0.69759	3D 1.35632	0.17093
3P 2.02870	-0.00034	0.06442		

CHROMIUM K(2)L(8)3S(2)3P(6)4S(2)3D(4), 3H  
T.E.= -0.10432223D+04 P.E.= -0.20864438D+04 K.E.= 0.10432214D+04 V.T.= -0.20000009D+01

S	1S	2S	3S	4S
BASIS/ORB E	-220.61053	-26.46006	-3.51365	-0.24131
1S 24.06730	-0.94212	-0.28648	-0.10820	-0.02403
1S 37.48750	-0.01739	-0.00315	0.00073	0.00008
2S 21.07680	-0.05066	-0.16164	-0.05675	-0.01302
2S 10.61970	-0.00177	0.84728	0.31788	0.07202
3S 9.77905	0.00023	0.30490	0.27829	0.06629
3S 5.98021	0.00025	0.02255	-0.19829	-0.04045
3S 4.31311	-0.00017	-0.00088	-0.81383	-0.23578
4S 3.52059	0.00008	-0.00013	-0.18380	-0.01075
4S 1.84447	-0.00002	0.00036	-0.00525	0.43284
4S 1.13430	0.00002	-0.00027	0.00250	0.56637
4S 0.77196	-0.00001	0.00011	-0.00096	0.10806

P	2P	3P	D	3D
BASIS/ORB E	-22.38591	-2.26214	BASIS/ORB E	-0.53224
2P 9.58945	0.84599	-0.31247	3D 3.40360	0.37488
2P 16.49360	0.10707	-0.03504	3D 10.66370	0.02479
3P 7.42348	0.08843	-0.17856	3D 5.54649	0.24020
3P 5.65702	-0.00766	0.49279	3D 2.16743	0.36227
3P 3.37910	0.00240	0.69713	3D 1.35615	0.16045
3P 2.02850	-0.00034	0.06456		

CHROMIUM K(2)L(8)3S(2)3P(6)4S(2)3D(4), 3G  
T.E.= -0.10431993D+04 P.E.= -0.20863978D+04 K.E.= 0.10431985D+04 V.T.= -0.20000008D+01

S	1S	2S	3S	4S
BASIS/ORB E	-220.61537	-26.46537	-3.51729	-0.24171
1S 24.06800	-0.94210	-0.28646	-0.10822	-0.02407
1S 37.49010	-0.01737	-0.00316	0.00073	0.00008
2S 21.07790	-0.05070	-0.16164	-0.05676	-0.01305
2S 10.62040	-0.00176	0.84710	0.31787	0.07216
3S 9.77978	0.00022	0.30508	0.27845	0.06637
3S 5.98063	0.00025	0.02255	-0.19809	-0.04023
3S 4.31340	-0.00017	-0.00087	-0.81450	-0.23673
4S 3.52083	0.00008	-0.00013	-0.18329	-0.01031
4S 1.84459	-0.00002	0.00036	-0.00525	0.43426
4S 1.13438	0.00002	-0.00027	0.00250	0.56573
4S 0.77201	-0.00001	0.00011	-0.00096	0.10716

P	2P	3P	D	3D
BASIS/ORB E	-22.39117	-2.26547	BASIS/ORB E	-0.52243
2P 9.58879	0.84615	-0.31265	3D 3.40180	0.37473
2P 16.49460	0.10705	-0.03504	3D 10.66440	0.02472
3P 7.41857	0.08841	-0.17939	3D 5.54839	0.23980
3P 5.65919	-0.00780	0.49352	3D 2.16709	0.35895
2P 3.38062	0.00241	0.69734	3D 1.35625	0.16560
3P 2.02861	-0.00034	0.06448		

See page 183 for Explanation of Tables and Notes for Tables 32, 42, and 43

## ROOTHAAN-HARTREE-FOCK ATOMIC WAVEFUNCTIONS

TABLE 1 (15). HARTREE-FOCK FUNCTIONS FOR NEUTRAL ATOMS.

CHROMIUM K(2)L(8)3S(2)3P(6)4S(2)3D(4), 1G				
T.E.= -0.10431087D+04 P.E.= -0.20862161D+04 K.E.= 0.10431074D+04 V.T.= -0.20000013D+01				
S	1S	2S	3S	4S
BASIS/ORB E	-220.63573	-26.48779	-3.53296	-0.24349
1S 24.07490	-0.94190	-0.28625	-0.10829	-0.02424
1S 37.51280	-0.01725	-0.00320	0.00073	0.00007
2S 21.09000	-0.05108	-0.16164	-0.05675	-0.01316
2S 10.62690	-0.00173	0.84535	0.31735	0.07261
3S 9.78667	0.00019	0.3C669	0.27936	0.06697
3S 5.98440	0.00028	0.02262	-0.19632	-0.03563
3S 4.31599	-0.00019	-0.00086	-0.81776	-0.24017
4S 3.52297	0.00008	-0.00014	-0.18144	-0.00534
4S 1.84770	-0.00003	0.00036	-0.00531	0.43971
4S 1.13509	0.00002	-0.00027	0.00250	0.56438
4S 0.77248	-0.00001	0.00011	-0.00096	0.10301
P	2P	3P	D	3D
BASIS/ORB E	-22.41332	-2.27582	BASIS/ORB E	-0.48469
2P 9.58938	0.84643	-0.31259	3D 3.25790	0.40484
2P 16.50510	0.10681	-0.03519	3D 11.02570	0.02265
3P 7.42495	0.08821	-0.18750	3D 5.50006	0.25750
3P 5.71030	-0.00754	0.49212	3D 2.02776	0.33286
3P 3.39984	0.00223	0.70521	3D 1.30509	0.15144
3P 2.02965	-0.00029	0.06554		
CHROMIUM K(2)L(8)3S(2)3P(6)4S(2)3D(4), 3F				
T.E.= -0.10431421D+04 P.E.= -0.20862834D+04 K.E.= 0.10431413D+04 V.T.= -0.20000007D+01				
S	1S	2S	3S	4S
BASIS/ORB E	-220.62794	-26.47920	-3.52691	-0.24280
1S 24.07010	-0.94204	-0.28641	-0.10828	-0.02417
1S 37.49690	-0.01733	-0.00316	0.00073	0.00007
2S 21.08090	-0.05082	-0.16164	-0.05677	-0.01314
2S 10.62240	-0.00175	0.84657	0.31781	0.07254
3S 9.78196	0.00021	0.30558	0.27886	0.06659
3S 5.98176	0.00026	0.02256	-0.19752	-0.03565
3S 4.31417	-0.00018	-0.00087	-0.81628	-0.23927
4S 3.52147	0.00008	-0.00013	-0.18196	-0.00913
4S 1.84492	-0.00003	0.00036	-0.00525	0.43810
4S 1.13459	0.00002	-0.00027	0.00248	0.56402
4S 0.77215	-0.00001	0.00011	-0.00096	0.10474
P	2P	3P	D	3D
BASIS/ORB E	-22.40483	-2.27428	BASIS/ORB E	-0.49839
2P 9.58854	0.84638	-0.31230	3D 3.39705	0.37427
2P 16.49810	0.10696	-0.03526	3D 10.66640	0.02454
3P 7.40553	0.08912	-0.19340	3D 5.55375	0.23897
3P 5.72922	-0.00870	0.49598	3D 2.16620	0.34979
3P 3.40031	0.00241	0.70697	3D 1.35650	0.17950
3P 2.02892	-0.00033	0.06586		
CHROMIUM K(2)L(8)3S(2)3P(6)4S(2)3D(4), 1F				
T.E.= -0.10431110D+04 P.E.= -0.20862208D+04 K.E.= 0.10431097D+04 V.T.= -0.20000012D+01				
S	1S	2S	3S	4S
BASIS/ORB E	-220.63486	-26.48679	-3.53215	-0.24339
1S 24.07480	-0.94191	-0.28626	-0.10828	-0.02423
1S 37.51270	-0.01725	-0.00320	0.00073	0.00007
2S 21.08990	-0.05108	-0.16164	-0.05675	-0.01315
2S 10.62680	-0.00173	0.84537	0.31734	0.07257
3S 9.78661	0.00019	0.30666	0.27934	0.06695
3S 5.98437	0.00028	0.02262	-0.19637	-0.03568
3S 4.31598	-0.00019	-0.00086	-0.81761	-0.23993
4S 3.52296	0.00008	-0.00014	-0.18156	-0.00545
4S 1.84769	-0.00003	0.00036	-0.00531	0.43933
4S 1.13509	0.00002	-0.00027	0.00250	0.56454
4S 0.77248	-0.00001	0.00011	-0.00096	0.10325

See page 183 for Explanation of Tables and Notes for Tables 32, 42, and 43

TABLE 1 (16). HARTREE-FOCK FUNCTIONS FOR NEUTRAL ATOMS.

P BASIS/ORB E	2P -22.41234	3P -2.27907	D BASIS/ORB E	3D -0.48543
2P 9.58945	0.84642	-0.31256	3D 3.25800	0.40564
2P 16.50510	0.10681	-0.03519	3D 11.02570	0.02267
3P 7.42523	0.08821	-0.18748	3D 5.50043	0.25722
3P 5.71031	-0.00753	0.49210	3D 2.02777	0.33308
3P 3.39957	0.00223	0.70519	3D 1.30509	0.15035
3P 2.02965	-0.00029	0.06556		

CHROMIUM K(2)L(8)3S(2)3P(6)4S(2)3D(4), 5D  
T.E.= -0.10433095D+04 P.E.= -0.20866188D+04 K.E.= 0.10433093D+04 V.T.= -0.20000002D+01

S BASIS/ORB E	1S -220.59153	2S -26.43914	3S -3.49912	4S -0.23975
1S 24.06330	-0.94223	-0.28657	-0.10811	-0.02388
1S 37.47690	-0.01746	-0.00314	0.00072	0.0009
2S 21.07150	-0.05043	-0.16162	-0.05673	-0.01287
2S 10.61670	-0.00180	0.84808	0.31797	0.07145
3S 9.77606	0.00026	0.30412	0.27767	0.06597
3S 5.97845	0.00023	0.02259	-0.19915	-0.04135
3S 4.31189	-0.00015	-0.00091	-0.81110	-0.23195
4S 3.51959	0.00007	-0.00011	-0.18585	-0.01254
4S 1.84395	-0.00002	0.00035	-0.00522	0.42719
4S 1.13396	0.00002	-0.00026	0.00249	0.56890
4S 0.77174	-0.00001	0.00011	-0.00095	0.11158

P BASIS/ORB E	2P -22.36526	3P -2.24E5	D BASIS/ORB E	3D -0.56920
2P 9.62465	0.84099	-0.30904	3D 3.20848	0.44978
2P 16.50080	0.10620	-0.03502	3D 11.29070	0.02041
3P 7.58114	0.09230	-0.16453	3D 5.57635	0.25732
3P 5.63920	-0.00500	0.47285	3D 2.01453	0.30403
3P 3.37943	0.00237	0.69890	3D 1.35576	0.12567
3P 2.02801	-0.00037	0.06564		

CHROMIUM K(2)L(8)3S(2)3P(6)4S(2)3D(4), 3D  
T.E.= -0.10431672D+04 P.E.= -0.20863337D+04 K.E.= 0.10431665D+04 V.T.= -0.20000007D+01

S BASIS/ORB E	1S -220.62217	2S -26.47285	3S -3.52241	4S -0.24228
1S 24.06920	-0.94207	-0.28643	-0.10825	-0.02412
1S 37.49390	-0.01735	-0.00316	0.00073	0.0009
2S 21.07960	-0.05077	-0.16164	-0.05677	-0.01310
2S 10.62150	-0.00176	0.84681	0.31784	0.07236
3S 9.78091	0.00022	0.30535	0.27868	0.06649
3S 5.98127	0.00026	0.02254	-0.19780	-0.03993
3S 4.31384	-0.00017	-0.00086	-0.81544	-0.23807
4S 3.52119	0.00008	-0.00013	-0.18258	-0.00568
4S 1.84478	-0.00002	0.00036	-0.00526	0.43628
4S 1.13450	0.00002	-0.00027	0.00250	0.56483
4S 0.77209	-0.00001	0.00011	-0.00096	0.10590

P BASIS/ORB E	2P -22.39855	3P -2.27C16	D BASIS/ORB E	3D -0.50881
2P 9.58872	0.84635	-0.31290	3D 3.39912	0.37477
2P 16.49770	0.10696	-0.03501	3D 10.66550	0.02463
3P 7.41121	0.08857	-0.18C77	3D 5.55152	0.23918
3P 5.66255	-0.00812	0.49470	3D 2.16659	0.35398
3P 3.38277	0.00244	0.65765	3D 1.35639	0.17295
3P 2.02879	-0.00035	0.06438		

See page 183 for Explanation of Tables and Notes for Tables 32, 42, and 43

## ROOTHAAN-HARTREE-FOCK ATOMIC WAVEFUNCTIONS

TABLE 1 (17). HARTREE-FOCK FUNCTIONS FOR NEUTRAL ATOMS.

CHROMIUM K(2)L(8)3S(2)3P(6)4S(2)3D(4), 1D  
 T.E.= -0.104304580+04 P.E.= -0.20860898D+04 K.E.= 0.10430440D+04 V.T.= -0.20000018D+01

S	1S	2S	3S	4S
BASIS/ORB E	-220.64974	-26.50302	-3.54359	-0.24479
1S 24.06670	-0.94213	-0.28654	-0.10844	-0.02435
1S 37.48080	-0.01740	-0.00313	0.00074	0.00005
2S 21.07330	-0.05064	-0.16165	-0.05687	-0.01334
2S 10.61780	-0.00176	0.84772	0.31870	0.07347
3S 9.77768	0.00022	0.30458	0.27894	0.06681
3S 5.97909	0.00026	0.02236	-0.19846	-0.03902
3S 4.31233	-0.00017	-0.00CE2	-0.81854	-0.24373
4S 3.51995	0.00008	-0.00015	-0.17889	-0.00657
4S 1.84414	-0.00002	0.00036	-0.00515	0.44579
4S 1.13408	0.00002	-0.00C27	0.00242	0.56058
4S 0.77182	-0.00001	0.00011	-0.00093	0.09977

P	2P	3P	D	3D
BASIS/ORB E	-22.42838	-2.28556	BASIS/ORB E	-0.45850
2P 9.55974	0.84901	-0.31475	3D 3.29950	0.36996
2P 16.49050	0.10817	-0.03544	3D 10.66180	0.02484
3P 7.43680	0.07961	-0.17061	3D 5.47621	0.25429
3P 5.63333	-0.00236	0.49094	3D 2.16832	0.31560
3P 3.37655	0.00105	0.69827	3D 1.35590	0.20824
3P 1.99019	0.00001	0.05894		

CHROMIUM K(2)L(8)3S(2)3P(6)4S(2)3D(4), 3P  
 T.E.= -0.10431421D+04 P.E.= -0.20862834D+04 K.E.= 0.10431413D+04 V.T.= -0.20000007D+01

S	1S	2S	3S	4S
BASIS/ORB E	-220.62794	-26.47920	-3.52691	-0.24280
1S 24.07010	-0.94204	-0.28641	-0.10828	-0.02417
1S 37.49690	-0.01733	-0.00316	0.00073	0.00007
2S 21.08090	-0.05082	-0.16164	-0.05677	-0.01314
2S 10.62240	-0.00175	0.84657	0.31781	0.07254
3S 9.78196	0.00021	0.30558	0.27886	0.06659
3S 5.98176	0.00026	0.02256	-0.19752	-0.03965
3S 4.31417	-0.00018	-0.00C87	-0.81628	-0.23927
4S 3.52147	0.00008	-0.00013	-0.18196	-0.00913
4S 1.84492	-0.00003	0.00036	-0.00525	0.43810
4S 1.13459	0.00002	-0.00027	0.00248	0.56402
4S 0.77215	-0.00001	0.00011	-0.00096	0.10474

P	2P	3P	D	3D
BASIS/ORB E	-22.40483	-2.27428	BASIS/ORB E	-0.49839
2P 9.58854	0.84638	-0.31230	3D 3.39705	0.37427
2P 16.49810	0.10696	-0.03526	3D 10.66640	0.02454
3P 7.40553	0.08912	-0.19340	3D 5.55375	0.23897
3P 5.72922	-0.00870	0.49558	3D 2.16520	0.34979
3P 3.40031	0.00241	0.70697	3D 1.35650	0.17950
3P 2.02892	-0.00033	0.06586		

CHROMIUM K(2)L(8)3S(2)3P(5)4S(2)3D(4), 1S  
 T.E.= -0.104300050+04 P.E.= -0.20859984D+04 K.E.= 0.10429979D+04 V.T.= -0.20000025D+01

S	1S	2S	3S	4S
BASIS/ORB E	-220.66058	-26.51508	-3.55224	-0.24590
1S 24.06620	-0.94214	-0.28655	-0.10851	-0.02445
1S 37.48070	-0.01741	-0.00313	0.00074	0.00004
2S 21.07350	-0.05061	-0.16162	-0.05689	-0.01343
2S 10.61780	-0.00177	0.84767	0.31884	0.07388
3S 9.77814	0.00023	0.30462	0.27914	0.06699
3S 5.97908	0.00025	0.02235	-0.19830	-0.03857
3S 4.31233	-0.00016	-0.00083	-0.81997	-0.24610
4S 3.51994	0.00008	-0.00015	-0.17756	-0.00541
4S 1.84414	-0.00002	0.00036	-0.00513	0.44967
4S 1.13408	0.00002	-0.00027	0.00239	0.55882
4S 0.77182	-0.00001	0.00011	-0.00092	0.09730

See page 183 for Explanation of Tables and Notes for Tables 32, 42, and 43

TABLE 1 (18). HARTREE-FOCK FUNCTIONS FOR NEUTRAL ATOMS.

P	2P	3P	D	3D
BASIS/ORB E	-22.44027	-2.29750	BASIS/ORB E	-0.44033
2P 9.50455	0.84942	-0.31488	3D 3.36041	0.37813
2P 16.34680	0.11344	-0.03743	3D 10.66180	0.02425
3P 7.38990	0.07176	-0.18497	3D 5.54664	0.24054
3P 5.70893	-0.00042	0.49611	3D 2.11387	0.34222
3P 3.39519	0.00062	0.70826	3D 1.30390	0.19148
3P 1.99018	0.00011	0.06012		

MANGANESE K(2)L(8)3S(2)3P(6)4S(1)3D(6), 6D  
T.E.= -0.11497432D+04 P.E.= -0.22994792D+04 K.E.= 0.11497360D+04 V.T.= -0.20000063D+01

S	1S	2S	3S	4S
BASIS/ORB E	-240.35373	-28.90915	-3.62139	-0.22691
1S 38.03710	-0.02069	-0.00006	0.00072	-0.00009
1S 24.89280	-0.94796	-0.29756	-0.11008	-0.02201
2S 21.35560	-0.04058	-0.16741	-0.06397	-0.01388
2S 10.79310	-0.00077	0.94034	0.36711	0.07703
3S 9.86759	-0.00023	0.22321	0.24647	0.05210
3S 5.79804	0.00049	0.01802	-0.40172	-0.07482
3S 4.19444	-0.00037	-0.00337	-0.67444	-0.20098
4S 3.46874	0.00014	0.00090	-0.13450	0.03641
4S 1.78550	-0.00004	0.00006	-0.00264	0.42209
4S 1.11627	0.00003	0.00005	0.00074	0.48789
4S 0.82105	-0.00002	0.00004	-0.00030	0.18163

P	2P	3P	D	3D
BASIS/ORB E	-24.61603	-2.29839	BASIS/ORB E	-0.38285
2P 16.38050	0.14410	-0.04540	3D 11.21860	0.02378
2P 9.58293	0.86565	-0.32939	3D 5.84280	0.23831
3P 9.11541	-0.00421	-0.03171	3D 3.68285	0.29512
3P 5.34168	0.03620	0.46691	3D 2.43860	0.36492
2P 3.67682	-0.01719	0.49006	3D 1.34276	0.27319
3P 2.58797	0.00540	0.20491		

MANGANESE K(2)L(8)3S(2)3P(6)4S(2)3D(5), 21  
T.E.= -0.11496629D+04 P.E.= -0.22993173D+04 K.E.= 0.11496544D+04 V.T.= -0.20000075D+01

S	1S	2S	3S	4S
BASIS/ORB E	-240.57281	-29.15243	-3.84578	-0.25077
1S 25.35020	-0.93785	-0.28497	-0.10619	-0.02295
1S 40.10350	-0.01132	-0.00240	-0.00023	-0.00023
2S 22.12910	-0.06421	-0.16574	-0.06364	-0.01465
2S 10.22070	0.00195	1.03753	0.40927	0.09204
3S 9.60340	-0.00325	0.05695	0.22381	0.05145
3S 6.11700	0.00346	0.02266	-0.36349	-0.07025
3S 4.42124	-0.00281	-0.00352	-0.65922	-0.21298
4S 3.89065	0.00103	0.00081	-0.20998	-0.00272
4S 1.89923	-0.00019	0.00017	-0.01142	0.45508
4S 1.15280	0.00013	-0.00015	0.00628	0.54392
4S 0.81659	-0.00006	0.00007	-0.00262	0.10698

P	2P	3P	D	3D
BASIS/ORB E	-24.85503	-2.50630	BASIS/ORB E	-0.57337
2P 9.70399	0.86801	-0.34218	3D 3.61204	0.37197
2P 16.69360	0.13039	-0.03846	3D 11.30040	0.02491
3P 6.47360	0.01501	-0.36813	3D 5.87236	0.25240
3P 5.86352	0.02382	0.72759	3D 2.30236	0.35563
3P 3.79561	-0.00978	0.54467	3D 1.43505	0.15946
3P 2.66547	0.00338	0.20449		

See page 183 for Explanation of Tables and Notes for Tables 32, 42, and 43

## ROOTHAAN-HARTREE-FOCK ATOMIC WAVEFUNCTIONS

TABLE 1 (19). HARTREE-FOCK FUNCTIONS FOR NEUTRAL ATOMS.

MANGANESE K(2)L(8)3S(2)3P(6)4S(2)3D(5), 2H  
 T.E.= -0.11496167D+04 P.E.= -0.22952252D+04 K.E.= 0.11496084D+04 V.T.= -0.20000073D+01

S	1S	2S	3S	4S
BASIS/ORB E	-240.58192	-29.16240	-3.85268	-0.25150
1S 25.35100	-0.93783	-0.28495	-0.10624	-0.02302
1S 40.11380	-0.01131	-0.00240	-0.00023	-0.00023
2S 22.13230	-0.06425	0.16569	-0.06363	-0.01471
2S 10.21770	0.00194	1.03E44	0.40957	0.09243
3S 9.60600	-0.00323	0.09620	0.22361	0.05140
3S 6.11854	0.00345	0.02284	-0.36263	-0.06963
3S 4.42235	-0.00280	-0.00363	-0.66087	-0.21503
4S 3.89162	0.00103	0.00C85	-0.20904	-0.00175
4S 1.89971	-0.00019	0.00016	-0.01142	0.45738
4S 1.15310	0.00013	-0.00015	0.00627	0.54294
4S 0.81680	-0.00006	0.00007	-0.00262	0.10549

P	2P	3P	D	3D
BASIS/ORB E	-24.86488	-2.51266	BASIS/ORB E	-0.55871
2P 9.70494	0.86806	-0.34234	3D 3.75304	0.35041
2P 16.69640	0.13027	-0.03845	3D 11.08340	0.02601
3P 6.47524	0.01535	-0.36567	3D 5.93683	0.23346
3P 5.86495	0.02352	0.72932	3D 2.39301	0.37136
3P 3.79653	-0.00974	0.54516	3D 1.46343	0.18488
3P 2.66617	0.00337	0.20367		

MANGANESE K(2)L(8)3S(2)3P(6)4S(2)3D(5), 4G  
 T.E.= -0.11497228D+04 P.E.= -0.22954372D+04 K.E.= 0.11497145D+04 V.T.= -0.20000072D+01

S	1S	2S	3S	4S
BASIS/ORB E	-240.56099	-29.13946	-3.83683	-0.24985
1S 25.35320	-0.93770	-0.28467	-0.10612	-0.02289
1S 40.18170	-0.01129	-0.00252	-0.00023	-0.00021
2S 22.16080	-0.06430	0.16529	-0.06321	-0.01444
2S 10.19810	0.00169	1.04165	0.40980	0.09166
3S 9.62350	-0.00300	0.09123	0.22148	0.05111
3S 6.12872	0.00323	0.02418	-0.35851	-0.07C21
3S 4.42967	-0.00263	-0.00432	-0.65964	-0.20985
4S 3.89805	0.00096	0.00106	-0.21355	-0.00580
4S 1.90293	-0.00017	0.00013	-0.01190	0.44560
4S 1.15506	0.00013	-0.00013	0.00659	0.54617
4S 0.81817	-0.00006	0.00006	-0.00276	0.11092

P	2P	3P	D	3D
BASIS/ORB E	-24.84221	-2.49807	BASIS/ORB E	-0.59242
2P 9.71126	0.86816	-0.34176	3D 3.56168	0.41951
2P 16.71160	0.12960	-0.03821	3D 11.41300	0.02365
3P 6.48614	0.01739	-0.36946	3D 5.93290	0.24762
3P 5.87442	0.02195	0.72545	3D 2.15408	0.36280
3P 3.80260	-0.00949	0.54371	3D 1.35393	0.10845
3P 2.67081	0.00331	0.20856		

MANGANESE K(2)L(8)3S(2)3P(6)4S(2)3D(5), 2G  
 T.E.= -0.11495515D+04 P.E.= -0.22990943D+04 K.E.= 0.11495429D+04 V.T.= -0.20000075D+01

S	1S	2S	3S	4S
BASIS/ORB E	-240.59427	-29.17578	-3.86170	-0.25245
1S 25.35270	-0.93775	-0.28484	-0.10629	-0.02309
1S 40.13350	-0.01129	-0.00244	-0.00023	-0.00024
2S 22.14160	-0.06433	-0.16559	-0.06356	-0.01478
2S 10.21200	0.00188	1.03935	0.40995	0.09293
3S 9.61110	-0.00317	0.09483	0.22333	0.05128
3S 6.12151	0.00339	0.02312	-0.36143	-0.06873
3S 4.42448	-0.00276	-0.00277	-0.66278	-0.21766
4S 3.89350	0.00101	0.00C89	-0.20820	-0.00058
4S 1.90065	-0.00018	0.00016	-0.01140	0.46005
4S 1.15367	0.00013	-0.00014	0.00628	0.54179
4S 0.81720	-0.00006	0.00007	-0.00263	0.10378

See page 183 for Explanation of Tables and Notes for Tables 32, 42, and 43

TABLE I (20). HARTREE-FOCK FUNCTIONS FOR NEUTRAL ATOMS.

P	2P	3P	D	3D
BASIS/ORB E	-24.87814	-2.52098	BASIS/ORB E	-0.53758
2P 9.70672	-0.86817	-0.34210	3D 3.60040	0.39343
2P 16.70170	-0.13004	-0.03859	3D 11.52910	0.02280
3P 6.47841	-0.01801	-0.31149	3D 5.93888	0.24676
3P 5.75771	-0.02167	0.69979	3D 2.20641	0.36670
3P 3.79830	0.01124	0.47632	3D 1.35216	0.13973
3P 2.77352	-0.00417	0.24279		

MANGANESE K(2)L(8)3S(2)3P(6)4S(2)3D(5), 4F  
T.E.= -0.114962680+04 P.E.= -0.229924520+04 K.E.= 0.114961840+04 V.T.= -0.20000073D+01

S	1S	2S	3S	4S
BASIS/ORB E	-240.57934	-29.15550	-3.85049	-0.25126
1S 25.35090	-0.93783	-0.28495	-0.10622	-0.02300
1S 40.11300	-0.01131	-0.00240	-0.00023	-0.00023
2S 22.13200	-0.06424	-0.16569	-0.06362	-0.01469
2S 10.21800	0.00194	1.03E39	0.40950	0.09230
3S 9.60580	-0.00323	0.09627	0.22362	0.05141
3S 6.11843	0.00345	0.022E3	-0.36278	-0.06984
3S 4.42226	-0.00280	-0.00361	-0.66039	-0.21430
4S 3.89155	0.00103	0.00084	-0.20940	-0.00213
4S 1.89968	-0.00019	0.00016	-0.01143	0.45654
4S 1.15307	0.00013	-0.00015	0.00628	0.54332
4S 0.81678	-0.00006	0.00007	-0.00262	0.10602

P	2P	3P	D	3D
BASIS/ORB E	-24.86202	-2.51065	BASIS/ORB E	-0.56149
2P 9.70483	0.86806	-0.34229	3D 3.75326	0.35131
2P 16.69610	0.13028	-0.03845	3D 11.08310	0.02605
3P 6.47512	0.01528	-0.36926	3D 5.93660	0.23310
3P 5.86485	0.02359	0.72878	3D 2.39311	0.37250
3P 3.79646	-0.00974	0.54500	3D 1.46340	0.18250
3P 2.66612	0.00337	0.20400		

MANGANESE K(2)L(8)3S(2)3P(6)4S(2)3D(5), 2F  
T.E.= -0.11496103D+04 P.E.= -0.22992121D+04 K.E.= 0.11496018D+04 V.T.= -0.20000073D+01

S	1S	2S	3S	4S
BASIS/ORB E	-240.58295	-29.16349	-3.85335	-0.25158
1S 25.35120	-0.93782	-0.28493	-0.10624	-0.02302
1S 40.11610	-0.01131	-0.00241	-0.00023	-0.00023
2S 22.13330	-0.06426	-0.16568	-0.06362	-0.01472
2S 10.21710	0.00193	1.03E54	0.40960	0.09247
3S 9.60660	-0.00322	0.09606	0.22358	0.05139
3S 6.11890	0.00344	0.02287	-0.36249	-0.06957
3S 4.42260	-0.00280	-0.00364	-0.66103	-0.21520
4S 3.89185	0.00102	0.00085	-0.20900	-0.00169
4S 1.89982	-0.00018	0.00016	-0.01142	0.45755
4S 1.15316	0.00013	-0.00015	0.00627	0.54290
4S 0.81685	-0.00006	0.00007	-0.00262	0.10535

P	2P	3P	D	3D
BASIS/ORB E	-24.86596	-2.51328	BASIS/ORB E	-0.55647
2P 9.70513	0.86808	-0.34236	3D 3.69129	0.34561
2P 16.69700	0.13024	-0.03845	3D 11.07960	0.02640
3P 6.47562	0.01539	-0.36984	3D 5.87577	0.24492
3P 5.86528	0.02349	0.72546	3D 2.39270	0.36221
3P 3.79674	-0.00973	0.54521	3D 1.46352	0.18723
3P 2.66633	0.00337	0.20363		

See page 183 for Explanation of Tables and Notes for Tables 32, 42, and 43

## ROOTHAAAN-HARTREE-FOCK ATOMIC WAVEFUNCTIONS

TABLE 1 (21). HARTREE-FOCK FUNCTIONS FOR NEUTRAL ATOMS.

MANGANESE K(2)L(8)3S(2)3P(6)4S(2)3D(5), 4D  
 T.E.= -0.11496879D+04 P.E.= -0.22993677D+04 K.E.= 0.11496798D+04 V.T.= -0.20000071D+01

S	1S	2S	3S	4S
BASIS/ORB E	-240.56729	-29.14634	-3.84142	-0.25027
1S 25.34990	-0.93787	-0.28499	-0.10617	-0.02291
1S 40.09990	-0.01132	-0.00239	-0.00023	-0.00022
2S 22.12760	-0.06420	-0.16576	-0.06364	-0.01461
2S 10.22180	0.00196	1.03775	0.40912	0.09179
3S 9.60240	-0.00326	0.09722	0.22385	0.05148
3S 6.11647	0.00347	0.02261	-0.36384	-0.07066
3S 4.42085	-0.00282	-0.00348	-0.65830	-0.21160
4S 3.89031	0.00103	0.00080	-0.21061	-0.00342
4S 1.89906	-0.00019	0.00017	-0.01144	0.45355
4S 1.15269	0.00013	-0.00015	0.00629	0.54450
4S 0.81652	-0.00006	0.00007	-0.00263	0.10808

P	2P	3P	D	3D
BASIS/ORB E	-24.84901	-2.50229	BASIS/ORB E	-0.58097
2P 9.70367	0.86799	-0.34208	3D 3.61309	0.40182
2P 16.69260	0.13043	-0.03845	3D 11.29930	0.02428
3P 6.47302	0.01490	-0.36730	3D 5.94694	0.24175
3P 5.86302	0.02393	0.72656	3D 2.26026	0.33803
3P 3.79529	-0.00979	0.54434	3D 1.46292	0.15650
3P 2.66522	0.00338	0.20508		

MANGANESE K(2)L(8)3S(2)3P(6)4S(2)3D(5), 2D  
 T.E.= -0.11495134D+04 P.E.= -0.22990123D+04 K.E.= 0.11494990D+04 V.T.= -0.20000125D+01

S	1S	2S	3S	4S
BASIS/ORB E	-240.60195	-29.16412	-3.86743	-0.25302
1S 24.86090	-0.95030	-0.28938	-0.10874	-0.02320
1S 39.36800	-0.01947	-0.00453	-0.00061	-0.00058
2S 22.09560	-0.03615	-0.15754	-0.05923	-0.01465
2S 10.42070	-0.00759	0.98829	0.38584	0.08962
3S 9.81220	0.00575	0.15264	0.23643	0.04985
3S 6.00217	-0.00424	0.01900	-0.37214	-0.05514
3S 4.33996	0.00361	-0.00103	-0.67051	-0.24772
4S 3.81892	-0.00130	-0.00025	-0.17656	0.03376
4S 1.82686	0.00025	0.00041	-0.01025	0.50241
4S 1.13180	-0.00021	-0.00040	0.00706	0.46925
4S 0.85129	0.00010	0.00020	-0.00329	0.12290

P	2P	3P	D	3D
BASIS/ORB E	-24.88636	-2.52626	BASIS/ORB E	-0.52564
2P 9.67761	-0.86675	-0.34289	3D 3.61836	0.34401
2P 16.61710	-0.13365	-0.03954	3D 10.87040	0.02917
3P 6.35913	-0.01687	-0.30984	3D 5.75763	0.25746
3P 5.64833	-0.01994	0.74240	3D 2.33461	0.35379
3P 3.65869	0.01103	0.47660	3D 1.43632	0.18561
3P 2.72083	-0.00443	0.19992		

MANGANESE K(2)L(8)3S(2)3P(6)4S(2)3D(5), 4P  
 T.E.= -0.11497010D+04 P.E.= -0.22993931D+04 K.E.= 0.11496920D+04 V.T.= -0.20000078D+01

S	1S	2S	3S	4S
BASIS/ORB E	-240.56553	-29.14442	-3.84030	-0.25020
1S 25.35300	-0.93771	-0.28470	-0.10614	-0.02291
1S 40.17340	-0.01129	-0.00250	-0.00022	-0.00021
2S 22.15730	-0.06430	-0.16534	-0.06326	-0.01449
2S 10.20050	0.00173	1.04126	0.40979	0.09183
3S 9.62140	-0.00303	0.05184	0.22180	0.05114
3S 6.12749	0.00326	0.02402	-0.35905	-0.06999
3S 4.42878	-0.00265	-0.00425	-0.65998	-0.21096
4S 3.89727	0.00097	0.08104	-0.21281	-0.00503
4S 1.90254	-0.00018	0.00014	-0.01181	0.45106
4S 1.15482	0.00013	-0.00013	0.00654	0.54562
4S 0.81800	-0.00006	0.00006	-0.00274	0.10986

See page 183 for Explanation of Tables and Notes for Tables 32, 42, and 43

TABLE 1 (22). HARTREE-FOCK FUNCTIONS FOR NEUTRAL ATOMS.

P	2P	3P	D	3D
BASIS/ORB E	-24.84711	-2.50127	BASIS/ORB E	-0.58560
2P 9.71051	0.86803	-0.34185	3D 3.52329	0.41217
2P 16.70990	0.12972	-0.03826	3D 11.76060	0.02142
3P 6.48481	0.02142	-0.30505	3D 5.93537	0.25640
3P 5.76327	0.01759	0.69164	3D 2.20356	0.33629
3P 3.73186	-0.00934	0.52394	3D 1.40963	0.13671
3P 2.67025	0.00348	0.15754		

MANGANESE K(2)L(8)3S(2)3P(6)4S(2)3D(5), 2P  
T.E.= -0.11494126D+04 P.E.= -0.22988144D+04 K.E.= 0.11494018D+04 V.T.= -0.20000094D+01

S	1S	2S	3S	4S
BASIS/ORB E	-240.62180	-29.20575	-3.88240	-0.25489
1S 25.04010	-0.94895	-0.29451	-0.11105	-0.02448
1S 39.99390	-0.01457	-0.00027	0.00111	0.00011
2S 21.58590	-0.04656	-0.16525	-0.06110	-0.01420
2S 10.67240	-0.00068	0.95129	0.36770	0.08368
3S 9.97508	-0.00032	0.19816	0.25084	0.05898
3S 6.10056	0.00060	0.02925	-0.30146	-0.05821
3S 4.49441	-0.00046	-0.00514	-0.70124	-0.22187
4S 3.88027	0.00017	0.00266	-0.20858	-0.00827
4S 1.93103	-0.00003	-0.00024	-0.01161	0.44854
4S 1.17163	0.00002	0.00014	0.00616	0.55471
4S 0.81437	-0.00001	-0.00006	-0.00250	0.10516

P	2P	3P	D	3D
BASIS/ORB E	-24.90777	-2.54006	BASIS/ORB E	-0.49383
2P 9.69368	0.86796	-0.34269	3D 3.61381	0.37678
2P 16.66960	0.13144	-0.03912	3D 11.26870	0.02418
3P 6.45600	0.01075	-0.39027	3D 5.92198	0.24496
3P 5.84823	0.02752	0.76474	3D 2.25021	0.36217
3P 3.78580	-0.01085	0.52227	3D 1.34702	0.16769
3P 2.71097	0.00386	0.21127		

MANGANESE K(2)L(8)3S(2)3P(6)4S(2)3D(5), 6S  
T.E.= -0.114986570D+04 P.E.= -0.22957227D+04 K.E.= 0.11498570D+04 V.T.= -0.20000075D+01

S	1S	2S	3S	4S
BASIS/ORB E	-240.53386	-29.10973	-3.81661	-0.24784
1S 25.35890	-0.93746	-0.28436	-0.10595	-0.02239
1S 40.22850	-0.01123	-0.00262	-0.00022	-0.00035
2S 22.18590	-0.06458	-0.16507	-0.06286	-0.01473
2S 10.18450	0.00156	1.04380	0.40954	0.09217
3S 9.63560	-0.00288	0.08766	0.22020	0.04683
3S 6.13576	0.00310	0.02502	-0.35686	-0.05743
3S 4.43473	-0.00251	-0.00473	-0.65559	-0.22417
4S 3.90249	0.00092	0.00119	-0.21920	0.00628
4S 1.86815	-0.00017	0.00012	-0.01240	0.45255
4S 1.15642	0.00013	-0.00012	0.00736	0.52136
4S 0.81912	-0.00005	0.00006	-0.00303	0.12840

P	2P	3P	D	3D
BASIS/ORB E	-24.81281	-2.47548	BASIS/ORB E	-0.63884
2P 9.71579	0.86804	-0.34099	3D 3.63884	0.40990
2P 16.72170	0.12920	-0.03805	3D 11.55660	0.02214
3P 6.51366	0.02225	-0.29351	3D 5.02189	0.23736
3P 5.77096	0.01728	0.67446	3D 2.28340	0.35035
3P 3.73980	-0.00920	0.52325	3D 1.46766	0.13622
3P 2.67402	0.00343	0.20373		

See page 183 for Explanation of Tables and Notes for Tables 32, 42, and 43

## ROOTHAAN-HARTREE-FOCK ATOMIC WAVEFUNCTIONS

TABLE 1 (23). HARTREE-FOCK FUNCTIONS FOR NEUTRAL ATOMS.

MANGANESE K(2)L(8)3S(2)3P(6)4S(2)3C(5), 2S  
 T.E.= -0.11495597D+04 P.E.= -0.22991099D+04 K.E.= 0.11495503D+04 V.T.= -0.20000082D+01

	1S	2S	3S	4S
BASIS/ORB E	-240.59253	-29.17385	-3.86029	-0.25232
1S 25.35250	-0.93776	-0.28487	-0.10628	-0.02308
1S 40.13150	-0.01129	-0.00243	-0.00023	-0.00024
2S 22.13970	-0.06432	-0.16560	-0.06357	-0.01477
2S 10.21260	0.00189	1.03928	0.40993	0.05286
3S 9.61060	-0.00319	0.09495	0.22330	0.05130
3S 6.12121	0.00341	0.02311	-0.36145	-0.06888
3S 4.42426	-0.00277	-0.00377	-0.66263	-0.21724
4S 3.89331	0.00101	0.00089	-0.20829	-0.00079
4S 1.90055	-0.00018	0.00016	-0.01142	0.45963
4S 1.15361	0.00013	-0.00014	0.00628	0.54200
4S 0.81716	-0.00006	0.00007	-0.00263	0.10402

	2P	3P	D	3D
BASIS/ORB E	-24.87623	-2.51968	BASIS/ORB E	-0.54008
2P 9.70655	0.86803	-0.34249	3D 3.60149	0.39388
2P 16.70120	0.13011	-0.03845	3D 11.52850	0.02283
3P 6.47809	0.02023	-0.30626	3D 5.93912	0.24656
3P 5.75743	0.01845	0.69614	3D 2.20668	0.36739
3P 3.72812	-0.00951	0.52543	3D 1.35209	0.13835
3P 2.66739	0.00353	0.19281		

IRON K(2)L(8)3S(2)3P(6)4S(1)3D(7), 5F  
 T.E.= -0.12623763D+04 P.E.= -0.25247203D+04 K.E.= 0.12623440D+04 V.T.= -0.20300256D+01

	1S	2S	3S	4S
BASIS/ORB E	-261.17279	-31.71379	-3.95726	-0.23013
1S 39.03330	0.02500	0.00300	0.00141	0.00006
1S 25.64990	0.95463	-0.30930	-0.11439	-0.02200
2S 21.49470	0.02697	-0.17650	-0.07102	-0.01479
2S 11.09700	0.00253	1.01804	0.40951	0.08261
3S 9.57638	-0.00200	0.17531	0.30648	0.06130
3S 7.04409	0.00145	-0.01169	-0.33646	-0.05983
3S 4.67338	-0.00072	0.01056	-0.79119	-0.20737
4S 3.75688	0.00023	-0.00252	-0.17818	0.00950
4S 1.92542	-0.00007	0.00081	-0.00419	0.38130
4S 1.16347	0.00005	-0.00046	0.00114	0.55408
4S 0.80510	-0.00002	0.00024	-0.00052	0.17020

	2P	3P	D	3D
BASIS/ORB E	-27.19588	-2.54507	BASIS/ORB E	-0.40639
2P 17.15460	-0.12045	-0.03800	3D 11.54390	0.02601
2P 11.49160	0.67287	-0.25619	3D 6.18854	0.23679
3P 10.24270	0.24344	-0.12309	3D 4.02512	0.27992
3P 5.48104	0.01464	0.52113	3D 2.62070	0.38759
3P 3.63388	-0.00247	0.48986	3D 1.41267	0.26599
3P 2.55735	0.00067	0.13139		

IRON K(2)L(8)3S(2)3P(6)4S(2)3C(6), 1I  
 T.E.= -0.12622944D+04 P.E.= -0.25245729D+04 K.E.= 0.12622785D+04 V.T.= -0.20300126D+01

	1S	2S	3S	4S
BASIS/ORB E	-261.40016	-31.96471	-4.18917	-0.26016
1S 25.73310	0.95991	-0.30597	-0.11327	-0.02397
1S 41.39290	0.01809	0.00187	0.00060	-0.00009
2S 21.90370	0.02749	-0.16569	-0.06838	-0.01583
2S 10.62130	0.00603	1.07286	0.44616	0.09563
3S 9.55841	-0.00769	0.03806	0.25278	0.05157
3S 7.46043	0.00618	0.04083	-0.21267	-0.02579
3S 5.04798	-0.00247	-0.00520	-0.82199	-0.23712
4S 4.02944	0.00071	0.00236	-0.26129	-0.02467
4S 2.00805	-0.00019	-0.00051	-0.00405	0.42834
4S 1.23298	0.00014	0.00037	0.00110	0.53625
4S 0.85393	-0.00006	-0.00016	-0.00032	0.14685

See page 183 for Explanation of Tables and Notes for Tables 32, 42, and 43

TABLE 1 (24). HARTREE-FOCK FUNCTIONS FOR NEUTRAL ATOMS.

P	2P	3P	D	3D
BASIS/ORB E	-27.44258	-2.76044	BASIS/ORB E	-0.60918
2P 10.266680	0.87104	-0.34636	3D 3.88906	0.37901
2P 17.61340	0.11992	-0.03518	3D 12.21510	0.02165
3P 6.91312	0.04529	-0.29826	3D 6.36274	0.24613
3P 6.05752	-0.00342	0.70917	3D 2.45266	0.36169
3P 3.77573	-0.00397	0.57210	3D 1.48685	0.15899
3P 2.62244	0.00189	0.12412		

IRON            K(2)L(8)3S(2)3P(6)4S(2)3D(6), 3H  
T.E.= -0.12623437D+04 P.E.= -0.25246713D+04 K.E.= 0.12623276D+04 V.T.= -0.20000128D+01

S	1S	2S	3S	4S
BASIS/ORB E	-261.39130	-31.95507	-4.18256	-0.25949
1S 25.73230	0.95993	-0.30600	-0.11324	-0.02392
1S 41.38950	0.01810	0.00188	0.00060	-0.00009
2S 21.90190	0.02744	-0.16568	-0.06835	-0.01576
2S 10.62030	0.00603	1.09313	0.44610	0.09929
3S 9.55759	-0.00770	0.03760	0.25264	0.05170
3S 7.45982	0.00619	0.04107	-0.21298	-0.03035
3S 5.04758	-0.00248	-0.00528	-0.82100	-0.23567
4S 4.02910	0.00072	0.00238	-0.26200	-0.02526
4S 2.00788	-0.00019	-0.00052	-0.00410	0.42619
4S 1.23288	0.00014	0.00038	0.00114	0.53690
4S 0.85386	-0.00006	-0.00016	-0.00034	0.14848

P	2P	3P	D	3D
BASIS/ORB E	-27.43304	-2.75433	BASIS/ORB E	-0.62164
2P 10.26640	0.87100	-0.34618	3D 3.89436	0.38806
2P 17.61170	0.11998	-0.03518	3D 12.23390	0.02169
3P 6.91256	0.04522	-0.25791	3D 6.36872	0.24409
3P 6.05704	-0.00336	0.70877	3D 2.40848	0.37282
3P 3.77371	-0.00397	0.57188	3D 1.45673	0.13937
3P 2.62222	0.00189	0.12445		

IRON            K(2)L(8)3S(2)3P(6)4S(2)3D(6), 3G  
T.E.= -0.12623173D+04 P.E.= -0.25246187D+04 K.E.= 0.12623014D+04 V.T.= -0.20000126D+01

S	1S	2S	3S	4S
BASIS/ORB E	-261.39550	-31.95961	-4.18550	-0.25965
1S 25.73280	0.95992	-0.30598	-0.11325	-0.02394
1S 41.39180	0.01809	0.00188	0.00060	-0.00009
2S 21.90310	0.02747	-0.16569	-0.06836	-0.01579
2S 10.62090	0.00603	1.09297	0.44611	0.09943
3S 9.55815	-0.00769	0.03787	0.25270	0.05163
3S 7.46024	0.00618	0.04092	-0.21279	-0.03008
3S 5.04785	-0.00247	-0.00522	-0.82149	-0.23630
4S 4.02933	0.00071	0.00237	-0.26166	-0.02498
4S 2.00800	-0.00019	-0.00052	-0.00410	0.42706
4S 1.23295	0.00014	0.00038	0.00114	0.53643
4S 0.85391	-0.00006	-0.00016	-0.00034	0.14807

P	2P	3P	D	3D
BASIS/ORB E	-27.43754	-2.75704	BASIS/ORB E	-0.61459
2P 10.26670	0.87103	-0.34626	3D 3.89123	0.38846
2P 17.61280	0.11994	-0.03517	3D 12.23450	0.02179
3P 6.91294	0.04527	-0.29817	3D 6.36785	0.24351
3P 6.05736	-0.00340	0.70906	3D 2.45022	0.34266
3P 3.77473	-0.00397	0.57192	3D 1.54681	0.16883
3P 2.62237	0.00189	0.12435		

See page 183 for Explanation of Tables and Notes for Tables 32, 42, and 43

## ROOTHAAAN-HARTREE-FOCK ATOMIC WAVEFUNCTIONS

TABLE 1 (25). HARTREE-FOCK FUNCTIONS FOR NEUTRAL ATOMS.

IRON K(2)L(8)3S(2)3P(6)4S(2)3D(6), 1G  
 T.E.= -0.12622129D+04 P.E.= -0.25244116D+04 K.E.= 0.12621988D+04 V.T.= -0.20000112D+01

S	1S	2S	3S	4S
BASIS/ORB E	-261.41422	-31.98004	-4.19948	-0.26110
1S 25.72300	-0.96070	-0.30762	-0.11547	-0.02473
1S 41.21150	-0.01808	0.00260	0.00165	0.00023
2S 21.43280	-0.02762	-0.18182	-0.07133	-0.01620
2S 11.26570	-0.00341	0.99130	0.39556	0.08783
3S 9.71909	0.00382	0.21710	0.33745	0.07487
3S 7.43145	-0.00331	-0.02424	-0.27515	-0.05078
3S 5.02893	0.00158	0.01565	-0.75898	-0.21913
4S 4.17330	-0.00049	-0.00347	-0.28259	-0.03631
4S 2.03978	0.00011	0.00079	-0.01233	0.42427
4S 1.22802	-0.00008	-0.00054	0.00617	0.56056
4S 0.85062	0.00003	0.00023	-0.00249	0.12987

P	2P	3P	D	3D
BASIS/ORB E	-27.45774	-2.76997	BASIS/ORB E	-0.58831
2P 10.24490	0.87058	-0.34701	3D 4.09634	0.38203
2P 17.55260	0.12222	-0.05587	3D 11.74900	0.02472
3P 6.88622	0.03878	-0.28909	3D 6.45507	0.21236
3P 6.03475	0.00203	0.70141	3D 2.43123	0.40354
3P 3.81860	-0.00550	0.54494	3D 1.45105	0.14664
3P 2.71568	0.00244	0.15073		

IRON K(2)L(8)3S(2)3P(6)4S(2)3D(6), 3F  
 T.E.= -0.12622514D+04 P.E.= -0.25244864D+04 K.E.= 0.12622350D+04 V.T.= -0.20000131D+01

S	1S	2S	3S	4S
BASIS/ORB E	-261.40746	-31.97258	-4.19441	-0.26070
1S 25.72740	0.96001	-0.30627	-0.11339	-0.02403
1S 41.36310	0.01821	0.00197	0.00062	-0.00010
2S 21.88770	0.02720	-0.16559	-0.06844	-0.01591
2S 10.61290	0.00608	1.09511	0.44745	0.10021
3S 9.55116	-0.00778	0.03467	0.25175	0.05105
3S 7.45509	0.00625	0.04233	-0.21336	-0.02931
3S 5.04446	-0.00250	-0.00577	-0.82306	-0.23862
4S 4.02646	0.00072	0.00252	-0.25955	-0.02355
4S 2.00653	-0.00020	-0.00056	-0.00392	0.43088
4S 1.23207	0.00014	0.00041	0.00103	0.53542
4S 0.85332	-0.00006	-0.00017	-0.00029	0.14484

P	2P	3P	D	3D
BASIS/ORB E	-27.45037	-2.76530	BASIS/ORB E	-0.59808
2P 10.26280	0.87096	-0.34656	3D 3.89681	0.34859
2P 17.60230	0.12034	-0.03531	3D 11.73520	0.02576
3P 6.90816	0.04431	-0.29753	3D 6.22838	0.25411
3P 6.05332	-0.00273	0.70981	3D 2.49803	0.37282
3P 3.77433	-0.00408	0.57199	3D 1.48578	0.16752
3P 2.62046	0.00191	0.12303		

IRON K(2)L(8)3S(2)3P(6)4S(2)3D(6), 1F  
 T.E.= -0.12622156D+04 P.E.= -0.25244171D+04 K.E.= 0.12622015D+04 V.T.= -0.20000111D+01

S	1S	2S	3S	4S
BASIS/ORB E	-261.41342	-31.97913	-4.19876	-0.26102
1S 25.72300	-0.96070	-0.30762	-0.11547	-0.02472
1S 41.21150	-0.01808	0.00260	0.00165	0.00023
2S 21.43290	-0.02762	-0.18182	-0.07132	-0.01619
2S 11.26570	-0.00341	0.99129	0.39553	0.08778
3S 9.71911	0.00382	0.21710	0.33746	0.07489
3S 7.43147	-0.00331	-0.02424	-0.27521	-0.05C85
3S 5.02894	0.00158	0.01565	-0.75884	-0.21895
4S 4.17330	-0.00049	-0.00347	-0.28269	-0.03638
4S 2.03978	0.00011	0.00079	-0.01234	0.42401
4S 1.22802	-0.00008	-0.00054	0.00618	0.56065
4S 0.85062	0.00003	0.00023	-0.00249	0.13006

See page 183 for Explanation of Tables and Notes for Tables 32, 42, and 43

TABLE 1 (26). HARTREE-FOCK FUNCTIONS FOR NEUTRAL ATOMS.

P	2P	3P	D	3D
BASIS/ORB E	-27.45685	-2.76930	BASIS/ORB E	-0.58875
2P 10.24490	0.87058	-0.34699	3D 4.09631	0.38249
2P 17.55250	0.12223	-0.03586	3D 11.74840	0.02473
3P 6.88623	0.03878	-0.28899	3D 6.45569	0.21213
3P 6.03476	0.00203	0.70126	3D 2.43131	0.40363
3P 3.81861	-0.00549	0.54491	3D 1.45106	0.14611
3P 2.71568	0.00244	0.15082		

IRON            K(2)L(8)3S(2)3P(6)4S(2)3D(6), 5D  
T.E.= -0.12624432D+04 P.E.= -0.25248698D+04 K.F.= 0.12624266D+04 V.T.= -0.20000131D+01

S	1S	2S	3S	4S
BASIS/ORB E	-261.37361	-31.93584	-4.16943	-0.25815
1S 25.73090	0.95996	-0.30606	-0.11318	-0.02381
1S 41.38410	0.01813	0.00190	0.00061	-0.00007
2S 21.89900	0.02737	-0.16565	-0.06828	-0.01561
2S 10.61880	0.00605	1.09354	0.44592	0.09861
3S 9.55626	-0.00773	0.03690	0.25239	0.05201
3S 7.45884	0.00621	0.04145	-0.21356	-0.03147
3S 5.04693	-0.00249	-0.00540	-0.81903	-0.23277
4S 4.02856	0.00072	0.00242	-0.26346	-0.02645
4S 2.00760	-0.00019	-0.00053	-0.00422	0.42197
4S 1.23271	0.00014	0.00039	0.00122	0.53816
4S 0.85375	-0.00006	-0.00016	-0.00037	0.15172

P	2P	3P	D	3D
BASIS/ORB E	-27.41400	-2.74217	BASIS/ORB E	-0.64689
2P 10.26560	0.87094	-0.34563	3D 3.90292	0.39452
2P 17.60900	0.12008	-0.03518	3D 12.23240	0.02192
3P 6.91165	0.04500	-0.25719	3D 6.37125	0.24207
3P 6.05627	-0.00315	0.70788	3D 2.40608	0.37020
3P 3.76984	-0.00400	0.57147	3D 1.48653	0.13365
3P 2.62185	0.00190	0.12516		

IRON            K(2)L(8)3S(2)3P(6)4S(2)3D(6), 3D  
T.E.= -0.126228050D+04 P.E.= -0.25245451D+04 K.F.= 0.12622646D+04 V.T.= -0.20000126D+01

S	1S	2S	3S	4S
BASIS/ORB E	-261.40205	-31.96674	-4.19038	-0.26027
1S 25.73360	0.95990	-0.30595	-0.11327	-0.02398
1S 41.39530	0.01808	0.00187	0.00060	-0.00009
2S 21.90500	0.02751	-0.16570	-0.06838	-0.01584
2S 10.62190	0.00602	1.09270	0.44611	0.09567
3S 9.55899	-0.00768	0.03632	0.25289	0.05157
3S 7.46086	0.00617	0.04070	-0.21261	-0.02571
3S 5.04825	-0.00247	-0.00515	-0.82214	-0.23734
4S 4.02968	0.00071	0.00234	-0.26121	-0.02460
4S 2.00818	-0.00019	-0.00051	-0.00404	0.42865
4S 1.23306	0.00014	0.00037	0.00109	0.53615
4S 0.85398	-0.00006	-0.00016	-0.00032	0.14662

P	2P	3P	D	3D
BASIS/ORB E	-27.44460	-2.76156	BASIS/ORB E	-0.60527
2P 10.26710	0.87106	-0.34639	3D 3.88655	0.37927
2P 17.61430	0.11989	-0.03517	3D 12.21760	0.02163
3P 6.91352	0.04536	-0.29840	3D 6.36260	0.24610
3P 6.05785	-0.00347	0.70928	3D 2.45360	0.36040
3P 3.77620	-0.00396	0.57214	3D 1.48693	0.16030
3P 2.62260	0.00188	0.12408		

See page 183 for Explanation of Tables and Notes for Tables 32, 42, and 43

## ROOTHAAN-HARTREE-FOCK ATOMIC WAVEFUNCTIONS

TABLE 1 (27). HARTREE-FOCK FUNCTIONS FOR NEUTRAL ATOMS.

IRON      K(2)L(8)3S(2)3P(6)4S(2)3D(6), 1D  
 T.E.= -0.12621399D+04 P.E.= -0.25242666D+04 K.E.= 0.12621267D+04 V.T.= -0.20000105D+01

	S	1S	2S	3S	4S
BASIS/ORB E	-261.42708	-31.99394	-4.20895	-0.26220	
1S 25.72510	-0.96067	-0.30757	-0.11551	-0.02481	
1S 41.22160	-0.01803	0.00259	0.00165	0.00022	
2S 21.43410	-0.02774	-0.18189	-0.07139	-0.01631	
2S 11.26860	-0.00336	0.99077	0.39553	0.08824	
3S 9.72154	0.00376	0.21789	0.33768	0.07486	
3S 7.43326	-0.00326	-0.02451	-0.27438	-0.0509	
3S 5.03012	0.00155	0.01575	-0.76049	-0.22117	
4S 4.17431	-0.00049	-0.00350	-0.28171	-0.03562	
4S 2.04029	0.00011	0.00079	-0.01222	0.42728	
4S 1.22833	-0.00008	-0.00054	0.00609	0.55987	
4S 0.85083	0.00003	0.00023	-0.00245	0.12738	

	P	2P	3P	D	3D
BASIS/ORB E	-27.47152	-2.77874	BASIS/ORB E	-0.56982	
2P 10.24630	0.87065	-0.34722	3D 3.94828	0.37991	
2P 17.55680	0.12206	-0.03585	3D 11.96220	0.02275	
3P 6.88790	0.03916	-0.29055	3D 6.40350	0.23387	
3P 6.03617	0.00170	0.70329	3D 2.43549	0.37330	
3P 3.81951	-0.00544	0.54536	3D 1.45103	0.16240	
3P 2.71635	0.00248	0.14513			

IRON      K(2)L(8)3S(2)3P(6)4S(2)3D(6), 3P  
 T.E.= -0.12622514D+04 P.E.= -0.25244864D+04 K.E.= 0.126223500+04 V.T.= -0.20000131D+01

	S	1S	2S	3S	4S
BASIS/ORB E	-261.40746	-31.97258	-4.19441	-0.26070	
1S 25.72740	0.96001	-0.30627	-0.11339	-0.02403	
1S 41.36310	0.01821	0.00157	0.00062	-0.00010	
2S 21.88770	0.02720	-0.16559	-0.06844	-0.01591	
2S 10.61290	0.00608	1.09511	0.44745	0.10021	
3S 9.55116	-0.00778	0.03467	0.25175	0.05105	
3S 7.45509	0.00625	0.04233	-0.21336	-0.02931	
3S 5.04446	-0.00250	-0.03577	-0.82306	-0.23862	
4S 4.02646	0.00072	0.00252	-0.25955	-0.02355	
4S 2.00653	-0.00020	-0.00056	-0.00392	0.43088	
4S 1.23207	0.00014	0.00041	0.00103	0.53542	
4S 0.85332	-0.00006	-0.00017	-0.00029	0.14484	

	P	2P	3P	D	3D
BASIS/ORB E	-27.45037	-2.76530	BASIS/ORB E	-0.59808	
2P 10.26280	0.87096	-0.34656	3D 3.89681	0.34859	
2P 17.60230	0.12034	-0.03531	3D 11.73520	0.02576	
3P 6.90816	0.04431	-0.25753	3D 6.22838	0.25411	
3P 6.05332	-0.00273	0.70581	3D 2.49803	0.37282	
3P 3.77433	-0.00408	0.57199	3D 1.48578	0.16752	
3P 2.62046	0.00191	0.12303			

IRON      K(2)L(8)3S(2)3P(6)4S(2)3D(6), 1S  
 T.E.= -0.12620871D+04 P.E.= -0.25241611D+04 K.E.= 0.126207400+04 V.T.= -0.20000104D+01

	S	1S	2S	3S	4S
BASIS/ORB E	-261.43695	-32.00469	-4.21641	-0.26301	
1S 25.72660	-0.96065	-0.30755	-0.11555	-0.02488	
1S 41.22920	-0.01799	0.00260	0.00165	0.00021	
2S 21.43360	-0.02782	-0.18197	-0.07144	-0.01640	
2S 11.27070	-0.00332	0.99044	0.39556	0.08858	
3S 9.72340	0.00371	0.21839	0.33776	0.07480	
3S 7.43463	-0.00322	-0.02463	-0.27369	-0.04945	
3S 5.03102	0.00153	0.01579	-0.76178	-0.22285	
4S 4.17507	-0.00048	-0.00351	-0.28097	-0.03503	
4S 2.04068	0.00011	0.00080	-0.01215	0.42968	
4S 1.22856	-0.00008	-0.00054	0.00604	0.55912	
4S 0.85098	0.00003	0.00023	-0.00243	0.12562	

See page 183 for Explanation of Tables and Notes for Tables 32, 42, and 43

TABLE I (28). HARTREE-FOCK FUNCTIONS FOR NEUTRAL ATOMS.

P BASIS/ORB E	2P -27.48215	3P -2.78565	D BASIS/ORB E	3D -0.55687
2P 10.24740	0.87070	-0.34737	3D 3.94450	0.37796
2P 17.56020	0.12193	-0.03584	3D 11.96430	0.02265
3P 6.88917	0.03946	-0.29181	3D 6.40334	0.23441
3P 6.03724	0.00145	0.70491	3D 2.43813	0.37038
3P 3.82019	-0.00540	0.54562	3D 1.44920	0.16859
3P 2.71686	0.00242	0.14897		

COBALT K(2)L(8)3S(2)3P(6)4S(1)3D(8), 4F  
T.E.= -0.138137500+04 P.E.= -0.276273750+04 K.E.= 0.138136250+04 V.T.= -0.200000910+01

S BASIS/ORB E	1S -282.85035	2S -34.62579	3S -4.29857	4S -0.23266
1S 42.04550	-0.02458	0.00101	0.00068	-0.00002
1S 26.37570	-0.96785	-0.31200	-0.11614	-0.02150
2S 22.36780	-0.00665	-0.17503	-0.07004	-0.01391
2S 11.95990	-0.01283	0.94350	0.37803	0.07296
3S 10.73090	0.01016	0.24459	0.25853	0.04997
3S 6.38758	-0.01334	0.00811	-0.31313	-0.03259
3S 5.29530	0.01148	0.00412	-0.59632	-0.18195
4S 4.29211	-0.00218	-0.00089	-0.31652	-0.02548
4S 2.07123	0.00040	0.00040	-0.00978	0.34131
4S 1.22938	-0.00026	-0.00021	0.00328	0.57111
4S 0.82667	0.00011	0.00012	-0.00134	0.20483

P BASIS/ORB E	2P -29.88594	3P -2.79621	D BASIS/ORB E	3D -0.43394
2P 19.37300	0.08595	-0.02461	3D 12.96590	0.01878
2P 11.15270	0.86614	-0.33658	3D 6.86293	0.21901
3P 8.58893	0.08134	-0.08442	3D 4.30923	0.32641
3P 5.97118	-0.00018	0.53832	3D 2.74770	0.37036
3P 3.82593	-0.00007	0.53219	3D 1.49723	0.26151
3P 2.63314	0.00071	0.11623		

COBALT K(2)L(8)3S(2)3P(6)4S(2)3D(7), 2H  
T.E.= -0.138130190+04 P.E.= -0.276259290+04 K.E.= 0.138129110+04 V.T.= -0.200000780+01

S BASIS/ORB E	1S -283.08384	2S -34.88793	3S -4.53727	4S -0.26854
1S 26.83620	-0.96113	-0.30363	-0.11403	-0.02397
1S 44.30130	-0.01413	0.00076	0.00068	0.00008
2S 22.96430	-0.03041	-0.17660	-0.06654	-0.01447
2S 12.12260	-0.00552	0.87781	0.34727	0.07461
3S 11.32000	0.00400	0.28132	0.25188	0.05647
3S 6.73299	-0.00431	0.05513	0.03072	0.02745
3S 5.58580	0.00356	-0.02661	-0.91606	-0.25621
4S 4.26182	-0.00061	0.00374	-0.30628	-0.04534
4S 2.16041	0.00016	-0.00066	-0.00192	0.38836
4S 1.30858	-0.00010	0.00041	-0.00061	0.57194
4S 0.86701	0.00004	-0.00016	0.00037	0.16055

P BASIS/ORB E	2P -30.13960	3P -3.01831	D BASIS/ORB E	3D -0.65170
2P 11.15970	0.86453	-0.33971	3D 4.11980	0.38109
2P 19.34890	0.08615	-0.02530	3D 12.43670	0.02473
3P 8.63126	0.06275	-0.10422	3D 6.64608	0.25020
3P 6.06815	-0.00005	0.51990	3D 2.55890	0.35688
3P 3.93549	-0.00020	0.54154	3D 1.57942	0.15479
3P 2.79017	0.00073	0.12967		

See page 183 for Explanation of Tables and Notes for Tables 32, 42, and 43

## ROOTHAAN-HARTREE-FOCK ATOMIC WAVEFUNCTIONS

TABLE 1 (29). HARTREE-FOCK FUNCTIONS FOR NEUTRAL ATOMS.

COBALT K(2)L(8)3S(2)3P(6)4S(2)3D(7), 26  
 T.E.= -0.138132980+04 P.E.= -0.27626489D+04 K.E.= 0.13813191D+04 V.T.= -0.20300077D+01

	1S	2S	3S	4S
BASIS/ORB E	-283.07973	-34.88352	-4.53445	-0.26839
1S 26.82670	-0.96142	-0.30422	-0.11493	-0.02405
1S 44.25080	-0.01426	0.00057	0.00110	0.00012
2S 22.91000	-0.02996	-0.17114	-0.06502	-0.01437
2S 12.10780	-0.00549	0.88253	0.34490	0.07459
3S 11.30650	0.00402	0.27698	0.25990	0.05701
3S 6.72522	-0.00450	0.05706	-0.03173	0.02002
3S 5.57938	-0.00379	-0.02878	-0.83748	-0.24666
4S 4.36784	-0.00067	0.00427	-0.32631	-0.04688
4S 2.15595	0.00015	-0.00066	-0.00863	0.38777
4S 1.30710	-0.00010	0.00041	0.00328	0.57201
4S 0.86602	0.00004	-0.00016	-0.00114	0.15982

	2P	3P	D	3D
BASIS/ORB E	-30.13522	-3.01568	BASIS/ORB E	-0.65786
2P 11.15810	0.86471	-0.33963	3D 4.20829	0.36040
2P 19.34810	0.08619	-0.02527	3D 12.37440	0.02548
3P 8.62189	0.08262	-0.10372	3D 6.63584	0.24599
3P 6.05996	-0.00021	0.52215	3D 2.58303	0.39648
3P 3.92740	-0.00016	0.54046	3D 1.51357	0.14002
3P 2.78684	0.00072	0.12820		

COBALT K(2)L(8)3S(2)3P(6)4S(2)3D(7), 4F  
 T.E.= -0.13814142D+04 P.E.= -0.27628194D+04 K.E.= 0.13814051D+04 V.T.= -0.20000066D+01

	1S	2S	3S	4S
BASIS/ORB E	-283.06587	-34.86557	-4.52440	-0.26746
1S 26.83210	-0.96126	-0.30396	-0.11474	-0.02395
1S 44.27070	-0.01419	0.00089	0.00105	0.00012
2S 22.93140	-0.03023	-0.17558	-0.06499	-0.01425
2S 12.11360	-0.00546	0.88074	0.34417	0.07402
3S 11.31180	0.00399	0.27856	0.25970	0.05705
3S 6.72828	-0.00444	0.05672	-0.02690	0.01936
3S 5.58191	0.00374	-0.02838	-0.84188	-0.24460
4S 4.36115	-0.00068	0.00418	-0.32635	-0.04774
4S 2.15692	0.00015	-0.00064	-0.00831	0.38442
4S 1.30768	-0.00010	0.00041	0.00309	0.57290
4S 0.86641	0.00004	-0.00016	-0.00106	0.16252

	2P	3P	D	3D
BASIS/ORB E	-30.12040	-3.00633	BASIS/ORB E	-0.67548
2P 11.15900	0.86458	-0.33549	3D 4.18799	0.38834
2P 19.34770	0.08618	-0.02527	3D 13.17460	0.01895
3P 8.62558	0.08273	-0.10400	3D 6.85725	0.23761
3P 6.06638	-0.00014	0.52001	3D 2.61143	0.36586
3P 3.93006	-0.00016	0.54134	3D 1.57829	0.15535
3P 2.78815	0.00071	0.12972		

COBALT K(2)L(8)3S(2)3P(6)4S(2)3D(7), 2F  
 T.E.= -0.13812182D+04 P.E.= -0.27624276D+04 K.E.= 0.13812094D+04 V.T.= -0.20000064D+01

	1S	2S	3S	4S
BASIS/ORB E	-283.09705	-34.90213	-4.54680	-0.26953
1S 26.83540	-0.96116	-0.30365	-0.11535	-0.02405
1S 44.29790	-0.01414	0.00077	0.00129	0.00007
2S 22.96060	-0.03036	-0.17668	-0.06344	-0.01458
2S 12.12160	-0.00555	0.87823	0.33987	0.07504
3S 11.31910	0.00406	0.28085	0.26849	0.05649
3S 6.73246	-0.00454	0.05638	-0.07134	0.02731
3S 5.58536	0.00384	-0.02824	-0.78430	-0.25430
4S 4.44098	-0.00067	0.00417	-0.34350	-0.03998
4S 2.07625	0.00013	-0.00052	-0.01212	0.44922
4S 1.23348	-0.00010	0.00038	0.00647	0.54984
4S 0.86695	0.00005	-0.00017	-0.00277	0.11377

See page 183 for Explanation of Tables and Notes for Tables 32, 42, and 43

TABLE 1 (30). HARTREE-FOCK FUNCTIONS FOR NEUTRAL ATOMS.

P	2P	3P	D	3D
BASIS/ORB E	-30.15367	-3.02716	BASIS/ORB E	-0.63398
2P 11.15930	0.86460	-0.34001	3D 4.11806	0.37743
2P 19.34950	0.08615	-0.02530	3D 12.45640	0.02430
3P 8.63063	0.08268	-0.10355	3D 6.65742	0.25041
3P 6.06414	-0.00006	0.52104	3D 2.556329	0.36144
3P 3.93538	-0.00021	0.54106	3D 1.54996	0.15656
3P 2.78995	0.00074	0.12872		

COBALT K(2)L(8)3S(2)3P(6)4S(2)3D(7), 2D  
T.E.= -0.13811996D+04 P.E.= -0.27623905D+04 K.E.= 0.13811909D+04 V.T.= -0.20000063D+01

S	1S	2S	3S	4S
BASIS/ORB E	-283.10045	-34.90584	-4.54942	-0.26979
1S 26.83430	-0.96119	-0.30367	-0.11537	-0.02408
1S 44.29700	-0.01415	0.00077	0.00129	0.00007
2S 22.95970	-0.03029	-0.17066	-0.06345	-0.01461
2S 12.12130	-0.00558	0.87830	0.33994	0.07516
3S 11.31890	0.00408	0.28079	0.26850	0.05647
3S 6.73233	-0.00457	0.05638	-0.07128	0.02777
3S 5.58525	0.00387	-0.02825	-0.78463	-0.25716
4S 4.44127	-0.00068	0.00417	-0.34223	-0.03971
4S 2.07620	0.00013	-0.00052	-0.01210	0.45008
4S 1.23345	-0.00010	0.00038	0.00645	0.54951
4S 0.86693	0.00005	-0.00017	-0.00276	0.11318

P	2P	3P	D	3D
BASIS/ORB E	-30.15735	-3.02959	BASIS/ORB E	-0.63038
2P 11.15930	0.86460	-0.34008	3D 4.11933	0.38252
2P 19.34970	0.08615	-0.02530	3D 12.67870	0.02256
3P 8.63046	0.08268	-0.10389	3D 6.70497	0.24879
3P 6.06304	-0.00008	0.52136	3D 2.55763	0.35921
3P 3.93536	-0.00021	0.54092	3D 1.54861	0.15759
3P 2.78989	0.00074	0.12848		

COBALT K(2)L(8)3S(2)3P(6)4S(2)3D(7), 4P  
T.E.= -0.13813300D+04 P.E.= -0.27626494D+04 K.E.= 0.13813193D+04 V.T.= -0.20000078D+01

S	1S	2S	3S	4S
BASIS/ORB E	-283.07881	-34.88243	-4.53341	-0.26817
1S 26.83640	-0.96113	-0.30361	-0.11401	-0.02394
1S 44.30230	-0.01413	0.00076	0.00068	0.00008
2S 22.96540	-0.03042	-0.17059	-0.06652	-0.01444
2S 12.12290	-0.00552	0.87772	0.34716	0.07444
3S 11.32030	0.00400	0.28139	0.25184	0.05645
3S 6.73314	-0.00431	0.05513	0.03063	0.02701
3S 5.58592	0.00356	-0.02660	-0.91557	-0.25524
4S 4.26149	-0.00061	0.00374	-0.30667	-0.04561
4S 2.16046	0.00016	-0.00066	-0.00193	0.38716
4S 1.30861	-0.00010	0.00041	-0.00060	0.57224
4S 0.86704	0.00004	-0.00016	0.00037	0.16150

P	2P	3P	D	3D
BASIS/ORB E	-30.13416	-3.01472	BASIS/ORB E	-0.65724
2P 11.15980	0.86451	-0.33561	3D 4.11949	0.38191
2P 19.34870	0.08615	-0.02530	3D 12.43290	0.02482
3P 8.63145	0.08276	-0.10432	3D 6.64341	0.25018
3P 6.06975	-0.00004	0.51945	3D 2.55792	0.35798
3P 3.93547	-0.00020	0.54175	3D 1.57945	0.15205
3P 2.79024	0.00073	0.13002		

See page 183 for Explanation of Tables and Notes for Tables 32, 42, and 43

## ROOTHAAAN-HARTREE-FOCK ATOMIC WAVEFUNCTIONS

TABLE 1 (31). HARTREE-FOCK FUNCTIONS FOR NEUTRAL ATOMS.

COBALT K(2)L(8)3S(2)3P(6)4S(2)3D(7), 2P  
 T.E.= -0.13813019D+04 P.E.= -0.27625929D+04 K.E.= 0.13812911D+04 V.T.= -0.20000078D+01

	1S	2S	3S	4S
BASIS/ORB E	-283.08384	-34.88793	-4.53727	-0.26854
1S 26.83620	-0.96113	-0.30363	-0.11403	-0.02397
1S 44.30130	-0.01413	0.00076	0.00068	0.00008
2S 22.96430	-0.03041	-0.1760	-0.06654	-0.01447
2S 12.12260	-0.00552	0.87781	0.34727	0.07461
3S 11.32000	0.00400	0.28132	0.25188	0.05647
3S 6.73299	-0.00431	0.05513	0.03072	0.02745
3S 5.58580	0.00356	-0.02661	-0.91606	-0.25621
4S 4.26182	-0.00061	0.00374	-0.30628	-0.04534
4S 2.16041	0.00016	-0.00066	-0.00192	0.38836
4S 1.30858	-0.00010	0.00041	-0.00061	0.57194
4S 0.86701	0.00004	-0.00016	0.00037	0.16055

	2P	3P	D	3D
BASIS/ORB E	-30.13960	-3.01831	BASIS/ORB E	-0.65170
2P 11.15970	0.86453	-0.33971	3D 4.11980	0.38109
2P 19.34890	0.08615	-0.02530	3D 12.43670	0.02473
3P 8.63126	0.08275	-0.10422	3D 6.64608	0.25020
3P 6.06815	-0.00005	0.51990	3D 2.55890	0.35688
3P 3.93549	-0.00020	0.54154	3D 1.57942	0.15479
3P 2.79017	0.00073	0.12967		

NICKEL K(2)L(8)3S(2)3P(6)4S(1)3D(9), 3D  
 T.E.= -0.15068224D+04 P.E.= -0.30136314D+04 K.E.= 0.15068090D+04 V.T.= -0.20000089D+01

	1S	2S	3S	4S
BASIS/ORB E	-305.29483	-37.67074	-4.65409	-0.23576
1S 41.39530	-0.02771	0.0067	0.00216	0.00039
1S 27.50200	-0.95823	-0.32019	-0.11906	-0.02149
2S 22.43750	-0.01910	-0.19744	-0.08251	-0.01505
2S 12.52050	-0.00309	0.98225	0.40374	0.07354
3S 10.82530	0.00236	0.24000	0.27229	0.05440
3S 6.83997	-0.00310	-0.01707	-0.33533	-0.05768
3S 5.57363	0.00254	0.01990	-0.58528	-0.14534
4S 4.52162	-0.00049	-0.00299	-0.33156	-0.04181
4S 2.21327	0.00009	0.00061	-0.01055	0.31587
4S 1.27722	-0.00005	-0.00033	0.00314	0.58993
4S 0.84488	0.00002	0.00015	-0.00128	0.22002

	2P	3P	D	3D
BASIS/ORB E	-32.69900	-3.05579	BASIS/ORB E	-0.45730
2P 18.54110	0.13236	-0.03965	3D 11.84520	0.03219
2P 11.45370	0.80317	-0.32222	3D 6.96821	0.21853
3P 10.93120	0.07733	-0.04933	3D 4.58757	0.30420
3P 5.94694	0.03748	0.52515	3D 2.95021	0.37397
3P 4.39883	-0.02213	0.29124	3D 1.58997	0.26745
3P 3.23023	0.00672	0.32070		

NICKEL K(2)L(8)3S(2)3P(6)4S(2)3D(8), 1G  
 T.E.= -0.15067560D+04 P.E.= -0.30135044D+04 K.E.= 0.15067483D+04 V.T.= -0.20000051D+01

	1S	2S	3S	4S
BASIS/ORB E	-305.63609	-37.93617	-4.90002	-0.27736
1S 27.67460	-0.96283	-0.31540	-0.11899	-0.02452
1S 43.73640	-0.01871	0.00471	0.00217	0.00033
2S 22.82970	-0.02439	-0.18754	-0.07580	-0.01646
2S 12.23000	-0.00304	1.00442	0.40756	0.08678
3S 11.00270	0.00278	0.18044	0.25724	0.05599
3S 7.22960	-0.00354	0.02920	-0.18957	-0.01925
3S 5.88231	0.00276	-0.01108	-0.67276	-0.20130
4S 4.73490	-0.00051	0.00265	-0.38276	-0.06288
4S 2.27679	0.00009	-0.00034	-0.01516	0.37399
4S 1.35122	-0.00006	0.00022	0.00620	0.60017
4S 0.86733	0.00002	-0.00009	-0.00219	0.15068

See page 183 for Explanation of Tables and Notes for Tables 32, 42, and 43

TABLE 1 (32). HARTREE-FOCK FUNCTIONS FOR NEUTRAL ATOMS.

P	2P	3P	D	3D
BASIS/ORB E	-32.95995	-3.28904	BASIS/ORB E	-0.68660
2P 11.54260	0.84450	-0.33128	3D 4.37307	0.36659
2P 19.37000	0.10395	-0.03286	3D 12.81280	0.02645
3P 10.32760	0.06048	-0.07478	3D 6.94849	0.25529
3P 6.56896	0.03382	0.37197	3D 2.69088	0.37970
3P 4.54190	-0.01317	0.55310	3D 1.58554	0.14280
3P 3.13019	0.00403	0.23379		

NICKEL K(2)L(8)3S(2)3P(6)4S(2)3D(8), 3F  
T.E.= -0.15068705D+04 P.E.= -0.30137323D+04 K.E.= 0.15068618D+04 V.T.= -0.20000057D+01

S	1S	2S	3S	4S
BASIS/ORB E	-305.61882	-37.91793	-4.88783	-0.27624
1S 27.70810	-0.96109	-0.31249	-0.11762	-0.02413
1S 43.60820	-0.01879	0.00353	0.00162	0.00021
2S 23.22390	-0.02605	-0.17653	-0.07249	-0.01568
2S 11.93940	-0.00362	1.03779	0.42204	0.08946
3S 10.96830	0.00324	0.12533	0.23460	0.05112
3S 7.20834	-0.00380	0.04318	-0.19094	-0.02007
3S 5.86511	0.00293	-0.01953	-0.67309	-0.20008
4S 4.72090	-0.00053	0.00383	-0.37926	-0.06158
4S 2.27022	0.00009	-0.00050	-0.01470	0.37388
4S 1.34716	-0.00006	0.00031	0.00597	0.60023
4S 0.86480	0.00002	-0.00012	-0.00210	0.15044

P	2P	3R	D	3D
BASIS/ORB E	-32.94182	-3.27764	BASIS/ORB E	-0.70693
2P 11.57800	0.83639	-0.32814	3D 4.39854	0.35554
2P 19.26870	0.10552	-0.09327	3D 12.88330	0.02557
3P 10.31320	0.06952	-0.07993	3D 6.97998	0.25412
3P 6.67054	0.02932	0.34654	3D 2.79684	0.36406
3P 4.58463	-0.00937	0.58559	3D 1.67922	0.16885
3P 3.09195	0.00281	0.22929		

NICKEL K(2)L(8)3S(2)3P(6)4S(2)3D(8), 1D  
T.E.= -0.15067973D+04 P.E.= -0.30135870D+04 K.E.= 0.15067897D+04 V.T.= -0.20000051D+01

S	1S	2S	3S	4S
BASIS/ORB E	-305.63010	-37.92976	-4.89580	-0.27697
1S 27.67510	-0.96284	-0.31537	-0.11897	-0.02448
1S 43.74190	-0.01869	0.00470	0.00218	0.00034
2S 22.83050	-0.02441	-0.18756	-0.07576	-0.01642
2S 12.23180	-0.00304	1.00410	0.40726	0.08656
3S 11.00410	0.00277	0.18082	0.25744	0.05604
3S 7.23052	-0.00353	0.02914	-0.18991	-0.01970
3S 5.88305	0.00276	-0.01102	-0.67171	-0.20027
4S 4.73555	-0.00050	0.00264	-0.38348	-0.06322
4S 2.27707	0.00009	-0.00034	-0.01526	0.37268
4S 1.35140	-0.00006	0.00022	0.00625	0.60050
4S 0.86744	0.00002	-0.00009	-0.00221	0.15170

P	2P	3P	D	3D
BASIS/ORB E	-32.95359	-3.26511	BASIS/ORB E	-0.69405
2P 11.54420	0.84438	-0.33109	3D 4.37081	0.36647
2P 19.37220	0.10387	-0.03285	3D 12.80150	0.02660
3P 10.32900	0.06067	-0.07497	3D 6.94158	0.25600
3P 6.57227	0.03381	0.37128	3D 2.69010	0.38059
3P 4.54242	-0.01313	0.55345	3D 1.58575	0.14050
3P 3.12993	0.00402	0.23423		

See page 183 for Explanation of Tables and Notes for Tables 32, 42, and 43

## ROOCHAAN-HARTREE-FOCK ATOMIC WAVEFUNCTIONS

TABLE 1 (33). HARTREE-FOCK FUNCTIONS FOR NEUTRAL ATOMS.

NICKEL K(2)L(8)3S(2)3P(6)4S(2)3D(8), 3P  
 T.E.= -0.15067817D+04 P.E.= -0.30135558D+04 K.E.= 0.15067740D+04 V.T.= -0.20000051D+01

	1S	2S	3S	4S
BASIS/ORB E	-305.63194	-37.93166	-4.89691	-0.27707
1S 27.67490	-0.96283	-0.31538	-0.11898	-0.02449
1S 43.73900	-0.01870	0.00471	0.00217	0.00034
2S 22.83030	-0.02441	-0.18154	-0.07577	-0.01643
2S 12.23080	-0.00304	1.00427	0.40739	0.08663
3S 11.00340	0.00277	0.1861	0.25734	0.05602
3S 7.23004	-0.00353	0.02517	-0.18989	-0.01961
3S 5.88266	0.00276	-0.01105	-0.67199	-0.20052
4S 4.73521	-0.00050	0.00264	-0.38324	-0.06311
4S 2.27692	0.00009	-0.00034	-0.01523	0.37305
4S 1.35130	-0.00006	0.00022	0.00623	0.60041
4S 0.86738	0.00002	-0.00009	-0.00220	0.15141
P	2P	3P	D	3D
BASIS/ORB E	-32.95549	-3.2E614	BASIS/ORB E	-0.69089
2P 11.54340	0.84444	-0.33116	3D 4.37201	0.36689
2P 19.37110	0.10391	-0.03285	3D 12.80620	0.02654
3P 10.32830	0.06057	-0.07488	3D 6.94472	0.25549
3P 6.57080	0.03381	0.37160	3D 2.69051	0.38023
3P 4.54206	-0.01315	0.55320	3D 1.58564	0.14116
3P 3.13008	0.00402	0.23412		

NICKEL K(2)L(8)3S(2)3P(6)4S(2)3D(8), 1S  
 T.E.= -0.15065894D+04 P.E.= -0.30131704D+04 K.E.= 0.15065810D+04 V.T.= -0.20000056D+01

	1S	2S	3S	4S
BASIS/ORB E	-305.66129	-37.96350	-4.91838	-0.27910
1S 27.70200	-0.96037	-0.30928	-0.11641	-0.02407
1S 43.57300	-0.01934	0.00182	0.00089	0.00004
2S 23.61670	-0.02532	-0.17119	-0.06977	-0.01533
2S 11.67820	-0.00574	1.07233	0.43721	0.09383
3S 10.95880	0.00533	0.07307	0.21319	0.04650
3S 7.20251	-0.00588	0.05145	-0.18584	-0.01636
3S 5.86040	0.00446	-0.02373	-0.68144	-0.20769
4S 4.71678	-0.00080	0.00423	-0.37430	-0.05920
4S 2.26842	0.00014	-0.00051	-0.01400	0.38339
4S 1.34604	-0.00009	0.00031	0.00559	0.59760
4S 0.86410	0.00003	-0.00012	-0.00196	0.14320
P	2P	3P	D	3D
BASIS/ORB E	-32.98701	-3.30617	BASIS/ORB E	-0.65760
2P 11.59700	0.83534	-0.32830	3D 4.40449	0.36741
2P 19.29570	0.10450	-0.03298	3D 12.93220	0.02447
3P 10.30370	0.07241	-0.08141	3D 7.05067	0.24705
3P 6.66514	0.02843	0.34932	3D 2.75601	0.36072
3P 4.58692	-0.00907	0.58613	3D 1.64175	0.17368
3P 3.09478	0.00273	0.22669		

COPPER K(2)L(8)3S(2)3P(6)4S(1)3D(10), 2S  
 T.E.= -0.16389628D+04 P.E.= -0.32779229D+04 K.E.= 0.16389601D+04 V.T.= -0.20000016D+01

	1S	2S	3S	4S
BASIS/ORB E	-328.79173	-40.81804	-5.01126	-0.23795
1S 28.48390	-0.95789	-0.31805	-0.11906	-0.02267
1S 42.50560	-0.02856	0.00412	0.00160	0.00143
2S 23.54780	-0.01759	-0.19769	-0.08169	-0.00941
2S 13.26670	-0.00457	0.93663	0.38342	0.05604
3S 11.52060	0.00440	0.25775	0.28466	0.08953
3S 8.09772	-0.00584	-0.04582	0.04973	-0.11580
3S 6.70827	0.00407	0.04067	-0.83111	-0.03551
4S 5.07948	-0.00063	-0.00460	-0.44639	-0.15751
4S 3.19095	0.00015	0.00127	-0.03257	0.17463
4S 1.53564	-0.00003	-0.00028	0.00086	0.66426
4S 0.87051	0.00001	0.00010	-0.00037	0.34469

See page 183 for Explanation of Tables and Notes for Tables 32, 42, and 43

TABLE 1 (34). HARTREE-FOCK FUNCTIONS FOR NEUTRAL ATOMS.

P	2P	3P	D	3D
BASIS/ORB E	-35.61699	-3.32415	BASIS/ORB E	-0.49074
2P 11.88610	0.84302	-0.32074	3D 5.21851	0.29853
2P 19.58060	0.11714	-0.04070	3D 12.96880	0.02649
3P 10.83980	0.04499	-0.10529	3D 7.61139	0.18625
3P 7.30670	0.03012	0.37164	3D 3.18734	0.42214
3P 4.57017	-0.00511	0.67096	3D 1.66248	0.26291
3P 2.89365	0.00182	0.14959		

COPPER K(2)L(8)3S(2)3P(6)4S(2)3D(9), 2D  
T.E.= -0.16389496D+04 P.E.= -0.32778900D+04 K.E.= 0.16389404D+04 V.T.= -0.20000056D+01

S	1S	2S	3S	4S
BASIS/ORB E	-329.03384	-41.08457	-5.26032	-0.28460
1S 28.21170	-0.96437	-0.31453	-0.11966	-0.02337
1S 43.00190	-0.03209	-0.00034	0.00059	-0.00043
2S 23.81960	-0.00138	-0.19276	-0.07709	-0.01795
2S 13.42030	-0.01240	0.90724	0.36661	0.07953
3S 11.65060	0.00909	0.31562	0.30550	0.05836
3S 6.80495	-0.01786	-0.05869	-0.50961	-0.00178
3S 5.96241	0.01641	0.06338	-0.33870	-0.23026
4S 4.92700	-0.00231	-0.00892	-0.39948	-0.02662
4S 2.18662	0.00029	0.00131	-0.01241	0.45956
4S 1.27996	-0.00021	-0.00096	0.00630	0.54963
4S 0.88067	0.00010	0.00044	-0.00263	0.10328

P	2P	3P	D	3D
BASIS/ORB E	-35.87888	-3.55663	BASIS/ORB E	-0.74000
2P 12.53960	0.79142	-0.30541	3D 4.96685	0.35220
2P 20.26500	0.09141	-0.03064	3D 13.27730	0.02608
3P 11.13030	0.13861	-0.11810	3D 7.54224	0.21390
3P 6.97516	0.01996	0.39990	3D 3.01000	0.40481
3P 4.50090	-0.00341	0.64144	3D 1.75517	0.17294
3P 2.92823	0.00125	0.12562		

ZINC K(2)L(8)3S(2)3P(6)4S(2)3D(10), 1S  
T.E.= -0.17778477D+04 P.E.= -0.35556901D+04 K.E.= 0.17778424D+04 V.T.= -0.20000029D+01

S	1S	2S	3S	4S
BASIS/ORB E	-353.30398	-44.36188	-5.63777	-0.29249
1S 29.48600	-0.95504	-0.31973	-0.11970	-0.02302
1S 43.28590	-0.03057	0.00458	0.00113	-0.00032
2S 24.73990	-0.01886	-0.18330	-0.07840	-0.01758
2S 13.15510	-0.00384	1.00556	0.41934	0.08850
3S 12.00720	0.00264	0.17770	0.23499	0.04466
3S 7.19899	-0.00287	0.03350	-0.35224	-0.02731
3S 5.90512	0.00246	-0.01651	-0.58692	-0.21465
4S 4.83215	-0.00049	0.00305	-0.29127	-0.00882
4S 2.30295	0.00009	-0.00035	-0.00539	0.41428
4S 1.39478	-0.00006	0.00024	0.00164	0.52676
4S 0.94264	0.00002	-0.00010	-0.00050	0.17422

P	2P	3P	D	3D
BASIS/ORB E	-38.92494	-3.83931	BASIS/ORB E	-0.78256
2P 12.37110	0.87225	-0.35894	3D 5.02809	0.38099
2P 20.71820	0.10237	-0.02667	3D 14.55740	0.02036
3P 8.82555	0.06399	-0.14269	3D 8.00450	0.22908
3P 6.89964	-0.01065	0.64545	3D 3.05216	0.38095
3P 4.13660	0.00203	0.58274	3D 1.78869	0.16037
3P 2.20119	-0.00007	0.02297		

See page 183 for Explanation of Tables and Notes for Tables 32, 42, and 43

## ROOTHAAN-HARTREE-FOCK ATOMIC WAVEFUNCTIONS

TABLE 1 (35). HARTREE-FOCK FUNCTIONS FOR NEUTRAL ATOMS.

GALLIUM K(2)L(8)M(18)4S(2)4P(1), 2P  
 T.E.= -0.19232604D+04 P.E.= -0.38465139D+04 K.E.= 0.19232535D+04 V.T.= -0.20000035D+01

	S	1S	2S	3S	4S
BASIS/ORB E	-378.81805	-48.16849	-6.39460	-0.42446	
1S	28.81010	0.74710	0.30472	-0.11978	-0.03229
1S	35.61210	0.25535	0.02593	-0.00728	0.00156
2S	26.15790	0.00008	0.15106	-0.06164	-0.01150
2S	13.27810	0.00169	-1.03361	0.42524	0.09475
3S	12.54240	-0.00014	-0.12909	0.23678	0.07128
3S	7.45372	-0.00033	-0.02392	-0.54469	-0.16710
3S	4.91188	0.00015	0.00424	-0.67749	-0.16344
4S	2.62926	-0.00005	-0.00119	-0.00788	0.44141
4S	1.58911	0.00004	0.00084	0.00186	0.57985
4S	1.03307	-0.00002	-0.00034	-0.00049	0.10455

	P	2P	3P	4P	D	3D
BASIS/ORB E	-42.49412	-4.48235	-0.20849	BASIS/ORB E	-1.19332	
2P	12.51630	0.89110	0.35639	3D	3.49966	0.42542
2P	20.94950	0.11879	0.04000	3D	2.08524	0.14613
3P	12.15290	-0.01678	0.05337	3D	5.57215	0.31824
3P	7.64617	0.04239	-0.37284	3D	8.17656	0.23367
3P	4.93738	-0.01281	-0.71286	3D	14.38050	0.02762
4P	3.55119	0.00488	-0.08520		0.02852	
4P	1.98803	-0.00227	0.00550		0.39484	
4P	1.18954	0.00163	-0.00441		0.46618	
4P	0.86212	-0.00076	0.00191		0.24077	

GERMANIUM K(2)L(8)M(18)4S(2)4P(2), 3P  
 T.E.= -0.20753591D+04 P.E.= -0.41507190D+04 K.E.= 0.20753599D+04 V.T.= -0.19999996D+01

	S	1S	2S	3S	4S
BASIS/ORB E	-405.24403	-52.15019	-7.19090	-0.55331	
1S	30.02100	0.75815	0.30153	0.11337	-0.03022
1S	36.80580	0.23936	0.02606	0.01215	-0.00226
2S	27.00910	0.00627	0.16087	0.07053	-0.01741
2S	13.79970	0.00058	-1.03666	-0.43821	0.11165
3S	12.88370	0.00059	-0.13209	-0.24038	0.07481
3S	7.89859	-0.00062	-0.02214	0.49626	-0.16000
3S	5.27181	0.00028	0.00323	0.72784	-0.21325
4S	2.87538	-0.00010	-0.00097	0.01467	0.46131
4S	1.79597	0.00009	0.00081	-0.00665	0.53115
4S	1.29724	-0.00004	-0.00036	0.00270	0.13401

	P	2P	3P	4P	D	3D	
BASIS/ORB E	-46.23602	-5.16148	-0.28729	BASIS/ORB E	-1.63475		
2P	13.35370	0.86134	0.34590	3D	3.82993	0.44017	
2P	22.09880	0.10385	0.09597	3D	2.34719	0.12938	
3P	12.89370	0.02927	0.07589	3D	6.11651	0.33840	
3P	8.12507	0.04517	-0.33604	-0.07467	3D	8.86174	0.20172
3P	5.26670	-0.01327	-0.74958	-0.16721	3D	14.92730	0.02653
4P	3.74374	0.00507	-0.08490	0.03395			
4P	2.16483	-0.00240	0.00762	0.48432			
4P	1.27537	0.00147	-0.00478	0.53214			
4P	0.88029	-0.00063	0.00190	0.07195			

GERMANIUM K(2)L(8)M(18)4S(2)4P(2), 1D  
 T.E.= -0.20753208D+04 P.E.= -0.41506415D+04 K.E.= 0.20753207D+04 V.T.= -0.20000000D+01

	S	1S	2S	3S	4S
BASIS/ORB E	-405.25624	-52.16209	-7.20265	-0.56082	
1S	30.11030	0.75685	0.30271	-0.11385	-0.02936
1S	36.75400	0.23839	0.02425	-0.01145	-0.00289
2S	26.97020	0.00937	0.16255	-0.07125	-0.01836
2S	13.81980	-0.00014	-1.03537	0.43796	0.11307
3S	12.86500	0.00108	-0.13496	0.24190	0.07361
3S	7.88735	-0.00083	-0.02166	-0.50141	-0.15840
3S	5.26432	0.00038	0.00219	-0.72340	-0.21765
4S	2.95609	-0.00014	-0.00099	-0.01414	0.41079
4S	1.88171	0.00011	0.00073	0.00521	0.55583
4S	1.29537	-0.00004	-0.00029	-0.00179	0.16322

See page 183 for Explanation of Tables and Notes for Tables 32, 42, and 43

TABLE 1 (36). HARTREE-FOCK FUNCTIONS FOR NEUTRAL ATOMS.

P	2P	3P	4P	D	3D
BASIS/ORB E	-46.24792	-5.17311	-0.25179	BASIS/ORB E	-1.64646
2P 13.33500	0.86102	0.34354	0.06898	3D 3.82320	0.43574
2P 22.03540	0.10550	0.03732	0.00655	3D 2.34388	0.12862
3P 12.87500	0.02851	0.0847	0.01443	3D 6.03378	0.33101
3P 8.11355	0.04382	-0.35395	-0.07298	3D 8.79423	0.21499
3P 5.20226	-0.01249	-0.74431	-0.16979	3D 15.06150	0.02578
4P 3.71097	0.00488	-0.07299	0.04795		
4P 2.16180	-0.00221	0.00405	0.45729		
4P 1.27350	0.00110	-0.00237	0.54099		
4P 0.77799	-0.00039	0.00061	0.09789		

ARSENIC K(2)L(8)M(18)4S(2)4P(3), 4S  
T.E.= -0.22342382D+04 P.E.= -0.44684756D+04 K.E.= 0.22342374D+04 V.T.= -0.20000003D+01

S	1S	2S	3S	4S
BASIS/ORB E	-432.58580	-56.30582	-8.02962	-0.68589
1S 31.34600	0.80944	0.35297	-0.13676	-0.03678
1S 38.60770	0.18590	-0.01548	0.00550	0.00086
2S 26.26730	0.00949	0.18189	-0.08033	-0.02303
2S 14.94890	-0.00069	-0.98989	0.42323	0.11843
3S 13.45360	0.00121	-0.22138	0.27579	0.08597
3S 8.13994	-0.00083	-0.01725	-0.49356	-0.16171
3S 5.53193	0.00039	0.00209	-0.72763	-0.24575
4S 3.14867	-0.00014	-0.00065	-0.01353	0.45102
4S 2.01557	0.00012	0.00050	0.00483	0.54525
4S 1.42236	-0.00005	-0.00020	-0.00178	0.13765

P	2P	3P	4P	D	3D
BASIS/ORB E	-50.15375	-5.88C68	-0.36946	BASIS/ORB E	-2.11262
2P 14.05460	0.83284	0.33887	0.07735	3D 4.15670	0.44874
2P 22.78430	0.10192	0.03589	0.00736	3D 2.56420	0.11466
3P 13.52830	0.06278	0.08838	0.01932	3D 6.36170	0.30600
3P 8.37724	0.04654	-0.33676	-0.08004	3D 9.09175	0.22855
3P 5.57821	-0.01655	-0.73040	-0.19430	3D 15.54610	0.02710
4P 4.34244	0.00612	-0.09452	0.02331		
4P 2.42567	-0.00205	-0.00136	0.50866		
4P 1.45140	0.00109	-0.00010	0.53655		
4P 0.91898	-0.00039	0.00004	0.05044		

ARSENIC K(2)L(8)M(18)4S(2)4P(3), 2D  
T.E.= -0.22341718D+04 P.E.= -0.4468420D+04 K.E.= 0.22341702D+04 V.T.= -0.20000007D+01

S	1S	2S	3S	4S
BASIS/ORB E	-432.60186	-56.32522	-8.04466	-0.69515
1S 31.67020	0.83573	0.35422	0.13846	-0.03830
1S 39.00520	0.15475	-0.02015	-0.00821	0.00230
2S 26.53930	0.01615	0.17749	0.07651	-0.02118
2S 14.79200	-0.00252	-0.99509	-0.42112	0.11673
3S 13.58960	0.00234	-0.20147	-0.26824	0.08596
3S 8.22467	-0.00125	-0.02457	0.45881	-0.15391
3S 5.58946	0.00058	0.00472	0.75602	-0.25236
4S 3.13890	-0.00020	-0.00149	0.01720	0.44755
4S 2.04110	0.00017	0.00119	-0.00716	0.53273
4S 1.43098	-0.00007	-0.00047	0.00256	0.15183

P	2P	3P	4P	D	3D
BASIS/ORB E	-50.16918	-5.89554	-0.33013	BASIS/ORB E	-2.12759
2P 14.47740	0.82224	0.336C5	0.07648	3D 4.22038	0.45364
2P 23.69180	0.07849	0.02630	0.00508	3D 2.59035	0.12284
3P 13.13570	0.10438	0.10910	0.02235	3D 6.31604	0.27411
3P 8.46406	0.04080	-0.32224	-0.07003	3D 8.96525	0.24688
3P 5.74756	-0.01479	-0.71C89	-0.19704	3D 15.55490	0.02754
4P 4.63726	0.00533	-0.13644	0.01282		
4P 2.44756	-0.00139	-0.00424	0.50406		
4P 1.43823	0.00080	0.00032	0.52618		
4P 0.94100	-0.00032	-0.00027	0.07986		

See page 183 for Explanation of Tables and Notes for Tables 32, 42, and 43

## ROOTHAAN-HARTREE-FOCK ATOMIC WAVEFUNCTIONS

TABLE 1 (37). HARTREE-FOCK FUNCTIONS FOR NEUTRAL ATOMS.

ARSENIC K(2)L(8)M(18)4S(2)4P(3), 2P  
 T.E.= -0.22341283D+04 P.E.= -0.44682543D+04 K.E.= 0.22341259D+04 V.T.= -0.20000011D+01

	S	1S	2S	3S	4S
BASIS/ORB E	-432.61273	-56.33585	-8.05500	-0.70156	
1S	31.38020	0.81237	0.35319	-0.13698	-0.03929
1S	38.64970	0.18249	-0.01604	0.00582	0.00262
2S	26.29600	0.01016	0.18134	-0.07989	-0.02102
2S	14.93230	-0.00087	-0.99030	0.42296	0.11566
3S	13.46800	0.00132	-0.21933	0.27502	0.09099
3S	8.14889	-0.00088	-0.01808	-0.48987	-0.16993
3S	5.53801	0.00042	0.00240	-0.73071	-0.23812
4S	3.12362	-0.00016	-0.00080	-0.01431	0.44027
4S	2.07906	0.00013	0.00061	0.00547	0.52281
4S	1.42468	-0.00005	-0.00022	-0.00176	0.16806

	P	2P	3P	4P	D	3D
BASIS/ORB E	-50.17980	-5.90578	-0.30501	BASIS/ORB E	-2.13792	
2P	14.03920	0.83684	0.33987	0.07736	3D	4.25244
2P	22.83290	0.10092	0.03568	0.00697	3D	2.59440
3P	13.54270	0.05872	0.08733	0.01747	3D	6.66243
3P	8.38641	0.04794	-0.33511	-0.07526	3D	9.10169
3P	5.58429	-0.01749	-0.73C14	-0.19725	3D	15.41460
4P	4.36629	0.00658	-0.09579	0.02920		0.02872
4P	2.42832	-0.00230	-0.00252	0.49787		
4P	1.45294	0.00145	-0.00029	0.46586		
4P	1.02097	-0.00063	-0.00026	0.14476		

SELENIUM K(2)L(8)M(18)4S(2)4P(4), 3P  
 T.E.= -0.23998658D+04 P.E.= -0.47557310D+04 K.E.= 0.23998653D+04 V.T.= -0.20000002D+01

	S	1S	2S	3S	4S
BASIS/ORB E	-460.86751	-60.66916	-8.93244	-0.83750	
1S	32.00980	0.84307	0.34872	-0.13350	-0.03934
1S	40.79540	0.16359	-0.0C786	0.00048	0.00037
2S	27.17130	-0.00790	0.17658	-0.08308	-0.02419
2S	15.13520	0.00666	-1.03246	0.45513	0.13351
3S	13.62030	-0.00349	-0.17253	0.26080	0.09050
3S	8.41955	0.00127	-0.01678	-0.51814	-0.18446
3S	5.75207	-0.00060	0.00228	-0.71665	-0.25805
4S	3.33167	0.00018	-0.00069	-0.00820	0.47154
4S	2.19374	-0.00013	0.00050	0.00114	0.54554
4S	1.45697	0.00005	-0.00016	-0.00034	0.11764

	P	2P	3P	4P	D	3D
BASIS/ORB E	-54.26928	-6.66187	-0.40299	BASIS/CRB E	-2.64972	
2P	14.75700	0.80693	0.33247	0.08386	3D	4.59417
2P	23.48300	0.10012	0.03580	0.00743	3D	2.84235
3P	14.16660	0.09287	0.101C8	0.02171	3D	5.27029
3P	8.69278	0.04670	-0.33254	-0.07972	3D	9.42659
3P	5.83188	-0.01717	-0.74258	-0.22666	3D	19.54570
4P	4.54856	0.00658	-0.08364	0.04165		
4P	2.59061	-0.00276	-0.00162	0.54173		
4P	1.63458	0.00213	-0.00C34	0.36695		
4P	1.25528	-0.00101	-0.000C7	0.18340		

SELENIUM K(2)L(8)M(18)4S(2)4P(4), 1D  
 T.E.= -0.23998185D+04 P.E.= -0.47557314D+04 K.E.= 0.23998129D+04 V.T.= -0.20000023D+01

	S	1S	2S	3S	4S
BASIS/ORB E	-460.87697	-60.67832	-8.94116	-0.84286	
1S	31.62030	0.84643	0.34569	-0.13313	-0.03796
1S	41.03150	0.17055	-0.00136	0.00145	-0.00113
2S	27.33060	-0.02272	0.16667	-0.07784	-0.02406
2S	15.04660	0.01188	-1.03383	0.45317	0.13547
3S	13.69700	-0.00689	-0.16232	0.25716	0.08573
3S	8.46853	0.00271	-0.01984	-0.49905	-0.17C96
3S	5.78570	-0.00126	0.00324	-0.73256	-0.27223
4S	3.35115	0.00039	-0.00094	-0.01006	0.47920
4S	2.17158	-0.00029	0.00C69	0.00211	0.55220
4S	1.47824	0.00011	-0.00025	-0.00071	0.10932

See page 183 for Explanation of Tables and Notes for Tables 32, 42, and 43

TABLE 1 (38). HARTREE-FOCK FUNCTIONS FOR NEUTRAL ATOMS.

P	2P	3P	4P	D	3D
BASIS/ORB E	-54.27832	-6.67046	-0.38217	BASIS/ORB E	-2.65867
2P 14.84560	0.80569	0.33285	0.08317	3D 4.59578	0.48194
2P 23.61880	0.09531	0.03357	0.00713	3D 2.86913	0.11874
3P 14.00140	0.10131	0.10636	0.02399	3D 7.16922	0.30646
3P 8.74354	0.04317	-0.32837	-0.08029	3D 9.76019	0.17962
3P 5.86611	-0.01478	-0.74348	-0.22390	3D 15.82680	0.02876
4P 4.59972	0.00547	-0.09050	0.03329		
4P 2.60473	-0.00193	-0.00196	0.55232		
4P 1.55132	0.00134	-0.00084	0.44111		
4P 1.16732	-0.00066	-0.00001	0.10771		

SELENIUM K(2)L(8)M(18)4S(2)4P(4), 1S  
T.E.=-0.23997466D+04 P.E.=-0.47994864D+04 K.E.= 0.23997398D+04 V.T.=-0.20000028D+01

S	1S	2S	3S	4S
BASIS/ORB E	-460.89241	-60.65323	-8.95557	-0.85172
1S 31.70270	0.84542	0.34615	-0.13321	-0.03931
1S 40.98160	0.16929	-0.00259	-0.00104	-0.00016
2S 27.29690	-0.01952	0.16880	-0.07889	-0.02314
2S 15.06540	0.01083	-1.03352	0.45347	0.13368
3S 13.68080	-0.00622	-0.16443	0.25809	0.08969
3S 8.45817	0.00248	-0.01934	-0.50330	-0.17910
3S 5.77859	-0.00118	0.00316	-0.72901	-0.26464
4S 3.36126	0.00042	-0.00105	-0.00987	0.44469
4S 2.28997	-0.00032	0.00080	0.00206	0.51600
4S 1.57271	0.00011	-0.00027	-0.00061	0.17774

P	2P	3P	4P	D	3D
BASIS/ORB E	-54.29326	-6.68470	-0.35240	BASIS/ORB E	-2.67306
2P 14.82680	0.80593	0.33264	0.08381	3D 4.64823	0.48180
2P 23.59010	0.09633	0.03405	0.00695	3D 2.89094	0.12584
3P 14.03630	0.09949	0.10525	0.02226	3D 6.98191	0.25599
3P 8.73281	0.04398	-0.32928	-0.07733	3D 9.47732	0.22363
3P 5.85888	-0.01530	-0.74273	-0.22773	3D 15.99710	0.02825
4P 4.59410	0.00569	-0.08918	0.03788		
4P 2.63520	-0.00197	-0.00258	0.51857		
4P 1.58654	0.00106	-0.00126	0.46674		
4P 1.06699	-0.00042	-0.00023	0.12348		

BROMINE K(2)L(8)M(18)4S(2)4P(5), 2P  
T.E.=-0.257244080D+04 P.E.=-0.51448726D+04 K.E.= 0.257243190D+04 V.T.=-0.20000034D+01

S	1S	2S	3S	4S
BASIS/ORB E	-490.05997	-65.20006	-9.67188	-0.99263
1S 32.58640	0.81095	0.37448	-0.14513	-0.04178
1S 41.35570	0.20011	-0.02121	0.00582	-0.00013
2S 26.53420	-0.01554	0.19595	-0.09653	-0.03333
2S 15.87920	0.01020	-1.05505	0.47805	0.15368
3S 13.79510	-0.00540	-0.18909	0.27859	0.09132
3S 8.78775	0.00246	-0.00887	-0.52656	-0.17533
3S 6.01958	-0.00115	-0.00028	-0.72544	-0.30447
4S 3.65032	0.00037	-0.00002	-0.00594	0.46075
4S 2.39212	-0.00025	0.00005	-0.00099	0.56685
4S 1.63837	0.00009	-0.00001	0.00027	0.12548

P	2P	3P	4P	D	3D
BASIS/ORB E	-58.55431	-7.47821	-0.45703	BASIS/ORB E	-3.22020
2P 15.81260	0.74854	0.31389	0.08539	3D 4.81505	0.47817
2P 24.12670	0.09604	0.03407	0.00721	3D 3.01772	0.09572
3P 14.74150	0.16709	0.12804	0.02963	3D 7.36217	0.31609
3P 8.64224	0.04123	-0.41337	-0.10120	3D 10.19710	0.19151
3P 5.90145	-0.01974	-0.66676	-0.24356	3D 16.62740	0.02657
4P 5.18209	0.00780	-0.06708	0.05048		
4P 2.82688	-0.00154	-0.01083	0.56500		
4P 1.70190	0.00090	0.00362	0.45389		
4P 1.21513	-0.00039	-0.00184	0.08536		

See page 183 for Explanation of Tables and Notes for Tables 32, 42, and 43

## ROOTHAAN-HARTREE-FOCK ATOMIC WAVEFUNCTIONS

TABLE 1 (39). HARTREE-FOCK FUNCTIONS FOR NEUTRAL ATOMS.

KRYPTON K(2)L(8)M(18)4S(2)4P(6), 1S  
 T.E.= -0.27520546D+04 P.E.= -0.55041027D+04 K.E.= 0.27520481D+04 V.T.= -0.20000024D+01

S	1S	2S	3S	4S
BASIS/ORB E	-520.16529	-69.90320	-10.84949	-1.15288
1S 32.83510	0.71521	0.38139	-0.14543	-0.04349
1S 40.94470	0.29911	-0.01623	0.00181	-0.00148
2S 27.45800	-0.01854	0.17175	-0.09037	-0.03219
2S 16.06660	0.00897	-1.07160	0.49528	0.16451
3S 14.29620	-0.00464	-0.14913	0.25451	0.08852
3S 9.10937	0.00190	-0.01920	-0.48504	-0.16671
3S 6.37181	-0.00088	0.00401	-0.75593	-0.33291
4S 3.84546	0.00026	-0.00122	-0.01203	0.46913
4S 2.57902	-0.00018	0.00092	0.00218	0.55106
4S 1.77192	0.00006	-0.00031	-0.00085	0.13572

P	2P	3P	4P	C	3D
BASIS/ORB E	-63.00992	-8.33152	-0.52412	BASIS/CRB E	-3.82526
2P 17.03660	0.72322	0.30165	0.08488	3D 5.30650	0.50854
2P 26.04380	0.06774	0.02508	0.00571	3D 3.36240	0.11070
3P 15.51000	0.22056	0.15903	0.04169	3D 7.54963	0.24778
3P 9.49403	0.04478	-0.28475	-0.07425	3D 10.35430	0.20584
3P 6.57275	-0.01672	-0.76440	-0.26866	3D 17.11420	0.02863
4P 5.38507	0.00609	-0.10670	0.01341		
4P 3.15603	-0.00195	-0.00562	0.51241		
4P 2.02966	0.00111	0.00137	0.42557		
4P 1.42733	-0.00040	-0.00053	0.18141		

RUBIDIUM K(2)L(8)M(18)4S(2)4P(6)5S(1), 2S  
 T.E.= -0.29383470D+04 P.E.= -0.58766002D+04 K.E.= 0.29382533D+04 V.T.= -0.20300319D+01

S	1S	2S	3S	4S	5S
BASIS/ORB E	-551.45887	-75.04574	-12.13354	-1.52359	-0.13785
1S 38.05890	0.84819	0.03144	-0.00977	-0.00320	0.00066
1S 26.17890	0.16950	0.46742	-0.19461	-0.06591	0.01390
2S 17.87590	-0.05364	-0.21527	-0.24622	-0.10599	0.02262
2S 15.13760	0.03990	-0.96951	0.91735	0.34496	-0.07316
3S 9.32726	-0.00642	-0.03122	-0.37076	-0.13569	0.02802
3S 6.80548	0.00366	0.06888	-0.82244	-0.37869	0.08360
4S 3.91418	-0.00114	-0.00192	-0.02077	0.57680	-0.14618
4S 2.58977	0.00087	0.00141	0.00720	0.54775	-0.11134
5S 1.88043	-0.00043	-0.00065	-0.00302	0.02430	0.12653
5S 1.15468	0.00021	0.00031	0.00130	-0.00036	0.53476
5S 0.74153	-0.00008	-0.00011	-0.00044	0.00032	0.46820

P	2P	3P	4P	D	3D
BASIS/ORB E	-67.90640	-9.48807	-0.81013	BASIS/ORB E	-4.73194
2P 24.46350	-0.13089	0.03396	0.00899	3D 12.29820	0.21496
2P 15.28570	-0.87175	0.42037	0.12897	3D 6.79196	0.64623
3P 8.24457	-0.03211	-0.65799	-0.22816	3D 4.05372	0.23414
3P 5.69739	0.01381	-0.46125	-0.16836		
4P 3.64326	-0.00454	-0.00094	0.47521		
4P 2.33347	0.00282	-0.00215	0.55302		
4P 1.56570	-0.00100	0.00069	0.11614		

STRONTIUM K(2)L(8)M(18)4S(2)4P(6)5S(2), 1S  
 T.E.= -0.31315379D+04 P.E.= -0.62630144D+04 K.E.= 0.31314765D+04 V.T.= -0.20000196D+01

S	1S	2S	3S	4S	5S
BASIS/ORB E	-583.66810	-80.39092	-13.47508	-1.89685	-0.17843
1S 39.08880	0.84790	0.02971	0.00938	0.00295	0.00062
1S 26.96480	0.16977	0.46986	0.19693	0.07068	0.01846
2S 18.30310	-0.05879	-0.18491	0.30385	0.13168	0.03309
2S 15.69910	0.04531	-0.99718	-0.98235	-0.38559	-0.09869
3S 9.88651	-0.00684	-0.03413	0.30498	0.10711	0.02485
3S 7.19156	0.00375	0.00908	0.88822	0.44139	0.12228
4S 4.16674	-0.00114	-0.00189	0.02426	-0.57030	-0.18773
4S 2.84586	0.00078	0.00126	-0.00773	-0.56603	-0.13437
5S 1.83155	-0.00037	-0.00055	0.00289	-0.01778	0.30164
5S 1.20420	0.00025	0.00037	-0.00180	0.00438	0.55277
5S 0.81729	-0.00009	-0.00014	0.00064	-0.00119	0.28152

See page 183 for Explanation of Tables and Notes for Tables 32, 42, and 43

TABLE 1 (40). HARTREE-FOCK FUNCTIONS FOR NEUTRAL ATOMS.

P	2P	3P	4P	D	3D
BASIS/ORB E	-72.99584	-10.70003	-1.09821	BASIS/CRB E	-5.69411
2P 25.13250	-0.12972	0.03329	0.00945	3D 13.08380	0.19034
2P 15.76700	-0.87247	0.42673	0.14075	3D 7.35453	0.62984
3P 8.48946	-0.03347	-0.67785	-0.24994	3D 4.48799	0.26961
3P 5.91883	0.01577	-0.44895	-0.18689		
4P 3.96255	-0.00568	0.00118	0.45397		
4P 2.64250	0.00338	-0.00291	0.57921		
4P 1.77261	-0.00107	0.00085	0.11558		

YTTRIUM K(2)L(8)M(18)4S(2)4P(6)5S(1)4D(2), 4F  
T.E.= -0.333165500D+04 P.E.= -0.666318160D+04 K.E.= 0.333152660D+04 V.T.= -0.200003850D+01

S	1S	2S	3S	4S	5S
BASIS/ORB E	-616.65791	-85.71190	-14.65929	-2.07097	-0.19233
1S 40.08530	0.85223	-0.02986	-0.00908	0.00319	0.00056
1S 27.58290	0.16533	-0.47340	-0.20077	0.07364	0.01912
2S 18.66340	-0.06231	0.21408	-0.32652	0.14999	0.03566
2S 16.13290	0.04910	0.97C72	1.01692	-0.41658	-0.10323
3S 10.36790	-0.00701	0.03398	-0.27771	0.10C34	0.02099
3S 7.50901	0.00362	-0.00818	-0.92176	0.46995	0.13017
4S 4.28620	-0.00105	0.00158	-0.02324	-0.64305	-0.21485
4S 2.93376	0.00071	-0.00105	0.00734	-0.50000	-0.09701
5S 1.84017	-0.00032	0.00045	-0.00267	-0.01815	0.35987
5S 1.19254	0.00025	-0.00034	0.00188	0.00E28	0.53005
5S 0.85045	-0.00011	0.00014	-0.00076	-0.00200	0.23643

P	2P	3P	4P	D	3D	4D
BASIS/ORB E	-78.06632	-11.75568	-1.21465	BASIS/ORB E	-6.50135	-0.19375
2P 25.72410	-0.13098	0.03342	0.00961	3D 12.92070	0.23868	-0.04579
2P 16.22790	-0.87137	0.43245	0.14837	3D 7.04305	0.74269	-0.14380
3P 8.76281	-0.03241	-0.68333	-0.26366	4D 4.68556	0.11582	0.06558
3P 6.20312	0.01475	-0.44303	-0.19102	4D 2.53176	-0.00659	0.50656
4P 4.03822	-0.00439	-0.00128	0.56094	4D 1.18894	0.00174	0.60960
4P 2.61826	0.00241	-0.00132	0.53673			
4P 1.65639	-0.00073	0.00030	0.05561			

YTTRIUM K(2)L(8)M(18)4S(2)4P(6)5S(2)4D(1), 2D  
T.E.= -0.333167120D+04 P.E.= -0.66622133D+04 K.E.= 0.33315421D+04 V.T.= -0.20000387D+01

S	1S	2S	3S	4S	5S
BASIS/ORB E	-616.75119	-85.81091	-14.75890	-2.16815	-0.19578
1S 40.08530	0.85224	-0.02987	-0.00910	0.00305	0.00053
1S 27.58290	0.16531	-0.47339	-0.20077	0.07437	0.02021
2S 18.66340	-0.06221	0.21397	-0.32696	0.14901	0.03676
2S 16.13290	0.04899	0.97C86	1.01756	-0.41701	-0.10770
3S 10.36790	-0.00696	0.03390	-0.27826	0.09906	0.02124
3S 7.50901	0.00357	-0.00811	-0.92142	0.47540	0.13811
4S 4.28620	-0.00100	0.00152	-0.02305	-0.65361	-0.22997
4S 2.93376	0.00065	-0.00098	0.00706	-0.49519	-0.09756
5S 1.80195	-0.00027	0.00037	-0.00230	-0.00740	0.45781
5S 1.12467	0.00021	-0.00028	0.00161	0.00148	0.54223
5S 0.80163	-0.00009	0.00013	-0.00071	-0.00048	0.13081

P	2P	3P	4P	D	3D	4D
BASIS/ORB E	-78.16422	-11.85424	-1.30054	BASIS/ORB E	-6.59860	-0.24987
2P 25.72410	-0.13095	0.03341	0.00961	3D 12.92070	0.23859	-0.05149
2P 16.22790	-0.87140	0.43251	0.14998	3D 7.04305	0.74282	-0.16246
3P 8.76281	-0.03230	-0.68360	-0.26819	4D 4.66942	0.11663	0.07689
3P 6.20312	0.01459	-0.44268	-0.18882	4D 2.55392	-0.00782	0.55325
4P 3.99693	-0.00432	-0.00160	0.58611	4D 1.29851	0.00217	0.53220
4P 2.60040	0.00241	-0.00105	0.52213			
4P 1.63935	-0.00073	0.00030	0.03958			

See page 183 for Explanation of Tables and Notes for Tables 32, 42, and 43

## ROOTHAAN-HARTREE-FOCK ATOMIC WAVEFUNCTIONS

TABLE 1 (41). HARTREE-FOCK FUNCTIONS FOR NEUTRAL ATOMS.

ZIRCONIUM K(2)L(8)M(18)4S(2)4P(6)5S(0)4D(4), 5D  
 T.E.= -0.35389172D+04 P.E.= -0.7C777148D+04 K.E.= 0.35387976D+04 V.T.= -0.20300338D+01

S	1S	2S	3S	4S	P	2P	3P	4P	D	3D	4D
BASIS/ORB E	-650.51704	-91.17658	-15.85266	-2.22109	BASIS/ORB E	-83.27941	-12.81955	-1.31144	BASIS/ORB E	-7.31725	-0.17258
1S 41.10980	0.85247	0.02845	-0.00876	-0.00256	2P 26.41180	-0.12935	0.03251	0.00963	3D 13.34840	0.24006	-0.04840
1S 28.34320	0.16501	0.47587	-0.20300	-0.07699	2P 16.71350	-0.87250	0.43847	0.15442	3D 7.30972	0.75146	-0.15899
2S 19.09090	-0.06953	-0.17555	-0.39741	-0.17468	3P 9.01670	-0.03401	-0.65763	-0.27104	4D 4.79790	0.10110	0.10412
2S 16.70750	0.05660	-1.00280	1.09384	0.44791	3P 6.44970	0.01681	-0.42540	-0.20816	4D 2.54864	-0.00733	0.55842
3S 10.93860	-0.00768	-0.03724	-0.22901	-0.07C17	4S 4.50854	-0.00153	-0.00219	-0.02878	4D 1.17646	0.00191	0.54433
3S 7.86993	0.00393	0.00655	-0.56986	-0.51752	4P 4.37811	-0.00538	-0.00C57	0.51601			
4S 3.22075	-0.00167	0.00230	0.01525	0.37855	4P 2.91510	0.00295	-0.00179	0.54453			
4S 2.58348	-0.00077	-0.00101	-0.00610	0.13901	4P 1.92247	-0.00087	0.00026	0.10855			

ZIRCONIUM K(2)L(8)M(18)4S(2)4P(6)5S(1)4D(3), 5F  
 T.E.= -0.35389957D+04 P.E.= -0.7C778643D+04 K.E.= 0.35388685D+04 V.T.= -0.20300359D+01

S	1S	2S	3S	4S	5S	P	2P	3P	4P	D	3D	4D
BASIS/ORB E	-650.59359	-91.25643	-15.93519	-2.30344	-0.20396	BASIS/ORB E	-83.36018	-12.90107	-1.38406	BASIS/ORB E	-7.39771	-0.24854
1S 41.10980	0.85252	0.02848	0.00869	-0.00283	0.00043	2P 26.41180	-0.12933	0.03249	0.00964	3D 13.34840	0.24019	-0.05413
1S 28.34320	0.16505	0.47581	0.20314	-0.07702	0.02026	2P 16.71350	-0.87254	0.43852	0.15558	3D 7.30972	0.75087	-0.16609
2S 19.09090	-0.06900	-0.17909	0.39668	-0.17571	0.04284	3P 9.01670	-0.03387	-0.65788	-0.27429	4D 4.79321	0.10307	0.08174
2S 16.70750	0.05603	-1.00333	-1.09311	0.45523	-0.11334	3P 6.44970	0.01660	-0.42906	-0.20663	4D 2.76946	-0.00893	0.53541
3S 10.93860	-0.00741	-0.03693	0.22849	-0.07407	0.01374	4S 4.49276	-0.00113	-0.00168	0.02614	4D 1.36146	0.00208	0.55698
3S 7.86993	0.00367	0.00826	0.97069	-0.51684	0.14493	4S 3.09333	0.00081	0.00119	-0.00898	4D 0.48637	-0.09640	
4S 3.09333	-0.00081	0.00019	-0.00898	0.48637		5S 2.03548	-0.00039	-0.00054	0.00343	4D 0.01877	0.29705	
5S 2.03548	-0.00039	-0.00054	0.00343	0.01877		5S 1.35801	0.00026	0.00035	-0.00208	4D 0.00725	0.51987	
5S 1.35801	0.00026	0.00035	-0.00208	-0.00725		5S 0.91842	-0.00009	-0.00012	0.00069	4D 0.00042	0.31820	

ZIRCONIUM K(2)L(8)M(18)4S(2)4P(6)5S(2)4D(2), 3F  
 T.E.= -0.35389821D+04 P.E.= -0.7C778365D+04 K.E.= 0.35388544D+04 V.T.= -0.20000361D+01

S	1S	2S	3S	4S	5S	P	2P	3P	4P	D	3D	4D
BASIS/ORB E	-650.70678	-91.37772	-16.05512	-2.41864	-0.20702	BASIS/ORB E	-83.36018	-12.90107	-1.38406	BASIS/ORB E	-7.39771	-0.24854
1S 41.10980	0.85254	-0.02851	-0.00865	0.00270	0.00045	2P 26.41180	-0.12933	0.03249	0.00964	3D 13.34840	0.24019	-0.05413
1S 28.34320	0.16501	-0.47578	-0.20325	0.07773	0.02106	2P 16.71350	-0.87254	0.43852	0.15558	3D 7.30972	0.75087	-0.16609
2S 19.09090	-0.06875	0.17870	-0.39597	0.17870	0.04449	3P 9.01670	-0.03387	-0.65788	-0.27429	4D 4.79321	0.10307	0.08174
2S 16.70750	0.05576	1.00379	1.09237	-0.45559	-0.11775	3P 6.44970	0.01660	-0.42906	-0.20663	4D 2.76946	-0.00893	0.53541
3S 10.92390	-0.00732	0.03687	-0.22935	0.07311	0.01421	4P 4.34059	-0.00523	-0.00089	0.53758	4D 1.36146	0.00208	0.55698
3S 7.86993	0.00361	-0.00828	-0.56970	0.52174	0.15092	4P 2.88014	0.00290	-0.00159	0.54273	4D 0.48637	-0.09727	
4S 4.49276	-0.00105	0.00159	-0.02588	-0.67253	-0.23665	5S 1.96589	-0.00030	0.00041	-0.00280	4D 0.01877	0.40630	
4S 3.09333	0.00071	-0.00106	0.00847	-0.48277	-0.09727	5S 1.24093	0.00020	-0.00027	0.00170	4D 0.00100	0.55801	
5S 1.24093	-0.00008	0.00011	-0.00066	-0.00025	0.17512	5S 0.84334	-0.00008	0.00011	-0.00066			

See page 183 for Explanation of Tables and Notes for Tables 32, 42, and 43

TABLE 1 (42). HARTREE-FOCK FUNCTIONS FOR NEUTRAL ATOMS.

P	2P	3P	4P	C	3D	4D
BASIS/ORB E	-83.47832	-13.01992	-1.48711	BASIS/ORB E	-7.51511	-0.33654
2P 26.41190	-0.12930	0.03248	0.00970	3D 13.34840	0.24002	-0.05884
2P 16.71350	-0.87258	0.43659	0.15714	3D 7.30972	0.75132	-0.18499
3P 9.01670	-0.03374	-0.65819	-0.27770	4D 4.76501	0.10371	0.10562
3P 6.44970	0.01642	-0.42866	-0.20724	4D 2.71988	-0.01048	0.58930
4P 4.32282	-0.00507	-0.00124	0.55207	4D 1.45115	0.00280	0.46133
4P 2.86362	0.00271	-0.00131	0.55148			
4P 1.82585	-0.00077	0.00029	0.05792			

NIOBIUM K(2)L(8)M(18)4S(2)4P(6)5S(1)4D(5), 6S  
T.E.= -0.37535403D+04 P.E.= -0.75C69759D+04 K.E.= 0.37534357D+04 V.T.= -0.20000279D+01

S	1S	2S	3S	4S
BASIS/ORB E	-685.33896	-96.86225	-17.13391	-2.42682
1S 42.11660	0.85560	0.02925	-0.00919	-0.00260
1S 28.90030	0.16254	0.47555	-0.20601	-0.08011
2S 19.62750	-0.07275	-0.19030	-0.40058	-0.17678
2S 17.17410	0.05949	-0.95513	1.10532	0.45866
3S 11.48940	-0.00807	-0.03782	-0.19287	-0.05C30
3S 8.21250	0.00391	0.00774	-1.00717	-0.55493
4S 4.70554	-0.00146	-0.00166	-0.03012	0.67C38
4S 3.34203	0.00154	0.00190	0.01542	0.38647
4S 2.64850	-0.00069	-0.00C81	-0.00603	0.11569

P	2P	3P	4P	D	3D	4D
BASIS/ORB E	-88.71141	-13.96943	-1.45798	BASIS/ORB E	-8.21784	-0.21225
2P 27.03590	-0.12946	0.03215	0.00968	3D 13.82720	0.23725	-0.05397
2P 17.18580	-0.87224	0.44395	0.16081	3D 7.61214	0.75915	-0.17792
3P 9.27353	-0.03444	-0.71115	-0.28168	4D 4.93415	0.09355	0.12564
3P 6.70608	0.01762	-0.41611	-0.21806	4D 2.73772	-0.00925	0.57951
4P 4.61304	-0.00547	-0.00148	0.52814	4D 1.31126	0.00221	0.49494
4P 3.08219	0.00289	-0.00142	0.53963			
4P 2.03253	-0.00083	0.00010	0.11041			

NIOBIUM K(2)L(8)M(18)4S(2)4P(6)5S(1)4D(4), 6D  
T.E.= -0.37539845D+04 P.E.= -0.75C70475D+04 K.E.= 0.375346300+04 V.T.= -0.20000324D+01

S	1S	2S	3S	4S	5S
BASIS/ORB E	-685.44324	-96.97275	-17.24464	-2.53443	-0.21422
1S 42.11660	0.85563	0.02527	0.00916	-0.00282	0.00046
1S 28.90030	0.16249	0.47952	0.20609	-0.08032	0.02113
2S 19.62750	-0.07243	-0.19002	0.40041	-0.18123	0.04367
2S 17.17410	0.05915	-0.99546	-1.10525	0.46559	-0.11668
3S 11.48940	-0.00791	-0.03764	0.19280	-0.05325	0.00850
3S 8.21250	0.00376	0.00758	1.00754	-0.55615	0.15583
4S 4.69787	-0.00120	-0.00156	0.02810	0.68008	-0.23123
4S 3.24460	0.00089	0.00116	-0.01005	0.47540	-0.09812
5S 2.19942	-0.00045	-0.00054	0.00394	0.01922	0.27410
5S 1.48175	0.00029	0.00034	-0.00224	-0.00680	0.48854
5S 0.99373	-0.00010	-0.00011	0.00070	-0.00039	0.37851

P	2P	3P	4P	D	3D	4D
BASIS/ORB E	-88.82070	-14.07907	-1.55415	BASIS/ORB E	-8.32624	-0.29876
2P 27.03600	-0.12943	0.03213	0.00975	3D 13.82720	0.23751	-0.05860
2P 17.18580	-0.87227	0.44402	0.16206	3D 7.61214	0.75807	-0.18605
3P 9.27353	-0.03434	-0.71146	-0.28415	4D 4.95791	0.09496	0.11018
3P 6.70608	0.01748	-0.41572	-0.21922	4D 2.90204	-0.00966	0.56843
4P 4.59632	-0.00534	-0.00177	0.54274	4D 1.46959	0.00223	0.49649
4P 3.05676	0.00281	-0.00122	0.54768			
4P 2.00120	-0.00081	0.00013	0.08484			

See page 183 for Explanation of Tables and Notes for Tables 32, 42, and 43

## ROOTHAAAN-HARTREE-FOCK ATOMIC WAVEFUNCTIONS

TABLE 1 (43). HARTREE-FOCK FUNCTIONS FOR NEUTRAL ATOMS.

NIOBIUM K(2)L(8)M(18)4S(2)4P(6)5S(2)4D(3), 4F  
 T.E.= -0.37535394D+04 P.E.= -0.75069333D+04 K.E.= 0.37533939D+04 V.T.= -0.20000388D+01

S	1S	2S	3S	4S	5S	
BASIS/ORB E	-685.57332	-97.1C985	-17.38199	-2.66484	-0.21636	
1S 42.11660	0.84974	-0.01324	-0.00254	0.00017	-0.00020	
1S 29.90330	0.16406	-0.48208	-0.20680	0.08116	0.02174	
2S 19.62750	-0.05108	0.11828	-0.43418	0.19440	0.04863	
2S 17.17410	0.04140	1.05690	1.13504	-0.47861	-0.12323	
3S 11.48940	-0.00520	0.02702	-0.19889	0.05482	0.00937	
3S 8.21250	0.00236	-0.00182	-1.00409	0.55547	0.15992	
4S 4.69787	-0.00068	-0.00056	-0.02894	-0.68834	-0.23984	
4S 3.24460	0.00047	0.00045	0.01033	-0.47320	-0.09705	
5S 2.12323	-0.00020	-0.00025	-0.00365	-0.00790	0.36172	
5S 1.35601	0.00013	0.00017	0.00212	0.00059	0.55055	
5S 0.90940	-0.00005	-0.00007	-0.00078	-0.00009	0.23338	
P	2P	3P	4P	D	3D	4D
BASIS/ORB E	-88.95671	-14.21532	-1.67185	BASIS/ORB E	-8.46101	-0.40560
2P 27.03600	-0.12941	0.03212	0.00979	3D 13.82720	0.23753	-0.06302
2P 17.18580	-0.87231	0.44409	0.16369	3D 7.61214	0.75785	-0.20248
3P 9.27353	-0.03423	-0.71179	-0.28806	4D 4.95700	0.09543	0.12643
3P 6.70608	0.01732	-0.41533	-0.21901	4D 2.89109	-0.01024	0.60975
4P 4.57466	-0.00524	-0.00206	0.55657	4D 1.57252	0.00261	0.41963
4P 3.04566	0.00272	-0.00099	0.55259			
4P 1.95922	-0.00076	0.00015	0.06208			

MOLYBDENUM K(2)L(8)M(18)4S(2)4P(6)5S(0)4D(6), 5D  
 T.E.= -0.39753889D+04 P.E.= -0.750506177D+04 K.E.= 0.39752287D+04 V.T.= -0.20000403D+01

S	1S	2S	3S	4S		
BASIS/ORB E	-721.11290	-102.75449	-18.48544	-2.66260		
1S 43.14050	0.85545	0.02700	-0.00779	-0.00191		
1S 29.78150	0.16200	0.48043	-0.20866	-0.08302		
2S 19.66010	-0.09988	-0.10550	-0.68733	-0.29904		
2S 17.88260	0.08783	-1.06818	1.39929	0.58858		
3S 12.22990	-0.00821	-0.04327	-0.15808	-0.03267		
3S 8.55027	0.00345	0.00733	-1.04571	-0.58892		
4S 4.88931	-0.00112	-0.00160	-0.02859	0.70190		
4S 3.38113	0.00096	0.00138	0.01149	0.42909		
4S 2.47192	-0.00037	-0.00050	-0.00381	0.04737		
P	2P	3P	4P	D	3D	4D
BASIS/ORB E	-94.34872	-15.18671	-1.63387	BASIS/ORB E	-9.18670	-0.22696
2P 27.64310	-0.13000	0.03175	0.00968	3D 14.06420	0.25465	-0.06416
2P 17.65560	-0.87155	0.44954	0.16709	3D 7.73842	0.76438	-0.18676
3P 9.58870	-0.03452	-0.69289	-0.27809	4D 4.69545	0.06746	0.20149
3P 7.09084	0.01750	-0.43175	-0.23776	4D 2.77739	-0.01089	0.55816
4P 4.80266	-0.00456	-0.00714	0.56157	4D 1.36991	0.00244	0.44671
4P 3.16931	0.00229	0.00060	0.53754			
4P 2.04386	-0.00064	-0.00043	0.08356			

MOLYBDENUM K(2)L(8)M(18)4S(2)4P(6)5S(1)4D(5), 7S  
 T.E.= -0.39755338D+04 P.E.= -0.750508874D+04 K.E.= 0.39753536D+04 V.T.= -0.20000453D+01

S	1S	2S	3S	4S	5S	
BASIS/ORB E	-721.20539	-102.85269	-18.58499	-2.76119	-0.22198	
1S 43.14050	0.85545	0.02700	0.00780	-0.00221	0.00027	
1S 29.78150	0.16200	0.48044	0.20867	-0.08302	0.02174	
2S 19.66010	-0.09989	-0.10544	0.68779	-0.30793	0.07347	
2S 17.88260	0.08784	-1.06825	-1.39988	0.60009	-0.14784	
3S 12.22990	-0.00822	-0.04323	0.15831	-0.03681	0.00387	
3S 8.55027	0.00345	0.00731	1.04572	-0.58811	0.16365	
4S 4.85752	-0.00110	-0.00157	0.02845	0.72364	-0.24513	
4S 3.32874	0.00083	0.00119	-0.01018	0.44046	-0.08389	
5S 2.29197	-0.00042	-0.00056	0.00398	0.01389	0.28570	
5S 1.51663	0.00025	0.00033	-0.00213	-0.00543	0.50505	
5S 1.00605	-0.00008	-0.00011	0.00067	-0.00083	0.35518	
P	2P	3P	4P	D	3D	4D

See page 183 for Explanation of Tables and Notes for Tables 32, 42, and 43

TABLE 1 (44). HARTREE-FOCK FUNCTIONS FOR NEUTRAL ATOMS.

P	2P	3P	4P	D	3D	4D
BASIS/ORB E	-94.44572	-15.28713	-1.72206	BASIS/ORB E	-9.28394	-0.35683
2P 27.64310	-0.12999	0.03174	0.00971	3D 14.06420	0.25477	-0.06836
2P 17.65560	-0.87156	0.44558	0.16815	3D 7.73842	0.76389	-0.19807
3P 9.58870	-0.03453	-0.69309	-0.28042	4D 4.70906	0.06850	0.20450
3P 7.09084	0.01752	-0.43147	-0.23806	4D 2.85675	-0.01188	0.56575
4P 4.79603	-0.00461	-0.00740	0.56544	4D 1.52600	0.00254	0.40851
4P 3.17901	0.00237	0.00080	0.53860			
4P 2.07183	-0.00067	-0.00042	0.07560			

MOLYBDENUM K(2)L(8)M(18)4S(2)4P(6)5S(2)4D(4), 5D  
T.E.= -0.35754280D+04 P.E.= -0.79506883D+04 K.E.= 0.39752603D+04 V.T.= -0.20000422D+01

S	1S	2S	3S	4S	5S
BASIS/ORB E	-721.35638	-103.01048	-18.74319	-2.90999	-0.22455
1S 43.14050	0.85547	-0.02702	-0.00779	0.00209	0.00022
1S 29.78150	0.16196	-0.48041	-0.20871	0.08372	0.02228
2S 19.66010	-0.09947	0.10904	-0.68801	0.30676	0.07365
2S 17.88260	0.08740	1.06870	1.40026	-0.60026	-0.14941
3S 12.22990	-0.00809	0.04307	-0.15850	0.03547	0.00310
3S 8.55027	0.00335	-0.00719	-1.04578	0.59339	0.16818
4S 4.85792	-0.00099	0.00142	-0.02774	-0.73350	-0.25565
4S 3.32874	0.00068	-0.00100	0.00914	-0.43635	-0.07428
5S 2.16167	-0.00030	0.00040	-0.00310	-0.00398	0.39031
5S 1.36655	0.00019	-0.00025	0.00179	-0.00035	0.54305
5S 0.91953	-0.00007	0.00010	-0.00067	0.00018	0.20971

P	2P	3P	4P	D	3D	4D
BASIS/ORB E	-94.60227	-15.44424	-1.85724	BASIS/ORB E	-9.43943	-0.46992
2P 27.64310	-0.12997	0.03173	0.00975	3D 14.06420	-0.25458	-0.07287
2P 17.65560	-0.87160	0.44564	0.16989	3D 7.73842	-0.76434	-0.21197
3P 9.58870	-0.03437	-0.69334	-0.28474	4D 4.65923	-0.06952	0.23725
3P 7.09084	0.01730	-0.43123	-0.23739	4D 2.80795	0.01390	0.60297
4P 4.76487	-0.00446	-0.00759	0.58502	4D 1.59468	-0.00356	0.32059
4P 3.15475	0.00223	0.00099	0.54063			
4P 1.99061	-0.00060	-0.00036	0.04970			

TECHNETIUM K(2)L(8)M(18)4S(2)4P(6)5S(0)4D(7), 4F  
T.E.= -0.42046768D+04 P.E.= -0.84092185D+04 K.E.= 0.42045416D+04 V.T.= -0.20000322D+01

S	1S	2S	3S	4S
BASIS/ORB E	-757.78883	-108.80181	-19.86139	-2.89136
1S 44.15280	0.85478	0.01965	-0.00459	-0.00054
1S 30.92560	0.16084	0.48392	-0.21159	-0.08574
2S 20.10150	-0.09675	-0.01355	-0.82240	-0.35724
2S 18.44720	0.08629	-1.15942	1.53752	0.65220
3S 12.78620	-0.00717	-0.04027	-0.13289	-0.01755
3S 8.88272	0.00280	0.00459	-1.07131	-0.61777
4S 5.07803	-0.00085	-0.00055	-0.03045	0.72306
4S 3.48991	0.00070	0.00043	0.01219	0.42386
4S 2.49311	-0.00026	-0.00013	-0.00396	0.03666

P	2P	3P	4P	D	3D	4D
BASIS/ORB E	-100.14022	-16.43142	-1.80431	BASIS/ORB E	-10.17849	-0.24964
2P 28.24940	-0.13053	0.03144	0.00970	3D 14.59380	0.24524	-0.06518
2P 18.12530	-0.87093	0.45461	0.17267	3D 8.11647	0.76749	-0.20224
3P 9.86474	-0.03488	-0.65412	-0.28021	4D 5.04274	0.07094	0.20088
2P 7.40530	0.01808	-0.42949	-0.25277	4D 2.98629	-0.01056	0.57555
4P 5.03978	-0.00434	-0.01011	0.56849	4D 1.46829	0.00249	0.43106
4P 3.32695	0.00210	0.00152	0.53911			
4P 2.14087	-0.00057	-0.00070	0.08247			

See page 183 for Explanation of Tables and Notes for Tables 32, 42, and 43

## ROOTHAAN-HARTREE-FOCK ATOMIC WAVEFUNCTIONS

TABLE 1 (45). HARTREE-FOCK FUNCTIONS FOR NEUTRAL ATOMS.

TECHNETIUM K(2)L(8)M(18)4S(2)4P(6)5S(1)4D(6), 6D  
 T.E.= -0.42047669D+04 P.E.= -0.84093624D+04 K.E.= 0.42045955D+04 V.T.= -0.20000408D+01

S	1S	2S	3S	4S	5S	
BASIS/ORB E	-757.90370	-108.92295	-19.98293	-3.00901	-0.22198	
1S 44.15280	0.85476	0.01957	0.00480	-0.00082	-0.00015	
1S 30.92560	0.16087	0.48404	0.21126	-0.08575	0.02181	
2S 20.10150	-0.09726	-0.01600	0.83049	-0.36706	0.08348	
2S 18.44720	0.08687	-1.15664	-1.54686	0.66459	-0.15656	
3S 12.88620	-0.00715	-0.04013	0.13252	-0.02070	-0.00105	
3S 8.88272	0.00268	0.00395	1.07356	-0.61829	0.16698	
4S 5.05896	-0.00080	-0.00041	0.02944	0.73599	-0.24406	
4S 3.46214	0.00056	0.0028	-0.00993	0.43510	-0.07317	
5S 2.30341	-0.00024	-0.00008	0.00343	0.01180	0.33035	
5S 1.43970	0.00014	0.00004	-0.00181	-0.00410	0.56067	
5S 0.94238	-0.00005	-0.00001	0.00065	-0.00002	0.25868	
P	2P	3P	4P	D	3D	4D
BASIS/ORB E	-100.26013	-16.55189	-1.91094	BASIS/ORB E	-10.29779	-0.37650
2P 28.24940	-0.13052	0.03143	0.00973	3D 14.59380	0.24564	-0.06937
2P 18.12530	-0.87094	0.45466	0.17383	3D 8.11647	0.76607	-0.21148
3P 9.86474	-0.03487	-0.69439	-0.28286	4D 5.11590	0.07175	0.17998
3P 7.40530	0.01808	-0.42918	-0.25287	4D 3.16955	-0.01008	0.55987
4P 5.03118	-0.00437	-0.01035	0.57330	4D 1.66661	0.00205	0.43005
4P 3.33395	0.00216	0.00172	0.54123			
4P 2.15951	-0.00059	-0.00069	0.07234			

TECHNETIUM K(2)L(8)M(18)4S(2)4P(6)5S(2)4D(5), 6S  
 T.E.= -0.42047753D+04 P.E.= -0.84C94168D+04 K.E.= 0.42046415D+04 V.T.= -0.20000318D+01

S	1S	2S	3S	4S	5S	
BASIS/ORB E	-758.04447	-109.06567	-20.13200	-3.15177	-0.23107	
1S 44.15280	0.85740	0.02691	0.00790	-0.00190	0.00016	
1S 30.42560	0.16030	0.48335	0.21115	-0.08647	0.02260	
2S 20.10150	-0.11332	-0.07213	0.80442	-0.35342	0.08317	
2S 18.44720	0.10132	-1.10509	-1.52278	0.65277	-0.15899	
3S 12.88620	-0.00848	-0.04553	0.12990	-0.01760	-0.00167	
3S 8.88272	0.00322	0.00634	1.07483	-0.62432	0.17353	
4S 5.05896	-0.00096	-0.00124	0.02873	0.74588	-0.25566	
4S 3.46214	0.00066	0.00088	-0.00928	0.43015	-0.07102	
5S 2.25854	-0.00028	-0.00035	0.00306	0.003E3	0.38177	
5S 1.41055	0.00017	0.00021	-0.00168	0.00037	0.55683	
5S 0.93382	-0.00007	-0.00008	0.00062	-0.00018	0.20792	
P	2P	3P	4P	D	3D	4D
BASIS/ORB E	-100.40558	-16.69981	-2.04087	BASIS/ORB E	-10.44409	-0.54372
2P 28.24940	-0.13050	0.02142	0.00977	3D 14.59380	-0.24496	-0.07374
2P 18.12530	-0.87097	0.45469	0.17528	3D 8.11647	-0.76834	-0.22371
3P 9.86474	-0.03478	-0.65449	-0.28617	4D 4.92916	-0.07475	0.23233
3P 7.40530	0.01795	-0.42907	-0.25296	4D 3.05653	0.01696	0.59271
4P 5.00727	-0.00430	-0.01C54	0.58857	4D 1.75674	-0.00422	0.33208
4P 3.31663	0.00211	0.00191	0.54234			
4P 2.12022	-0.00057	-0.00063	0.05228			

RUTHENIUM K(2)L(8)M(18)4S(2)4P(6)5S(0)4D(8), 3F  
 T.E.= -0.44414632D+04 P.E.= -0.88828226D+04 K.E.= 0.44413594D+04 V.T.= -0.20000234D+01

S	1S	2S	3S	4S	
BASIS/ORB E	-795.38229	-115.02129	-21.27432	-3.12119	
1S 45.16680	0.85895	0.02642	-0.00778	-0.00155	
1S 31.10290	0.15891	0.48605	-0.21350	-0.08827	
2S 20.48290	-0.13672	-0.00366	-1.01634	-0.43343	
2S 19.04240	0.12495	-1.17235	1.74026	0.73466	
3S 13.49850	-0.00895	-0.04834	-0.10981	-0.00268	
3S 9.19966	0.00319	0.00588	-1.09572	-0.64462	
4S 5.27372	-0.00102	-0.00122	-0.02933	0.73928	
4S 3.61594	0.00086	0.00105	0.01097	0.41355	
4S 2.61880	-0.00033	-0.00038	-0.00360	0.03670	

See page 183 for Explanation of Tables and Notes for Tables 32, 42, and 43

TABLE 1 (46). HARTREE-FOCK FUNCTIONS FOR NEUTRAL ATOMS.

P	2P	3P	4P	D	3D	4D
BASIS/ORB E	-106.10254	-17.71030	-1.57676	BASIS/ORB E	-11.20573	-0.27434
2P 28.84240	-0.13144	0.03136	0.00975	3D 15.16420	0.23594	-0.06582
2P 18.59030	-0.87011	0.45921	0.17779	3D 8.46851	0.77526	-0.21592
3P 10.09130	-0.03490	-0.72337	-0.29430	4D 5.25471	0.07010	0.22128
3P 7.62287	0.01872	-0.40101	-0.25682	4D 3.12928	-0.01073	0.57990
4P 5.28410	-0.00442	-0.01044	0.57575	4D 1.54972	0.00266	0.40775
4P 3.48206	0.00203	0.00147	0.54294			
4P 2.23147	-0.00053	-0.00073	0.08114			

RUTHENIUM K(2)L(8)M(18)4S(2)4P(6)5S(2)4D(6),5D  
T.E.= -0.44414746D+04 P.E.= -0.88828698D+04 K.E.= 0.44043952D+04 V.T.= -0.20000179D+01

S	1S	2S	3S	4S	5S
BASIS/ORB E	-795.66933	-115.32118	-21.57724	-3.41016	-0.23915
1S 45.16680	0.85897	0.02643	-0.00777	0.00171	-0.00001
1S 31.10290	0.15887	0.48604	-0.21356	0.08898	0.02321
2S 20.48290	-0.13610	-0.00309	-1.01686	0.44374	0.09931
2S 19.04240	0.12429	-1.17299	1.74101	-0.74884	-0.17534
3S 13.49850	-0.00881	-0.04816	-0.11005	0.00479	-0.00650
3S 9.19966	0.00309	0.00576	-1.09591	0.64977	0.18009
4S 5.24666	-0.00090	-0.00108	-0.02849	-0.76639	-0.26429
4S 3.57817	0.00059	0.00075	0.00866	-0.41615	-0.05657
5S 2.28762	-0.00024	-0.00028	-0.00273	-0.00282	0.41306
5S 1.40886	0.00015	0.00017	0.00153	-0.00039	0.55411
5S 0.93218	-0.00006	-0.00007	-0.00059	0.00019	0.17669

P	2P	3P	4P	D	3D	4D
BASIS/ORB E	-106.39990	-18.01090	-2.24038	BASIS/ORB E	-11.50329	-0.56821
2P 28.84240	-0.13143	0.03133	0.01000	3D 15.16420	-0.23545	-0.07296
2P 18.59030	-0.87012	0.45932	0.18010	3D 8.46851	-0.77676	-0.23724
3P 10.09130	-0.03499	-0.72396	-0.29615	4D 5.10000	-0.07340	0.27795
3P 7.62287	0.01888	-0.40023	-0.26486	4D 3.10000	0.01750	0.59162
4P 5.28427	-0.00463	-0.01110	0.59075	4D 1.80000	-0.00494	0.29416
4P 3.50086	0.00234	0.00213	0.53783			
4P 2.40421	-0.00071	-0.00086	0.06745			

RUTHENIUM M K(2)L(8)M(18)4S(2)4P(6)5S(1)4D(7),5F  
T.E.= -0.44415264D+04 P.E.= -0.88829545D+04 K.E.= 0.44414281D+04 V.T.= -0.20000221D+01

S	1S	2S	3S	4S	5S
BASIS/ORB E	-795.51327	-115.15E47	-21.41291	-3.25556	-0.22164
1S 45.16680	0.85945	0.02311	-0.00350	-0.00018	-0.00037
1S 31.10290	0.15807	0.49170	-0.22084	-0.09107	0.02241
2S 20.48290	-0.08804	-0.44580	-0.36914	-0.17031	0.03301
2S 18.04240	0.07805	-0.74818	1.12104	0.48666	-0.10721
3S 13.49850	-0.01086	-0.02584	-0.14662	-0.02406	-0.00189
3S 9.19966	0.00363	-0.00077	-1.08415	-0.63755	0.16700
4S 5.24666	-0.00105	0.00080	-0.03258	0.75256	-0.24404
4S 3.57817	0.00070	-0.00051	0.01163	0.42448	-0.05795
5S 2.32116	-0.00029	0.00024	-0.00411	0.00982	0.34577
5S 1.43167	0.00017	-0.00015	0.00231	-0.00295	0.55573
5S 0.93706	-0.00007	0.00006	-0.00088	0.00023	0.24706

P	2P	3P	4P	D	3D	4D
BASIS/ORB E	-106.23861	-17.84779	-2.09982	BASIS/ORB E	-11.34191	-0.41165
2P 28.84240	-0.13144	0.03134	0.00984	3D 15.16420	0.23583	-0.06973
2P 18.59030	-0.87010	0.45927	0.17884	3D 8.46851	0.77557	-0.22449
3P 10.09130	-0.03503	-0.72369	-0.29614	4D 5.20000	0.07205	0.22987
3P 7.62287	0.01893	-0.40C59	-0.25809	4D 3.20000	-0.01361	0.57674
4P 5.26010	-0.00477	-0.01104	0.58912	4D 1.70000	0.00326	0.37794
4P 3.51264	0.00258	0.00232	0.50524			
4P 2.48583	-0.00083	-0.00107	0.10136			

See page 183 for Explanation of Tables and Notes for Tables 32, 42, and 43

## ROOTHIAAN-HARTREE-FOCK ATOMIC WAVEFUNCTIONS

TABLE 1 (47). HARTREE-FOCK FUNCTIONS FOR NEUTRAL ATOMS.

RHODIUM K(2)L(8)M(18)4S(2)4P(6)5S(1)4D(9), 2D  
 T.E.= -0.468583080D+04 P.E.= -0.93715316D+04 K.E.= 0.46857009D+04 V.T.= -0.20300277D+01

S	1S	2S	3S	4S	P	2P	3P	4P	D	3D	4D			
BASIS/ORB E	-833.88889	-121.40782	-22.71969	-3.34764	BASIS/ORB E	-112.23084	-19.02076	-2.14676	BASIS/ORB E	-12.26371	-0.29655			
1S 46.16090	0.86311	0.02783	-0.00899	-0.00174	2P 29.44820	-0.13195	0.03112	0.00972	3D 15.67055	0.23156	-0.06872			
1S 31.53901	0.15559	0.49098	-0.21595	-0.09095	2P 19.05914	-0.86963	0.46372	0.18255	3D 8.78548	0.78059	-0.22274			
2S 21.40055	-0.10500	-0.12280	-0.66348	-0.27594	3P 14.15310	-0.00911	-0.04682	-0.08599	0.01424	3S 9.52913	0.00298	0.00410	-1.11817	-0.67886
2S 19.34869	0.09251	-1.05970	1.39307	0.58129	4S 5.48810	-0.00094	-0.00073	-0.03043	0.73917	4S 3.76374	0.00074	0.00062	0.01063	0.42255
3S 14.15310	-0.00911	-0.04682	-0.08599	0.01424	4S 2.664216	-0.00026	-0.00020	-0.00324	0.03335	4S 2.664216	-0.00026	-0.00020	-0.00324	0.03335
3S 9.52913	0.00298	0.00410	-1.11817	-0.67886	4P 5.55328	-0.00473	-0.01160	0.56909	4D 5.40496	0.06800	0.21676			
4S 5.48810	-0.00094	-0.00073	-0.03043	0.73917	4P 3.68055	0.00209	0.00175	0.54821	4D 3.43781	-0.01188	0.54488			
4S 3.76374	0.00074	0.00062	0.01063	0.42255	4P 2.38196	-0.00053	-0.00086	0.09286	4D 1.73097	0.00271	0.43752			

RHODIUM K(2)L(8)M(18)4S(2)4P(6)5S(1)4D(8), 4F  
 T.E.= -0.468588330D+04 P.E.= -0.93716320D+04 K.E.= 0.46857487D+04 V.T.= -0.20000287D+01

S	1S	2S	3S	4S	5S	P	2P	3P	4P	D	3D	4D
BASIS/ORB E	-834.03798	-121.56271	-22.87695	-3.50026	-0.22040	BASIS/ORB E	-112.38459	-19.17702	-2.28782	BASIS/ORB E	-12.41852	-0.45126
1S 46.16090	0.86309	0.02782	-0.00904	0.00202	0.00027	2P 29.44820	-0.13194	0.03111	0.00972	3D 15.67050	0.23157	-0.07078
1S 31.53900	0.15562	0.49100	-0.21589	0.09091	0.02110	2P 19.05910	-0.86963	0.46375	0.18367	3D 8.78548	0.78055	-0.23660
2S 21.40050	-0.10528	-0.12288	-0.66465	0.28398	0.06126	3P 10.31520	-0.03534	-0.75427	-0.30938	4D 5.41999	0.06731	0.25232
2S 19.34870	0.09282	-1.05962	1.39443	-0.59171	-0.13125	3P 7.83910	0.01977	-0.37446	-0.26076	4D 3.32956	-0.01165	0.57706
3S 14.15310	-0.00920	-0.04684	-0.08648	-0.01102	-0.00706	4S 5.46427	-0.00100	-0.00077	-0.03095	-0.75276	-0.22528	
3S 9.52913	0.00304	0.00413	-1.11789	0.67074	0.16515	4S 3.74091	0.00075	0.00062	0.01047	-0.42700	-0.07709	
4S 5.46427	-0.00100	-0.00077	-0.03095	-0.75276	-0.22528	5S 2.67135	-0.00033	-0.00024	-0.00361	-0.01385	0.22788	
4S 3.74091	0.00075	0.00062	0.01047	-0.42700	-0.07709	5S 1.64780	0.00015	0.00011	0.00143	0.00165	0.55161	
5S 1.64780	0.00015	0.00011	0.00143	0.00165	0.55161	5S 1.01924	-0.00005	-0.00003	-0.00045	-0.00012	0.38449	
5S 1.01924	-0.00005	-0.00003	-0.00045	-0.00012	0.38449	4P 5.56514	-0.00477	-0.01184	0.56800	4D 1.78783	0.00283	0.35745
4P 3.69486	0.00211	0.00186	0.55902	4P 2.40205	-0.00054	-0.00082	0.08129	4P 2.40205	-0.00054	-0.00082	0.08129	

RHODIUM K(2)L(8)M(18)4S(2)4P(6)5S(2)4D(7), 4F  
 T.E.= -0.46857892D+04 P.E.= -0.93714856D+04 K.E.= 0.46856563D+04 V.T.= -0.20000198D+01

S	1S	2S	3S	4S	5S	P	2P	3P	4P	D	3D	4D
BASIS/ORB E	-834.20952	-121.74179	-23.05743	-3.66E16	-0.24693	BASIS/ORB E	-112.78920	-19.25072	-2.28782	BASIS/ORB E	-12.41852	-0.45126
1S 46.16090	0.86312	0.02783	-0.00902	-0.00190	0.00008	2P 29.44820	-0.13194	0.03111	0.00972	3D 15.67050	0.23157	-0.07078
1S 31.53900	0.15557	0.49098	-0.21594	-0.09170	0.02355	2P 19.05910	-0.86963	0.46375	0.18367	3D 8.78548	0.78055	-0.23660
2S 21.40050	-0.10484	-0.12262	-0.66467	-0.28275	0.06238	3P 10.31520	-0.03534	-0.75427	-0.30938	4D 5.41999	0.06731	0.25232
2S 19.34870	0.09235	-1.05992	1.39458	0.59200	-0.13863	3P 7.83910	0.01983	-0.37016	-0.26353	4D 3.32956	-0.01165	0.57706
3S 14.15310	-0.00907	-0.04674	-0.08654	0.01256	-0.01029	4S 5.46427	-0.00090	-0.00069	-0.03017	-0.76294	-0.25842	
3S 9.52913	0.00295	0.00406	-1.11806	-0.57667	0.18444	4S 3.74091	0.00061	0.00051	0.00932	0.42385	-0.06493	
4S 5.46427	-0.00090	-0.00069	-0.03017	-0.76294	-0.25842	5S 2.44604	-0.00025	-0.00019	-0.00300	0.00453	0.36787	
5S 2.44604	0.00015	0.00011	0.00159	0.00012	0.55138	5S 1.52450	0.00015	0.00011	0.00159	0.00012	0.55138	
5S 0.99690	-0.00006	-0.00004	-0.00008	-0.00008	0.23120	5S 0.99690	-0.00006	-0.00004	-0.00008	-0.00008	0.23120	

See page 183 for Explanation of Tables and Notes for Tables 32, 42, and 43

TABLE 1 (48). HARTREE-FOCK FUNCTIONS FOR NEUTRAL ATOMS.

P	2P	3P	4P	D	3D	4D
BASIS/ORB E	-112.56220	-19.35612	-2.44063	BASIS/ORB E	-12.59579	-0.61113
2P 29.44820	-0.13192	0.03110	0.00980	3D 15.67050	-0.23104	-0.07434
2P 19.05910	-0.86966	0.46379	0.18529	3D 8.78548	-0.78225	-0.24552
3P 10.31520	-0.03521	-0.75443	-0.31384	4D 5.26085	-0.06943	0.30167
3P 7.83910	0.01965	-0.37005	-0.26222	4D 3.23302	0.01666	0.58420
4P 5.53288	-0.00468	-0.01199	0.58388	4D 1.85255	-0.00458	0.28268
4P 3.67444	0.00206	0.00205	0.56064			
4P 2.35018	-0.00052	-0.00075	0.05982			

PALLADIUM K{2}L{8}M{18}4S{2}14P{6}5S{0}4D{10}, 1S  
T.E.= -0.49379071D+04 P.E.= -0.98756762D+04 K.E.= 0.49377691D+04 V.T.= -0.20300280D+01

S	1S	2S	3S	4S
BASIS/ORB E	-873.31281	-127.96408	-24.20458	-3.58134
1S 47.17760	0.86380	0.02643	-0.00814	-0.00117
1S 32.33280	0.15453	0.49240	-0.21823	-0.09331
2S 21.43550	-0.16870	0.05505	-1.26063	-0.51384
2S 20.13080	0.15729	-1.23058	1.99543	0.82277
3S 14.88960	-0.00977	-0.05335	-0.07270	0.02416
3S 9.83750	0.00285	0.00379	-1.13346	-0.68978
4S 5.67422	-0.00095	-0.00073	-0.03059	0.75458
4S 3.89395	0.00083	0.00068	0.01125	0.40375
4S 2.87094	-0.00033	-0.00025	-0.00382	0.04127

P	2P	3P	4P	D	3D	4D
BASIS/ORB E	-118.52793	-20.36985	-2.32440	BASIS/ORB E	-13.35887	-0.33124
2P 30.03560	-0.13288	0.03084	0.00968	3D 16.11630	0.23017	-0.06849
2P 19.52630	-0.86863	0.46826	0.18704	3D 9.10001	0.78114	-0.23809
3P 10.61360	-0.03590	-0.73861	-0.29731	4D 5.79000	0.06224	0.23909
3P 8.24787	0.02034	-0.38299	-0.28295	4D 3.47691	-0.00726	0.58889
4P 5.80312	-0.00417	-0.01739	0.56281	4D 1.73789	0.00134	0.38367
4P 3.85593	0.00178	0.00331	0.55483			
4P 2.49634	-0.00044	-0.00127	0.09703			

PALLADIUM K{2}L{8}M{18}4S{2}14P{6}5S{1}4D{9}, 3D  
T.E.= -0.49378815D+04 P.E.= -0.98756408D+04 K.E.= 0.49377593D+04 V.T.= -0.20000247D+01

S	1S	2S	3S	4S	5S
BASIS/ORB E	-873.48106	-128.13806	-24.38095	-3.75075	-0.22014
1S 47.17760	0.86381	0.02643	-0.00812	0.00150	0.00001
1S 32.33280	0.15451	0.49240	-0.21828	0.09216	0.02099
2S 21.43550	-0.16841	0.05522	-1.26011	0.53017	0.10471
2S 20.13080	0.15699	-1.23077	1.99492	-0.84174	-0.17223
3S 14.88960	-0.00972	-0.05330	-0.07256	-0.02039	-0.01038
3S 9.83752	0.00281	0.00376	-1.13374	0.68920	0.16429
4S 5.64584	-0.00090	-0.00068	-0.03012	-0.77122	-0.22653
4S 3.84282	0.00064	0.00054	0.00935	-0.41551	-0.05785
5S 2.62554	-0.00029	-0.00022	-0.00325	-0.01155	0.24560
5S 1.66217	0.00016	0.00011	0.00153	0.00182	0.49942
5S 1.05115	-0.00005	-0.00004	-0.00049	-0.00054	0.41064

P	2P	3P	4P	D	3D	4D
BASIS/ORB E	-118.70081	-20.54525	-2.48184	BASIS/ORB E	-13.53280	-0.48835
2P 30.03560	-0.13287	0.03083	0.00973	3D 16.11630	0.22938	-0.07274
2P 19.52630	-0.86865	0.46829	0.18823	3D 9.10001	0.78303	-0.24516
3P 10.61360	-0.03586	-0.73872	-0.29948	4D 5.55936	0.06552	0.28400
3P 8.24787	0.02029	-0.38288	-0.28425	4D 3.42997	-0.01253	0.56690
4P 5.79214	-0.00414	-0.01752	0.57150	4D 1.86178	0.00343	0.33769
4P 3.84224	0.00178	0.00344	0.56106			
4P 2.49146	-0.00044	-0.00123	0.07939			

See page 183 for Explanation of Tables and Notes for Tables 32, 42, and 43

## ROOTHAAN-HARTREE-FOCK ATOMIC WAVEFUNCTIONS

TABLE 1 (49). HARTREE-FOCK FUNCTIONS FOR NEUTRAL ATOMS.

PALLADIUM K(2)L(8)M(18)4S(2)4P(6)5S(2)4D(8),3F						
T.E.= -0.49377709D+04 P.E.= -0.98754328D+04 K.E.= 0.49376619D+04 V.T.= -0.20000221D+01						
S	1S	2S	3S	4S	5S	
BASIS/ORB E	-873.66372	-128.32862	-24.57224	-3.92718	-0.25349	
1S 47.17760	0.86383	0.02644	-0.00811	-0.00133	-0.00016	
1S 32.33280	0.15447	0.49239	-0.21833	-0.09405	0.02395	
2S 21.43550	-0.16777	0.05567	-1.26068	-0.52654	0.11098	
2S 20.13080	0.15631	-1.23127	1.99566	0.83548	-0.18646	
3S 14.88960	-0.00961	-0.05220	-0.07274	0.02244	-0.01378	
3S 9.83752	0.00274	0.00371	-1.13384	-0.69564	0.18757	
4S 5.64584	-0.00082	-0.00062	-0.02949	0.78261	-0.26391	
4S 3.84828	0.00054	0.00046	0.00850	0.41028	-0.05217	
5S 2.46530	-0.00022	-0.00016	-0.02624	0.00281	0.39721	
5S 1.51096	0.00013	0.00010	0.00142	0.00050	0.55445	
5S 0.98781	-0.00005	-0.00004	-0.00054	-0.00022	0.19650	
P	2P	3P	4P	D	3D	4D
BASIS/ORB E	-118.88981	-20.73510	-2.64263	BASIS/ORB E	-13.72079	-0.65717
2P 30.03230	-0.13290	0.03076	0.00971	3D 16.06610	-0.23244	-0.07698
2P 19.52700	-0.86855	0.46847	0.18993	3D 9.07378	-0.78260	-0.25306
3P 10.65990	-0.03586	-0.70566	-0.29045	4D 5.42837	-0.06402	0.33334
3P 8.35200	0.01989	-0.41073	-0.29267	4D 3.32363	0.01498	0.57654
4P 5.73125	-0.00368	-0.01969	0.59171	4D 1.91117	-0.00429	0.26312
4P 3.80564	0.00161	0.00439	0.55559			
4P 2.42822	-0.00039	-0.00132	0.05676			
SILVER	K(2)L(8)M(18)4S(2)4P(6)5S(1)4D(10),2S					
T.E.= -0.51976852D+04 P.E.= -0.103951980+05 K.E.= 0.51975130D+04 V.T.= -0.20300331D+01						
S	1S	2S	3S	4S	5S	
BASIS/ORB E	-913.83799	-134.881C3	-25.91889	-4.00076	-0.21972	
1S 48.27140	0.85321	0.01541	0.00405	-0.00037	-0.00019	
1S 34.04940	0.16287	0.48955	0.21698	-0.09248	0.01987	
2S 21.93670	-0.28452	1.81227	3.45888	-1.55C34	0.31024	
2S 21.32090	0.27326	-2.97601	-4.17359	1.86019	-0.37499	
3S 14.14920	-0.00757	-0.05501	0.04946	0.04C19	-0.01483	
3S 10.13800	0.00328	0.01094	1.13958	-0.71940	0.16544	
4S 5.87182	-0.00088	-0.00178	0.02993	0.77034	-0.21760	
4S 3.98770	0.00058	0.00118	-0.00847	0.42464	-0.05567	
5S 2.66401	-0.00024	-0.00045	0.00277	0.01133	0.25280	
5S 1.65008	0.00013	0.00024	-0.00132	-0.00164	0.51023	
5S 1.04186	-0.00005	-0.00008	0.00044	0.00C74	0.39485	
P	2P	3P	4P	D	3D	4D
BASIS/ORB E	-125.18357	-21.94657	-2.67611	BASIS/ORB E	-14.67909	-0.53667
2P 30.61540	-0.13383	0.03049	0.00947	3D 16.46200	0.23488	-0.07446
2P 19.99580	-0.86745	0.47268	0.19286	3D 9.36028	0.78019	-0.25709
3P 11.00880	-0.03675	-0.65496	-0.26069	4D 5.93684	0.05511	0.29070
3P 8.86584	0.02046	-0.46200	-0.32251	4D 3.53384	-0.00618	0.60532
4P 5.90958	-0.00291	-0.02649	0.59654	4D 1.88607	0.00117	0.30158
4P 3.92436	0.00130	0.00687	0.53658			
4P 2.55069	-0.00032	-0.00213	0.07101			
SILVER	K(2)L(8)M(18)4S(2)4P(6)5S(2)4D(9),2D					
T.E.= -0.51975029D+04 P.E.= -0.10394903D+05 K.E.= 0.51973999D+04 V.T.= -0.20000198D+01						
S	1S	2S	3S	4S	5S	
BASIS/ORB E	-914.03294	-135.08352	-26.12256	-4.18897	-0.25924	
1S 48.27140	0.85323	0.01542	-0.00405	-0.00017	-0.00048	
1S 34.04940	0.16284	0.48953	-0.21702	-0.09341	0.02345	
2S 21.93670	-0.28353	1.81339	-3.46001	-1.54579	0.34035	
2S 21.32090	0.27225	-2.97719	4.17487	1.85712	-0.41472	
3S 14.14920	-0.00747	-0.05465	-0.04966	0.04288	-0.02049	
3S 10.13800	0.00321	0.01C81	-1.13961	-0.72693	0.19573	
4S 5.87182	-0.00081	-0.00166	-0.02943	0.78256	-0.26288	
4S 3.98770	0.00050	0.00103	0.00782	0.41854	-0.04906	
5S 2.51063	-0.00019	-0.00036	-0.00232	0.00320	0.41076	
5S 1.51827	0.00011	0.00021	0.00125	0.00006	0.55965	
5S 0.98459	-0.00004	-0.00008	-0.00048	-0.00005	0.17806	

See page 183 for Explanation of Tables and Notes for Tables 32, 42, and 43

TABLE 1 (50). HARTREE-FOCK FUNCTIONS FOR NEUTRAL ATOMS.

P	2P	3P	4P	D	3D	4D
BASIS/ORB E	-125.38460	-22.14672	-2.64759	BASIS/ORB E	-14.87921	-0.70637
2P 30.61540	-0.13382	0.03049	0.01081	3D 16.46200	-0.23358	-0.07980
2P 19.99580	-0.86748	0.47271	0.19155	3D 9.36028	-0.78364	-0.25896
3P 11.00880	-0.03661	-0.65508	-0.22928	4D 5.51852	-0.05911	0.38627
3P 8.86584	0.02029	-0.46195	-0.37499	4D 3.32364	0.01438	0.56720
4P 5.94295	-0.00268	-0.02549	0.67069	4D 1.92368	-0.00457	0.22241
4P 3.66775	0.00121	0.00645	0.54966			
4P 2.57495	-0.00042	-0.00257	-0.00236			

CADMIUM K(2)L(8)M(18)4S(2)4P(6)5S(2)4D(10),1S  
T.E.= -0.54650722D+04 P.E.= -0.10929188D+05 K.E.= 0.54641159D+04 V.T.= -0.20001750D+01

S	1S	2S	3S	4S	5S
BASIS/ORB E	-955.36086	-142.06579	-27.73669	-4.45149	-0.26500
1S 49.23600	0.86581	0.03257	-0.01227	-0.00350	0.00006
1S 33.05620	0.15625	0.49876	-0.22108	-0.05634	0.02428
2S 23.46380	-0.10878	-0.02627	-0.62069	-0.27657	0.05165
2S 21.02170	0.09218	-1.16538	1.35240	0.59663	-0.12614
3S 14.73870	-0.01008	-0.05725	-0.03310	0.05511	-0.02625
3S 10.45450	0.00412	0.01172	-1.15754	-0.74768	0.20087
4S 6.08432	-0.00103	-0.00223	-0.02824	0.78190	-0.26528
4S 4.13285	0.00061	0.00136	0.00644	0.42395	-0.03745
5S 2.48431	-0.00021	-0.00046	-0.00168	0.00409	0.46040
5S 1.46842	0.00013	0.00029	0.00096	-0.00053	0.54846
5S 0.97250	-0.00006	-0.00013	-0.00040	0.00017	0.13333

P	2P	3P	4P	D	3D	4D
BASIS/ORB E	-132.10352	-23.62612	-3.05432	BASIS/ORB E	-16.10029	-0.76357
2P 31.22510	-0.13405	0.02966	0.00951	3D 16.76950	0.26158	-0.09052
2P 20.47030	-0.86694	0.47797	0.19809	3D 9.29293	0.78571	-0.26251
3P 11.48860	-0.03642	-0.53438	-0.19508	4D 5.52892	0.00683	0.48577
3P 9.46699	0.01955	-0.58057	-0.39801	4D 3.19716	0.01135	0.54271
4P 6.02421	-0.00198	-0.03359	0.65712	4D 1.85909	-0.00522	0.16015
4P 3.97808	0.00123	0.01488	0.44871			
4P 3.17360	-0.00049	-0.00691	0.09355			

INDIUM K(2)L(8)M(18)4S(2)4P(6)5S(2)4D(10)5P(1),2P  
T.E.= -0.57401570D+04 P.E.= -0.11480219D+05 K.E.= 0.57400617D+04 V.T.= -0.20000166D+01

S	1S	2S	3S	4S	5S
BASIS/ORB E	-997.79915	-149.39500	-29.62430	-4.97642	-0.37247
1S 51.54130	0.68966	0.00637	0.01992	0.00732	-0.00289
1S 39.87640	0.33380	0.42568	0.16143	-0.09231	0.02621
2S 33.32180	-0.03659	0.21484	0.17298	-0.03719	0.00769
2S 23.91180	0.01539	-1.09387	-0.61974	0.21817	-0.05563
3S 20.59930	-0.00358	-0.25842	-0.26956	0.18834	-0.05530
3S 10.91620	0.00040	-0.00484	1.20459	-0.73739	0.21149
4S 6.09269	-0.00025	0.00168	0.04834	0.85938	-0.29992
4S 3.99176	0.00028	-0.00158	-0.02795	0.36057	-0.08229
5S 3.34341	-0.00019	0.00101	0.01503	-0.03686	0.22314
5S 2.16245	0.00007	-0.00037	-0.00474	0.00921	0.57994
5S 1.34820	-0.00002	0.00010	0.00124	-0.00212	0.36972

P	2P	3P	4P	5P	D	3D	4D
BASIS/ORB E	-139.17047	-25.37401	-3.50707	-0.19709	BASIS/ORB E	-17.58918	-1.06301
2P 30.25110	0.18582	-0.04630	0.01563	-0.00266	3D 17.48610	-0.22219	-0.08085
2P 20.51010	0.82208	-0.47317	0.20165	-0.04107	3D 10.04430	-0.79160	-0.28228
3P 11.80560	0.01213	0.60312	-0.23651	0.05254	4D 5.99670	-0.05960	0.40630
3P 9.54601	-0.00107	0.52528	-0.38218	0.07303	4D 3.68324	0.01615	0.56839
4P 6.32791	-0.00196	0.02725	0.62892	-0.13994	4D 2.22477	-0.00457	0.19205
4P 4.19372	0.00137	-0.00687	0.55232	-0.13391			
5P 3.04380	-0.00060	0.00244	0.02880	0.17634			
5P 1.69398	0.00029	-0.00080	0.00185	0.60102			
5P 0.99207	-0.00008	0.00028	-0.00028	0.40498			

See page 183 for Explanation of Tables and Notes for Tables 32, 42, and 43

## ROOTHAAAN-HARTREE-FOCK ATOMIC WAVEFUNCTIONS

TABLE 1 (51). HARTREE-FOCK FUNCTIONS FOR NEUTRAL ATOMS.

TIN K(2)L(8)M(18)4S(2)4P(6)5S(2)4D(10)5P(2),3P  
 T.E.= -0.60229220D+04 P.E.= -0.12045784D+05 K.E.= 0.60228622D+04 V.T.= -0.20000099D+01

	1S	2S	3S	4S	5S
BASIS/ORB E	-1041.22246	-156.97756	-31.59897	-5.51246	-0.47635
1S 51.24680	0.86794	0.02601	-0.00917	-0.00179	0.00011
1S 34.83590	0.15221	0.50368	-0.22572	-0.10183	0.03050
2S 24.80250	-0.08713	-0.03064	-0.52275	-0.23112	0.06165
2S 21.88120	0.07211	-1.16236	1.25758	0.56002	-0.15719
3S 15.46340	-0.00947	-0.05107	0.00855	0.09440	-0.03936
3S 11.12930	0.00410	0.00582	-1.19334	-0.81085	0.26268
4S 6.54571	-0.00119	-0.00176	-0.03711	0.75650	-0.30750
4S 4.60056	0.00082	0.00123	0.01165	0.45490	-0.10069
5S 3.04899	-0.00034	-0.00048	-0.00364	0.00540	0.42410
5S 1.98832	0.00021	0.00029	0.00201	-0.00020	0.53970
5S 1.33764	-0.00008	-0.00011	-0.00068	0.00013	0.18408

	2P	3P	4P	5P	D	3D	4D
BASIS/ORB E	-146.48852	-27.20901	-3.96903	-0.26498	BASIS/ORB E	-19.16337	-1.36905
2P 32.40500	0.13594	0.02578	-0.00945	-0.00220	3D 18.08490	-0.21195	-0.07987
2P 21.39340	0.86581	0.48457	-0.20942	-0.04885	3D 10.42740	-0.79714	-0.29974
3P 11.60720	0.03802	-0.79049	0.31227	0.06630	4D 6.32865	-0.06387	0.39274
3P 9.53813	-0.02353	-0.32592	0.33166	0.09376	4D 3.95998	0.01730	0.58769
4P 6.69982	0.00312	-0.02114	-0.61022	-0.18763	4D 2.43189	-0.00475	0.17966
4P 4.42649	-0.00105	0.00632	-0.59925	-0.12451			
5P 2.68092	0.00027	-0.00212	-0.02215	0.33186			
5P 1.66952	-0.00015	0.00130	0.00368	0.56925			
5P 1.07438	0.00006	-0.00048	-0.00125	0.24890			

ANTIMONY K(2)L(8)M(18)4S(2)4P(6)5S(2)4D(10)5P(3),4S  
 T.E.= -0.63134755D+04 P.E.= -0.12626867D+05 K.E.= 0.63133915D+04 V.T.= -0.20000133D+01

	1S	2S	3S	4S	5S
BASIS/ORB E	-1085.58854	-164.75823	-33.63648	-6.06325	-0.58172
1S 52.29670	0.86330	0.01937	-0.00764	-0.00114	-0.00016
1S 36.20580	0.15526	0.50197	-0.22350	-0.10212	0.03259
2S 25.71070	-0.07402	0.00546	-0.54484	-0.24575	0.07002
2S 22.55570	0.05984	-1.26797	1.27093	0.57541	-0.17174
3S 15.58310	-0.00834	-0.05240	0.04021	0.12287	-0.05298
3S 11.47010	0.00398	0.01161	-1.21742	-0.85090	0.29518
4S 6.78464	-0.00114	-0.00182	-0.03927	0.74241	-0.32558
4S 4.84462	0.00077	0.00122	0.01231	0.47295	-0.11697
5S 3.16711	-0.00031	-0.00044	-0.00347	0.00678	0.48369
5S 2.07061	0.00020	0.00027	0.00200	-0.00075	0.52328
5S 1.42099	-0.00007	-0.00010	-0.00070	0.00035	0.14041

	2P	3P	4P	5P	D	3D	4D
BASIS/ORB E	-154.00335	-29.10637	-4.44479	-0.33467	BASIS/ORB E	-20.79840	-1.68795
2P 33.03150	0.13557	0.62906	-0.00927	-0.00242	3D 18.49620	-0.21216	-0.08297
2P 21.87460	0.86582	0.48854	-0.21481	-0.05549	3D 10.72730	-0.79764	-0.31179
3P 11.96880	0.04245	-0.68889	0.23840	0.05008	4D 6.51769	-0.06093	0.42124
3P 10.26190	-0.02726	-0.42290	0.40998	0.12884	4D 4.09028	0.01660	0.59520
4P 6.89427	0.00222	-0.03555	-0.60342	-0.20961	4D 2.53196	-0.00452	0.13979
4P 4.63326	-0.00075	0.00927	-0.60017	-0.13867			
5P 2.79439	0.00016	-0.00289	-0.01976	0.40191			
5P 1.76190	-0.00009	0.00185	0.00377	0.56336			
5P 1.16248	0.00003	-0.00070	-0.00113	0.17854			

TELLURIUM K(2)L(8)M(18)4S(2)4P(6)5S(2)4D(10)5P(4),3P  
 T.E.= -0.66117748D+04 P.E.= -0.13223469D+05 K.E.= 0.66116943D+04 V.T.= -0.20000122D+01

	1S	2S	3S	4S	5S
BASIS/ORB E	-1130.91649	-172.75583	-35.75517	-6.64708	-0.70051
1S 53.30360	0.86565	0.02046	0.00798	-0.00145	0.00002
1S 36.73090	0.15343	0.50474	0.22599	-0.10429	0.03485
2S 26.32940	-0.07363	0.06342	0.51512	-0.23842	0.07290
2S 22.99520	0.05884	-1.25086	-1.24602	0.57522	-0.18253
3S 15.68090	-0.00904	-0.05401	-0.06539	0.14987	-0.06577
3S 11.81490	0.00470	0.01466	1.24125	-0.89185	0.32633
4S 7.00022	-0.00134	-0.00241	0.04294	0.74034	-0.34170
4S 5.06510	0.00094	0.00166	-0.01459	0.47870	-0.13619
5S 3.35991	-0.00038	-0.00062	0.00416	0.00727	0.49466
5S 2.24531	0.00025	0.00039	-0.00243	-0.00069	0.50924
5S 1.56178	-0.00009	-0.00014	0.00082	0.00040	0.14903

See page 183 for Explanation of Tables and Notes for Tables 32, 42, and 43

TABLE 1 (52). HARTREE-FOCK FUNCTIONS FOR NEUTRAL ATOMS.

P	2P	3P	4P	5P	D	3D	4D
BASIS/ORB E	-161.73407	-31.08428	-4.95263	-0.35979	BASIS/ORB E	-22.51278	-2.03837
2P 33.61480	0.13646	0.02892	-0.00925	-0.00256	3D 19.01070	-0.20691	-0.08333
2P 22.33970	0.86508	0.4920C	-C.22003	-0.06108	3D 11.07400	-0.80067	-0.32504
3P 12.13790	0.04592	-0.73999	0.23812	0.05069	4D 6.78484	-0.06239	0.42109
3P 10.60150	-0.03121	-C.36618	0.42691	0.14705	4D 4.32877	0.01730	0.60165
4P 7.18478	0.00220	-0.04487	-0.58604	-0.22060	4D 2.71371	-0.00457	0.13026
4P 4.88471	-0.00070	0.01C84	-0.62258	-0.16305			
5P 2.97927	0.00013	-0.00316	-0.02040	0.43602			
5P 1.87617	-0.00006	0.00155	0.00313	0.54689			
5P 1.22654	0.00002	-0.00072	-0.00118	0.17212			
<b>IODINE</b> K(2)L(8)M(18)4S(2)4P(6)5S(2)4D(10)5P(5),2P							
T.E.= -0.69179727D+04	P.E.= -0.13835882D+05	K.E.= 0.69179098D+04	V.T.= -0.20000091D+01				
S	1S	2S	3S	4S	5S		
BASIS/ORB E	-1177.18523	-180.94951	-37.93448	-7.24439	-0.82107		
1S 54.36390	0.86126	0.01765	0.00837	0.00162	0.00021		
1S 37.74000	0.15804	0.50429	0.22392	0.10461	0.03616		
2S 27.61050	-0.06219	0.08968	0.43590	0.20465	0.06726		
2S 23.54300	0.04662	-1.27320	-1.15839	-0.54189	-0.18201		
3S 15.58780	-0.00954	-0.06038	-0.15019	-0.22E57	-0.09791		
3S 12.25910	0.00584	0.02196	1.31242	0.97929	0.37340		
4S 7.32866	-0.00164	-0.00355	0.05294	-0.66288	-0.31712		
4S 5.44922	0.00118	0.00246	-0.01960	-0.55328	-0.19780		
5S 3.65514	-0.00046	-0.00C87	0.00521	-0.01661	0.44715		
5S 2.50677	0.00029	0.00053	-0.00294	0.00329	0.53230		
5S 1.72722	-0.00009	-0.00017	0.00089	-0.00117	0.18598		
P	2P	3P	4P	5P	D	3D	4D
BASIS/ORB E	-169.65990	-33.12224	-5.47339	-0.40313	BASIS/ORB E	-24.28594	-2.40128
2P 34.23150	0.13634	0.02843	-0.00924	-0.00269	3D 19.61210	-0.19762	-0.08133
2P 22.81720	0.86504	0.49543	-0.22471	-0.06630	3D 11.45840	-0.80541	-0.33938
3P 12.34330	0.05825	-0.71406	0.13850	0.01473	4D 7.12795	-0.06695	0.39632
3P 11.20990	-0.04344	-0.39019	0.53800	0.19920	4D 4.64351	0.01855	0.61735
4P 7.49817	0.00182	-0.05302	-0.55045	-0.22156	4D 2.93955	-0.00465	0.13703
4P 5.16592	-0.00052	0.01321	-0.65717	-0.19441			
5P 3.17551	0.00005	-0.00360	-0.02336	0.45661			
5P 2.00372	-0.00001	0.00216	0.00330	0.54348			
5P 1.30484	0.00000	-0.00077	-0.00149	0.16224			
<b>XENON</b> K(2)L(8)M(18)4S(2)4P(6)5S(2)4D(10)5P(6),1S							
T.E.= -0.72321302D+04	P.E.= -0.14464177D+05	K.E.= 0.7232C470D+04	V.T.= -0.20003115D+01				
S	1S	2S	3S	4S	5S		
BASIS/ORB E	-1224.39718	-189.34093	-40.17583	-7.85620	-0.94433		
1S 55.30720	0.87059	0.02107	-0.00868	0.00237	0.00070		
1S 37.80730	0.14926	0.51209	-0.23044	0.10784	0.03815		
2S 27.92970	-0.06259	-0.01873	-0.38195	0.19149	0.06768		
2S 23.69210	0.04643	-1.18386	1.12481	-0.54498	-0.19267		
3S 15.03530	-0.01383	-0.06502	0.23955	-0.35456	-0.15274		
3S 12.67230	0.01030	0.03432	-1.41092	1.13006	C.44776		
4S 7.60195	-0.00254	-0.00469	-0.06111	-0.63451	-0.30543		
4S 5.73899	0.00201	0.00352	0.02591	-0.58291	-0.24664		
5S 4.17583	-0.00085	-0.00136	-0.00759	-0.02272	0.27675		
5S 2.99772	0.00045	0.00C69	0.00353	0.00218	0.59862		
5S 1.98532	-0.00011	-0.00C17	-0.00076	-0.00092	0.30408		
P	2P	3P	4P	5P	D	3D	4D
BASIS/ORB E	-177.78252	-35.22174	-6.00824	-0.45719	BASIS/ORB E	-26.11939	-2.77780
2P 34.88440	0.13527	0.02765	-0.00908	-0.00277	3D 20.08240	-0.19493	-0.08265
2P 23.30470	0.86575	0.49883	-0.22945	-0.07C54	3D 11.78600	-0.80743	-0.34860
3P 12.54120	0.11362	-0.48416	-0.34216	-0.18148	4D 7.30842	-0.06830	0.40928
3P 12.02300	-0.09833	-0.61656	1.02476	0.40692	4D 4.88400	0.02129	0.59391
4P 7.72390	0.00123	-0.05586	-0.53369	-0.22741	4D 3.19850	-0.00536	0.14481
4P 5.40562	-0.00028	0.01605	-0.67016	-0.21144			
5P 3.32661	-0.00003	-0.00407	-0.02313	0.49354			
5P 2.09341	0.00004	0.00238	0.00433	0.53529			
5P 1.36686	-0.00002	-0.00087	-0.00136	0.13666			

See page 183 for Explanation of Tables and Notes for Tables 32, 42, and 43

## ROOTHAAN-HARTREE-FOCK ATOMIC WAVEFUNCTIONS

TABLE 2 (1). HARTREE-FOCK FUNCTIONS FOR POSITIVE IONS.

LITHIUM 1S(2),1S  
 T.E.= -0.72364140D+01  
 P.E.= -0.14472633D+02  
 K.E.= 0.72362190D+01  
 V.T.= -0.20000269D+01

S	1S
BASIS/ORB E	-2.79238
1S	2.46376
1S	4.70359
1S	6.46694
1S	1.35790
	0.89459
	0.11839
	-0.00232
	0.00445

BERYLLIUM 1S(2)2S(1), 3-2S  
 T.E.= -0.14277391D+02 P.E.= -0.26555234D+02  
 K.E.= 0.14277843D+02 V.T.= -0.19999684D+01

S	1S	2S
BASIS/ORB E	-5.13829	-0.66615
1S	3.49771	0.92264
1S	6.50227	0.07879
2S	1.18383	0.00052
2S	2.62771	0.01148
		-0.20462
		-0.01566
		1.1C808
		-0.13290

BORON 1S(2)2S(2), 4-1S  
 T.E.= -0.24237566D+02 P.E.= -0.4E474924D+02  
 K.E.= 0.24237358D+02 V.T.= -0.20000086D+01

S	1S	2S
BASIS/ORB E	-8.18593	-0.87381
1S	4.42994	0.92801
1S	7.86336	0.08063
2S	1.59241	0.00320
2S	4.01022	-0.00081
2S	1.25021	-0.00198
		-0.20288
		-0.01942
		0.73490
		-0.09218
		0.34527

CARBON 1S(2)2S(2)2P(1), 5-2P  
 T.E.= -0.37292215D+02 P.E.= -0.74584349D+02  
 K.E.= 0.37292134D+02 V.T.= -0.20000022D+01

S	1S	2S	P	2P
BASIS/ORB E	-11.89824	-1.15375	BASIS/ORB E	-0.90476
1S	5.54099	0.92321	2P	1.87782
1S	9.68937	0.06002	2P	3.07800
2S	2.14468	0.00270	2P	1.39268
2S	4.96979	0.02758	2P	0.51189
2S	1.56842	-0.00102	2P	7.01117
		0.60483		0.00780

NITROGEN 1S(2)2S(2)2P(2), 6-3P  
 T.E.= -0.53887988D+02 P.E.= -0.1C777559D+03  
 K.E.= 0.53887603D+02 V.T.= -0.20000071D+01

S	1S	2S	P	2P
BASIS/ORB E	-16.28455	-1.46247	BASIS/ORB E	-1.11006
1S	6.42321	0.91648	2P	1.97595
1S	10.61430	0.07678	2P	3.38577
2S	2.53445	0.00539	2P	1.47888
2S	6.15603	0.01393	2P	8.00193
2S	1.79167	-0.00200	2P	0.00884
		0.56449		

OXYGEN 1S(2)2S(2)2P(3), 7-4S  
 T.E.= -0.74372598D+02 P.E.= -0.14E74491D+03  
 K.E.= 0.74372308D+02 V.T.= -0.20000039D+01

S	1S	2S	P	2P
BASIS/ORB E	-21.34632	-1.80C78	BASIS/ORB E	-1.32692
1S	7.63820	0.92666	2P	2.24453
1S	13.11140	0.04270	2P	3.84166
2S	3.20134	0.00319	2P	1.64132
2S	6.68310	0.04204	2P	8.59404
2S	2.10186	-0.00041	2P	0.01072
		0.68872		

See page 183 for Explanation of Tables and Notes for Tables 32, 42, and 43

TABLE 2 (2). HARTREE-FOCK FUNCTIONS FOR POSITIVE IONS.

FLUORINE	1S{2}2S{2}2P{4}, 8-3P					
T.E.=	-0.98831699D+02	P.E.=	-0.15766275D+03			
K.E.=	0.98831054D+02	V.T.=	-0.2000C0065D+01			
S	1S	2S	P	2P		
BASIS/ORB E	-27.14132	-2.19484	BASIS/ORB E	-1.44410		
1S 8.61501	0.93580	-0.23141	2P 2.33167	0.60326		
1S 14.80480	0.03872	-0.00618	2P 4.24798	0.29135		
2S 3.74689	0.00360	0.42C22	2P 1.64224	0.16094		
2S 7.35807	0.03539	-0.11425	2P 9.53227	0.01107		
2S 2.36945	-0.00032	0.70036				
NEDN	1S{2}2S{2}2P{5}, 9-2P					
T.E.=	-0.12781777D+03	P.E.=	-0.25563410D+03			
K.E.=	0.12781633D+03	V.T.=	-0.20000113D+01			
S	1S	2S	P	2P		
BASIS/ORB E	-33.61233	-2.61911	BASIS/ORB E	-1.60658		
1S 9.86116	0.91448	-0.22341	2P 2.57103	0.58722		
1S 16.78310	0.03022	-0.00647	2P 4.72364	0.30522		
2S 3.87930	0.00507	0.52587	2P 1.75238	0.16718		
2S 8.83998	0.06892	-0.10559	2P 9.81100	0.01385		
2S 2.52757	-0.00107	0.57763				
SODIUM	1S{2}2S{2}2P{6}, 10-1S					
T.E.=	-0.16167692D+03	P.E.=	-0.32335484D+03			
K.E.=	0.16167793D+03	V.T.=	-0.19999938D+01			
S	1S	2S	P	2P		
BASIS/ORB E	-40.75964	-3.07365	BASIS/ORB E	-1.79715		
1S 9.60854	1.04471	-0.23717	2P 2.89481	0.54279		
1S 16.19560	0.06184	-0.02342	2P 5.26509	0.30481		
2S 4.38717	0.00584	0.48735	2P 1.95889	0.21629		
2S 10.20650	-0.11882	-0.07038	2P 10.69400	0.01413		
2S 2.81650	-0.00106	0.61604				
MAGNESIUM	K{2}L{8}3S{1} - 2S					
T.E.=	-0.19937151D+03	P.E.=	-0.39874194D+03			
K.E.=	0.19937042D+03	V.T.=	-0.20000C055D+01			
S	1S	2S	3S	P	2P	
BASIS/ORB E	-49.35642	-4.08567	-0.54128	BASIS/ORB E	-2.60298	
1S 12.16010	0.89679	-0.22539	0.05115	2P 2.83019	0.60377	
1S 19.88220	0.02391	-0.00661	0.00160	2P 5.12522	0.42107	
2S 4.52530	0.00483	0.83C69	-0.20582	2P 9.56577	0.04058	
2S 10.93280	0.09625	-0.11655	0.02873			
3S 1.41355	0.00054	-0.00C77	0.65000			
3S 1.06321	-0.00035	0.00129	0.40655			
3S 3.55363	-0.00115	0.29691	-0.09583			
ALUMINUM	K{2}L{8}3S{2} - 1S					
T.E.=	-0.24167433D+03	P.E.=	-0.48334741D+03			
K.E.=	0.24167309D+03	V.T.=	-0.20000051D+01			
S	1S	2S	3S	P	2P	
BASIS/ORB E	-58.81218	-5.21754	-0.65209	BASIS/ORB E	-3.52263	
1S 13.41920	0.87459	-0.22161	0.05386	2P 3.28098	0.60412	
1S 20.82510	0.02490	-0.00597	0.00304	2P 5.69821	0.41354	
2S 4.83620	0.00538	0.88725	-0.24286	2P 10.42940	0.04012	
2S 12.17030	0.12018	-0.12545	0.03467			
3S 1.77513	0.00069	-0.00308	0.55460			
3S 1.25381	-0.00038	0.00148	0.52628			
3S 3.88799	-0.00171	0.23144	-0.09809			
SILICON	K{2}L{8}3S{2}3P{1} - 2P					
T.E.=	-0.28857288D+03	P.E.=	-0.5713930D+03	K.E.=	0.28856642D+03	
V.T.=	-0.20000224D+01					
S	1S	2S	3S	P	2P	3P
BASIS/ORB E	-69.17485	-6.51253	-0.83853	BASIS/ORB E	-4.60963	-0.58590
1S 14.37600	0.88733	-0.23583	0.06283	2P 5.78133	0.67042	-0.16576
1S 22.84810	0.02220	-0.00611	0.00225	2P 11.00520	0.04869	-0.01132
2S 5.03531	0.00541	0.99217	-0.29911	3P 1.70780	0.00819	0.61271
2S 13.04660	0.10842	-0.12132	0.03699	3P 1.14775	-0.00222	0.44999
2S 2.34292	0.00171	-0.02360	0.47721	3P 4.27372	0.35965	-0.08952
3S 1.51148	-0.00057	0.00590	0.68147			
3S 3.68465	-0.00279	0.13132	-0.14132			

See page 183 for Explanation of Tables and Notes for Tables 32, 42, and 43

## ROOTHAAN-HARTREE-FOCK ATOMIC WAVEFUNCTIONS

TABLE 2 (3). HARTREE-FOCK FUNCTIONS FOR POSITIVE IONS.

PHOSPHORUS K(2)L(8)3S(2)3P(2) -3P						
T.E.= -0.34034959D+03 P.E.= -0.68C69365D+03 K.E.= 0.34034406D+03 V.T.= -0.20000163D+01						
S	1S	2S	3S	P	2P	3P
BASIS/ORB E	-80.38155	-7.91509	-1.03401	BASIS/ORB E	-5.80262	-0.72003
1S 15.29030	0.90282	-0.24446	0.06967	2P 6.46199	0.66290	-0.17746
1S 24.54860	0.02003	-0.00585	0.00208	2P 12.31770	0.03698	-0.00971
2S 5.68698	0.00496	0.93148	-0.29598	3P 2.02237	0.00931	0.58876
2S 13.77400	0.09302	-0.12784	0.04078	3P 1.34371	-0.00224	0.48308
3S 2.40272	0.00062	0.00160	0.60037	3P 4.84290	0.37205	-0.10429
3S 1.62738	-0.00029	-0.00011	0.51897			
3S 4.76941	-0.00182	0.18734	-0.12664			
SULFUR K(2)L(8)3S(2)3P(3) -4S						
T.E.= -0.39717296D+03 P.E.= -0.79434200D+03 K.E.= 0.39716904D+03 V.T.= -0.20000099D+01						
S	1S	2S	3S	P	2P	3P
BASIS/ORB E	-92.43411	-9.42767	-1.24006	BASIS/CRB E	-7.10393	-0.86169
1S 16.61110	0.87854	-0.23309	0.06764	2P 6.87921	0.68387	-0.19398
1S 24.51550	0.02262	-0.01175	0.00501	2P 12.94140	0.04332	-0.01134
2S 6.02289	0.00411	0.97585	-0.32790	3P 2.33228	0.00627	0.57242
2S 15.00660	0.11829	-0.14C80	0.04816	3P 1.53607	-0.00094	0.50786
3S 2.72748	0.00037	0.00C85	0.60312	3P 5.26386	0.34162	-0.10538
3S 1.82072	-0.00015	0.00051	0.53665			
3S 5.04320	-0.00137	0.13894	-0.12860			
CHLORINE K(2)L(8)3S(2)3P(4) - 3P						
T.E.= -0.45904841D+03 P.E.= -0.91809217D+03 K.E.= 0.45904376D+03 V.T.= -0.20000101D+01						
S	1S	2S	3S	P	2P	3P
BASIS/ORB E	-105.36099	-11.07623	-1.47010	BASIS/ORB E	-8.53913	-0.93879
1S 16.41090	0.91179	-0.26596	-0.08505	2P 7.49526	0.67402	-0.19950
1S 23.56000	0.06669	-0.01276	-0.00283	2P 13.71160	0.04201	-0.01120
2S 7.13038	0.00610	0.82157	0.27571	3P 2.64828	0.00879	0.57298
2S 14.87010	0.02736	-0.12810	-0.04157	3P 1.65706	-0.00104	0.52126
3S 2.93941	0.00050	0.00866	-0.63782	3P 5.82970	C.34845	-0.11454
3S 1.97300	-0.00025	-0.00165	-0.49262			
3S 6.16710	-0.00208	0.32495	0.19392			
ARGON K(2)L(8)3S(2)3P(5) - 2P						
T.E.= -0.52627435D+03 P.E.= -0.10525452D+04 K.E.= 0.52627086D+03 V.T.= -0.20000066D+01						
S	1S	2S	3S	P	2P	3P
BASIS/ORB E	-119.13381	-12.83628	-1.71135	BASIS/ORB E	-10.08383	-1.04543
1S 18.25010	0.92239	0.26244	0.08447	2P 7.95043	0.68234	-0.20940
1S 29.44590	0.01582	0.00433	0.00137	2P 14.19760	0.04695	-0.01291
2S 7.26099	0.00286	-0.90535	-0.31873	3P 2.95647	0.00922	0.57519
2S 16.15690	0.07578	0.14294	0.04957	3P 1.79986	-0.00048	0.52964
3S 3.29566	0.00003	-0.00758	0.61185	3P 6.30014	0.33055	-0.11664
3S 2.18528	-0.00003	0.00072	0.53681			
3S 6.40657	-0.00068	-0.22485	-0.17615			
POTASSIUM K(2)L(8)3S(2)3P(6) - 1S						
T.E.= -0.59901730D+03 P.E.= -0.11980285D+04 K.E.= 0.59901120D+03 V.T.= -0.20000102D+01						
S	1S	2S	3S	P	2P	3P
BASIS/ORB E	-133.75338	-14.70914	-1.96444	BASIS/ORB E	-11.73922	-1.17109
1S 18.98260	0.93931	-0.27701	0.08889	2P 8.61735	0.67152	-0.20999
1S 31.39050	0.01789	-0.00171	0.00173	2P 15.19580	0.04224	-0.01178
2S 7.30079	0.00420	1.04665	-0.39368	3P 3.24817	0.01009	0.58221
2S 16.70010	0.05305	-0.13733	0.05415	3P 1.94563	-0.00196	0.52976
3S 3.88331	0.00135	-0.00664	0.64114	3P 6.88378	0.34429	-0.12638
3S 2.40881	-0.00037	0.00268	0.61485			
3S 5.70995	-0.00255	0.08655	-0.21575			

See page 183 for Explanation of Tables and Notes for Tables 32, 42, and 43

TABLE 2 (4). HARTREE-FOCK FUNCTIONS FOR POSITIVE IONS.

CALCIUM K(2)L(8)3S(2)3P(6)4S(1), 2S T.E.= -0.67656989D+03 P.E.= -0.13531385D+04 K.E.= 0.67656863D+03 V.T.= -0.20000019D+01							
S	1S	2S	3S	4S	P	2P	3P
BASIS/ORB E	-149.60939	-17.06681	-2.48511	-0.41632	BASIS/ORB E	-13.87423	-1.58162
1S 19.97610	-0.94180	-0.28206	0.09893	-0.02780	2P 9.12850	0.67668	-0.22488
1S 32.14530	-0.01800	-0.00095	-0.00055	0.00012	2P 15.91600	0.04326	-0.01326
2S 17.24190	-0.05095	-0.15043	0.05325	-0.01522	3P 7.38744	0.33394	-0.13928
2S 8.40484	-0.00210	0.85576	-0.32893	0.09358	3P 3.67247	0.01296	0.52031
3S 7.46798	0.00046	0.25703	-0.22503	0.06910	3P 2.38393	-0.00491	0.54690
3S 3.95877	0.00002	0.00926	0.71538	-0.20373	3P 1.72715	0.00156	0.04753
2S 3.01613	-0.00002	0.00151	0.09977	-0.10885			
4S 3.09060	0.00004	-0.00196	0.36973	-0.05597			
4S 1.42597	-0.00001	0.00075	0.01979	0.60382			
4S 1.00258	0.00002	-0.00116	-0.02197	0.53477			
4S 0.86831	-0.00001	0.00069	0.01261	-0.06591			
SCANDIUM K(2)L(8)3S(2)3P(6)4S(0)3D(2), 3F T.E.= -0.75950974D+03 P.E.= -0.15190209D+04 K.E.= 0.75951114D+03 V.T.= -0.19999981D+01							
S	1S	2S	3S				
BASIS/ORB E	-165.98191	-19.13262	-2.63251				
1S 20.89120	-0.94637	0.28925	0.10129				
1S 33.33330	-0.01935	-0.00030	-0.00049				
2S 17.88050	-0.04400	0.15321	0.05754				
2S 8.53919	-0.00212	-1.00086	-0.38003				
3S 7.32747	0.00084	-0.15731	-0.23497				
3S 4.70217	-0.00039	0.00571	0.47311				
3S 3.23133	0.00037	-0.00591	0.49288				
3S 2.63303	-0.00016	0.00378	0.26476				
P	2P	3P	D	3D			
BASIS/ORB E	-15.72595	-1.66608	BASIS/ORB E	-0.45481			
2P 9.59010	0.68831	-0.23003	3D 3.47301	0.29546			
2P 16.58910	0.04512	-0.01454	3D 8.60700	0.02387			
3P 7.84754	0.31662	-0.14450	3D 4.90755	0.06672			
3P 4.17069	0.01309	0.42309	3D 1.80631	0.50176			
3P 2.82651	-0.00359	0.49102	3D 1.03675	0.29574			
3P 2.08275	0.00114	0.21546					
SCANDIUM K(2)L(8)3S(2)3P(6)4S(1)3D(1), 3D T.E.= -0.75953901D+03 P.E.= -0.15190750D+04 K.E.= 0.75953596D+03 V.T.= -0.20000040D+01							
S	1S	2S	3S	4S			
BASIS/ORB E	-166.15494	-19.33312	-2.81674	-0.44926			
1S 33.41930	-0.02013	-0.00030	-0.00051	-0.00019			
1S 20.88410	-0.94517	-0.28815	-0.10064	-0.02826			
2S 18.18200	-0.04336	-0.14388	-0.05750	-0.01651			
2S 8.22724	-0.00464	1.06367	0.41717	0.11907			
3S 7.00657	0.00419	0.06288	0.22427	0.07368			
3S 4.78088	-0.00432	0.02294	-0.48782	-0.15769			
3S 3.23961	0.00391	-0.01416	-0.65129	-0.23290			
4S 3.05930	-0.00191	0.00754	-0.11598	-0.00630			
4S 1.58481	0.00039	-0.00153	-0.01082	0.52583			
4S 1.11478	-0.00029	0.00120	0.00539	0.55054			
4S 0.79972	0.00010	-0.00040	-0.00165	-0.00105			
P	2P	3P	D	3D			
BASIS/ORB E	-15.92174	-1.82564	BASIS/ORB E	-0.59990			
2P 16.63080	0.04478	-0.01459	3D 9.45240	0.01448			
2P 9.57942	0.69039	-0.23497	3D 5.84497	0.06475			
3P 7.83531	0.31504	-0.14639	3D 3.43076	0.38139			
3P 4.19994	0.01240	0.40592	3D 1.79500	0.52752			
3P 2.87080	-0.00303	0.54785	3D 1.13169	0.16732			
3P 2.09354	0.00075	0.17227					

See page 183 for Explanation of Tables and Notes for Tables 32, 42, and 43

## ROOTHAAN-HARTREE-FOCK ATOMIC WAVEFUNCTIONS

TABLE 2 (5). HARTREE-FOCK FUNCTIONS FOR POSITIVE IONS.

SCANDIUM K(2)L(8)3S(2)3P(6)4S(2), 1S  
 T.E.= -0.75946197D+03 P.E.= -0.15189209D+04 K.E.= 0.75945892D+03 V.T.= -0.20000040D+C1

S	1S	2S	3S	4S	P	2P	3P
BASIS/ORB E	-166.38407	-19.59985	-3.04420	-0.48719	BASIS/ORB E	-16.18202	-2.02885
1S 20.88410	-0.94512	-0.28803	0.10244	-0.03036	2P 9.57942	0.68959	-0.24065
1S 33.41930	-0.02014	-0.00037	0.00052	-0.00048	2P 16.63080	0.04493	-0.01482
2S 18.18200	-0.04337	-0.14402	0.05852	-0.01894	3P 7.84217	0.31583	-0.14826
2S 8.22724	-0.00478	1.06370	-0.42458	0.13252	3P 4.13447	0.01290	0.43667
3S 7.00657	0.00454	0.06309	-0.23055	0.07084	3P 2.87076	-0.00416	0.56662
3S 4.78088	-0.00534	0.02416	0.49736	-0.12704	3P 2.09616	0.00095	0.11758
3S 3.23961	0.00585	-0.01880	0.67800	-0.35865			
4S 3.25751	-0.00311	0.01053	0.08064	0.07325			
4S 1.58924	0.00029	-0.00097	0.00797	0.72742			
4S 1.07089	-0.00020	0.00068	-0.00403	0.36798			
4S 0.73186	0.00007	-0.00023	0.00117	-0.01953			

TITANIUM K(2)L(8)3S(2)3P(6)4S(0)3D(3), 4F  
 T.E.= -0.84818639D+03 P.E.= -0.16963743D+04 K.E.= 0.84818787D+03 V.T.= -0.19999983D+01

S	1S	2S	3S
BASIS/ORB E	-183.35059	-21.47055	-2.93668
1S 21.99140	-0.94468	0.28891	0.10302
1S 34.90540	-0.01721	0.00018	-0.00045
2S 18.88570	-0.04887	0.15783	0.05911
2S 9.13379	-0.00085	-0.96944	-0.36984
3S 8.15958	-0.00027	-0.16454	-0.22543
3S 4.87702	0.00047	-0.00863	0.45482
3S 3.41148	-0.00035	-0.00080	0.57532
3S 2.62460	0.00015	0.00003	0.17406

P	2P	3P	D	3D
BASIS/ORB E	-17.84503	-1.87885	BASIS/ORB E	-0.52472
2P 10.06340	0.68764	-0.23134	3D 2.03289	0.48212
2P 16.63140	0.05305	-0.01892	3D 9.18612	0.02831
3P 8.29658	0.30949	-0.15889	3D 4.44554	0.23576
3P 4.52656	0.00797	0.47386	3D 3.36221	0.15127
3P 2.75253	0.00057	0.64939	3D 1.17302	0.28115
3P 1.35410	-0.00016	0.02231		

TITANIUM K(2)L(8)3S(2)3P(6)4S(1)3D(2), 4F  
 T.E.= -0.84820321D+03 P.E.= -0.16964038D+04 K.E.= 0.84820055D+03 V.T.= -0.20000031D+01

S	1S	2S	3S	4S
BASIS/ORB E	-183.53834	-21.68555	-3.13375	-0.47570
1S 35.00210	0.01598	-0.00159	-0.00057	0.00037
1S 22.05210	0.94305	0.29112	0.10399	-0.02943
2S 18.93820	0.05253	0.15117	0.05961	-0.01609
2S 8.71313	0.00027	-1.06497	-0.41911	0.11630
3S 7.65091	0.00071	-0.06740	-0.22325	0.07860
3S 4.89030	-0.00059	-0.01726	0.74595	-0.25651
3S 0.34209	0.00001	0.00015	-0.00085	0.00074
4S 3.71676	0.00022	0.00327	0.51925	-0.15379
4S 1.74243	-0.00015	-0.00246	0.03152	0.47235
4S 1.19237	0.00022	0.00328	-0.02685	0.60003
4S 0.95979	-0.00013	-0.00194	0.01374	0.01135

P	2P	3P	D	3D
BASIS/ORB E	-18.05524	-2.05717	BASIS/ORB E	-0.70682
2P 17.00010	0.05046	-0.01681	3D 9.27716	0.02475
2P 10.01400	0.69764	-0.24262	3D 5.04931	0.17057
3P 8.29641	0.29921	-0.14740	3D 3.24307	0.34756
3P 4.47215	0.01224	0.45627	3D 1.99277	0.41393
3P 2.89817	-0.00243	0.61707	3D 1.31603	0.19433
3P 1.88859	0.00060	0.05570		

See page 183 for Explanation of Tables and Notes for Tables 32, 42, and 43

TABLE 2 (6). HARTREE-FOCK FUNCTIONS FOR POSITIVE IONS.

TITANIUM K(2)L(8)3S(2)3P(6)4S(2)3D(1), 2D  
 T.E.= -0.848056220+03 P.E.= -0.16961104D+04 K.E.= 0.84805420D+03 V.T.= -0.203000240+01

S	1S	2S	3S	4S
BASIS/ORB E	-183.78639	-21.97103	-3.37617	-0.51149
1S 35.00210	-0.01600	-0.00150	-0.00039	0.00022
1S 22.05210	-0.94297	0.29096	0.10532	-0.03135
2S 18.93820	-0.05258	0.15138	0.06121	-0.01794
2S 8.71313	-0.00030	-1.06517	-0.42748	0.12682
3S 7.65091	-0.00070	-0.06736	-0.22330	0.08142
3S 4.89030	0.00062	-0.01729	0.75158	-0.27212
3S 0.34209	-0.00001	0.00013	-0.00057	0.00097
4S 3.79619	-0.00024	0.00356	0.51362	-0.17331
4S 1.81698	0.00016	-0.00232	0.02391	0.54486
4S 1.22208	-0.00023	0.00336	-0.02110	0.56754
4S 1.00617	0.00014	-0.00205	0.01130	-0.01525

P	2P	3P	D	3D
BASIS/ORB E	-18.33392	-2.27565	BASIS/ORB E	-0.89266
2P 17.00010	0.05079	-0.01710	3D 10.06030	0.01915
2P 10.01400	0.69635	-0.24774	3D 5.41178	0.15815
3P 8.31203	0.29994	-0.14879	3D 3.33037	0.42503
3P 4.41964	0.01330	0.47843	3D 2.03531	0.41644
3P 2.93900	-0.00370	0.60651	3D 1.46121	0.10753
3P 1.91312	0.00082	0.04263		

VANADIUM K(2)L(8)3S(2)3P(6)4S(C)3D(4), 5D  
 T.E.= -0.94266936D+03 P.E.= -0.18853290D+04 K.E.= 0.94265961D+03 V.T.= -0.20000103D+01

S	1S	2S	3S
BASIS/ORB E	-201.57752	-23.91907	-3.24461
1S 22.51160	-0.95577	0.30630	0.10866
1S 35.22130	-0.02853	-0.00277	-0.00053
2S 19.21270	-0.01955	0.14883	0.06154
2S 9.23988	-0.00765	-1.07091	-0.42860
3S 8.02855	0.00674	-0.07128	-0.21199
3S 5.23391	-0.00649	-0.02673	0.50868
3S 3.93990	0.00554	0.01638	0.25824
3S 3.13236	-0.00194	-0.00656	0.47612

P	2P	3P	D	3D
BASIS/ORB E	-20.07280	-2.10106	BASIS/ORB E	-0.58442
2P 10.58920	0.67432	-0.21949	3D 2.93145	0.33876
2P 16.78480	0.06245	-0.02686	3D 9.75240	0.02740
3P 8.86537	0.30944	-0.19392	3D 4.89947	0.26091
3P 5.31114	0.01004	0.38646	3D 1.93482	0.31459
3P 3.11403	0.00193	0.73704	3D 1.26261	0.23526
3P 1.70944	-0.00048	0.04788		

VANADIUM K(2)L(8)3S(2)3P(6)4S(1)3D(3), 5F  
 T.E.= -0.94267593D+03 P.E.= -0.18853538D+04 K.E.= 0.94267788D+03 V.T.= -0.19999979D+01

S	1S	2S	3S	4S
BASIS/ORB E	-201.77805	-24.14768	-3.45375	-0.50013
1S 22.83270	-0.95080	-0.29262	-0.10507	-0.02781
1S 36.53570	-0.01947	-0.00106	-0.00071	-0.00081
2S 19.80900	-0.03707	-0.15561	-0.06346	-0.01985
2S 9.31485	-0.00495	1.04370	0.41933	0.12236
3S 7.99464	0.00448	0.11106	0.24515	0.05658
3S 5.19818	-0.00616	-0.00934	-0.64532	-0.07788
3S 3.95445	0.00592	0.01549	-0.27101	-0.30837
4S 3.71727	-0.00208	-0.00506	-0.36208	0.04133
4S 1.60643	0.00019	0.00069	-0.01139	0.77255
4S 1.03018	-0.00014	-0.00039	0.00584	0.31012
4S 0.70069	0.00005	0.00017	-0.00212	-0.02935

See page 183 for Explanation of Tables and Notes for Tables 32, 42, and 43

## ROOTHAAN-HARTREE-FOCK ATOMIC WAVEFUNCTIONS

TABLE 2 (7). HARTREE-FOCK FUNCTIONS FOR POSITIVE IONS.

P	2P	3P	D	3D
BASIS/ORB E	-20.29644	-2.29152	BASIS/ORB E	-0.78563
2P 10.68040	0.66204	-0.22875	3D 3.21449	0.28709
2P 17.06310	0.05992	-0.02233	3D 9.62920	0.03174
3P 9.02274	0.32028	-0.169C4	3D 4.89289	0.26651
3P 4.99846	0.01985	0.39E52	3C 2.05006	0.45566
3P 3.15462	-0.00393	0.69260	3D 1.24288	0.11128
3P 1.83417	0.00092	0.051C3		

VANADIUM K(2)L(8)3S(2)3P(6)4S(2)3D(2), 3F  
 T.E.= -0.9424982D+03 P.E.= -0.1884994D+04 K.E.= 0.94249573D+03 V.T.= -0.20000026D+01

S	1S	2S	3S	4S
BASIS/ORB E	-202.03719	-24.44261	-3.70594	-0.53327
1S 36.53570	-0.01947	-0.00108	0.00079	-0.00071
1S 22.83270	-0.95077	-0.29260	0.10648	-0.02982
2S 19.80900	-0.03707	-0.15560	0.06458	-0.02C55
2S 9.31485	-0.00510	1.04342	-0.42584	0.12859
3S 7.99464	0.00480	0.11227	-0.24925	0.06687
3S 5.19818	-0.00740	-0.01377	0.66636	-0.11141
3S 3.95445	0.00781	0.02158	0.25228	-0.29122
4S 3.82415	-0.00302	-0.00808	0.36142	0.01750
4S 1.73257	0.00022	0.00699	0.00824	0.73590
4S 1.12927	-0.00014	-0.00044	-0.00358	0.35146
4S 0.68917	0.00004	0.00013	0.00091	-0.01703

P	2P	3P	D	3D
BASIS/ORB E	-20.58510	-2.52048	BASIS/ORB E	-1.01239
2P 17.06310	0.05999	-0.02124	3D 9.72325	0.03239
2P 10.68040	0.66164	-0.23695	3D 4.96821	0.28760
3P 9.01847	0.32178	-0.16204	3D 3.04042	0.41731
3P 4.78925	0.02004	0.45333	3D 2.01687	0.34326
3P 3.15262	-0.00595	0.63758	3D 1.36759	0.04544
3P 1.93549	0.00133	0.03998		

CHROMIUM K(2)L(8)3S(2)3P(6)4S(0)3D(5), 6S  
 T.E.= -0.10431388D+04 P.E.= -0.2C862725D+04 K.E.= 0.10431337D+04 V.T.= -0.20300049D+01

S	1S	2S	3S
BASIS/ORB E	-220.65383	-26.46991	-3.55058
1S 23.91730	-0.93447	-0.27807	0.10216
1S 35.53690	-0.02799	-0.00558	0.00246
2S 21.61760	-0.04518	-0.15343	0.05680
2S 10.07520	-0.00622	0.93624	-0.35805
3S 9.63943	0.00371	0.194E4	-0.21888
3S 5.66524	-0.00185	0.03051	0.21875
3S 4.39352	0.00141	-0.00935	0.62978
3S 3.07388	-0.00030	0.00185	0.33407

P	2P	3P	D	3D
BASIS/ORB E	-22.40208	-2.32147	BASIS/ORB E	-0.64925
2P 10.82120	0.68145	-0.23274	3D 3.22269	C.31097
2P 16.87160	0.08244	-0.03141	3D 10.51780	0.02544
3P 9.34648	0.27459	-0.16773	3D 5.35538	0.25990
3P 5.57901	0.01576	0.34907	3D 2.38079	0.26295
3P 3.48331	-0.00019	0.68539	3D 1.46678	0.31458
3P 2.21454	0.00010	0.12689		

CHROMIUM K(2)L(8)3S(2)3P(6)4S(1)3D(4), 6D  
 T.E.= -0.10430963D+04 P.E.= -0.20861939D+04 K.E.= 0.1043C977D+04 V.T.= -0.19999986D+01

S	1S	2S	3S	4S
BASIS/ORB E	-220.87676	-26.72180	-3.77932	-0.52337
1S 24.13360	-0.92896	0.27714	-0.10403	-0.02781
1S 35.41620	-0.02412	0.00805	-0.00122	-0.00070
2S 21.54520	-0.05786	0.158C7	-0.05789	-0.01674
2S 9.76558	-0.00236	-1.01698	0.39115	0.10967
3S 9.34904	0.00062	-0.10933	0.21804	0.06257
3S 5.87559	0.00032	-0.02453	-0.31231	-0.07645
3S 4.07495	-0.00027	0.00347	-0.77822	-0.29944
4S 3.38790	0.00013	-0.00085	-0.12404	0.04120
4S 1.71453	-0.00005	-0.00C26	-0.00574	0.72477
4S 1.03048	0.00009	0.00015	0.00628	0.61180
4S 0.92348	-0.00007	-0.00016	-0.00479	-0.28370

See page 183 for Explanation of Tables and Notes for Tables 32, 42, and 43

TABLE 2 (8). HARTREE-FOCK FUNCTIONS FOR POSITIVE IONS.

P BASIS/ORB E	2P -22.64881	3P -2.53073	D BASIS/ORB E	3D -0.85459
2P 10.80450	0.65758	-0.22357	3D 3.54136	0.33377
2P 16.56190	0.09546	-0.03799	3D 10.27090	0.03055
3P 9.52663	0.28041	-0.17387	3D 5.39230	0.24129
3P 5.61370	0.02414	0.34378	3D 2.15663	0.44969
3P 3.45763	-0.00333	0.74418	3D 1.30491	0.09761
3P 1.98991	0.00082	0.06783		

CHROMIUM K(2)L(8)3S(2)3P(6)4S(2)3D(3), 4F  
T.E.= -0.10428897D+04 P.E.= -0.20E57770D+04 K.E.= 0.10428873D+04 V.T.= -0.20300024D+01

S BASIS/ORB E	1S -221.14735	2S -27.02719	3S -4.04226	4S -0.55402
1S 35.41620	-0.02420	-0.00787	-0.00164	-0.00044
1S 24.13360	-0.92879	-0.27745	-0.10471	-0.02960
2S 21.54520	-0.05801	-0.15767	-0.05973	-0.01755
2S 9.76558	-0.00222	1.01596	0.39959	0.11755
3S 9.34904	0.00155	0.10395	0.18137	-0.07883
3S 5.87559	-0.00553	0.06030	-0.11698	0.66331
3S 4.07495	0.00106	-0.01C87	-0.89719	-0.53905
4S 2.99588	-0.00018	0.00233	-0.06374	0.17961
4S 1.63394	0.00005	-0.00063	0.00472	0.79159
4S 1.10115	-0.00002	0.00024	-0.00160	0.19038
4S 7.38768	0.00398	-0.02486	-0.10763	-0.46209

P BASIS/ORB E	2P -22.94804	3P -2.77094	D BASIS/ORB E	3D -1.10143
2P 16.56190	0.09572	-0.036C7	3D 10.42790	0.02987
2P 10.80450	0.65673	-0.23378	3D 5.48965	0.25862
3P 9.51962	0.28298	-0.16166	3D 3.42419	0.41725
3P 5.31521	0.02401	0.39597	3D 2.17775	0.38147
3P 3.43201	-0.00586	0.69397	3D 1.39827	0.04047
3P 2.07412	0.00132	0.05123		

MANGANESE K(2)L(8)3S(2)3P(6)4S(0)3D(6), 5D  
T.E.= -0.11495205D+04 P.E.= -0.22990304D+04 K.E.= 0.11495098D+04 V.T.= -0.20000093D+01

S BASIS/ORB E	1S -240.63259	2S -29.18004	3S -3.89721
1S 25.35960	-0.93786	-0.28772	0.10779
1S 38.74670	-0.01159	-0.00096	-0.00123
2S 21.74770	-0.06613	-0.17426	0.06297
2S 10.99850	0.00586	0.89172	-0.33882
3S 10.05060	-0.00526	0.27194	-0.27099
3S 5.90450	0.00362	0.01743	0.37111
3S 4.27100	-0.00287	-0.00180	0.57596
3S 3.19300	0.00097	0.00062	0.25522

P BASIS/ORB E	2P -24.88890	3P -2.57906	D BASIS/ORB E	3D -0.66729
2P 9.67526	-0.86762	-0.33546	3D 3.61648	0.39420
2P 16.63330	-0.13343	-0.03952	3D 10.18720	0.03436
2P 6.26300	0.00343	-1.15102	3D 5.78370	0.21646
3P 5.97500	-0.03850	1.56691	3D 2.10220	0.34577
3P 3.53200	0.00945	0.53284	3D 1.41200	0.18803
3P 2.58598	-0.00412	0.16135		

MANGANESE K(2)L(8)3S(2)3P(6)4S(1)3D(5), 7S  
T.E.= -0.11496485D+04 P.E.= -0.22992794D+04 K.E.= 0.11496309D+04 V.T.= -0.20000154D+C1

S BASIS/ORB E	1S -240.82852	2S -29.40196	3S -4.10603	4S -0.54431
1S 38.06800	-0.02027	0.00112	0.00035	-0.00C60
1S 24.91310	-0.94753	-0.29535	-0.10982	-0.02839
2S 21.37620	-0.04170	-0.16258	-0.06588	-0.02011
2S 10.24180	-0.00059	1.05459	0.42529	0.12124
3S 9.37620	-0.00040	0.08845	0.20994	0.05137
3S 5.80268	0.00083	0.03091	-0.48141	-0.08176
3S 4.19777	-0.00073	-0.01595	-0.57312	-0.31570
4S 3.80451	0.00030	0.00584	-0.17665	0.07774
4S 1.77031	-0.00005	-0.00051	-0.00868	0.72401
4S 1.12926	0.00004	0.00065	0.00374	0.35793
4S 0.79778	-0.00002	-0.00023	-0.00162	-0.03281

See page 183 for Explanation of Tables and Notes for Tables 32, 42, and 43

## ROOTHAAN-HARTREE-FOCK ATOMIC WAVEFUNCTIONS

TABLE 2 (9). HARTREE-FOCK FUNCTIONS FOR POSITIVE IONS.

P	2P	3P	D	3D
BASIS/ORB E	-25.10589	-2.77060	BASIS/ORB E	-0.93322
2P 16.39570	0.14443	-0.04354	3D 11.08340	0.02942
2P 9.57457	0.86549	-0.34031	3D 5.67214	0.26923
3P 7.07710	-0.01192	-0.09881	3D 3.69353	0.32263
3P 5.54740	0.04255	0.51928	3D 2.31586	0.42428
3P 3.60258	-0.01672	0.53520	3D 1.43825	0.10664
3P 2.62989	0.00601	0.15646		

MANGANESE K(2)L(8)3S(2)3P(6)4S(2)3D(4) 5D  
 T.E.= -0.11493687D+04 P.E.= -0.22987276D+04 K.E.= 0.11493589D+04 V.T.= -0.20300086D+01

S	1S	2S	3S	4S
BASIS/ORB E	-241.11838	-29.72683	-4.38616	-0.57393
1S 38.06800	-0.02029	0.00110	-0.00015	-0.00048
1S 24.91310	-0.94748	-0.29932	-0.11029	-0.02966
2S 21.37620	-0.04172	-0.16257	-0.06825	-0.02037
2S 10.24180	-0.00065	1.05472	0.43444	0.12438
3S 9.37620	-0.00033	0.08918	0.20344	0.05751
3S 5.80268	0.00071	0.02892	-0.43687	-0.10743
3S 4.19777	-0.00057	-0.01307	-0.68231	-0.28904
4S 3.57000	0.00022	0.00447	-0.10579	0.05328
4S 1.87622	-0.00006	-0.00101	0.00216	0.68521
4S 1.21958	0.00004	0.00067	-0.00194	0.39053
4S 0.84637	-0.00002	-0.00024	0.00078	-0.02132

F	2P	3P	D	3D
BASIS/ORB E	-25.42458	-3.02787	BASIS/CRB E	-1.18079
2P 16.39570	0.14313	-0.04783	3D 10.91510	0.03060
2P 9.57457	0.86932	-0.33308	3D 5.82945	0.26434
3P 9.34029	-0.00777	-0.03954	3D 3.63996	0.41433
3P 5.44951	0.03561	0.42617	3D 2.32880	0.36466
3P 3.69768	-0.01597	0.58270	3D 1.56178	0.05577
3P 2.63511	0.00501	0.12953		

IRON K(2)L(8)3S(2)3P(6)4S(0)3D(7), 4F  
 T.E.= -0.12622208D+04 P.E.= -0.25244161D+04 K.E.= 0.12621953D+04 V.T.= -0.200002020D+01

S	1S	2S	3S
BASIS/ORB E	-261.44787	-31.97969	-4.23202
1S 25.64570	-0.95477	-0.30896	0.11308
1S 39.05820	-0.02504	0.00279	-0.00082
2S 21.50810	-0.02669	-0.17658	0.07277
2S 11.10400	-0.00266	1.01666	-0.41261
3S 9.57945	0.00210	0.17708	-0.28501
3S 7.04857	-0.00152	-0.01278	0.26762
2S 3.48518	-0.00017	-0.00153	0.38558
2S 4.98635	0.00075	0.01094	0.62569

P	2P	3P	D	3D
BASIS/ORB E	-27.46389	-2.82515	BASIS/ORB E	-0.71284
2P 10.08990	-0.86577	-0.34654	3D 3.73410	0.36676
2P 17.16540	-0.13925	-0.03974	3D 11.40830	0.02845
3P 6.53068	-0.00764	-0.15962	3D 6.06825	0.25671
3P 5.60563	-0.02317	0.68776	3D 2.26526	0.35649
3P 3.48315	0.01092	0.49273	3D 1.41442	0.17372
3P 2.57346	-0.00474	0.09895		

IRON K(2)L(8)3S(2)3P(6)4S(1)3D(6), 6D  
 T.E.= -0.12622122D+04 P.E.= -0.25244046D+04 K.E.= 0.12621924D+04 V.T.= -0.20000157D+01

S	1S	2S	3S	4S
BASIS/ORB E	-261.67767	-32.23678	-4.46877	-0.56020
1S 39.07900	0.02618	0.00199	0.00056	-0.00049
1S 25.59940	0.95520	-0.30831	-0.11375	-0.02862
2S 21.70570	0.02386	-0.16945	-0.07040	-0.02077
2S 10.88620	0.00479	1.04779	0.42878	0.11847
3S 9.40162	-0.00493	0.12893	0.29966	0.06931
3S 7.05231	0.00389	-0.00295	-0.34588	-0.05909
3S 4.71260	-0.00180	0.00704	-0.78849	-0.30754
4S 3.83931	0.00058	-0.00142	-0.18359	0.03399
4S 1.86530	-0.00016	0.00061	-0.00270	0.67548
4S 1.19327	0.00012	-0.00026	-0.00028	0.40294
4S 0.83151	-0.00005	0.00013	-0.00001	-0.02787

See page 183 for Explanation of Tables and Notes for Tables 32, 42, and 43

TABLE 2 (10). HARTREE-FOCK FUNCTIONS FOR POSITIVE IONS.

P	2P	3P	D	3D
BASIS/ORB E	-27.71594	-3.04362	BASIS/ORB E	-0.95085
2P 17.17450	0.13902	-0.04169	3D 11.71760	0.02727
2P 10.08050	0.86766	-0.34590	3D 6.21570	0.24232
3P 7.97384	-0.00158	-0.05221	3D 4.06451	0.33339
3P 5.61991	0.03336	0.53387	3D 2.54111	0.39868
3P 3.60890	-0.01432	0.54522	3D 1.60897	0.15526
3P 2.57237	0.00524	0.08665		

IRON            K(2)L(8)3S(2)3P(6)4S(2)3D(5), 6S  
T.E.= -0.12621252D+04 P.E.= -0.25242269D+04 K.E.= 0.12621018D+04 V.T.= -0.20300185D+01

S	1S	2S	3S	4S
BASIS/ORB E	-261.94402	-32.53491	-4.73373	-0.59255
1S 39.07930	0.02618	0.00197	0.00061	-0.00066
1S 25.59940	0.95517	-0.3C827	-0.11500	-0.02955
2S 21.70570	0.02387	-0.16546	-0.07095	-0.02216
2S 10.88620	0.00486	1.04761	0.43269	0.12474
3S 9.40162	-0.00508	0.12555	0.30558	0.06818
3S 7.05231	0.00410	-0.00376	-0.35339	-0.05340
3S 4.71260	-0.00198	0.00762	-0.79735	-0.33277
4S 3.93268	0.00066	-0.00174	-0.16878	0.04032
4S 1.91411	-0.00016	0.00046	-0.00180	0.72993
4S 1.20297	0.00012	-0.00034	0.00068	0.35787
4S 0.83151	-0.00005	0.00014	-0.00021	-0.02988

P	2P	3P	D	3D
BASIS/ORB E	-28.00815	-3.28748	BASIS/ORB E	-1.27368
2P 17.17450	0.13902	-0.04148	3D 11.53690	0.03003
2P 10.08050	0.86741	-0.35235	3D 6.24694	0.25007
3P 7.42180	-0.00086	-0.06539	3D 4.04217	0.38148
3P 5.60775	0.03294	0.56995	3D 2.55225	0.40934
3P 3.61859	-0.01469	0.54479	3D 1.60788	0.06021
3P 2.62611	0.00539	0.06626		

COBALT            K(2)L(8)3S(2)3P(6)4S(C)3D(8), 3F  
T.E.= -0.138111282D+04 P.E.= -0.27622475D+04 K.E.= 0.13811193D+04 V.T.= -0.20000054D+01

S	1S	2S	3S
BASIS/ORB E	-283.15239	-34.92573	-4.59802
1S 26.49780	-0.96415	-0.31241	0.11656
1S 41.86020	-0.02321	0.00234	-0.00139
2S 22.26840	-0.01479	-0.17772	0.66991
2S 11.86770	-0.00854	0.96368	-0.38280
3S 10.68120	0.00674	0.22015	-0.26588
3S 7.08540	-0.00457	0.01387	0.22682
3S 5.15265	0.00277	0.00153	0.64409
3S 3.60786	-0.00068	0.00036	0.35474

P	2P	3P	D	3D
BASIS/ORB E	-30.18352	-3.09974	BASIS/ORB E	-0.73473
2P 11.13470	0.87718	-0.34380	3D 4.99975	0.30194
2P 19.55780	0.08223	-0.02297	3D 11.56820	0.02985
3P 7.84410	0.09482	-0.13568	3D 7.01733	0.13832
3P 5.96817	-0.02589	0.63154	3D 2.97339	0.43113
3P 3.59800	0.00580	0.56483	3D 1.62864	C.28419
3P 2.22684	-0.00100	0.03548		

COBALT            K(2)L(8)3S(2)3P(6)4S(2)3D(6), 5D  
T.E.= -0.13810089D+04 P.E.= -0.27619576D+04 K.E.= 0.13809887D+04 V.T.= -0.20000146D+01

S	1S	2S	3S	4S
BASIS/ORB E	-283.66414	-35.49504	-5.11290	-0.61337
1S 42.07870	-0.02489	-0.00007	0.00015	-0.00066
1S 26.35390	-0.96837	-0.31027	-0.11698	-0.02571
2S 22.38560	-0.00549	-0.17869	-0.07366	-0.02276
2S 11.93290	-0.01309	0.95879	0.39360	0.11220
3S 10.40270	0.01138	0.24768	0.28312	0.06573
3S 6.39267	-0.01817	-0.04397	-0.48164	-0.00851
3S 5.29950	0.01632	0.04701	-0.41204	-0.32203
4S 4.55432	-0.00344	-0.00554	-0.36306	-0.00634
4S 2.03932	0.00045	0.00138	-0.00833	0.68076
4S 1.29045	-0.00031	-0.00095	0.00398	0.40726
4S 0.83159	0.00011	0.00034	-0.00125	-0.01829

See page 183 for Explanation of Tables and Notes for Tables 32, 42, and 43

## ROOCHAAN-HARTREE-FOCK ATOMIC WAVEFUNCTIONS

TABLE 2 (11). HARTREE-FOCK FUNCTIONS FOR POSITIVE IONS.

P	2P	3P	D	3D
BASIS/ORB E	-30.74193	-3.57576	BASIS/ORB E	-1.29179
2P 19.71750	0.07982	-0.02295	3D 12.43560	0.02408
2P 11.14750	0.87864	-0.35035	3D 6.90277	C.22866
2P 7.96114	0.09227	-0.15112	3D 4.28989	0.42411
3P 6.12059	-0.02128	0.58937	3D 2.68142	0.35890
3P 3.86380	0.00408	0.58090	3D 1.83300	0.10105
3P 2.67925	-0.00055	0.06844		

NICKEL K(2)L(8)3S(2)3P(6)4S(C)3D(9), 2D  
 T.E.= -0.15065903D+04 P.E.= -0.30131781D+04 K.E.= 0.15065878D+04 V.T.= -0.20000016D+01

S	1S	2S	3S
BASIS/ORB E	-305.70319	-37.97248	-4.96011
1S 27.45160	-0.95953	-0.32451	0.12109
1S 41.46910	-0.02838	0.00795	-0.00318
2S 22.12550	-0.01652	-0.20037	0.08235
2S 12.49710	-0.00366	0.99579	-0.40541
3S 10.84510	0.00280	0.22474	-0.28080
3S 7.33471	-0.00207	0.00266	0.28960
3S 5.30118	0.00127	0.00461	0.61346
3S 3.75824	-0.00032	-0.00014	0.34474

P	2P	3P	D	3D
BASIS/ORB E	-33.00252	-3.36587	BASIS/ORB E	-0.76920
2P 11.47350	0.82345	-0.31862	3D 4.75253	C.33129
2P 19.06180	0.11781	-0.03806	3D 12.83200	0.02520
3P 11.48690	0.05987	-0.05489	3D 7.12077	0.20378
3P 6.33446	0.05874	0.33635	3D 2.78709	0.41773
3P 4.83042	-0.03258	0.45125	3D 1.57027	0.21053
3P 3.26358	0.00723	0.34528		

NICKEL K(2)L(8)3S(2)3P(6)4S(2)3D(7), 4F  
 T.E.= -0.15064317D+04 P.E.= -0.30128479D+04 K.E.= 0.15064161D+04 V.T.= -0.20000104D+01

S	1S	2S	3S	4S
BASIS/ORB E	-306.23660	-38.56427	-5.49597	-0.63285
1S 41.52310	-0.02822	0.00459	0.00093	-0.00067
1S 27.48100	-0.95816	-0.31785	-0.11858	-0.02929
2S 22.96760	-0.01746	-0.17777	-0.07834	-0.02392
2S 11.87030	-0.00554	1.06334	0.45159	0.12671
3S 10.33090	0.00543	0.11814	0.25305	0.05115
3S 6.86116	-0.00772	0.01287	-0.45277	-0.00370
3S 5.59077	0.00621	-0.00340	-0.46895	-0.31577
4S 4.73983	-0.00126	0.00130	-0.36250	-0.01020
4S 2.12892	0.00017	-0.00010	-0.00806	0.65684
4S 1.34549	-0.00011	0.00007	0.00358	0.42817
4S 0.83170	0.00004	-0.00002	-0.00103	-0.01320

P	2P	3P	D	3D
BASIS/ORB E	-33.58319	-3.86690	BASIS/ORB E	-1.33551
2P 18.37300	0.14472	-0.04808	3D 12.64120	0.02792
2P 11.64690	0.74104	-0.29446	3D 7.13558	0.23508
3P 11.61210	0.12529	-0.07882	3D 4.52387	0.41433
3P 6.13983	0.05276	0.42E50	3D 2.72992	0.39562
3P 4.72317	-0.03270	0.35197	3D 1.73362	0.6800
3P 3.46175	0.00831	0.35027		

COPPER K(2)L(8)3S(2)3P(6)4S(0)3D(10), 1S  
 T.E.= -0.16387276D+04 P.E.= -0.32774473D+04 K.E.= 0.16387196D+04 V.T.= -0.20000049D+01

S	1S	2S	3S
BASIS/ORB E	-329.10745	-41.12805	-5.32511
1S 28.45300	-0.95851	-0.32587	0.12160
1S 42.53270	-0.02906	0.00819	-0.00297
2S 23.10340	-0.01709	-0.15715	0.08245
2S 13.01550	-0.00297	0.98177	-0.40335
3S 11.52770	0.00168	0.23C62	-0.25689
3S 6.72990	-0.00089	0.01499	0.55723
3S 4.61704	0.00078	-0.00405	0.54604
3S 3.53495	-0.00031	0.00191	0.11723

See page 183 for Explanation of Tables and Notes for Tables 32, 42, and 43

TABLE 2 (12). HARTREE-FOCK FUNCTIONS FOR POSITIVE IONS.

P	2P	3P	D	3D
BASIS/ORB E	-35.92860	-3.64181	BASIS/ORB E	-0.81009
2P 12.36430	0.76853	-0.28521	3D 4.70557	0.33575
2P 19.52640	0.11626	-0.04270	3D 13.47820	0.02401
3P 11.52780	0.12971	-0.12476	3D 7.38627	0.23802
3P 7.15679	0.02772	0.37278	3D 2.93665	0.36175
3P 4.50992	-0.00468	0.66459	3D 1.69283	0.22921
3P 2.86886	0.00165	0.13142		

CUPRUM      K(2)L(8)3S(2)3P(6)4S(2)3D(8), 3F  
T.E.= -0.163847910+04 P.E.= -0.32769476D+04 K.E.= 0.16384685D+04 V.T.= -0.20300055D+01

S	1S	2S	3S	4S
BASIS/ORB E	-329.67225	-41.75098	-5.88844	-0.65195
1S 28.21170	-0.96437	-0.31456	-0.12065	-0.02888
1S 43.00190	-0.03209	-0.00033	0.00064	-0.00097
2S 23.81960	-0.00135	-0.19268	-0.07745	-0.02443
2S 13.42030	-0.01251	0.90692	0.36885	0.10427
3S 11.65060	0.00926	0.32027	0.30989	0.06709
3S 6.80495	-0.01896	-0.06288	-0.55099	0.06873
3S 5.96241	0.01771	0.06827	-0.29145	-0.38053
4S 5.01873	-0.00262	-0.01018	-0.40781	-0.00496
4S 2.17031	0.00031	0.00138	-0.01060	0.68667
4S 1.32762	-0.00023	-0.00103	0.00582	0.41405
4S 0.89707	0.00010	0.00043	-0.00222	-0.03153

P	2P	3P	D	3D
BASIS/ORB E	-36.54038	-4.16598	BASIS/ORB E	-1.38352
2P 12.53960	0.79000	-0.30631	3D 4.98629	0.37603
2P 20.26500	0.09183	-0.03168	3D 13.33850	0.02681
3P 11.18040	0.13867	-0.12183	3D 7.56839	0.22091
3P 6.98993	0.02143	0.40392	3D 2.99457	0.43480
3P 4.49957	-0.00417	0.65847	3D 1.78785	0.08646
3P 2.98275	0.00142	0.1C614		

ZINC      K(2)L(8)3S(2)3P(6)4S(1)3D(10), 2S  
T.E.= -0.17775666D+04 P.E.= -0.35551193D+04 K.E.= 0.17775526D+04 V.T.= -0.20000079D+01

S	1S	2S	3S	4S
BASIS/ORB E	-353.64651	-44.69892	-5.97654	-0.61157
1S 29.37180	-0.95931	-0.32111	-0.12009	-0.02598
1S 43.79180	-0.03080	0.00422	0.00100	-0.00074
2S 24.30800	-0.01241	-0.19718	-0.08539	-0.02340
2S 13.41410	-0.00592	0.99835	0.42015	0.10516
3S 11.61830	0.00448	0.22267	0.27000	0.05225
3S 6.94855	-0.00685	-0.02270	-0.69452	-0.04481
3S 5.70187	0.00647	0.02822	-0.19561	-0.25748
4S 5.04098	-0.00154	-0.00630	-0.37237	0.02367
4S 2.15231	0.00017	0.00078	-0.00991	0.60922
4S 1.32855	-0.00013	-0.00063	0.00525	0.48521
4S 0.93366	0.00006	0.00028	-0.00216	-0.02961

P	2P	3P	D	3D
BASIS/ORB E	-39.26347	-4.18115	BASIS/ORB E	-1.12468
2P 12.35290	0.85919	-0.34507	3D 4.99726	0.37547
2P 20.47910	0.10999	-0.03426	3D 13.69260	0.02796
3P 10.22320	0.04710	-0.09771	3D 7.75106	0.23644
3P 6.98237	0.01568	0.55640	3D 2.96150	0.39696
3P 4.17640	-0.00199	0.62430	3D 1.79216	0.12963
3P 1.88125	0.00056	0.01625		

See page 183 for Explanation of Tables and Notes for Tables 32, 42, and 43

## ROOTHAAN-HARTREE-FOCK ATOMIC WAVEFUNCTIONS

TABLE 2 (13). HARTREE-FOCK FUNCTIONS FOR POSITIVE IONS.

GALLIUM K{2}L{8}M{18}4S{2}, 1S  
 T.E.= -0.19230591D+04 P.E.= -0.38461065D+04 K.E.= 0.19230474D+04 V.T.= -0.20000051D+01

S	1S	2S	3S	4S
BASIS/ORB E	-379.12245	-48.47104	-6.69742	-0.68809
1S 28.53020	0.75004	0.30120	0.11921	-0.03526
1S 35.69370	0.26028	0.03159	0.00893	0.00186
2S 26.21850	-0.00997	0.14785	0.05975	-0.01110
2S 13.30840	0.00347	-1.02650	-0.42121	0.09917
3S 12.57040	-0.00127	-0.13639	-0.23974	0.07820
3S 7.43622	0.00004	-0.02346	0.54957	-0.18241
3S 4.90021	-0.00001	0.00411	0.67240	-0.17002
4S 2.61152	-0.00001	-0.00120	0.00702	0.48042
4S 1.61757	0.00001	0.00025	-0.00162	0.60152
4S 1.04163	-0.00000	-0.00032	0.00032	0.02181

P	2P	3P	D	3D
BASIS/ORB E	-42.79622	-4.78368	BASIS/ORB E	-1.49530
2P 12.55790	0.87929	-0.36120	3D 3.55434	0.41579
2P 20.88540	0.12092	-0.03787	3D 2.16536	0.16050
3P 11.08750	-0.00590	-0.06601	3D 5.63780	0.32817
3P 7.66322	0.04167	0.39042	3D 8.35144	0.21994
3P 5.07206	-0.01310	0.60888	3D 14.57690	0.02493
3P 3.50071	0.00417	0.17E55		

GERMANIUM K{2}L{8}M{18}4S{2}4P{1}, 2P  
 T.E.= -0.20750859D+04 P.E.= -0.41501711D+04 K.E.= 0.20750852D+04 V.T.= -0.20000003D+01

S	1S	2S	3S	4S
BASIS/ORB E	-405.58342	-52.48734	-7.52764	-0.84417
1S 29.96380	0.75913	0.30062	-0.11398	-0.03172
1S 36.83900	0.23993	0.02734	-0.01193	-0.00255
2S 27.03400	0.00427	0.15955	-0.06953	-0.01828
2S 13.78660	0.00100	-1.03781	0.43764	0.11786
3S 12.89570	0.00033	-0.12989	0.24070	0.07814
3S 7.90579	-0.00054	-0.02278	-0.49520	-0.16564
3S 5.27661	0.00026	0.00358	-0.72846	-0.23020
4S 3.02514	-0.00010	-0.00114	-0.01483	0.37569
4S 1.95836	0.00008	0.00078	0.00504	0.64633
4S 1.30000	-0.00003	-0.00028	-0.00146	0.09054

P	2P	3P	4P	C	3D
BASIS/ORB E	-46.57277	-5.49663	-0.56450	BASIS/ORB E	-1.97048
2P 13.36570	0.86138	0.34500	0.07853	3D 3.81341	0.44271
2P 22.13940	0.10286	0.03586	0.00745	3D 2.35796	0.12395
3P 12.90570	0.02999	0.07744	0.01716	3D 6.12204	0.34108
3P 8.13246	0.04567	-0.33649	-0.08119	3D 8.86986	0.20080
3P 5.27150	-0.01352	-0.74690	-0.19395	3D 14.94120	0.02644
4P 3.81319	0.00495	-0.08552	0.04704		
4P 2.10472	-0.00211	0.00488	0.61695		
4P 1.27657	0.00117	-0.00295	0.45663		
4P 0.77981	-0.00040	0.00092	-0.02522		

ARSENIC K{2}L{8}M{18}4S{2}4P{2}, 3P  
 T.E.= -0.22338878D+04 P.E.= -0.44677731D+04 K.E.= 0.22338853D+04 V.T.= -0.20000012D+01

S	1S	2S	3S	4S
BASIS/ORB E	-432.95904	-56.68045	-8.39903	-1.00311
1S 31.38330	0.81265	0.35320	-0.13711	-0.04051
1S 38.65360	0.18217	-0.01608	0.00591	0.00246
2S 26.29870	0.01022	0.18131	-0.07978	-0.02218
2S 14.93080	-0.00090	-0.99041	0.42288	0.12085
3S 13.46930	0.00134	-0.21909	0.27518	0.09384
3S 8.14971	-0.00089	-0.01216	-0.49007	-0.17500
3S 5.53857	0.00043	0.00245	-0.73058	-0.25069
4S 3.16196	-0.00016	-0.00082	-0.01402	0.43893
4S 2.09393	0.00013	0.00060	0.00510	0.60117
4S 1.42405	-0.00005	-0.00021	-0.00155	0.07998

See page 183 for Explanation of Tables and Notes for Tables 32, 42, and 43

TABLE 2 (14). HARTREE-FOCK FUNCTIONS FOR POSITIVE IONS.

P BASIS/ORB E	2P -50.52402	3P -6.24E40	4P -0.67339	D BASIS/ORB E	3D -2.4E098
2P 14.03770	0.83717	0.34060	0.08618	3D 4.21611	0.46465
2P 22.83730	0.10085	0.03546	0.00777	3D 2.62925	0.12058
3P 13.54400	0.05841	0.08613	0.01958	3D 6.56199	0.29583
3P 8.38725	0.04787	-0.33219	-0.08457	3D 9.10260	0.21415
3P 5.58485	-0.01726	-0.734E5	-0.21872	3D 15.41610	0.02856
4P 4.30457	0.00656	-0.05483	0.03268		
4P 2.41552	-0.00265	0.00011	0.56203		
4P 1.53533	0.00164	-0.00103	0.49701		
4P 1.03206	-0.00059	0.00029	0.00592		

ARSENIC K(2)L(8)M(18)4S(2)4P(2), 1D  
T.E.= -0.22338390D+04 P.E.= -0.44676762D+04 K.E.= 0.22338371D+04 V.T.= -0.20000008D+01

S BASIS/ORB E	1S -432.96814	2S -56.68E21	3S -8.40750	4S -1.00809
1S 31.35320	0.81009	0.35305	-0.13674	-0.03952
1S 38.61660	0.18516	-0.01562	0.00550	0.00194
2S 26.27340	0.00962	0.18177	-0.08033	-0.02285
2S 14.94540	-0.00072	-0.99002	0.42339	0.12196
3S 13.45660	0.00123	-0.22093	0.27551	0.09311
3S 8.14183	-0.00083	-0.01737	-0.49279	-0.17508
3S 5.53321	0.00039	0.00212	-0.72850	-0.25110
4S 3.10949	-0.00014	-0.00C69	-0.01359	0.48997
4S 2.01615	0.00012	0.00054	0.00548	0.57968
4S 1.42268	-0.00005	-0.00021	-0.00193	0.04959

P BASIS/ORB E	2P -50.53277	3P -6.25675	4P -0.62672	D BASIS/ORB E	3D -2.48944
2P 14.05140	0.83372	0.33942	0.08636	3D 4.14005	0.44484
2P 22.79450	0.10169	0.03569	0.00741	3D 2.59793	0.11247
3P 13.53130	0.06187	0.08735	0.01787	3D 6.35867	0.31295
3P 8.37917	0.04690	-0.33434	-0.08037	3D 9.09384	0.22544
3P 5.57949	-0.01675	-0.73342	-0.22312	3D 15.40150	0.02810
4P 4.30039	0.00637	-0.05427	0.04097		
4P 2.42623	-0.00256	0.00002	0.53702		
4P 1.53387	0.00156	-0.00131	0.50490		
4P 1.03108	-0.00057	0.00030	0.02643		

ARSENIC K(2)L(8)M(18)4S(2)4P(2), 1S  
T.E.= -0.22337677D+04 P.E.= -0.44675333D+04 K.E.= 0.22337656D+04 V.T.= -0.20000009D+C1

S BASIS/ORB E	1S -432.98250	2S -56.70299	3S -8.42079	4S -1.01602
1S 31.36110	0.81077	0.35311	-0.13675	-0.04060
1S 38.62630	0.18436	-0.01576	0.00554	0.00239
2S 26.28000	0.00977	0.18163	-0.08027	-0.02237
2S 14.94150	-0.00076	-0.59012	0.42341	0.12140
3S 13.45990	0.00125	-0.22046	0.27524	0.09453
3S 8.14390	-0.00084	-0.01754	-0.49180	-0.17759
3S 5.53462	0.00039	0.00218	-0.72937	-0.24908
4S 3.08811	-0.00014	-0.00C71	-0.01376	0.50161
4S 2.01343	0.00012	0.00057	0.00582	0.56468
4S 1.42304	-0.00005	-0.00022	-0.00206	0.05199

P BASIS/ORB E	2P -50.54657	3P -6.26988	4P -0.55968	D BASIS/ORB E	3D -2.50270
2P 14.04780	0.83472	0.34001	0.08263	3D 4.25373	0.46060
2P 22.80570	0.10144	0.03552	0.00827	3D 2.67129	0.12898
3P 13.53460	0.06082	0.08641	0.02268	3D 6.55732	0.28863
3P 8.38129	0.04736	-0.33219	-0.09117	3D 9.09614	0.21678
3P 5.58090	-0.01710	-0.73621	-0.20268	3D 15.40540	0.02850
4P 4.26354	0.00684	-0.09401	0.00893		
4P 2.57553	-0.00278	0.00123	0.48909		
4P 1.53426	0.00140	-0.00222	0.56707		
4P 1.03134	-0.00054	0.00C48	0.04545		

See page 183 for Explanation of Tables and Notes for Tables 32, 42, and 43

## ROOTHAAN-HARTREE-FOCK ATOMIC WAVEFUNCTIONS

TABLE 2 (15). HARTREE-FOCK FUNCTIONS FOR POSITIVE IONS.

SELENIUM K(2)L(8)M(18)4S(2)4P(3), 4S  
 T.E.= -0.23995581D+04 P.E.= -0.47951123D+04 K.E.= 0.23995542D+04 V.T.= -0.20000016D+01

	S	1S	2S	3S	4S
BASIS/ORB	E	-461.24923	-61.04879	-9.31085	-1.16698
1S	31.55230	0.84747	0.34531	-0.13314	-0.03998
1S	41.07280	0.17145	-0.00034	-0.00174	-0.00076
2S	27.35850	-0.02546	0.16498	-0.07695	-0.02385
2S	15.03120	0.01281	-1.03425	0.45295	0.13872
3S	13.71040	-0.00752	-0.16042	0.25655	0.09064
3S	8.47709	0.00298	-0.02038	-0.49597	-0.17980
3S	5.79158	-0.00140	0.00343	-0.73526	-0.27826
4S	3.33386	0.00046	-0.00106	-0.01049	0.49828
4S	2.19720	-0.00038	0.00085	0.00283	0.56808
4S	1.56897	0.00015	-0.00033	-0.00091	0.06129

	P	2P	3P	4P	D	3D
BASIS/ORB	E	-54.64843	-7.03876	-0.78638	BASIS/CRB	E
2P	14.86100	0.80055	0.33058	0.08584	3D	4.41508
2P	23.64250	0.09614	0.03397	0.00929	3D	2.82845
3P	14.22060	0.10314	0.10297	0.03264	3D	6.80527
3P	8.75241	0.04784	-0.31047	-0.10170	3D	9.84704
3P	5.87210	-0.01697	-0.76587	-0.21953	3D	16.31710
4P	4.27784	0.00767	-0.08996	-0.01202		0.02403
4P	2.79396	-0.00472	0.01325	0.53157		
4P	1.74032	0.00398	-0.01026	0.55369		
4P	1.46128	-0.00228	0.00566	0.01312		

SELENIUM K(2)L(8)M(18)4S(2)4P(3), 2D  
 T.E.= -0.23994774D+04 P.E.= -0.47989478D+04 K.E.= 0.23994703D+04 V.T.= -0.20000030D+01

	S	1S	2S	3S	4S
BASIS/ORB	E	-461.26216	-61.06124	-9.32259	-1.17358
1S	31.89310	0.84363	0.34769	-0.13323	-0.04161
1S	40.86620	0.16600	-0.00580	-0.00023	0.00077
2S	27.21910	-0.01219	0.17356	-0.08163	-0.02374
2S	15.10860	0.00819	-1.03276	0.45478	0.13680
3S	13.64330	-0.00445	-0.16556	0.25949	0.09642
3S	8.43423	0.00166	-0.01758	-0.51216	-0.19597
3S	5.76215	-0.00075	0.00246	-0.72197	-0.26112
4S	3.19905	0.00023	-0.00075	-0.00898	0.59468
4S	2.05429	-0.00022	0.00071	0.00303	0.51144
4S	1.56123	0.00011	-0.00033	-0.00123	0.01561

	P	2P	3P	4P	D	3D
BASIS/ORB	E	-54.66093	-7.05035	-0.73642	BASIS/ORB	E
2P	14.78360	0.80679	0.33295	0.08819	3D	4.48251
2P	23.52370	0.09859	0.03499	0.00883	3D	2.81399
3P	14.11710	0.09497	0.10187	0.02882	3D	7.14608
3P	8.70800	0.04636	-0.32906	-0.09831	3D	9.79695
3P	5.84215	-0.01718	-0.74649	-0.22661	3D	15.95090
4P	4.49523	0.00725	-0.08547	0.00983		0.02829
4P	2.74890	-0.00366	0.00132	0.53052		
4P	1.73154	0.00340	-0.00287	0.48069		
4P	1.45405	-0.00195	0.00125	0.07879		

SELENIUM K(2)L(8)M(18)4S(2)4P(3), 2P  
 T.E.= -0.23994245D+04 P.E.= -0.47988429D+04 K.E.= 0.23994184D+04 V.T.= -0.20000025D+01

	S	1S	2S	3S	4S
BASIS/ORB	E	-461.27073	-61.06940	-9.33040	-1.17822
1S	31.61260	0.84657	0.34565	-0.13315	-0.03992
1S	41.03620	0.17064	-0.00123	-0.00148	-0.00081
2S	27.33380	-0.02305	0.16650	-0.07776	-0.02436
2S	15.04490	0.01200	-1.03395	0.45324	0.13954
3S	13.69850	-0.00698	-0.16205	0.25714	0.09062
3S	8.46950	0.00276	-0.01992	-0.49896	-0.18059
3S	5.78637	-0.00129	0.00329	-0.73282	-0.27919
4S	3.33278	0.00043	-0.00102	-0.01010	0.50450
4S	2.19471	-0.00035	0.00082	0.00266	0.56431
4S	1.56760	0.00014	-0.00032	-0.00086	0.05964

See page 183 for Explanation of Tables and Notes for Tables 32, 42, and 43

TABLE 2 (16). HARTREE-FOCK FUNCTIONS FOR POSITIVE IONS.

P	2P	3P	4P	C	3D
BASIS/ORB E	-54.66908	-7.05805	-0.70401	BASIS/ORB E	-3.04694
2P 14.84730	0.80594	0.33338	0.08807	3D 4.54341	0.48825
2P 23.62150	0.09512	0.03333	0.00840	3D 2.82589	0.10548
3P 13.99810	0.10105	0.10539	0.02982	3D 7.17625	0.31835
3P 8.74454	0.04377	-0.32532	-0.09710	3D 9.82817	0.17567
3P 5.86679	-0.01547	-0.74841	-0.22655	3D 16.01890	0.02709
4P 4.51392	0.00651	-0.09024	0.00642		
4P 2.77227	-0.00324	0.00211	0.52160		
4P 1.73876	0.00294	-0.00416	0.45021		
4P 1.46000	-0.00170	0.00178	0.12457		

BROMINE K(2)L(8)M(18)4S(2)4P(4), 3P  
T.E.= -0.25720447D+04 P.E.= -0.51440795D+04 K.E.= 0.25720348D+04 V.T.= -0.20300038D+01

S	1S	2S	3S	4S
BASIS/ORB E	-490.47343	-65.61101	-10.28080	-1.34673
1S 32.61300	0.81113	0.37480	-0.14526	-0.04384
1S 41.34500	0.19937	-0.02176	0.00602	0.00042
2S 26.52740	-0.01461	0.19667	-0.09689	-0.03366
2S 15.88340	0.00975	-1.05532	0.47832	0.15723
3S 13.79150	-0.00511	-0.18942	0.27885	0.09673
3S 8.78548	0.00229	-0.00870	-0.52780	-0.18599
3S 6.01804	-0.00105	-0.00034	-0.72459	-0.30932
4S 3.62898	0.00032	-0.00001	-0.00584	0.48399
4S 2.37802	-0.00020	0.00004	-0.00063	0.61556
4S 1.51458	0.00006	-0.00001	0.00021	0.04328

P	2P	3P	4P	C	3D
BASIS/ORB E	-58.96492	-7.88555	-0.63788	BASIS/ORB E	-3.62820
2P 15.80840	0.74807	0.31586	0.08978	3D 4.82146	0.47512
2P 24.12050	0.09646	0.03341	0.00838	3D 3.06715	0.09763
3P 14.74930	0.16730	0.12438	0.03461	3D 7.36027	0.31587
3P 8.64003	0.03991	-0.40083	-0.12039	3D 10.19450	0.19186
3P 5.89994	-0.01694	-0.69385	-0.23742	3D 16.61900	0.02664
4P 4.72390	0.00677	-0.05631	0.03599		
4P 2.89088	-0.00262	-0.00332	0.56990		
4P 1.81889	0.00146	0.00014	0.49309		
4P 1.31753	-0.00058	-0.00020	0.01907		

BROMINE K(2)L(8)M(18)4S(2)4P(4), 1D  
T.E.= -0.25719871D+04 P.E.= -0.51439644D+04 K.E.= 0.25715774D+04 V.T.= -0.20000038D+01

S	1S	2S	3S	4S
BASIS/ORB E	-490.48170	-65.61887	-10.28820	-1.35096
1S 32.62800	0.81124	0.37498	-0.14531	-0.04379
1S 41.33900	0.19893	-0.02207	0.00612	0.00037
2S 26.52360	-0.01410	0.19707	-0.09709	-0.03388
2S 15.88570	0.00952	-1.05545	0.47845	0.15762
3S 13.78940	-0.00496	-0.18961	0.27893	0.09656
3S 8.78420	0.00222	-0.00861	-0.52831	-0.18596
3S 6.01717	-0.00101	-0.00036	-0.72420	-0.30976
4S 3.61920	0.00030	-0.00000	-0.00580	0.49279
4S 2.36724	-0.00019	0.00003	-0.00060	0.60945
4S 1.51436	0.00006	-0.00001	0.00020	0.04066

P	2P	3P	4P	C	3D
BASIS/ORB E	-58.97279	-7.89282	-0.81206	BASIS/ORB E	-3.63561
2P 15.80610	0.74784	0.31637	0.08921	3D 4.82075	0.47527
2P 24.11690	0.09668	0.03323	0.00864	3D 3.06671	0.09751
3P 14.75370	0.16735	0.12319	0.03560	3D 7.35919	0.31583
3P 8.63877	0.03954	-0.39743	-0.12376	3D 10.19310	0.19199
3P 5.89908	-0.01618	-0.69981	-0.23156	3D 16.61430	0.02667
4P 4.55851	0.00666	-0.05521	0.02998		
4P 2.92474	-0.00303	0.00002	0.55576		
4P 1.81862	0.00155	-0.00202	0.50771		
4P 1.31734	-0.00062	0.00044	0.02411		

See page 183 for Explanation of Tables and Notes for Tables 32, 42, and 43

## ROOTHAAAN-HARTREE-FOCK ATOMIC WAVEFUNCTIONS

TABLE 2 (17). HARTREE-FOCK FUNCTIONS FOR POSITIVE IONS.

BROMINE K(2)L(8)M(18)4S(2)4P(4), 1S  
 T.E.= -0.257190140D+04 P.E.= -0.51437941D+04 K.E.= 0.25718927D+04 V.T.= -0.20000034D+01

S	1S	2S	3S	4S
BASIS/ORB E	-490.49415	-65.63070	-10.29936	-1.35737
1S 32.55520	0.81076	0.37415	-0.14511	-0.04345
1S 41.36820	0.20097	-0.02059	0.00563	-0.00001
2S 26.54220	-0.01662	0.19512	-0.09609	-0.03405
2S 15.87430	0.01070	-1.05487	0.47784	0.15842
3S 13.79940	-0.00570	-0.18862	0.27863	0.09510
3S 8.79041	0.00262	-0.00903	-0.52609	-0.18152
3S 6.02138	-0.00122	-0.00023	-0.72598	-0.31651
4S 3.70258	0.00038	-0.00004	-0.00575	0.44749
4S 2.43249	-0.00023	0.00006	-0.00089	0.64533
4S 1.51543	0.00007	-0.00001	0.00024	0.05380

P	2P	3P	4P	C	3D
BASIS/ORB E	-58.98465	-7.90379	-0.77399	BASIS/CRB E	-3.64680
2P 15.81750	0.74830	0.31513	0.08972	3D 4.82417	0.47602
2P 24.13410	0.09587	0.03339	0.00839	3D 3.06885	0.09761
3P 14.73230	0.16798	0.12692	0.03547	3D 7.36440	0.31525
3P 8.76768	0.03707	-0.38266	-0.11622	3D 10.20020	0.19186
3P 5.90322	-0.01280	-0.72457	-0.24348	3D 16.63720	0.02647
4P 4.26147	0.00562	-0.05126	0.06318		
4P 2.87063	-0.00335	0.00483	0.53210		
4P 1.81991	0.00167	-0.00435	0.48212		
4P 1.31827	-0.00064	0.00092	0.05006		

KRYPTON K(2)L(8)M(18)4S(2)4P(5), 2P  
 T.E.= -0.27515670D+04 P.E.= -0.55031339D+04 K.E.= 0.27515669D+04 V.T.= -0.200000000D+01

S	1S	2S	3S	4S
BASIS/ORB E	-520.61003	-70.34474	-11.28835	-1.53137
1S 32.82330	0.71564	0.38146	-0.14484	-0.04539
1S 40.96840	0.29884	-0.01809	0.00130	-0.00108
2S 27.19930	-0.01920	0.18154	-0.09672	-0.03451
2S 16.21990	0.00951	-1.06909	0.49827	0.16905
3S 14.16200	-0.00482	-0.16814	0.26307	0.09635
3S 9.02411	0.00214	-0.01140	-0.52093	-0.18952
3S 6.31241	-0.00102	0.00107	-0.72686	-0.32845
4S 3.85573	0.00031	-0.00037	-0.00895	0.47329
4S 2.60208	-0.00021	0.00030	0.00086	0.59546
4S 1.75564	0.00007	-0.00009	-0.00035	0.07602

P	2P	3P	4P	C	3D
BASIS/ORB E	-63.45116	-8.76872	-0.91557	BASIS/CRB E	-4.26331
2P 16.56360	0.74143	0.31211	0.09065	3D 5.29877	0.49334
2P 25.56470	0.08281	0.03017	0.00872	3D 3.39672	0.11317
3P 15.65820	0.17792	0.13321	0.04258	3D 7.79894	0.25880
3P 9.31398	0.05916	-0.28871	-0.10038	3D 10.45830	0.20890
3P 6.51144	-0.02768	-0.76825	-0.25577	3D 17.22100	0.02679
4P 5.10297	0.01122	-0.09364	-0.02932		
4P 3.33850	-0.00475	0.00106	0.51715		
4P 2.06152	0.00188	-0.00236	0.57263		
4P 1.33176	-0.00059	0.00036	0.04091		

RUBIDIUM K(2)L(8)M(18)4S(2)4P(6), 1S  
 T.E.= -0.29382072D+04 P.E.= -0.58763529D+04 K.E.= 0.29381457D+04 V.T.= -0.20000209D+01

S	1S	2S	3S	4S
BASIS/ORB E	-551.66510	-75.25552	-12.34065	-1.72345
1S 38.06320	-0.84581	0.03288	0.01107	-0.00373
1S 26.02730	-0.17379	0.46892	0.19403	-0.06563
2S 18.17220	0.05748	-0.19595	0.21398	-0.09308
2S 15.15290	-0.04235	-0.98800	-0.88110	0.33070
3S 9.11875	0.01132	-0.03704	0.39815	-0.14521
3S 6.81163	-0.00962	0.01677	0.77912	-0.36464
4S 5.31210	0.00412	-0.00494	0.02187	0.00886
4S 3.78513	-0.00184	0.00182	0.00541	0.65104
4S 2.44518	0.00039	-0.00030	-0.00038	0.48260

See page 183 for Explanation of Tables and Notes for Tables 32, 42, and 43

TABLE 2 (18). HARTREE-FOCK FUNCTIONS FOR POSITIVE IONS.

P BASIS/ORB	E	2P -68.11257	3P -9.69535	4P -1.00984	D BASIS/ORB	E	3D -4.93799
2P 24.57940		-0.12760	0.03267	0.00875	3D 13.11290		0.15444
2P 15.31180		-0.87425	0.42138	0.12968	3D 7.38297		0.62662
3P 8.27716		-0.03466	-0.64055	-0.22041	3D 4.21200		0.31775
3P 5.75613		0.01634	-0.48241	-0.18114			
4P 3.83956		-0.00675	-0.00299	0.35299			
4P 2.69131		0.00450	-0.00199	0.48286			
4P 1.87579		-0.00139	0.00043	0.30792			

STRONTIUM K(2)L(8)M(18)4S(2)4P(6)5S(1),2S  
T.E.= -0.31313671D+04 P.E.= -0.62626682D+04 K.E.= 0.31312011D+04 V.T.= -0.20000211D+01

S BASIS/ORB	E	1S -583.90917	2S -80.61161	3S -13.69489	4S -2.11340	5S -0.37887
1S 39.C7750		-0.84987	0.03171	-0.01153	-0.00403	0.00128
1S 26.66250		-0.16976	0.47433	-0.19650	-0.06553	0.02113
2S 19.13200		0.04997	-0.17596	-0.18663	-0.08495	0.02698
2S 15.61730		-0.03413	-1.01779	0.85759	0.33596	-0.10372
3S 9.10433		0.01085	0.03603	-0.47822	-0.17877	0.05526
3S 6.93072		-0.00965	0.01749	-0.70874	-0.37166	0.11712
4S 4.16382		0.02472	-0.02490	-0.02635	0.60881	-0.17089
4S 2.82673		-0.09087	0.08832	0.04478	0.45552	-0.40251
5S 3.17454		0.07159	-0.06917	-0.03291	0.08128	0.21685
5S 1.67395		0.00103	-0.00114	-0.00134	0.01437	0.51965
5S 1.12943		-0.00029	0.00034	0.00052	-0.00276	0.57054

P BASIS/ORB	E	2P -73.21685	3P -10.92038	4P -1.31539	D BASIS/ORB	E	3D -5.91460
2P 25.24630		-0.12672	0.03217	0.00914	3D 13.26860		0.17794
2P 15.78900		-0.87491	0.42762	0.14134	3D 7.49528		0.61748
3P 8.52946		-0.03500	-0.65518	-0.24135	3D 4.57526		0.29417
3P 6.00502		0.01690	-0.46815	-0.19568			
4P 4.01920		-0.00649	-0.00364	0.41214			
4P 2.76930		0.00435	-0.00093	0.54279			
4P 1.97647		-0.00146	0.00021	0.18995			

YTTRIUM K(2)L(8)M(18)4S(2)4P(6)5S(2),1S  
T.E.= -0.33314661D+04 P.E.= -0.66628971D+04 K.E.= 0.33314310D+04 V.T.= -0.20000105D+01

S BASIS/ORB	E	1S -617.10467	2S -86.17499	3S -15.12060	4S -2.51795	5S -0.43486
1S 27.05240		-0.16190	-0.47772	-0.20189	-0.07580	-0.02418
1S 40.05530		-0.85779	-0.03530	-0.01184	-0.00395	-0.00157
2S 15.94770		-0.04507	0.92343	0.91421	0.37472	0.12762
2S 19.00340		0.06022	0.27536	-0.21858	-0.10253	-0.03773
3S 7.51479		-0.00522	-0.00772	-0.91243	-0.48113	-0.16062
3S 10.29590		0.00879	0.03045	-0.28573	-0.09965	-0.03548
4S 3.02849		-0.00387	-0.00318	0.01938	0.51996	0.23423
4S 4.32473		0.00297	0.00261	-0.03140	0.62522	0.23345
5S 2.65831		0.00293	0.00225	-0.01082	0.00249	-0.12096
5S 2.00435		-0.00124	-0.00090	0.00343	0.00596	-0.30435
5S 1.35356		0.00024	0.00017	-0.00052	-0.00039	-0.73556

P BASIS/ORB	E	2P -78.52679	3P -12.21480	4P -1.63468	D BASIS/ORB	E	3D -6.95809
2P 16.27030		-0.87612	0.43374	0.15210	3D 7.80781		0.63402
2P 25.93330		-0.12529	0.03149	0.00937	3D 13.84780		0.17300
3P 6.22524		0.01742	-0.44549	-0.20606	3D 4.80528		0.27829
3P 8.76369		-0.03533	-0.67899	-0.26440			
4P 2.82305		0.00352	-0.00062	0.59003			
4P 4.17957		-0.00600	-0.00292	0.48832			
4P 1.88671		-0.00106	0.00019	0.07191			

See page 183 for Explanation of Tables and Notes for Tables 32, 42, and 43

## ROOTHAAN-HARTREE-FOCK ATOMIC WAVEFUNCTIONS

TABLE 2 (19). HARTREE-FOCK FUNCTIONS FOR POSITIVE IONS.

ZIRCONIUM K(2)L(8)M(18)4S(2)4P(6)5S(0)4D(3), 4F  
 T.E.= -0.35387663D+04 P.E.= -0.7C776009D+04 K.E.= 0.35388345D+04 V.T.= -0.19999807D+01

S	1S	2S	3S	4S	P	2P	3P	4P	D	3D	4D
BASIS/ORB E	-650.80415	-91.46823	-16.15201	-2.52167	BASIS/ORB E	-83.56990	-13.11903	-1.60786	BASIS/ORB E	-7.61350	-0.47496
1S 41.07000	0.85942	0.03384	-0.01199	-0.00297	2P 25.59770	-0.14130	0.03535	0.01032	3D 12.36300	0.33226	-0.07524
1S 27.70420	0.16059	0.48281	-0.20428	-0.07906	2P 16.75060	-0.85552	0.43363	0.15408	3D 8.15419	0.35343	-0.09337
2S 20.08540	-0.05078	-0.21720	-0.18569	-0.07819	3P 9.01743	-0.05260	-0.68511	-0.27169	4D 7.34426	0.39031	-0.06069
2S 16.46690	0.03409	-0.98723	0.87827	0.34900	3S 7.64201	0.00528	0.01279	-0.80296	4D 3.31480	0.03833	0.45161
3S 9.90120	-0.00780	-0.03259	-0.38921	-0.10894	4S 4.72625	-0.00144	-0.00219	-0.01907	4D 1.63918	-0.00814	0.67376
3S 7.64201	0.00528	0.01279	-0.80296	-0.49385	4S 3.16484	0.00103	0.00149	0.00450	4S 2.26231	0.57136	
4S 4.72625	-0.00144	-0.00219	-0.01907	0.58991	4S 3.16484	0.00103	0.00149	0.00450	4S 2.26231	0.57136	
4S 3.16484	0.00103	0.00149	0.00450	0.57136	4S 2.26231	-0.00038	-0.00051	-0.00155	4S 2.26231	0.02379	
4S 2.26231	-0.00038	-0.00051	-0.00155	0.02379							

ZIRCONIUM K(2)L(8)M(18)4S(2)4P(6)5S(1)4D(2), 4F  
 T.E.= -0.35387956D+04 P.E.= -0.7C774709D+04 K.E.= 0.35386753D+04 V.T.= -0.20000340D+01

S	1S	2S	3S	4S	5S	P	2P	3P	4P	D	3D	4D
BASIS/ORB E	-650.94577	-91.61656	-16.29214	-2.65285	-0.44387	BASIS/ORB E	-83.71742	-13.25753	-1.72283	BASIS/ORB E	-7.75301	-0.57633
1S 41.07000	0.85941	0.03385	-0.01198	0.00471	0.00105	2P 26.59770	-0.12443	0.03093	0.00918	3D 13.36300	0.24167	-0.06244
1S 27.70420	0.16059	0.48279	-0.20435	0.07686	0.02481	2P 16.75060	-0.87665	0.43396	0.15755	3D 7.25419	0.76093	-0.18046
2S 20.08540	-0.05075	-0.21699	-0.18580	0.05425	0.02678	3P 9.01743	-0.03633	-0.69687	-0.27535	4D 4.41068	0.10523	0.08862
2S 16.46690	0.03405	-0.98752	0.87862	-0.37C77	-0.11331	3S 7.64201	0.00519	0.01248	-0.80334	0.45126	0.16204	
3S 9.90128	-0.00773	-0.03225	-0.38952	0.14560	0.03579	4S 4.51782	-0.00157	-0.00234	-0.02064	-0.65342	-0.28303	
3S 7.64201	0.00519	0.01248	-0.80334	0.45126	0.16204	4S 3.15135	0.00114	0.00162	0.00661	-0.49860	-0.10970	
4S 3.15135	0.00114	0.00162	0.00661	-0.49860	-0.10970	5S 1.93276	-0.00114	-0.00147	-0.00496	0.03506	0.49467	
5S 1.93276	-0.00114	-0.00147	-0.00496	0.03506	0.49467	5S 1.56654	0.00123	0.00156	0.00504	0.02947	0.13141	
5S 1.56654	0.00123	0.00156	0.00504	0.13141		5S 1.23614	-0.00041	-0.00051	-0.00159	-0.00778	0.47233	
5S 1.23614	-0.00041	-0.00051	-0.00159	0.47233								

P	2P	3P	4P	D	3D	4D
BASIS/ORB E	-83.71742	-13.25753	-1.72283	BASIS/ORB E	-7.75301	-0.57633
2P 26.59770	-0.12443	0.03093	0.00918	3D 13.36300	0.24167	-0.06244
2P 16.75060	-0.87665	0.43396	0.15755	3D 7.25419	0.76093	-0.18046
3P 9.01743	-0.03633	-0.69687	-0.27535	4D 4.41068	0.10523	0.08862
3P 6.49159	0.01865	-0.43322	-0.20822	4D 2.99803	-0.02571	0.46967
4P 4.34400	-0.00652	-0.00429	0.52634	4D 1.64755	0.00462	0.57667
4P 2.96592	0.00432	0.00022	0.51769			
4P 2.12967	-0.00149	-0.00025	0.11336			

ZIRCONIUM K(2)L(8)M(18)4S(2)4P(6)5S(2)4D(1), 2D  
 T.E.= -0.35386948D+04 P.E.= -0.7C773447D+04 K.E.= 0.35386499D+04 V.T.= -0.20000127D+01

S	1S	2S	3S	4S	5S	P	2P	3P	4P	D	3D	4D
BASIS/ORB E	-651.08869	-91.76767	-16.44480	-2.79361	-0.46027	BASIS/ORB E	-83.71742	-13.25753	-1.72283	BASIS/ORB E	-7.75301	-0.57633
1S 41.07000	0.85941	0.03384	-0.01201	0.00452	0.00136	2P 26.59770	-0.12443	0.03093	0.00918	3D 13.36300	0.24167	-0.06244
1S 27.70420	0.16058	0.48281	-0.20435	0.07804	0.02549	2S 20.08540	-0.05071	-0.21700	-0.18621	0.09336	0.03031	
2S 16.46690	0.03402	-0.98755	0.87929	-0.37240	-0.12124	3S 9.90128	-0.00770	-0.03217	-0.39058	0.14334	0.04181	
3S 7.64201	0.00516	0.01242	-0.80247	0.46100	0.16443	4S 4.51782	-0.00156	-0.00230	-0.02073	-0.67208	-0.28689	
4S 4.51782	0.00112	0.00159	0.00674	-0.48959	-0.13938	4S 3.15135	0.00112	0.00159	0.00674	-0.00428	0.50991	
5S 2.05416	-0.00066	-0.00085	-0.00301	-0.00004	0.43024	5S 1.37661	0.00113	0.00142	0.00458	-0.00004	0.43024	
5S 1.37661	0.00113	0.00142	0.00458	-0.00004		5S 1.23725	-0.00078	-0.00098	-0.00312	0.00020	0.17923	
5S 1.23725	-0.00078	-0.00098	-0.00312	0.00020								

See page 183 for Explanation of Tables and Notes for Tables 32, 42, and 43

TABLE 2 (20). HARTREE-FOCK FUNCTIONS FOR POSITIVE IONS.

P BASIS/ORB E	2P -83.86691	3P -13.4048	4P -1.84586	D BASIS/ORB E	3D -7.90152	4D -0.65676
2P 26.59770	-0.12440	0.03091	0.00918	3D 13.36300	-0.24038	-0.06620
2P 16.75060	-0.87671	0.43943	0.16001	3D 7.25419	-0.76532	-0.19758
3P 9.01743	-0.03610	-0.69120	-0.28256	4D 4.17511	-0.11053	0.18763
3P 6.49159	0.01831	-0.43285	-0.20441	4D 2.70839	0.04127	0.48746
4P 4.27166	-0.00645	-0.00479	0.56706	4D 1.70038	-0.01212	0.44986
4P 2.93340	0.00449	0.00078	0.50009			
4P 2.12232	-0.00158	-0.00029	0.08391			

NIOBIUM K(2)L(8)M(18)4S(2)4P(6)5S(1)4D(4), 5D  
T.E.= -0.37533773D+04 P.E.= -0.75066373D+04 K.E.= 0.37532600D+04 V.T.= -0.20000312D+01

S BASIS/ORB E	1S -685.68185	2S -97.20529	3S -17.47988	4S -2.77065
1S 42.08350	0.86110	0.03308	-0.01183	-0.00417
1S 28.36340	0.15907	0.48638	-0.20717	-0.07984
2S 20.69320	-0.05083	-0.20583	-0.18865	-0.09211
2S 16.94400	0.03388	-0.99708	0.88724	0.37370
3S 10.09090	-0.00842	-0.03444	-0.39700	-0.13060
3S 7.92723	0.00597	0.01493	-0.79563	-0.48467
4S 4.79723	-0.00186	-0.00285	-0.02131	0.63863
4S 3.38191	0.00175	0.00252	0.00831	0.44953
4S 2.65938	-0.00075	-0.00102	-0.00324	0.09397

P BASIS/ORB E	2P -89.05797	3P -14.31540	4P -1.79562	D BASIS/ORB E	3D -8.56339	4D -0.54035
2P 27.13020	-0.12708	0.03142	0.00949	3D 13.92240	0.23265	-0.05959
2P 17.20310	-0.87429	0.44433	0.16197	3D 7.62257	0.76477	-0.19245
3P 9.27346	-0.03566	-0.70659	-0.28181	4D 4.86892	0.09549	0.11717
3P 6.73590	0.01873	-0.41833	-0.22002	4D 2.94814	-0.01274	0.54406
4P 4.62800	-0.00622	-0.00401	0.51469	4D 1.59441	0.00296	0.49506
4P 3.15673	0.00375	-0.00011	0.51852			
4P 2.23926	-0.00121	-0.00032	0.13885			

NIOBIUM K(2)L(8)M(18)4S(2)4P(6)5S(1)4D(3), 5F  
T.E.= -0.37533505D+04 P.E.= -0.75655852D+04 K.E.= 0.37532348D+04 V.T.= -0.20000308D+01

S BASIS/ORB E	1S -685.82117	2S -97.35711	3S -17.62759	4S -2.90837	5S -0.46850
1S 42.08350	0.86103	0.03302	-0.01030	0.00375	0.00111
1S 28.36340	0.15918	0.48649	-0.20989	0.08144	0.02563
2S 20.69320	-0.05124	-0.21030	-0.17444	0.08827	0.02811
2S 16.94400	0.03434	-0.95655	0.87007	-0.37147	-0.11742
3S 10.09090	-0.00935	-0.03617	-0.31603	0.09134	0.02308
3S 8.12723	0.00678	0.01642	-0.86280	0.51965	0.17849
4S 4.76016	-0.00189	-0.00264	-0.04127	-0.64604	-0.26291
4S 3.32504	0.00155	0.00202	0.02165	-0.51148	-0.15660
5S 2.39349	-0.00097	-0.00116	-0.01212	-0.01597	0.25084
5S 1.72388	0.00070	0.00080	0.00834	0.00256	0.46779
5S 1.27701	-0.00024	-0.00027	-0.00279	0.00110	0.40860

P BASIS/ORB E	2P -89.20414	3P -14.46148	4P -1.91682	D BASIS/ORB E	3D -8.70753	4D -0.65431
2P 27.13020	-0.12705	0.03140	0.00959	3D 13.92240	0.23236	-0.06389
2P 17.20310	-0.87434	0.44443	0.16382	3D 7.62257	0.76575	-0.19935
3P 9.27346	-0.03547	-0.70745	-0.28518	4D 4.76508	0.10093	0.10759
3P 6.73590	0.01845	-0.41781	-0.22246	4D 3.11070	-0.01997	0.51652
4P 4.61309	-0.00588	-0.00432	0.53260	4D 1.74615	0.00410	0.51483
4P 3.11228	0.00337	0.00009	0.55020			
4P 2.14536	-0.00105	-0.00023	0.08691			

See page 183 for Explanation of Tables and Notes for Tables 32, 42, and 43.

## ROOCHAAN-HARTREE-FOCK ATOMIC WAVEFUNCTIONS

TABLE 2 (21). HARTREE-FOCK FUNCTIONS FOR POSITIVE IONS.

NIOBIUM K(2)L(8)M(18)4S(2)4P(6)5S(2)4D(2), 3F  
 T.E.= -0.37532028D+04 P.E.= -0.7564383D+04 K.E.= 0.37532355D+04 V.T.= -0.19999913D+01

S	1S	2S	3S	4S	5S	
BASIS/ORB E	-685.97420	-97.51756	-17.79201	-3.06010	-0.48144	
1S 42.08350	0.86110	0.03307	-0.01186	-0.00441	0.00127	
1S 28.36340	0.15905	0.48641	-0.20719	-0.08110	0.02630	
2S 20.69320	-0.05076	-0.20584	-0.18921	-0.05544	0.03047	
2S 15.94400	0.03382	-0.95712	0.88822	0.38281	-0.12324	
3S 10.09090	-0.00835	-0.03425	-0.39862	-0.13711	0.03751	
3S 7.92723	0.00589	0.01476	-0.79444	-0.48541	0.17533	
4S 4.76016	-0.00175	-0.00267	-0.02114	0.67450	-0.28772	
4S 3.32504	0.00128	0.00185	0.00665	0.49753	-0.14340	
5S 2.25610	-0.00072	-0.00095	-0.00283	0.00498	0.38948	
5S 1.57893	0.00059	0.00075	0.00204	0.00071	0.51415	
5S 1.20371	-0.00024	-0.00030	-0.00079	-0.00041	0.22277	
P	2P	3P	4P	D	3D	4D
BASIS/ORB E	-89.36306	-14.62417	-2.05063	BASIS/ORB E	-8.86741	-0.76546
2P 27.13020	-0.12703	0.03138	0.00962	3D 13.92240	-0.22998	-0.06872
2P 17.20310	-0.87438	0.44446	0.16615	3D 7.62257	-0.77388	-0.21062
3P 9.27346	-0.03530	-0.70765	-0.29158	4D 4.27003	-0.11857	0.21457
3P 6.73590	0.01821	-0.41755	-0.22005	4D 2.87810	0.05367	0.50678
4P 4.56170	-0.00581	-0.00473	0.55845	4D 1.79115	-0.01491	0.40377
4P 3.10273	0.00337	0.00050	0.54259			
4P 2.11208	-0.00102	-0.00022	0.06341			

MOLYBDENUM K(2)L(8)M(18)4S(2)4P(6)5S(1)4D(5), 6S  
 T.E.= -0.39753179D+04 P.E.= -0.79504403D+04 K.E.= 0.39751224D+04 V.T.= -0.20000492D+01

S	1S	2S	3S	4S		
BASIS/ORB E	-721.45444	-103.09898	-18.82988	-3.00748		
1S 43.12360	0.85919	0.03153	-0.01001	-0.00247		
1S 29.32550	0.16004	0.48368	-0.20963	-0.08415		
2S 19.87150	-0.09221	-0.25982	-0.46829	-0.19742		
2S 17.62300	0.07929	-0.92651	1.19006	0.48566		
3S 12.75010	-0.00934	-0.04033	-0.13963	-0.02323		
3S 8.59826	0.00326	0.00368	-1.06926	-0.59878		
4S 4.90907	-0.00106	-0.00076	-0.03102	0.68560		
4S 3.38649	0.00083	0.00063	0.01178	0.46363		
4S 2.33398	-0.00028	-0.00020	-0.00342	0.02610		
P	2P	3P	4P	D		
BASIS/ORB E	-94.69285	-15.53314	-1.97374	BASIS/ORB E	-9.53080	-0.60863
2P 27.41400	-0.12769	0.03143	0.00966	3D 14.14050	-0.25009	-0.07015
2P 17.66940	-0.87381	0.44908	0.16762	3D 7.76000	-0.76797	-0.19833
3P 9.46970	-0.03574	-0.75305	-0.30406	4D 4.61732	-0.07580	0.17570
3P 6.86820	0.01995	-0.37480	-0.22199	4D 3.15735	0.01900	0.47221
4P 4.92122	-0.00696	-0.00156	0.50651	4D 1.77289	-0.00304	0.50499
4P 3.36913	0.00382	-0.00072	0.53106			
4P 2.37008	-0.00116	-0.00029	0.14904			

MOLYBDENUM K(2)L(8)M(18)4S(2)4P(6)5S(1)4D(4), 6D  
 T.E.= -0.39752362D+04 P.E.= -0.79502752D+04 K.E.= 0.39750390D+04 V.T.= -0.20000496D+01

S	1S	2S	3S	4S	5S
BASIS/ORB E	-721.61390	-103.26744	-18.99796	-3.16205	-0.49057
1S 43.12360	0.85907	0.03150	-0.01023	0.00288	0.00063
1S 29.32550	0.16024	0.42374	-0.20929	0.08432	0.02682
2S 19.87150	-0.09370	-0.26028	-0.47283	0.20780	0.06116
2S 17.62300	0.08095	-0.92602	1.19546	-0.50444	-0.15360
3S 12.75010	-0.00992	-0.04052	-0.14208	0.02885	0.00374
3S 8.59826	0.00369	0.00386	-1.06747	0.59514	0.26183
4S 4.85083	-0.00174	-0.00113	-0.03540	-0.72396	-0.29609
4S 3.38062	0.00182	0.00118	0.01840	-0.43180	-0.12059
5S 2.71541	-0.00121	-0.00072	-0.00915	-0.01853	0.13268
5S 1.93981	0.00061	0.00035	0.00382	0.00458	0.53899
5S 1.32768	-0.00016	-0.00009	-0.00089	0.00058	0.45671

See page 183 for Explanation of Tables and Notes for Tables 32, 42, and 43

TABLE 2 (22). HARTREE-FOCK FUNCTIONS FOR POSITIVE IONS.

P	2P	3P	4P	C	3D	4D
BASIS/ORB E	-94.85956	-15.69955	-2.11066	BASIS/ORB E	-9.69512	-0.72681
2P 27.74100	-0.12767	0.03141	0.00974	3D 14.14050	-0.24996	-0.07307
2P 17.66940	-0.87384	0.44919	0.16962	3D 7.76000	-0.76826	-0.20953
3P 9.46970	-0.03569	-0.75357	-0.30843	4D 4.58713	-0.07594	0.21440
3P 6.86826	0.01990	-0.37418	-0.22316	4D 3.04885	0.02028	0.49450
4P 4.91535	-0.00696	-0.00195	0.51160	4D 1.81005	-0.00427	0.43737
4P 3.37518	0.00382	-0.00044	0.54932			
4P 2.36618	-0.00114	-0.00026	0.12274			

MOLYBDENUM K(2)L(8)M(18)4S(2)4P(6)5S(2)4D(3), 4F  
T.E.= -0.39750459D+04 P.E.= -0.79499053D+04 K.E.= 0.39748594D+04 V.T.= -0.20300459D+01

S	1S	2S	3S	4S	5S
BASIS/ORB E	-721.78688	-103.44489	-19.17876	-3.32401	-0.50022
1S 43.12360	0.85909	0.03150	-0.01027	0.00283	0.00066
1S 29.32550	0.16019	0.48374	-0.20929	0.08516	0.02744
2S 19.87150	-0.09334	-0.26002	-0.47395	0.20834	0.06307
2S 17.62300	0.08056	-0.92633	1.19699	-0.50732	-0.15783
3S 12.75010	-0.00979	-0.04039	-0.14279	0.02828	0.00390
3S 8.59826	0.00359	0.00379	-1.06730	0.60557	0.20711
4S 4.85083	-0.00157	-0.00102	-0.03440	-0.73584	-0.30731
4S 3.38062	0.00151	0.00099	0.01656	-0.43211	-0.11907
5S 2.55953	-0.00106	-0.00063	-0.00851	0.00020	0.21603
5S 1.88115	0.00066	0.00038	0.00458	-0.00215	0.51388
5S 1.32245	-0.00018	-0.00010	-0.00115	0.00032	0.40152

P	2P	3P	4P	D	3D	4D
BASIS/ORB E	-95.04022	-15.87866	-2.25455	BASIS/ORB E	-9.87210	-0.85445
2P 27.74100	-0.12764	0.03139	0.00977	3D 14.14050	-0.24992	-0.07705
2P 17.66940	-0.87389	0.44931	0.17185	3D 7.76000	-0.76836	-0.22312
3P 9.46970	-0.03553	-0.75416	-0.31467	4D 4.57743	-0.07562	0.24735
3P 6.86826	0.01967	-0.37355	-0.22098	4D 2.95998	0.02114	0.54689
4P 4.87241	-0.00690	-0.00230	0.53130	4D 1.85925	-0.00542	0.34083
4P 3.36428	0.00387	-0.00011	0.55238			
4P 2.34740	-0.00114	-0.00022	0.09522			

TECHNETIUM K(2)L(8)M(18)4S(2)4P(6)5S(0)4D(6), 5D  
T.E.= -0.42045228D+04 P.E.= -0.84C85053D+04 K.E.= 0.42039825D+04 V.T.= -0.20001285D+01

S	1S	2S	3S	4S
BASIS/ORB E	-758.18812	-109.21562	-20.25388	-3.26675
1S 44.13490	-0.86005	0.03138	0.00826	-0.00549
1S 29.94420	-0.16030	0.48711	0.21561	-0.08152
2S 20.36180	0.11790	-0.26C89	0.44355	-0.30249
2S 18.12600	-0.10779	-0.92598	-1.16070	0.62050
3S 13.33450	0.02131	-0.04351	0.05014	-0.11250
3S 7.90000	-0.02897	0.0C829	1.89683	-0.65753
4S 5.75511	-0.00095	-0.00030	0.00057	0.67474
4S 3.62684	0.00019	0.00015	0.00183	0.63318
4S 8.61263	0.02083	-0.00446	-0.78256	-0.01207

P	2P	3P	4P	D	3D	4D
BASIS/ORB E	-100.55224	-16.82400	-2.17356	BASIS/ORB E	-10.57018	-0.63805
2P 28.30000	-0.12916	0.03228	0.00968	3D 14.85810	-0.24566	-0.07171
2P 18.13000	-0.87269	0.45234	0.17357	3D 7.95000	-0.79170	-0.21493
3P 9.60000	-0.03472	-0.82834	-0.35408	4D 4.53922	-0.03833	0.31972
3P 6.90000	0.01976	-0.29964	-0.18025	4D 2.93131	0.00046	0.44288
4P 4.89762	-0.00678	-0.00316	0.64395	4D 1.76001	0.00182	0.40534
4P 3.18771	0.00381	0.00165	0.48373			
4P 2.26455	-0.00136	-0.00118	0.05618			

See page 183 for Explanation of Tables and Notes for Tables 32, 42, and 43

## ROOTHAAN-HARTREE-FOCK ATOMIC WAVEFUNCTIONS

TABLE 2 (23). HARTREE-FOCK FUNCTIONS FOR POSITIVE IONS.

TECHNETIUM K(2)L(8)M(18)4S(2)4P(6)5S(1)4D(5), 7S  
 T.E.= -0.42045831D+04 P.E.= -0.84090351D+04 K.E.= 0.42044520D+04 V.T.= -0.20000312D+01

S	1S	2S	3S	4S	5S	
BASIS/ORB E	-758.30899	-109.33528	-20.39469	-3.41174	-0.50944	
1S 44.13490	0.86085	0.03134	0.01041	-0.00214	0.00068	
1S 29.94420	0.15893	0.48718	0.21181	-0.08818	0.02734	
2S 20.36180	-0.10329	-0.26106	0.50692	-0.20535	0.06619	
2S 18.12500	-0.09101	-0.92590	-1.23677	0.50610	-0.16033	
3S 13.33450	-0.01176	-0.042E3	0.12520	-0.00789	0.00102	
3S 8.91426	0.00471	0.00375	1.08559	-0.63474	0.20755	
4S 5.03711	-0.00684	-0.00287	0.05079	0.88657	-0.27074	
4S 3.94770	0.01115	0.00447	-0.04312	-0.09103	-0.14710	
5S 3.97845	-0.00583	-0.00222	0.01708	0.39576	0.04400	
5S 2.17099	0.00030	0.00010	0.00023	0.01303	0.55200	
5S 1.40763	-0.00010	-0.00002	-0.00014	-0.00529	0.53580	
P	2P	3P	4P	D	3D	4D
BASIS/ORB E	-100.67134	-16.96302	-2.30205	BASIS/ORB E	-10.70798	-0.80820
2P 28.30070	-0.12936	0.03138	0.00976	3D 14.85810	0.22820	-0.06863
2P 18.13020	-0.87223	0.45429	0.17525	3D 8.23587	0.77447	-0.22762
3P 9.75353	-0.03503	-0.75544	-0.31388	4D 5.19427	0.08554	0.16350
3P 7.17120	0.01922	-0.37207	-0.23237	4D 3.32399	-0.01540	0.56356
4P 5.06891	-0.00584	-0.00421	0.56565	4D 1.92025	0.00320	0.42067
4P 3.40474	0.00304	0.00002	0.54352			
4P 2.33940	-0.00091	-0.00030	0.07996			

TECHNETIUM K(2)L(8)M(18)4S(2)4P(6)5S(2)4D(4), 5D  
 T.E.= -0.42043129D+04 P.E.= -0.84085031D+04 K.E.= 0.42041903D+04 V.T.= -0.20000292D+01

S	1S	2S	3S	4S	5S	
BASIS/ORB E	-758.49971	-109.53545	-20.59295	-3.58779	-0.51743	
1S 44.13490	0.86105	0.03138	-0.01038	-0.00391	0.00061	
1S 29.94420	0.15859	0.48712	-0.21193	-0.08580	0.02795	
2S 20.36180	-0.10028	-0.26025	-0.50662	-0.24596	0.06530	
2S 18.12600	0.08765	-0.92686	1.23663	0.55548	-0.16067	
3S 13.33450	-0.01058	-0.04243	-0.12501	-0.03069	-0.00041	
3S 8.91426	0.00376	0.00344	-1.08639	-0.61573	0.21310	
4S 5.03711	-0.00221	-0.00119	-0.03958	0.64737	-0.30314	
4S 3.94770	0.00195	0.00107	0.01900	0.46110	-0.09089	
5S 2.54460	-0.00143	-0.00067	-0.00783	0.15698	0.07535	
5S 2.15709	0.00115	0.00053	0.00564	-0.10656	0.50652	
5S 1.41796	-0.00017	-0.00007	-0.00068	0.01364	0.51890	
P	2P	3P	4P	D	3D	4D
BASIS/ORB E	-100.86974	-17.15962	-2.45958	BASIS/ORB E	-10.90242	-0.93787
2P 29.30070	-0.12933	0.03136	0.00975	3D 14.85810	-0.22790	-0.07226
2P 18.13020	-0.87230	0.45441	0.17758	3D 8.23587	-0.77543	-0.23910
3P 9.75353	-0.03473	-0.75557	-0.32150	4D 5.10708	-0.08784	0.19118
3P 7.17120	0.01878	-0.37160	-0.22745	4D 3.27771	0.01981	0.58931
4P 4.99831	-0.00559	-0.00445	0.60043	4D 1.96996	-0.00486	0.35594
4P 3.36362	0.00290	0.00034	0.53310			
4P 2.24692	-0.00083	-0.00025	0.04944			

RUTHENIUM K(2)L(8)M(18)4S(2)4P(6)5S(0)4D(7), 4F  
 T.E.= -0.44413115D+04 P.E.= -0.88825331D+04 K.E.= 0.44412216D+04 V.T.= -0.20000202D+01

S	1S	2S	3S	4S	
BASIS/ORB E	-795.77831	-115.42091	-21.67529	-3.52015	
1S 45.17170	0.85956	0.02947	0.00947	-0.00195	
1S 30.79900	0.15995	0.48787	0.21367	-0.08911	
2S 20.60400	-0.14011	-0.11421	0.85247	-0.34548	
2S 18.96490	0.12805	-1.06282	-1.57972	0.65050	
3S 14.07160	-0.01079	-0.05132	0.09126	0.00585	
3S 9.24888	0.00335	0.00367	1.11289	-0.64944	
4S 5.26552	-0.00162	-0.00116	0.03883	0.72777	
4S 3.82816	0.00215	0.00157	-0.02582	0.27819	
4S 3.22940	-0.00112	-0.00078	0.01179	0.17805	

See page 183 for Explanation of Tables and Notes for Tables 32, 42, and 43

TABLE 2 (24). HÄRTREE-FOCK FUNCTIONS FOR POSITIVE IONS.

P	2P	3P	4P	D	3D	4D
BASIS/ORB E	-106.50177	-18.11123	-2.36891	BASIS/ORB E	-11.60614	-0.68045
2P 28.90350	-0.13001	0.03109	0.00973	3D 15.40260	0.21959	-0.06500
2P 18.59920	-0.87150	0.45910	0.17870	3D 8.60709	0.77860	-0.23115
3P 10.02070	-0.03561	-0.76223	-0.31269	4D 5.49162	0.08640	0.17366
3P 7.47254	0.02018	-0.36391	-0.24750	4D 3.40390	-0.01385	0.57740
4P 5.37105	-0.00585	-0.00754	0.54046	4D 1.85342	0.00336	0.41659
4P 3.62965	0.00290	0.00095	0.54306			
4P 2.51446	-0.00084	-0.00073	0.11853			

RUTHENIUMM K(2)L(8)M(18)4S(2)4P(6)5S(1)4D(6), 6D  
T.E.= -0.44412678D+04 P.E.= -0.88824230D+04 K.E.= 0.44411553D+04 V.T.= -0.20000253D+01

S	1S	2S	3S	4S	5S
BASIS/ORB E	-795.94329	-115.59531	-21.84830	-3.67826	-0.51875
1S 45.17170	0.85966	0.02951	0.00928	0.00240	0.00011
1S 30.79900	0.15978	0.48781	0.21405	0.08907	0.02810
2S 20.60400	-0.13801	-0.11307	0.64756	0.36559	0.09354
2S 18.96490	0.12579	-1.06411	-1.57448	-0.67102	-0.18432
3S 14.07160	-0.01028	-0.05098	0.8965	-0.00101	-0.01008
3S 9.24888	0.00300	0.00345	1.11476	0.65036	0.21668
4S 5.24008	-0.00099	-0.00073	0.03304	-0.74774	-0.31522
4S 3.64109	0.00069	0.00056	-0.01160	-0.42528	-0.07257
5S 2.28474	-0.00032	-0.00023	0.00412	-0.01181	0.55684
5S 1.20838	-0.00029	-0.00021	0.00340	-0.00722	-0.08384
5S 1.40142	0.00043	0.00032	-0.00512	0.01220	0.63327

P	2P	3P	4P	D	3D	4D
BASIS/ORB E	-106.67433	-18.28257	-2.51023	BASIS/ORB E	-11.77572	-0.63993
2P 28.90350	-0.12998	0.03107	0.00976	3D 15.40260	0.21997	-0.06912
2P 18.59920	-0.87156	0.45920	0.18046	3D 8.60709	0.77741	-0.23618
3P 10.02070	-0.03541	-0.76267	-0.31749	4D 5.52456	0.08908	0.13248
3P 7.47254	0.01990	-0.36351	-0.24612	4D 3.70513	-0.01537	0.54611
4P 5.33081	-0.00567	-0.00774	0.56178	4D 2.08908	0.00273	0.46985
4P 3.58928	0.00282	0.00116	0.55113			
4P 2.46164	-0.00081	-0.00065	0.08522			

RUTHENIUMM K(2)L(8)M(18)4S(2)4P(6)5S(2)4D(5), 6S  
T.E.= -0.44411216D+04 P.E.= -0.88821350D+04 K.E.= 0.44410135D+04 V.T.= -0.20000243D+01

S	1S	2S	3S	4S	5S
BASIS/ORB E	-796.12586	-115.78727	-22.03941	-3.84999	-0.53274
1S 45.17170	0.85960	0.02949	0.00949	-0.00213	0.00037
1S 30.79900	0.15988	0.48785	0.21375	-0.09025	0.02831
2S 20.60400	-0.13920	-0.11339	0.85415	-0.36018	0.10393
2S 18.96490	0.12708	-1.06377	-1.58196	0.66658	-0.19780
3S 14.07160	-0.01057	-0.05106	0.09185	0.00413	-0.00743
3S 9.24888	0.00320	0.00354	1.11332	-0.65866	0.21934
4S 5.24008	-0.00126	-0.00089	0.03501	0.76454	-0.31423
4S 3.64109	0.00107	0.00080	-0.01482	0.41396	-0.10009
5S 2.60799	-0.00063	-0.00044	0.00659	0.00187	0.32747
5S 1.80631	0.00043	0.00029	-0.00394	0.00064	0.54066
5S 1.30840	-0.00016	-0.00010	0.00133	-0.00010	0.26163

P	2P	3P	4P	D	3D	4D
BASIS/ORB E	-106.86445	-18.47195	-2.66413	BASIS/ORB E	-11.96306	-1.03261
2P 28.90350	-0.12995	0.03105	C.00979	3D 15.40260	0.21980	-0.07223
2P 18.59920	-0.87161	0.45530	0.18239	3D 8.60709	0.77814	-0.24809
3P 10.02070	-0.03523	-0.76310	-0.32246	4D 5.46096	0.09091	0.15671
3P 7.47254	0.01965	-0.36311	-0.24546	4D 3.64846	-0.01913	0.55759
4P 5.30158	-0.00550	-0.00793	0.57834	4D 2.19814	0.00382	0.41013
4P 3.57168	0.00265	0.00135	0.55929			
4P 2.37257	-0.00072	-0.00055	0.05712			

See page 183 for Explanation of Tables and Notes for Tables 32, 42, and 43

## ROOTHAAN-HARTREE-FOCK ATOMIC WAVEFUNCTIONS

TABLE 2 (25). HARTREE-FOCK FUNCTIONS FOR POSITIVE IONS.

RHODIUM K(2)L(8)M(18)4S(2)4P(6)5S(0)4D(8), 3F  
 T.E.= -0.46856519D+04 P.E.= -0.93711693D+04 K.E.= 0.46855174D+04 V.T.= -0.20000287D+01

S	1S	2S	3S	4S
BASIS/ORB E	-834.31386	-121.83587	-23.15009	-3.77475
1S 46.16120	0.86420	0.03060	0.00975	-0.00164
1S 31.26650	0.15569	0.49249	0.21743	-0.09260
2S 21.12290	-0.13264	-0.23158	0.72604	-0.28489
2S 19.26920	0.12077	-0.95144	-1.46599	0.59256
3S 14.62120	-0.01151	-0.05044	0.08848	0.01540
3S 9.54463	0.00332	0.00283	1.12303	-0.67302
4S 5.48059	-0.00150	-0.00078	0.03571	0.74292
4S 3.86396	0.00223	0.00122	-0.02436	0.31127
4S 3.35394	-0.00132	-0.00069	0.01293	0.13734

P	2P	3P	4P	D	3D	4D
BASIS/ORB E	-112.65849	-19.45113	-2.56626	BASIS/ORB E	-12.69307	-0.72527
2P 29.47140	-0.13131	0.03053	0.00972	3D 15.63670	0.23408	-0.07253
2P 19.06500	-0.87012	0.46375	0.18359	3D 8.75986	0.78077	-0.23737
3P 10.30440	-0.03619	-0.75655	-0.31048	4D 5.30305	0.06555	0.28117
3P 7.83120	0.02085	-0.36520	-0.26310	4D 3.27492	-0.01339	0.55144
4P 5.61696	-0.00545	-0.01266	0.53823	4D 1.85478	0.00357	0.34500
4P 3.80524	0.00261	0.00246	0.54857			
4P 2.62160	-0.00072	-0.00115	0.12096			

RHODIUM K(2)L(8)M(18)4S(2)4P(6)5S(1)4D(7), 5F  
 T.E.= -0.46855672D+04 P.E.= -0.93709534D+04 K.E.= 0.46853862D+04 V.T.= -0.20000386D+01

S	1S	2S	3S	4S	5S
BASIS/ORB E	-834.49277	-122.02373	-23.33660	-3.94457	-0.52729
1S 46.16120	0.86415	0.03059	0.00981	-0.00224	0.00023
1S 31.26650	0.15577	0.49251	0.21737	-0.09225	0.02802
2S 21.12290	-0.13351	-0.23160	0.72818	-0.30530	0.07913
2S 19.26920	0.12172	-0.95144	-1.46857	0.61774	-0.17025
3S 14.62120	-0.01175	-0.05044	0.08921	0.00E01	-0.01016
3S 9.54463	0.00347	0.00286	1.12293	-0.67085	0.21565
4S 5.41154	-0.00173	-0.00085	0.03632	0.78642	-0.31203
4S 3.71214	0.00202	0.00104	-0.01960	0.38967	-0.07944
5S 3.17491	-0.00136	-0.00065	0.01005	0.01320	0.07122
5S 2.23507	0.00053	0.00024	-0.00301	-0.00252	0.52697
5S 1.44637	-0.00012	-0.00005	0.00059	0.00040	0.52365

P	2P	3P	4P	D	3D	4D
BASIS/ORB E	-112.84460	-19.63602	-2.71918	BASIS/ORB E	-12.87618	-0.89058
2P 29.47140	-0.13151	0.03103	0.00985	3D 15.63670	-0.23427	-0.07607
2P 19.06050	-0.87011	0.46381	0.18516	3D 8.75986	-0.78025	-0.24443
3P 10.30440	-0.03533	-0.75924	-0.31332	4D 5.30827	-0.06765	0.26902
3P 7.83122	0.01993	-0.36464	-0.26540	4D 3.45731	0.01540	0.52684
4P 5.58705	-0.00489	-0.01276	0.56318	4D 2.05239	-0.00353	0.36433
4P 3.73186	0.00221	0.00250	0.56925			
4P 2.49144	-0.00059	-0.00099	0.07350			

RHODIUM K(2)L(8)M(18)4S(2)4P(6)5S(2)4D(6), 5D  
 T.E.= -0.46853450D+04 P.E.= -0.93705181D+04 K.E.= 0.46851731D+04 V.T.= -0.20000367D+01

S	1S	2S	3S	4S	5S
BASIS/ORB E	-834.69059	-122.23154	-23.54270	-4.12779	-0.55009
1S 46.16120	0.86418	0.03060	-0.00983	0.00221	0.00042
1S 31.26650	0.15571	0.49250	-0.21737	0.09305	0.02880
2S 21.12290	-0.13287	-0.23121	-0.72963	0.30657	0.08747
2S 19.26920	0.12103	-0.95191	1.47042	-0.62134	-0.18283
3S 14.62120	-0.01158	-0.05030	-0.08978	-0.00863	-0.00865
3S 9.54463	0.00336	0.00279	-1.12292	0.67716	0.22276
4S 5.41154	-0.00153	-0.00C75	-0.03518	-0.79734	-0.32081
4S 3.71214	0.00160	0.00084	0.01727	-0.39108	-0.09819
5S 3.01774	-0.00105	-0.00051	-0.00855	0.00341	0.16888
5S 2.111734	0.00050	0.00023	0.00328	-0.00108	0.55263
5S 1.42904	-0.00013	-0.00006	-0.00078	-0.00018	0.41649

See page 183 for Explanation of Tables and Notes for Tables 32, 42, and 43

TABLE 2 (26). HARTREE-FOCK FUNCTIONS FOR POSITIVE IONS.

P	2P	3P	4P	D	3D	4D
BASIS/ORB E	-113.05047	-19.84030	-2.88368	BASIS/ORB E	-13.07837	-1.07081
2P 29.47140	-0.13148	0.03102	0.0984	3D 15.63670	-0.23431	-0.07690
2P 19.06050	-0.87016	0.46391	0.18723	3D 8.75986	-0.78022	-0.25570
3P 10.30440	-0.03516	-0.75965	-0.31992	4D 5.31486	-0.06729	0.29019
3P 7.83122	0.01971	-0.36434	-0.26182	4D 3.39727	0.01561	0.57151
4P 5.54217	-0.00482	-0.01297	0.58054	4D 2.10089	-0.00390	0.28727
4P 3.72603	0.00220	0.00285	0.56559			
4P 2.44699	-0.00056	-0.00094	0.05498			

PALLADIUM K(2)L(8)M(18)4S(2)4P(6)5S(0)4D(9), 2D  
T.E.= -0.493766250D+04 P.E.= -0.98751227D+04 K.E.= 0.49374602D+04 V.T.= -0.20300410D+01

S	1S	2S	3S	4S
BASIS/ORB E	-873.76547	-128.41556	-24.66107	-4.03099
1S 47.18200	0.86731	-0.03806	0.01231	-0.00241
1S 30.93790	0.15834	-0.50433	0.22532	-0.09766
2S 21.67970	-0.21910	0.41E24	0.68729	-0.21081
2S 19.88900	0.20977	0.75112	-1.42293	0.50767
3S 16.86780	-0.02151	0.08580	0.01814	0.05314
3S 9.99410	0.00331	0.00067	1.16285	-0.68468
4S 5.43729	-0.02469	0.00203	0.54019	1.29855
4S 5.32782	0.02459	-0.00219	-0.51331	-0.46540
4S 3.63435	-0.00063	0.00006	0.00899	0.34838

P	2P	3P	4P	D	3D	4D
BASIS/ORB E	-118.98299	-20.82629	-2.76587	BASIS/ORB E	-13.81422	-0.77188
2P 30.05800	-0.13239	0.03065	0.00970	3D 15.94220	0.24210	-0.07745
2P 19.53020	-0.86901	0.46842	0.18813	3D 8.99388	0.77828	-0.24432
3P 10.66190	-0.03645	-0.70365	-0.28074	4D 5.41872	0.05453	0.33113
3P 8.39312	0.02049	-0.41475	-0.29865	4D 3.29064	-0.00959	0.55061
4P 5.80736	-0.00386	-0.02245	0.55060	4D 1.87954	0.00282	0.30171
4P 3.91425	0.00180	0.00579	0.54836			
4P 2.68199	-0.00048	-0.00205	0.10721			

PALLADIUM K(2)L(8)M(18)4S(2)4P(6)5S(1)4D(8), 4F  
T.E.= -0.49375510D+04 P.E.= -0.98749240D+04 K.E.= 0.49373730D+04 V.T.= -0.20300361D+01

S	1S	2S	3S	4S	5S
BASIS/ORB E	-873.94939	-128.61323	-24.85475	-4.20824	-0.53340
1S 47.19200	0.86007	-0.01652	0.00242	0.00199	-0.00128
1S 32.93790	0.15638	-0.45566	0.22195	-0.09701	0.02906
2S 21.67970	-0.12940	0.1C875	0.81158	-0.25977	0.04617
2S 19.88900	0.12320	1.05254	-1.54141	0.55486	-0.12661
3S 16.86780	-0.01191	0.05153	0.02870	0.05158	-0.02593
3S 9.99411	0.00151	0.00680	1.16428	-0.69301	0.21611
4S 5.59763	-0.00074	-0.00384	0.06011	0.76073	-0.30250
4S 3.95172	0.00073	0.00383	-0.03836	0.40119	-0.06617
5S 2.99342	-0.00053	-0.00296	0.02415	0.02871	0.07698
5S 2.30636	0.00032	0.00179	-0.01362	-0.00834	0.48414
5S 1.48032	-0.00006	-0.00035	0.00246	0.00120	0.55031

P	2P	3P	4P	D	3D	4D
BASIS/ORB E	-119.17497	-21.01830	-2.92633	BASIS/ORB E	-14.00435	-0.94574
2P 30.05800	-0.13236	0.03C67	0.00953	3D 15.94220	-0.24215	-0.08040
2P 19.53020	-0.86906	0.46842	0.19023	3D 8.99368	-0.77829	-0.25286
3P 10.66190	-0.03617	-0.70320	-0.29090	4D 5.39500	-0.05582	0.34649
3P 8.39312	0.02012	-0.41566	-0.28824	4D 3.37128	0.01194	0.51748
4P 5.72272	-0.00367	-0.02217	0.57867	4D 2.09787	-0.00330	0.30103
4P 3.84855	0.00169	0.00586	0.55227			
4P 2.52879	-0.00042	-0.00180	0.06795			

See page 183 for Explanation of Tables and Notes for Tables 32, 42, and 43

## ROOTHAAN-HARTREE-FOCK ATOMIC WAVEFUNCTIONS

TABLE 2 (27). HARTREE-FOCK FUNCTIONS FOR POSITIVE IONS.

PALLADIUM K(2)L(8)M(18)4S(2)4P(6)5S(2)4D(7), 4F  
 T.E.= -0.49372737D+04 P.E.= -0.98743562D+04 K.E.= 0.49370825D+04 V.T.= -0.20000387D+01

S	1S	2S	3S	4S	5S	
BASIS/ORB E	-874.16486	-128.83850	-25.07722	-4.40431	-0.56565	
1S 47.18200	0.86747	0.03808	0.01167	-0.00188	0.00002	
1S 30.93790	0.15804	0.50430	0.22661	-0.10015	0.03113	
2S 21.67970	-0.21416	-0.41704	0.66204	-0.18870	0.03246	
2S 19.88900	0.20426	-0.75253	-1.39443	0.48619	-0.11836	
3S 16.86780	-0.02039	-0.08549	0.01105	0.06180	-0.02864	
3S 9.99411	0.00281	-0.00076	1.16824	-0.70174	0.22832	
4S 5.59763	-0.00140	0.00005	0.05564	0.77469	-0.31838	
4S 3.95172	0.00132	0.00011	-0.03243	0.39771	-0.08100	
5S 2.90622	-0.00092	-0.00008	0.01861	0.01355	0.20083	
5S 2.17581	0.00059	0.00006	-0.01119	-0.00407	0.48085	
5S 1.48032	-0.00015	-0.00001	0.00265	0.00095	0.44257	
P	2P	3P	4P	D	3D	4D
BASIS/ORB E	-119.39810	-21.23892	-3.10290	BASIS/CRB E	-14.22293	-1.12690
2P 30.05800	-0.13234	0.03064	0.00971	3D 15.94220	-0.24219	-0.08367
2P 19.53020	-0.86910	0.46656	0.19185	3D 8.99388	-0.77826	-0.26105
3P 10.66190	-0.03610	-0.70392	-0.29123	4D 5.39500	-0.05590	0.35533
3P 8.39312	0.02006	-0.41497	-0.29528	4D 3.37127	0.01212	0.56637
4P 5.72272	-0.00366	-0.02234	0.59213	4D 2.09787	-0.00325	0.23416
4P 3.84855	0.00168	0.00608	0.55489			
4P 2.52879	-0.00042	-0.00176	0.05166			

SILVER K(2)L(8)M(18)4S(2)4P(6)5S(0)4D(10), 1S  
 T.E.= -0.51974693D+04 P.E.= -0.10394772D+05 K.E.= 0.51973024D+04 V.T.= -0.20000321D+01

S	1S	2S	3S	4S
BASIS/ORB E	-914.12391	-135.16554	-26.20228	-4.28518
1S 48.21060	0.86501	0.03048	-0.00944	-0.00125
1S 32.55860	0.15588	0.49707	-0.22240	-0.09717
2S 21.74250	-0.27743	0.06763	-1.72062	-0.65839
2S 20.74280	0.26576	-1.24289	2.46078	0.96897
3S 15.83890	-0.01312	-0.06347	-0.04647	0.04343
3S 10.13110	0.00331	0.00345	-1.15454	-0.71239
4S 5.86653	-0.00141	-0.00104	-0.03708	0.75562
4S 4.10590	0.00178	0.00143	0.02165	0.34799
4S 3.44209	-0.00096	-0.00074	-0.01035	0.09255
P	2P	3P	4P	D
BASIS/ORB E	-125.46861	-22.23084	-2.96410	BASIS/GRB E
2P 30.59020	-0.13418	0.03088	0.00983	-14.96402
2P 19.99470	-0.86715	0.47193	0.19202	-0.23194
3P 10.81850	-0.03841	-0.77316	-0.30691	16.52270
3P 8.52037	0.02363	-0.34452	-0.29368	9.36471
4P 6.17800	-0.00520	-0.02429	0.51168	5.70437
4P 4.21499	0.00229	0.00586	0.56813	3.52868
4P 2.89007	-0.00058	-0.00210	0.14218	2.01046

SILVER K(2)L(8)M(18)4S(2)4P(6)5S(1)4D(9), 3D  
 T.E.= -0.51972612D+04 P.E.= -0.10394352D+05 K.E.= 0.5197C910D+04 V.T.= -0.20000327D+01

S	1S	2S	3S	4S	5S
BASIS/ORB E	-914.33177	-135.38231	-26.41845	-4.48146	-0.54195
1S 48.21060	0.86497	0.03047	0.00948	-0.00183	0.00008
1S 32.55860	0.15593	0.49709	0.22237	-0.09680	0.02784
2S 21.74250	-0.27865	0.06744	1.72374	-0.69982	0.17051
2S 20.74280	0.26705	-1.24271	-2.46423	1.01505	-0.25711
3S 15.83890	-0.01328	-0.06348	0.04692	0.03657	-0.01843
3S 10.18110	0.00340	0.00348	1.15464	-0.71061	0.21618
4S 5.79184	-0.00153	-0.00111	0.03748	0.80768	-0.30460
4S 3.93880	0.00161	0.00125	-0.01859	0.38148	-0.06533
5S 3.22791	-0.00108	-0.00080	0.00965	0.00811	0.09805
5S 2.27558	0.00048	0.00035	-0.00356	-0.00164	0.51597
5S 1.47401	-0.00011	-0.00008	0.00076	0.00102	0.50658

See page 183 for Explanation of Tables and Notes for Tables 32, 42, and 43

TABLE 2 (28). HARTREE-FOCK FUNCTIONS FOR POSITIVE IONS.

P BASIS/ORB E	2P 2P 30.59020	3P 2P 19.99470	4P 3P 10.81850	D BASIS/ORB E	3D 3D 16.52270	4D -0.23163
-125.68367	-0.13416	0.03088	0.00987	3D 16.52270	-0.23163	-0.07914
2P 30.59020	-0.13416	0.03088	0.00987	3D 9.36471	-0.78527	-0.26149
2P 19.99470	-0.86720	0.47197	0.19369	4D 5.61329	-0.05860	0.35289
3P 10.81850	-0.03816	-0.77307	-0.31133	4D 3.50433	0.01254	0.53523
3P 8.52037	0.02329	-0.34495	-0.29292	4D 2.10856	-0.00383	0.27770
4P 6.12749	-0.00500	-0.02404	0.53720			
4P 4.14244	0.00221	0.00597	0.58039			
4P 2.81778	-0.00057	-0.00201	0.10107			

SILVER      K(2)L(8)M(18)4S(2)4P(6)5S(2)4D(8),3F  
T.E.= -0.51969579D+04 P.E.= -0.10393765D+05 K.E.= 0.51568072D+04 V.T.= -0.203002900+01

S BASIS/ORB E	1S 1S 48.21060	2S 1S 32.55860	3S 2S 21.74250	4S 2S 20.74280	5S 3S 15.83890
-914.55186	0.86500	0.03048	0.00949	-0.00175	0.00021
1S 48.21060	0.86500	0.03048	0.00949	-0.00175	0.00021
1S 32.55860	0.15588	0.49707	0.22239	-0.09772	0.02952
2S 21.74250	-0.27733	0.06858	1.72618	-0.70008	0.18999
2S 20.74280	0.26567	-1.24355	-2.46703	1.01745	-0.28304
3S 15.83890	-0.01311	-0.06330	0.04736	0.03795	-0.01846
3S 10.18110	0.00330	0.00340	1.15476	-0.71770	0.23049
4S 5.79184	-0.00136	-0.00098	0.03627	0.82C41	-0.32522
4S 3.93880	0.00129	0.00101	-0.01634	0.37875	-0.07928
5S 3.04261	-0.00086	-0.00064	0.00832	-0.00590	0.22162
5S 2.15117	0.00048	0.00035	-0.00397	0.00220	0.52897
5S 1.47039	-0.00014	-0.00010	0.00104	-0.00016	0.38231

P BASIS/ORB E	2P 2P 30.59020	3P 2P 19.99470	4P 3P 10.81850	C BASIS/ORB E	3D 3D 16.52270	4D -0.23159
-125.91221	-0.13413	0.03087	0.00985	3D 9.36471	-0.78561	-0.27026
2P 30.59020	-0.13413	0.03087	0.00985	4D 5.58461	-0.05871	0.37957
2P 19.99470	-0.86724	0.47206	0.19570	4D 3.44845	0.01414	0.57015
3P 10.81850	-0.03796	-0.77330	-0.31825	4D 2.13078	-0.00425	0.20961
3P 8.52037	0.02304	-0.34499	-0.28885			
4P 6.07601	-0.00493	-0.02419	0.55503			
4P 4.12559	0.00222	0.00647	0.57980			
4P 2.78861	-0.00057	-0.00199	0.07922			

CADMIUM      K(2)L(8)M(18)4S(2)4P(6)5S(1)4D(10), 2S  
T.E.= -0.54648654D+04 P.E.= -0.10929491D+05 K.E.= 0.54646257D+04 V.T.= -0.203004390+01

S BASIS/ORB E	1S 1S 49.17740	2S 1S 33.11250	3S 2S 20.84450	4S 3S 15.89270	5S 3S 10.47290
-955.62367	0.87134	0.03100	0.00751	-0.00122	0.00015
1S 49.17740	0.87134	0.03100	0.00751	-0.00122	0.00015
1S 33.11250	0.14856	0.50037	0.22891	-0.10005	0.02748
2S 21.82640	-0.28246	-0.35648	1.61133	-0.67638	0.17377
2S 20.84450	0.27224	-0.82769	-2.37196	1.00469	-0.26242
3S 15.89270	-0.01399	-0.05901	0.06007	0.03430	-0.01514
3S 10.47290	0.00383	0.00464	1.1569	-0.72666	0.21298
4S 5.99770	-0.00153	-0.00141	0.03805	0.80958	-0.28900
4S 4.07408	0.00150	0.00148	-0.01846	0.38514	-0.08344
5S 3.33108	-0.00088	-0.00085	0.00892	0.00748	0.15038
5S 2.18832	0.00036	0.00034	-0.00309	-0.00066	0.54851
5S 1.44769	-0.00011	-0.00010	0.00086	0.00096	0.43663

P BASIS/ORB E	2P 2P 31.13020	3P 2P 20.43840	4P 3P 11.17220	D BASIS/CRB E	3D 3D 16.80950	4D -0.23990
-132.35322	-0.13694	0.03115	0.00991	3D 9.60576	-0.78112	-0.26681
2P 31.13020	-0.13694	0.03115	0.00991	4D 5.83238	-0.04847	0.37644
2P 20.43840	-0.86498	0.47627	0.19794	4D 3.55510	0.00868	0.55934
3P 11.17220	-0.03567	-0.72411	-0.28577	4D 2.11853	-0.00200	0.23621
3P 9.02438	0.02053	-0.39302	-0.32163			
4P 6.25149	-0.00296	-0.02816	0.57192			
4P 4.18757	0.00121	0.00714	0.56518			
4P 2.81791	-0.00028	-0.00228	0.07827			

See page 183 for Explanation of Tables and Notes for Tables 32, 42, and 43

## ROOTHAAN-HARTREE-FOCK ATOMIC WAVEFUNCTIONS

TABLE 2 (29). HARTREE-FOCK FUNCTIONS FOR POSITIVE IONS.

CADMUM K(2)L(8)M(18)4S(2)4P(6)5S(2)4D(9),2D  
 T.E.= -0.54644767D+04 P.E.= -0.10928730D+05 K.E.= 0.54642532D+04 V.T.= -0.20000439D+01

S	1S	2S	3S	4S	5S	
BASIS/ORB E	-955.85891	-142.55919	-28.25539	-4.96430	-0.59417	
1S 49.17740	0.87141	0.03103	0.00742	0.00110	-0.00010	
1S 33.11250	0.14844	0.50032	0.22913	0.10105	0.03029	
2S 21.82640	-0.27931	-0.35414	1.60721	0.67374	0.16976	
2S 20.84450	0.26893	-0.83021	-2.36779	-1.00410	-0.26462	
3S 15.89270	-0.01357	-0.05863	0.05942	-0.03622	-0.02028	
3S 10.47290	0.00358	0.00463	1.15665	0.73438	0.23514	
4S 5.99770	-0.00118	-0.00109	0.03526	-0.82341	-0.33010	
4S 4.07408	0.00091	0.00053	-0.01348	-0.38036	-0.05760	
5S 2.78167	-0.00059	-0.00058	0.00693	0.00539	0.40173	
5S 1.96115	0.00049	0.00047	-0.00526	-0.00407	0.39943	
5S 1.48237	-0.00019	-0.00019	0.00202	0.00127	0.31713	
P	2P	3P	4P	D	3D	4D
BASIS/ORB E	-132.59718	-24.14291	-3.54969	BASIS/ORB E	-16.61572	-1.25659
2P 31.13020	-0.13691	0.03116	0.00983	3D 16.80950	-0.23957	-0.08632
2P 20.43840	-0.86503	0.47632	0.20008	3D 9.60576	-0.78137	-0.27435
3P 11.17220	-0.03546	-0.72378	-0.29500	4D 5.73338	-0.05002	0.41812
3P 9.02438	0.02027	-0.39390	-0.31398	4D 3.48429	0.01015	0.56679
4P 6.16658	-0.00289	-0.02803	0.60352	4D 2.14523	-0.00323	0.17942
4P 4.13929	0.00122	0.00772	0.55170			
4P 2.74700	-0.00029	-0.00227	0.05413			

INDIUM K(2)L(8)M(18)4S(2)4P(6)5S(2)4D(10),1S  
 T.E.= -0.57399646D+04 P.E.= -0.11479687D+05 K.E.= 0.57397224D+04 V.T.= -0.20000422D+01

S	1S	2S	3S	4S	5S	
BASIS/ORB E	-998.07414	-149.66743	-29.89569	-5.24602	-0.60688	
1S 50.15070	0.86984	0.01440	-0.01057	-0.00283	0.00085	
1S 34.97610	0.14569	0.50458	-0.21400	-0.09452	0.02714	
2S 24.55580	-0.05141	-0.13212	-0.44604	-0.20465	0.06085	
2S 20.83330	0.04065	-1.06700	1.21694	0.54816	-0.16060	
3S 15.34990	-0.00715	-0.01686	-0.20750	-0.04061	0.00937	
3S 10.07610	0.00345	-0.00852	-1.10744	-0.74470	0.22959	
4S 6.24000	-0.00994	0.04055	0.58366	1.40335	-0.41351	
4S 4.39864	0.03122	-0.13043	-1.86048	-1.57045	0.18795	
5S 2.64214	-0.00015	0.00046	0.00829	0.01763	0.55617	
5S 1.62892	0.00002	-0.00004	-0.00114	-0.00315	0.54435	
5S 4.87386	-0.02341	0.09830	1.39535	1.50078	-0.16715	
P	2P	3P	4P	D	3D	4D
BASIS/ORB E	-139.44322	-25.64521	-3.77554	BASIS/ORB E	-17.86044	-1.33167
2P 31.80050	-0.13531	-0.02976	0.01000	3D 17.18530	-0.24029	-0.08709
2P 20.93160	-0.86597	-0.48115	0.20252	3D 9.91941	-0.77921	-0.27952
3P 11.49460	-0.04141	0.66664	-0.20590	4D 6.04509	-0.04908	0.39541
3P 9.66376	0.02603	0.43599	-0.42595	4D 3.72813	0.01005	0.56395
4P 7.30333	-0.00262	0.04313	0.29493	4D 2.29150	-0.00252	0.20448
4P 5.17808	0.00041	-0.00469	0.68070			
4P 3.50539	0.00006	0.00126	0.25325			

TIN K(2)L(8)M(18)4S(2)4P(6)5S(2)4D(10)5P(1),2P  
 T.E.= -0.60226685D+04 P.E.= -0.12045184D+05 K.E.= 0.60225154D+04 V.T.= -0.20000254D+01

S	1S	2S	3S	4S	5S	
BASIS/ORB E	-1041.52290	-157.277C7	-31.89573	-5.80693	-0.73091	
1S 51.22240	0.87190	0.02945	0.01028	0.00302	0.00060	
1S 34.30820	0.14967	0.50912	0.22895	0.10200	0.03206	
2S 24.72610	-0.08818	-0.18201	0.41293	0.19438	0.05574	
2S 21.52540	0.07246	-1.02428	-1.16373	-0.53270	-0.15969	
3S 15.57480	-0.01076	-0.04478	0.02177	-0.06542	-0.03062	
3S 11.07890	0.00443	0.00729	1.17740	0.78690	0.26745	
4S 6.40088	-0.00143	-0.00136	0.03445	-0.84109	-0.35544	
4S 4.37257	0.00119	0.00118	-0.01283	-0.37457	-0.07130	
5S 3.18008	-0.00080	-0.00075	0.00632	0.00588	0.31801	
5S 2.31060	0.00054	0.00049	-0.00370	-0.00209	0.48549	
5S 1.63503	-0.00016	-0.00015	0.00102	-0.00001	0.32425	
P	2P	3P	4P	D	3D	4D

See page 183 for Explanation of Tables and Notes for Tables 32, 42, and 43

TABLE 2 (30). HARTREE-FOCK FUNCTIONS FOR POSITIVE IONS.

P	2P	3P	4P	5P	D	3D	4D
BASIS/ORB E	-146.78785	-27.50535	-4.26237	-0.50746	BASIS/ORB E	-19.46023	-1.66249
2P 32.55760	-0.13264	-0.02915	0.00905	-0.00218	3D 18.02480	-0.21664	-0.08129
2P 21.41080	-0.86935	-0.4E459	0.20973	-0.05515	3D 10.38360	-0.79474	-0.30065
3P 11.36560	-0.03402	0.97128	-0.42666	0.11174	4D 6.40445	-0.05859	0.37427
3P 8.23469	0.02434	0.15681	-0.27559	0.08271	4D 4.05370	0.01318	0.57938
4P 6.83978	-0.00967	0.01626	0.66734	-0.21381	4D 2.54147	-0.00325	0.20640
4P 4.42240	0.00366	-0.00575	0.60220	-0.17092			
5P 3.51401	-0.00151	0.00330	0.01316	0.10870			
5P 2.24529	0.00050	-0.00124	0.01097	0.53803			
5P 1.43883	-0.00014	0.00036	-0.00231	0.49320			

ANTIMONY K(2)L(8)M(18)4S(2)4P(6)5S(2)4D(10)5P(2),3P  
T.E.= -0.63131565D+04 P.E.= -0.12626187D+05 K.E.= 0.63130305D+04 V.T.= -0.20300199D+01

S	1S	2S	3S	4S	5S
BASIS/ORB E	-1085.91223	-165.08143	-33.95714	-6.38176	-0.85581
1S 52.24950	0.86976	-0.02340	-0.00870	0.00262	0.00030
1S 35.61750	0.14974	-0.50737	-0.22720	0.10209	0.03413
2S 25.75090	-0.06741	0.07121	-0.40009	0.19749	0.05882
2S 22.11860	0.05202	1.12468	1.14273	-0.53894	-0.16934
3S 14.80440	-0.00945	0.04547	0.01146	-0.11582	-0.05686
3S 11.42790	0.00530	-0.01401	-1.20251	0.85680	0.31583
4S 6.72382	-0.00126	0.00181	-0.03627	-0.79037	-0.36658
4S 4.72815	0.00084	-0.00118	0.01112	-0.43134	-0.09054
5S 3.07208	-0.00036	0.00046	-0.00349	-0.00066	0.56585
5S 2.00557	0.00027	-0.00034	0.00239	-0.00121	0.50508
5S 1.48243	-0.00012	0.00015	-0.00100	0.00037	0.05317

P	2P	3P	4P	5P	D	3D	4D
BASIS/ORB E	-154.32635	-29.42652	-4.76209	-0.59695	BASIS/ORB E	-21.11921	-2.00528
2P 33.17040	-0.13190	0.02801	-0.00893	-0.00246	3D 18.54830	-0.21064	-0.08200
2P 21.90980	-0.86887	0.48871	-0.21461	-0.06085	3D 10.73240	-0.79881	-0.31421
3P 11.89620	-0.04858	-0.71308	0.23863	0.05737	4D 6.60673	-0.06023	0.39607
3P 10.30200	0.03313	-0.39460	0.40820	0.13689	4D 4.19906	0.01496	0.59149
4P 6.90314	-0.00304	-0.04600	-0.59763	-0.22197	4D 2.66650	-0.00386	0.16791
4P 4.65006	0.00128	0.01414	-0.60149	-0.16454			
5P 3.14513	-0.00048	-0.00678	-0.01989	0.21633			
5P 2.25954	0.00028	0.00440	-0.00144	0.50062			
5P 1.54254	-0.00007	-0.00125	0.00041	0.41C27			

TELLURIUM K(2)L(8)M(18)4S(2)4P(6)5S(2)4D(10)5P(3),4S  
T.E.= -0.66114951D+04 P.E.= -0.13222909D+05 K.E.= 0.66114143D+04 V.T.= -0.20300122D+01

S	1S	2S	3S	4S	5S
BASIS/ORB E	-1131.24476	-173.08385	-36.08108	-6.97158	-0.98305
1S 53.20830	0.87691	-0.02541	-0.00904	0.00310	0.00042
1S 35.87880	0.14276	-0.51401	-0.23220	0.10511	0.03672
2S 26.35740	-0.06117	0.16376	-0.31956	0.16871	0.05192
2S 22.29780	0.04514	1.05370	1.07709	-0.52378	-0.17192
3S 14.10170	-0.01228	0.04789	0.02118	-0.18916	-0.09906
3S 11.75490	0.00876	-0.02355	-1.21846	0.95884	0.38240
4S 7.07996	-0.00166	0.00243	-0.03874	-0.73190	-0.36392
4S 5.08066	0.00106	-0.00149	0.01129	-0.49981	-0.13069
5S 3.24449	-0.00043	0.00055	-0.00327	-0.00597	0.58171
5S 2.16995	0.00036	-0.00044	0.00247	0.00C82	0.46891
5S 1.65613	-0.00016	0.00020	-0.00106	-0.00C41	0.08030

P	2P	3P	4P	5P	D	3D	4D
BASIS/ORB E	-162.06190	-31.40968	-5.27604	-0.68883	BASIS/ORB E	-22.83877	-2.36178
2P 33.77710	-0.13206	0.02766	0.00903	-0.00255	3D 19.16700	-0.19989	-0.07983
2P 22.38550	-0.86855	0.49206	0.21938	-0.06617	3D 11.12990	-0.80403	-0.32932
3P 12.09940	-0.06204	-0.677C8	-0.14044	0.02744	4D 6.94873	-0.06635	0.37331
3P 10.93580	0.04647	-0.42391	-0.51792	0.18197	4D 4.51067	0.01712	0.60479
4P 7.22640	-0.00257	-0.05817	0.55382	-0.21568	4D 2.90235	-0.00431	0.17367
4P 4.95962	0.00100	0.01990	0.63920	-0.20E36			
5P 3.56240	-0.00025	-0.00854	0.02538	0.16815			
5P 2.49148	0.00009	0.00455	0.00293	0.56701			
5P 1.67160	-0.00002	-0.00125	-0.00081	0.40123			

See page 183 for Explanation of Tables and Notes for Tables 32, 42, and 43

## ROOTHAAN-HARTREE-FOCK ATOMIC WAVEFUNCTIONS

TABLE 2 (31). HARTREE-FOCK FUNCTIONS FOR POSITIVE IONS.

IODINE K(2)L(8)M(18)4S(2)4P(6)5S(2)4D(10)5P(4),3P  
 T.E.= -0.691761900+04 P.E.= -0.13835124D+05 K.E.= 0.69175055D+04 V.T.= -0.20000164D+01

S	1S	2S	3S	4S	5S
BASIS/ORB E	-1177.53707	-181.30065	-38.28320	-7.59061	-1.1213E
1S 54.17930	0.88276	-0.02762	-0.00965	0.00359	0.00071
1S 36.07530	0.13757	-0.52147	-0.23729	0.10838	0.03907
2S 26.93340	-0.05911	0.23684	-0.26076	0.14633	0.04760
2S 22.51240	0.04220	0.95529	1.03302	-0.51417	-0.17693
3S 13.64850	-0.01871	0.05716	0.04900	-0.33906	-0.18029
3S 12.09300	0.01552	-0.03755	-1.25189	1.13743	0.48767
4S 7.45966	-0.00216	0.00280	-0.04065	-0.67215	-0.35089
4S 5.41951	0.00131	-0.00161	0.01082	-0.57168	-0.16289
5S 3.43675	-0.00050	0.00054	-0.00279	-0.01057	0.59399
5S 2.31843	0.00042	-0.00044	0.00214	0.00256	0.45897
5S 1.78641	-0.00019	0.00020	-0.00091	-0.00111	0.08831

P	2P	3P	4P	5P	D	3D	4D
BASIS/ORB E	-170.01088	-33.47048	-5.81845	-0.72635	BASIS/ORB E	-24.63480	-2.74631
2P 34.38650	-0.13208	0.02710	-0.00887	-0.00273	3D 19.59770	-0.19937	-0.08200
2P 22.86520	-0.66820	0.49562	-0.22434	-0.07611	3D 11.43560	-0.80512	-0.33991
3P 12.55560	-0.07227	-0.35745	-0.09876	-0.06399	4D 7.15265	-0.06396	0.38985
3P 11.65480	0.05595	-0.74330	0.76128	0.28596	4D 4.69056	0.01657	0.60866
4P 7.36910	-0.00144	-0.06C43	-0.56387	-0.23566	4D 3.03621	-0.00400	0.15193
4P 5.13361	0.00045	0.02024	-0.62855	-0.20021			
5P 3.36110	-0.00001	-0.00889	-0.02377	0.32615			
5P 2.47098	-0.00004	0.00E31	0.00266	0.45387			
5P 1.73201	0.00002	-0.00182	-0.00077	0.35978			

XENON K(2)L(8)M(18)4S(2)4P(6)5S(2)4D(10)5P(5),2P  
 T.E.= -0.72317010D+04 P.E.= -0.14463294D+05 K.E.= 0.72315926D+04 V.T.= -0.20300150D+01

S	1S	2S	3S	4S	5S
BASIS/ORB E	-1224.77099	-189.71362	-40.54628	-8.22406	-1.26228
1S 55.62220	0.83440	0.0C838	0.00852	0.00019	-0.00118
1S 39.84110	0.18560	0.49397	0.21324	-0.10388	0.03943
2S 29.54330	-0.05875	0.24576	0.42862	-0.17907	0.05605
2S 24.68820	0.04283	-1.38386	-1.10528	0.49C98	-0.16743
3S 17.95710	-0.00757	-0.07411	-0.15574	0.18802	-0.08714
3S 12.52580	0.00313	0.01C82	1.28100	-0.91317	0.37013
4S 7.35659	-0.00140	-0.00259	0.05471	0.73091	-0.38722
4S 5.56174	0.00113	0.00203	-0.02315	0.47999	-0.15346
5S 3.63760	-0.00061	-0.00098	0.00769	0.01912	0.56099
5S 2.70265	0.0C056	0.00C87	-0.00629	-0.00918	0.30765
5S 2.12491	-0.00022	-0.00034	0.00228	0.00347	0.27739

P	2P	3P	4P	5P	D	3D	4D
BASIS/ORB E	-178.15510	-35.59174	-6.37487	-0.78618	BASIS/ORB E	-26.49001	-3.14450
2P 35.02500	0.13136	0.02634	-0.00875	-0.00285	3D 20.12230	-0.19398	-0.08155
2P 23.35320	0.86841	0.49903	-0.22879	-0.07493	3D 11.79100	-0.80768	-0.35168
3P 13.25210	0.06053	-0.01387	-0.25324	-0.11736	4D 7.45257	-0.06646	0.37518
3P 12.22860	-0.04340	-1.08E20	0.92085	0.35050	4D 4.98480	0.01747	0.61428
4P 7.52942	0.00049	-0.06372	-0.56836	-0.25483	4D 3.26786	-0.00401	0.15943
4P 5.33515	0.00003	0.02214	-0.62062	-0.20653			
5P 3.42626	-0.00020	-0.09833	-0.02337	0.43124			
5P 2.43132	0.00020	0.00623	0.00372	0.43178			
5P 1.77275	-0.00008	-0.00217	-0.00165	0.28316			

See page 183 for Explanation of Tables and Notes for Tables 32, 42, and 43

TABLE 3 (1). HARTREE-FOCK FUNCTIONS FOR He(<sup>1</sup>S) ISO-ELECTRONIC SERIES.

HELlUM	1S(2),1S	LITHIUM	1S(2),1S	BERYLliUM	1S(2),1S
T.E.= -0.28616784D+01		T.E.= -0.72364121D+01		T.E.= -0.13611297D+02	
P.E.= -0.57233458D+01		P.E.= -0.14473662D+02		P.E.= -0.27222506D+02	
K.E.= 0.28616674D+01		K.E.= 0.72372458D+01		K.E.= 0.13611211D+02	
V.T.= -0.20000038D+01		V.T.= -0.19998843D+01		V.T.= -0.20000063D+01	
S	1S	S	1S	S	1S
BASIS/ORB E	-0.91795	BASIS/ORB E	-2.79226	BASIS/ORB E	-5.66712
1S 1.45286	0.82958	1S 2.45055	0.89066	1S 3.43071	0.89855
1S 2.77954	0.18334	1S 4.57259	0.12328	1S 5.63150	0.09068
1S 4.34600	0.00824	1S 6.67032	0.00088	1S 7.35143	0.02158
BORON	1S(2),1S	CARBON	1S(2),1S	NITROGEN	1S(2),1S
T.E.= -0.21986232D+02		T.E.= -0.32361191D+02		T.E.= -0.44736162D+02	
P.E.= -0.43973056D+02		P.E.= -0.64722210D+02		P.E.= -0.89472723D+02	
K.E.= 0.21986824D+02		K.E.= 0.32361019D+02		K.E.= 0.44736561D+02	
V.T.= -0.19999731D+01		V.T.= -0.20000053D+01		V.T.= -0.19999911D+01	
S	1S	S	1S	S	1S
BASIS/ORB E	-9.54194	BASIS/ORB E	-14.41690	BASIS/ORB E	-20.29181
1S 4.44422	0.93036	1S 5.44726	0.94428	1S 6.45215	0.95445
1S 7.90274	0.07786	1S 9.80425	0.06382	1S 11.69880	0.05228
1S 11.31380	0.00013	1S 14.61460	-0.00125	1S 19.74440	-0.00096
OXYGEN	1S(2),1S	FLUCRINE	1S(2),1S	NEON	1S(2),1S
T.E.= -0.59111140D+02		T.E.= -0.75486124D+02		T.E.= -0.93861111D+02	
P.E.= -0.11822311D+03		P.E.= -0.15097018D+03		P.E.= -0.18771984D+03	
K.E.= 0.591111969D+02		K.E.= 0.75484053D+02		K.E.= 0.93858727D+02	
V.T.= -0.19999860D+01		V.T.= -0.20000274D+01		V.T.= -0.20000254D+01	
S	1S	S	1S	S	1S
BASIS/ORB E	-27.16675	BASIS/ORB E	-35.04182	BASIS/ORB E	-43.91679
1S 7.45601	0.96175	1S 8.44950	0.96398	1S 9.45544	0.96961
1S 13.66210	0.04445	1S 15.20300	0.04150	1S 17.36970	0.03573
1S 22.59050	-0.00121	1S 24.63050	-0.00103	1S 27.77710	-0.00138
SODIUM	1S(2),1S	MAGNESIUM	1S(2),1S	ALUMINUM	1S(2),1S
T.E.= -0.114236100D+03		T.E.= -0.13661109D+03		T.E.= -0.16098609D+03	
P.E.= -0.22846990D+03		P.E.= -0.27322000D+03		P.E.= -0.32197011D+03	
K.E.= 0.11423380D+03		K.E.= 0.13660891D+03		K.E.= 0.16098402D+03	
V.T.= -0.20000202D+01		V.T.= -0.20000160D+01		V.T.= -0.20000128D+01	
S	1S	S	1S	S	1S
BASIS/ORB E	-53.79177	BASIS/ORB E	-64.66674	BASIS/ORB E	-76.54172
1S 10.44750	0.96993	1S 11.44810	0.97261	1S 12.44850	0.97483
1S 18.64160	0.03476	1S 20.44990	0.03181	1S 22.27390	0.02946
1S 28.30950	-0.00109	1S 30.59270	-0.00113	1S 32.42660	-0.00125
SILICON	1S(2),1S	PHOSPHORUS	1S(2),1S	SULFUR	1S(2),1S
T.E.= -0.18736108D+03		T.E.= -0.21573607D+03		T.E.= -0.24611107D+03	
P.E.= -0.37471982D+03		P.E.= -0.43147008D+03		P.E.= -0.49222024D+03	
K.E.= 0.18735874D+03		K.E.= 0.21573401D+03		K.E.= 0.24610917D+03	
V.T.= -0.20000125D+01		V.T.= -0.20000096D+01		V.T.= -0.20000077D+01	
S	1S	S	1S	S	1S
BASIS/ORB E	-89.41671	BASIS/ORB E	-103.29165	BASIS/ORB E	-118.16667
1S 13.44850	0.97665	1S 14.44890	0.97830	1S 15.44920	0.97973
1S 24.09300	0.02754	1S 25.91690	0.02576	1S 27.78430	0.02437
1S 34.21320	-0.00139	1S 36.27310	-0.00144	1S 37.82710	-0.00165
CHLORINE	1S(2),1S	ARGON	1S(2),1S	POTASSIUM	1S(2),1S
T.E.= -0.27848606D+03		T.E.= -0.31286106D+03		T.E.= -0.34923606D+03	
P.E.= -0.55697024D+03		P.E.= -0.62572021D+03		P.E.= -0.69847036D+03	
K.E.= 0.27848418D+03		K.E.= 0.31285915D+03		K.E.= 0.34923430D+03	
V.T.= -0.20000068D+01		V.T.= -0.20000061D+01		V.T.= -0.20000050D+01	
S	1S	S	1S	S	1S
BASIS/ORB E	-134.04166	BASIS/ORB E	-150.91665	BASIS/ORB E	-168.79164
1S 16.44940	0.98097	1S 17.45040	0.98224	1S 18.45100	0.98329
1S 29.64730	0.02314	1S 31.64560	0.02200	1S 33.60020	0.02105
1S 39.57500	-0.00182	1S 41.48040	-0.00208	1S 43.31680	-0.00230

See page 183 for Explanation of Tables and Notes for Tables 32, 42, and 43

## ROOTHAAN-HARTREE-FOCK ATOMIC WAVEFUNCTIONS

 TABLE 3 (2). HARTREE-FOCK FUNCTIONS FOR He(<sup>1</sup>S) ISO-ELECTRONIC SERIES.

CALCIUM	1S(2),1S	SCANDIUM	1S(2),1S	TITANIUM	1S(2),1S
T.E.= -0.38761106D+03		T.E.= -0.42798605D+03		T.E.= -0.47036105D+03	
P.E.= -0.77522035D+03		P.E.= -0.85597049D+03		P.E.= -0.94072080D+03	
K.E.= 0.38760930D+03		K.E.= 0.42798443D+03		K.E.= 0.47035975D+03	
V.T.= -0.20000045D+01		V.T.= -0.20000038D+01		V.T.= -0.20000028D+01	
S	1S	S	1S	S	1S
BASIS/ORB E	-187.66664	BASIS/ORB E	-207.54163	BASIS/ORB E	-228.41662
1S 19.45300	0.98449	1S 20.45300	0.98523	1S 21.45430	0.98611
1S 35.80330	0.02004	1S 37.72940	0.01946	1S 39.88550	0.01880
1S 45.66780	-0.00259	1S 47.29890	-0.00285	1S 49.38710	-0.00315
VANADIUM	1S(2),1S	CHROMIUM	1S(2),1S	MANGANESE	1S(2),1S
T.E.= -0.51473605D+03		T.E.= -0.56111105D+03		T.E.= -0.60948604D+03	
P.E.= -0.10294707D+04		P.E.= -0.11222211D+04		P.E.= -0.12189713D+04	
K.E.= 0.51473464D+03		K.E.= 0.56111001D+03		K.E.= 0.60948528D+03	
V.T.= -0.20000027D+01		V.T.= -0.20000018D+01		V.T.= -0.20000013D+01	
S	1S	S	1S	S	1S
BASIS/ORB E	-250.29161	BASIS/ORB E	-273.16660	BASIS/ORB E	-297.04160
1S 22.45530	0.98687	1S 23.45690	0.98764	1S 24.45290	0.98758
1S 42.04130	0.01825	1S 44.32600	0.01772	1S 45.31270	0.01737
1S 51.49010	-0.00345	1S 53.77210	-0.00376	1S 54.52530	-0.00341
IRON	1S(2),1S	COBALT	1S(2),1S	NICKEL	1S(2),1S
T.E.= -0.65986104D+03		T.E.= -0.71223604D+03		T.E.= -0.76661104D+03	
P.E.= -0.13197213D+04		P.E.= -0.14244714D+04		P.E.= -0.15332219D+04	
K.E.= 0.65986030D+03		K.E.= 0.71223534D+03		K.E.= 0.76661089D+03	
V.T.= -0.20000011D+01		V.T.= -0.20000010D+01		V.T.= -0.20000002D+01	
S	1S	S	1S	S	1S
BASIS/ORB E	-321.91659	BASIS/ORB E	-347.79159	BASIS/ORB E	-374.66658
1S 25.45370	0.98817	1S 26.45460	0.98873	1S 27.45480	0.98915
1S 47.42210	0.01692	1S 45.53470	0.01637	1S 51.48940	0.01600
1S 56.67690	-0.00361	1S 59.04970	-0.00367	1S 60.97790	-0.00378
COPPER	1S(2),1S	ZINC	1S(2),1S	GALLIUM	1S(2),1S
T.E.= -0.82298604D+03		T.E.= -0.88136104D+03		T.E.= -0.94173604D+03	
P.E.= -0.16459720D+04		P.E.= -0.17627223D+04		P.E.= -0.18834724D+04	
K.E.= 0.82298594D+03		K.E.= 0.88136123D+03		K.E.= 0.94173641D+03	
V.T.= -0.20000001D+01		V.T.= -0.19999998D+01		V.T.= -0.19999996D+01	
S	1S	S	1S	S	1S
BASIS/ORB E	-402.54158	BASIS/ORB E	-431.41657	BASIS/ORB E	-461.29157
1S 28.45520	0.98957	1S 29.45710	0.99013	1S 30.45560	0.99028
1S 53.50200	0.01556	1S 55.93740	0.01508	1S 57.32130	0.01451
1S 63.18330	-0.00381	1S 65.95340	-0.00394	1S 67.74530	-0.00356
GERMANIUM	1S(2),1S	ARSENIC	1S(2),1S	SELENIUM	1S(2),1S
T.E.= -0.10041110D+04		T.E.= -0.10684860D+04		T.E.= -0.11346610D+04	
P.E.= -0.20082227D+04		P.E.= -0.21369727D+04		P.E.= -0.22697232D+04	
K.E.= 0.10041117D+04		K.E.= 0.10684867D+04		K.E.= 0.11348622D+04	
V.T.= -0.19999993D+01		V.T.= -0.19999994D+01		V.T.= -0.19999990D+01	
S	1S	S	1S	S	1S
BASIS/ORB E	-492.16656	BASIS/ORB E	-524.04156	BASIS/ORB E	-556.91556
1S 31.45560	0.99058	1S 32.45440	0.99074	1S 33.45270	0.99083
1S 59.15830	0.01402	1S 60.55150	0.01340	1S 61.75950	0.01291
1S 69.98870	-0.00341	1S 72.10310	-0.00298	1S 73.80030	-0.00262
BROMINE	1S(2),1S	KRYPTON	1S(2),1S		
T.E.= -0.12032360D+04	P.E.= -0.24064732D+04	T.E.= -0.12736110D+04	P.E.= -0.25472234D+04		
K.E.= 0.12032372D+04	V.T.= -0.19999990D+01	K.E.= 0.12736124D+04	V.T.= -0.19999989D+01		
S	1S	S	1S		
BASIS/ORB E	-590.79155	BASIS/ORB E	-625.66655		
1S 34.45160	0.99097	1S 35.44860	0.99091		
1S 63.13470	0.01239	1S 63.82420	0.01194		
1S 75.96420	-0.00227	1S 77.28000	-0.00178		

See page 183 for Explanation of Tables and Notes for Tables 32, 42, and 43

TABLE 4 (1). HARTREE-FOCK FUNCTIONS FOR Li(<sup>2</sup>S) ISO-ELECTRONIC SERIES.

LITHIUM	1S(2)2S(1), 3-2S	BERYLLIUM	1S(2)2S(1), 3-2S		
T.E.= -0.743272560+01	P.E.= -0.14865447D+02	T.E.= -0.14277391D+02	P.E.= -0.28555234D+02		
K.E.= 0.74327213D+01	V.T.= -0.20000060D+01	K.E.= 0.14277843D+02	V.T.= -0.19999684D+01		
S	1S	2S			
BASIS/ORB E	-2.47774	-0.19632	BASIS/ORB E	-5.13829	-0.66615
1S 2.47583	0.89675	-0.14500	1S 3.49771	0.92264	-0.20462
1S 4.68942	0.11224	-0.01575	1S 6.50227	0.07879	-0.01566
2S 0.76500	-0.00060	0.41679	2S 1.18383	0.00052	1.10808
2S 1.75300	0.00764	-0.07981	2S 2.62771	0.01148	-0.13290
2S 0.62711	0.00088	0.64613			
BORON	1S(2)2S(1), 3-2S	CARBON	1S(2)2S(1), 3-2S		
T.E.= -0.23375985D+02	P.E.= -0.46752537D+02	T.E.= -0.34726055D+02	P.E.= -0.69452783D+02		
K.E.= 0.23376552D+02	V.T.= -0.19999758D+01	K.E.= 0.34726728D+02	V.T.= -0.19999806D+01		
S	1S	2S	S	1S	2S
BASIS/ORB E	-8.80770	-1.38985	BASIS/ORB E	-13.48002	-2.36500
1S 4.50258	0.93765	-0.23923	1S 5.49312	0.94568	-0.26110
1S 8.27838	0.06214	-0.01356	1S 9.92427	0.05448	-0.01224
2S 1.68299	0.00064	1.15411	2S 2.17626	0.00083	1.18759
2S 3.40608	0.01054	-0.17788	2S 4.19258	0.00810	-0.20932
NITROGEN	1S(2)2S(1), 3-2S	OXYGEN	1S(2)2S(1), 3-2S		
T.E.= -0.48326843D+02	P.E.= -0.96655246D+02	T.E.= -0.64178042D+02	P.E.= -0.12835569D+03		
K.E.= 0.48328403D+02	V.T.= -0.19999677D+01	K.E.= 0.64178651D+02	V.T.= -0.19999905D+01		
S	1S	2S	S	1S	2S
BASIS/ORB E	-19.15366	-3.59086	BASIS/CRB E	-25.82812	-5.06710
1S 6.51869	0.95538	-0.27929	1S 7.48197	0.95787	-0.29233
1S 11.88210	0.04229	-0.00E40	1S 13.28360	0.04278	-0.00750
2S 2.67722	0.00027	1.22C21	2S 3.17458	0.00089	1.24518
2S 4.91820	0.01020	-0.23991	2S 5.65372	0.00521	-0.26116
FLUORINE	1S(2)2S(1), 3-2S	NEON	1S(2)2S(1), 3-2S		
T.E.= -0.82279488D+02	P.E.= -0.16456076D+03	T.E.= -0.10263110D+03	P.E.= -0.20526427D+03		
K.E.= 0.82281274D+02	V.T.= -0.19999783D+01	K.E.= 0.10263317D+03	V.T.= -0.19999759D+01		
S	1S	2S	S	1S	2S
BASIS/ORB E	-33.50292	-6.79359	BASIS/CRB E	-42.17806	-6.77023
1S 8.47703	0.96036	-0.30036	1S 9.48568	0.96489	-0.30704
1S 14.81170	0.04001	-0.00E80	1S 16.62160	0.03483	-0.00558
2S 3.66665	0.00073	1.25E71	2S 4.15827	0.00062	1.2714E
2S 6.45127	0.00491	-0.27483	2S 7.24920	0.00515	-0.28619
SODIUM	1S(2)2S(1), 3-2S	MAGNESIUM	1S(2)2S(1), 3-2S		
T.E.= -0.12523283D+03	P.E.= -0.25C46805D+03	T.E.= -0.15008465D+03	P.E.= -0.30017177D+03		
K.E.= 0.12523522D+03	V.T.= -0.19699809D+01	K.E.= 0.15008712D+03	V.T.= -0.19999835D+01		
S	1S	2S	S	1S	2S
BASIS/ORB E	-51.85339	-10.95699	BASIS/ORB E	-62.52888	-13.47383
1S 10.50110	0.96906	-0.31153	1S 11.50090	0.97173	-0.31822
1S 18.55720	0.02978	-0.00481	1S 20.30510	0.02723	-0.00315
2S 4.64647	0.00047	1.27E24	2S 5.14607	0.00042	1.29421
2S 8.07910	0.00582	-0.29322	2S 8.79224	0.00531	-0.30745
ALUMINUM	1S(2)2S(1), 3-2S	SILICON	1S(2)2S(1), 3-2S		
T.E.= -0.17718653D+03	P.E.= -0.35437581D+03	T.E.= -0.20653845D+03	P.E.= -0.41307991D+03		
K.E.= 0.17718929D+03	V.T.= -0.19959844D+01	K.E.= 0.20E54146D+03	V.T.= -0.19999854D+01		
S	1S	2S	S	1S	2S
BASIS/ORB E	-74.20446	-16.20073	BASIS/CRB E	-86.88013	-19.17767
1S 12.50980	0.97434	-0.321E1	1S 13.53950	0.97783	-0.32502
1S 22.19770	0.02424	-0.00256	1S 24.63260	0.01961	-0.00145
2S 5.63633	0.00034	1.30025	2S 6.13070	0.00009	1.30868
2S 9.59748	0.00548	-0.31343	2S 10.36880	0.00674	-0.32195

See page 183 for Explanation of Tables and Notes for Tables 32, 42, and 43

## ROOTHAAN-HARTREE-FOCK ATOMIC WAVEFUNCTIONS

 TABLE 4 (2). HARTREE-FOCK FUNCTIONS FOR Li(<sup>2</sup>S) ISO-ELECTRONIC SERIES.

PHOSPHORUS	1S(2)2S(1), 3-2S	SULFUR	1S(2)2S(1), 3-2S		
T.E.= -0.23814042D+03	P.E.= -0.47628395D+03	T.E.= -0.27199241D+03	P.E.= -0.54398817D+03		
K.E.= 0.23814353D+03	V.T.= -0.19999869D+01	K.E.= 0.27199576D+03	V.T.= -0.19999877D+C1		
S	1S	2S	S		
BASIS/ORB E	-100.55586	-22.40465	BASIS/CRB E	-115.23163	-25.88165
1S 14.53430	0.97900	-0.32800	1S 15.54800	0.98080	-0.32949
1S 26.28910	0.01878	-0.00105	1S 28.43680	0.01656	-0.00090
2S 6.62303	0.00014	1.31470	2S 7.11033	0.00006	1.31652
2S 11.15040	0.00604	-0.32732	2S 11.98C50	0.00638	-0.32957
CHLORINE	1S(2)2S(1), 3-2S	ARGON	1S(2)2S(1), 3-2S		
T.E.= -0.3C809443D+03	P.E.= -0.61618667D+03	T.E.= -0.34644647D+03	P.E.= -0.69289044D+03		
K.E.= 0.30809224D+03	V.T.= -0.20000C71D+01	K.E.= 0.34644398D+03	V.T.= -0.20000072D+01		
S	1S	2S	S		
BASIS/ORB E	-130.90753	-29.6C869	BASIS/CRB E	-147.58338	-33.58574
1S 16.54750	0.98327	-0.33265	1S 17.55420	0.98439	-0.33430
1S 30.87790	0.01465	-0.00015	1S 32.95650	0.01340	0.00009
2S 7.60843	C.00027	1.32524	2S 8.09970	0.00022	1.32880
2S 12.71230	0.00534	-0.33731	2S 13.50570	0.00535	-0.34079
POTASSIUM	1S(2)2S(1), 3-2S	CALCIUM	1S(2)2S(1), 3-2S		
T.E.= -0.38704852D+03	P.E.= -0.77409435D+03	T.E.= -0.42990060D+03	P.E.= -0.85979857D+03		
K.E.= 0.38704582D+03	V.T.= -0.20000070D+01	K.E.= 0.42985798D+03	V.T.= -0.20000061D+01		
S	1S	2S	S		
BASIS/ORB E	-165.25927	-37.81281	BASIS/CRB E	-183.93517	-42.28989
1S 18.54750	0.98503	-0.33653	1S 19.54590	0.98565	-0.33761
1S 34.58700	0.01309	0.00048	1S 36.34260	0.01257	0.00050
2S 8.59495	0.00026	1.33442	2S 9.08289	0.00027	1.33539
2S 14.26170	0.00478	-0.34569	2S 15.07920	0.00450	-0.34664
SCANDIUM	1S(2)2S(1), 3-2S	TITANIUM	1S(2)2S(1), 3-2S		
T.E.= -0.47500268D+03	P.E.= -0.95000281D+03	T.E.= -0.52235478D+03	P.E.= -0.10447069D+04		
K.E.= 0.47500013D+03	V.T.= -0.20000054D+01	K.E.= 0.52235212D+03	V.T.= -0.20000051D+C1		
S	1S	2S	S		
BASIS/ORB E	-203.61109	-47.01658	BASIS/ORB E	-224.28703	-51.99408
1S 20.53550	0.98600	-0.33914	1S 21.52620	0.98637	-0.34055
1S 37.77690	0.01259	C.00068	1S 39.25300	0.01255	0.00086
2S 9.57415	0.00032	1.33810	2S 10.06550	0.00037	1.34064
2S 15.86590	0.00389	-0.34888	2S 16.65180	0.00336	-0.35099
VANADIUM	1S(2)2S(1), 3-2S	CHROMIUM	1S(2)2S(1), 3-2S		
T.E.= -0.57195688D+03	P.E.= -0.11439111D+04	T.E.= -0.62380900D+03	P.E.= -0.12476150D+C4		
K.E.= 0.57195421D+03	V.T.= -0.20000047D+01	K.E.= 0.62380610D+03	V.T.= -0.20000048D+C1		
S	1S	2S	S		
BASIS/ORB E	-245.56299	-57.22119	BASIS/ORB E	-268.63896	-62.69831
1S 22.51800	0.98670	-0.34186	1S 23.51460	0.98715	-0.34286
1S 40.74420	0.01246	0.00105	1S 42.40640	0.01213	0.00118
2S 10.55710	0.00040	1.34308	2S 11.04750	0.00041	1.34477
2S 17.43570	0.00293	-0.35305	2S 18.23020	0.00270	-0.35456
MANGANESE	1S(2)2S(1), 3-2S	IRON	1S(2)2S(1), 3-2S		
T.E.= -0.67791111D+03	P.E.= -0.13558195D+04	T.E.= -0.73426324D+03	P.E.= -0.14685237D+04		
K.E.= 0.67790839D+03	V.T.= -0.20000040D+01	K.E.= 0.73426043D+03	V.T.= -0.20000038D+01		
S	1S	2S	S		
BASIS/ORB E	-292.31493	-68.42543	BASIS/ORB E	-316.99092	-74.40256
1S 24.50820	0.98747	-0.34401	1S 25.50650	0.98790	-0.34482
1S 43.93760	0.01198	0.00138	1S 45.64750	0.01161	0.00149
2S 11.53960	0.00042	1.34708	2S 12.03010	0.00042	1.34853
2S 19.01080	0.00239	-0.35655	2S 19.80530	0.00225	-0.35788

See page 183 for Explanation of Tables and Notes for Tables 32, 42, and 43

TABLE 4 (3). HARTREE-FOCK FUNCTIONS FOR Li(<sup>2</sup>S) ISO-ELECTRONIC SERIES.

COBALT            1S(2)2S(1), 3-2S			NICKEL            1S(2)2S(1), 3-2S		
T.E.= -0.79286536D+03 P.E.= -0.15E57271D+04			T.E.= -0.85371750D+03 P.E.= -0.17074313D+C4		
K.E.= 0.79286172D+03 V.T.= -0.20000046D+01			K.E.= 0.85371379D+03 V.T.= -0.20000043D+C1		
S	1S	2S	S	1S	2S
BASIS/ORB E	-342.66693	-80.62569	BASIS/CRB E	-369.34294	-87.10682
1S 26.50500	0.98838	-0.34662	1S 27.50350	0.98874	-0.34732
1S 47.42240	0.01120	0.00205	1S 49.12260	0.01088	0.00216
2S 12.53160	0.00041	1.35456	2S 13.02240	0.00041	1.35578
2S 20.51090	0.00209	-0.36318	2S 21.30270	0.00198	-0.36430
COPPER            1S(2)2S(1), 3-2S			ZINC            1S(2)2S(1), 3-2S		
T.E.= -0.91681963D+03 P.E.= -0.18336356D+C4			T.E.= -0.98217177D+03 P.E.= -0.19643394D+04		
K.E.= 0.91681592D+03 V.T.= -0.20000041D+01			K.E.= 0.98216764D+03 V.T.= -0.20000042D+01		
S	1S	2S	S	1S	2S
BASIS/ORB E	-397.01895	-93.83397	BASIS/ORB E	-425.69497	-100.81111
1S 28.50270	0.98911	-0.34804	1S 29.50340	0.98949	-0.34870
1S 50.86670	0.01054	0.00229	1S 52.67610	0.01015	0.00241
2S 13.51430	0.00040	1.35734	2S 14.00620	0.00039	1.35882
2S 22.08650	0.00189	-0.36573	2S 22.87000	0.00184	-0.36711
GALLIUM            1S(2)2S(1), 3-2S			GERMANIUM            1S(2)2S(1), 3-2S		
T.E.= -0.10457739D+04 P.E.= -0.20555436D+04			T.E.= -0.11196261D+04 P.E.= -0.22392476D+04		
K.E.= 0.10497697D+04 V.T.= -0.20000040D+01			K.E.= 0.11196215D+04 V.T.= -0.20000041D+01		
S	1S	2S	S	1S	2S
BASIS/ORB E	-455.37099	-108.03E26	BASIS/ORB E	-486.04702	-115.51541
1S 30.50410	0.98984	-0.34937	1S 31.50610	0.99021	-0.34996
1S 54.48280	0.00980	0.00255	1S 56.36820	0.00940	0.00267
2S 14.49900	0.00038	1.36053	2S 14.59180	0.00036	1.36213
2S 23.64710	0.00180	-0.36869	2S 24.42460	0.00179	-0.37021
ARSENIC            1S(2)2S(1), 3-2S			SELENIUM            1S(2)2S(1), 3-2S		
T.E.= -0.11917282D+04 P.E.= -0.23834520D+04			T.E.= -0.12660803D+04 P.E.= -0.25321610D+04		
K.E.= 0.11917238D+04 V.T.= -0.20000037C+01			K.E.= 0.12660807D+04 V.T.= -0.19999997D+01		
S	1S	2S	S	1S	2S
BASIS/ORB E	-517.72304	-123.24256	BASIS/CRB E	-550.39898	-131.21971
1S 32.50810	0.99056	-0.35051	1S 33.54140	0.99116	-0.34624
1S 58.26330	0.00903	0.00278	1S 61.48760	0.00774	0.00098
2S 15.48480	0.00034	1.36369	2S 15.92260	0.00023	1.34657
2S 25.20160	0.00178	-0.37169	2S 26.43500	0.00265	-0.35761
BROMINE            1S(2)2S(1), 3-2S			KRYPTON            1S(2)2S(1), 3-2S		
T.E.= -0.13426825D+04 P.E.= -0.26E53639D+04			T.E.= -0.14215347D+04 P.E.= -0.28430681D+04		
K.E.= 0.13426814D+04 V.T.= -0.2000009D+01			K.E.= 0.14215334D+04 V.T.= -0.20000009D+01		
S	1S	2S	S	1S	2S
BASIS/ORB E	-584.07505	-139.44688	BASIS/CRB E	-618.75109	-147.92404
1S 34.52730	0.99125	-0.3488	1S 35.52960	0.99156	-0.34881
1S 62.60870	0.00795	0.00157	1S 64.58930	0.00764	0.00177
2S 16.42770	0.00026	1.35238	2S 16.52320	0.00025	1.35484
2S 27.10370	0.00221	-0.36240	2S 27.85540	0.00219	-0.36462

See page 183 for Explanation of Tables and Notes for Tables 32, 42, and 43

## ROOTHAAN-HARTREE-FOCK ATOMIC WAVEFUNCTIONS

 TABLE 5 (1). HARTREE-FOCK FUNCTIONS FOR Be(<sup>1</sup>S) ISO-ELECTRONIC SERIES.

BERYLLIUM      1S(2)2S(2), 4-1S			BORON      1S(2)2S(2), 4-1S		
T.E.= -0.14573015D+02    P.E.= -0.29145870D+02			T.E.= -0.24237566D+02    P.E.= -0.48474924D+02		
K.E.= 0.14572855D+02	V.T.= -0.20C00110D+01		K.E.= 0.24237358D+02	V.T.= -0.20000086D+01	
S	1S	2S	S	1S	2S
BASIS/ORB E	-4.7327C	-0.30926	BASIS/CRB E	-8.18593	-0.67381
1S 3.49834	0.91117	-0.16385	1S 4.42994	0.92801	-0.20288
1S 6.38774	0.08527	-0.01659	1S 7.86336	0.08063	-0.01942
2S 1.20770	0.00095	0.51607	2S 1.59241	0.00320	0.73490
2S 3.07968	0.01673	-0.07243	2S 4.01022	-0.00081	-0.09218
2S 0.82055	-0.00048	0.55551	2S 1.25C21	-0.00198	0.34527
CARBON      1S(2)2S(2), 4-1S			NITROGEN      1S(2)2S(2), 4-1S		
T.E.= -0.364C8489D+02    P.E.= -0.72816655D+02			T.E.= -0.51082311D+02    P.E.= -0.10216413D+03		
K.E.= 0.36408167D+02	V.T.= -0.20000088D+01		K.E.= 0.51081823D+02	V.T.= -0.20000096D+01	
S	1S	2S	S	1S	2S
BASIS/ORB E	-12.65064	-1.69404	BASIS/ORB E	-18.12014	-2.76673
1S 5.43806	0.94114	-0.23411	1S 6.45100	0.94954	-0.25378
1S 9.62456	0.06483	-0.01534	1S 11.38700	0.05374	-0.01283
2S 2.05179	0.00453	0.61E29	2S 2.50371	0.00616	0.86015
2S 4.72768	0.00033	-0.11736	2S 5.53122	0.00230	-0.13747
2S 1.72221	-0.00313	0.2E540	2S 2.25623	-0.00486	0.26208
OXYGEN      1S(2)2S(2), 4-1S			FLUORINE      1S(2)2S(2), 4-1S		
T.E.= -0.68257705D+02    P.E.= -0.13651491D+03			T.E.= -0.87934048D+02    P.E.= -0.17586845D+03		
K.E.= 0.68257209D+02	V.T.= -0.20000073D+01		K.E.= 0.87934406D+02	V.T.= -0.19999959D+01	
S	1S	2S	S	1S	2S
BASIS/ORB E	-24.59210	-4.09C72	BASIS/CRB E	-32.06544	-5.66546
1S 7.47768	0.95638	-0.26887	1S 8.48913	0.95855	-0.27945
1S 13.26840	0.04363	-0.010C3	1S 14.87660	0.03945	-0.00876
2S 2.95696	0.00660	0.973E1	2S 3.41541	0.00012	1.15975
2S 6.30100	0.00553	-0.15750	2S 7.07468	0.00797	-0.17568
2S 2.76971	-0.00569	0.16791			
NEON      1S(2)2S(2), 4-1S			SODIUM      1S(2)2S(2), 4-1S		
T.E.= -0.11011100D+03    P.E.= -0.22022154D+03			T.E.= -0.13478839D+03    P.E.= -0.26957594D+03		
K.E.= 0.11011053D+03	V.T.= -0.20000043D+01		K.E.= 0.13478755D+03	V.T.= -0.20000062D+01	
S	1S	2S	S	1S	2S
BASIS/ORB E	-40.53980	-7.49C71	BASIS/CRB E	-50.01475	-9.56627
1S 9.49956	0.96494	-0.28655	1S 10.50300	0.96883	-0.29825
1S 16.88280	0.03298	-0.06667	1S 18.73480	0.02921	-0.00494
2S 3.90509	0.00014	1.17750	2S 4.39737	0.00009	1.19459
2S 7.82156	0.00747	-0.19252	2S 8.54355	0.00691	-0.20825
MAGNESIUM      1S(2)2S(2), 4-1S			ALUMINUM      1S(2)2S(2), 4-1S		
T.E.= -0.16156607D+03    P.E.= -0.32393152D+03			T.E.= -0.19164398D+03    P.E.= -0.38328803D+03		
K.E.= 0.16196545D+03	V.T.= -0.20000038D+01		K.E.= 0.19164405D+03	V.T.= -0.19999996D+01	
S	1S	2S	S	1S	2S
BASIS/ORB E	-60.49012	-11.89209	BASIS/CRB E	-71.96579	-14.46808
1S 11.51970	0.97220	-0.30213	1S 12.55450	0.97543	-0.30751
1S 20.75900	0.02505	-0.00399	1S 23.16130	0.02014	-0.00318
2S 4.88635	-0.00003	1.2C7C7	2S 5.37366	-0.00026	1.21680
2S 9.33296	0.00753	-0.22C51	2S 10.15320	0.00935	-0.23167
SILICON      1S(2)2S(2), 4-1S			PHOSPHORUS      1S(2)2S(2), 4-1S		
T.E.= -0.22382206D+03    P.E.= -0.44764391D+03			T.E.= -0.25850026D+03    P.E.= -0.51700158D+03		
K.E.= 0.22382185D+03	V.T.= -0.20C00009D+01		K.E.= 0.2585C132D+03	V.T.= -0.19999959D+01	
S	1S	2S	S	1S	2S
BASIS/ORB E	-84.44173	-17.29419	BASIS/CRB E	-97.91782	-20.37044
1S 13.56990	0.97794	-0.31205	1S 14.58860	0.97936	-0.31333
1S 25.42030	0.01729	-0.00224	1S 27.62840	0.01512	-0.00252
2S 5.86544	-0.00035	1.22E12	2S 6.34E39	-0.00041	1.23180
2S 10.91210	0.00955	-0.242E1	2S 11.81180	0.01022	-0.24766

See page 183 for Explanation of Tables and Notes for Tables 32, 42, and 43

TABLE 5 (2). HARTREE-FOCK FUNCTIONS FOR Be(<sup>1</sup>S) ISO-ELECTRONIC SERIES.

SULFUR            1S(2)2S(2), 4-1S			CHLORINE        1S(2)2S(2), 4-1S		
T.E.= -0.29567859D+03 P.E.= -0.59135769D+03			T.E.= -0.33535699D+03 P.E.= -0.67071518D+03		
K.E.= 0.29567910D+03 V.T.= -0.19999983D+01			K.E.= 0.33535819D+03 V.T.= -0.19999964D+01		
S	1S	2S	S	1S	2S
BASIS/ORB E	-112.39414	-23.65673	BASIS/ORB E	-127.87051	-27.27310
1S 15.54980	0.97993	-0.31755	1S 16.58800	0.98193	-0.31966
1S 28.53840	0.01663	-0.00214	1S 31.43250	0.01326	-0.00169
2S 6.84069	-0.00021	1.24246	2S 7.32740	-0.00040	1.24796
2S 12.53410	0.00741	-0.25631	2S 13.36630	0.00898	-0.26278
ARGON            1S(2)2S(2), 4-1S			POTASSIUM       1S(2)2S(2), 4-1S		
T.E.= -0.37753545D+03 P.E.= -0.755C7325D+03			T.E.= -0.42221398D+03 P.E.= -0.84443044D+03		
K.E.= 0.37753780D+03 V.T.= -0.19999938D+01			K.E.= 0.42221645D+03 V.T.= -0.19999942D+C1		
S	1S	2S	S	1S	2S
BASIS/ORB E	-144.34697	-31.09954	BASIS/CRB E	-161.82356	-35.17599
1S 17.60200	0.98293	-0.32080	1S 18.59330	0.98374	-0.32321
1S 33.67040	0.01188	-0.00177	1S 35.29640	0.01167	-0.00155
2S 7.81071	-0.00045	1.25124	2S 8.20093	-0.00039	1.25750
2S 14.23190	0.00930	-0.26675	2S 15.01440	0.00839	-0.27242
CALCIUM        1S(2)2S(2), 4-1S			SCANDIUM       1S(2)2S(2), 4-1S		
T.E.= -0.46939253D+03 P.E.= -0.93E78571D+03			T.E.= -0.51907123D+03 P.E.= -0.10381436D+04		
K.E.= 0.46939318D+03 V.T.= -0.19999986D+01			K.E.= C.51907236D+03 V.T.= -0.19999978D+C1		
S	1S	2S	S	1S	2S
BASIS/ORB E	-180.30019	-39.50250	BASIS/ORB E	-199.77695	-44.07899
1S 19.56940	0.98471	-0.32410	1S 20.55890	0.98507	-0.32949
1S 36.79960	0.01191	-0.00202	1S 38.04380	0.01204	-0.00042
2S 8.78182	-0.00014	1.25854	2S 9.29490	-0.00024	1.27414
2S 15.89890	0.00662	-0.27392	2S 16.44320	0.00603	-0.28649
TITANIUM       1S(2)2S(2), 4-1S			VANADIUM       1S(2)2S(2), 4-1S		
T.E.= -0.57124985D+03 P.E.= -0.11425039D+04			T.E.= -C.62592859D+03 P.E.= -C.12518562D+04		
K.E.= 0.57125409D+03 V.T.= -0.19999926D+01			K.E.= 0.62592764D+03 V.T.= -0.20000015D+01		
S	1S	2S	S	1S	2S
BASIS/ORB E	-220.25363	-48.90557	BASIS/ORB E	-241.73055	-53.98209
1S 21.57460	0.98567	-0.32658	1S 22.53990	0.98623	-0.33464
1S 40.24170	0.01095	-0.00112	1S 41.18660	0.01176	0.00068
2S 9.76864	-0.00028	1.27190	2S 10.28790	-0.00016	1.28871
2S 17.40340	0.00653	-0.28578	2S 17.88080	0.00473	-0.29913
CHROMIUM       1S(2)2S(2), 4-1S			MANGANESE      1S(2)2S(2), 4-1S		
T.E.= -0.68310731D+03 P.E.= -0.13662138D+04			T.E.= -0.74278605D+03 P.E.= -0.14855722D+04		
K.E.= 0.68310648D+03 V.T.= -0.20000012D+01			K.E.= 0.74278614D+03 V.T.= -0.19999999D+01		
S	1S	2S	S	1S	2S
BASIS/ORB E	-264.20738	-59.30869	BASIS/ORB E	-287.68423	-64.88532
1S 23.53680	0.98673	-0.33599	1S 24.51920	0.98675	-0.33688
1S 42.87870	0.01142	0.00084	1S 43.94970	0.01189	0.00072
2S 10.77860	-0.00015	1.29260	2S 11.26400	-0.00007	1.29411
2S 18.66760	0.00443	-0.30281	2S 19.50170	0.00371	-0.30419
IRON            1S(2)2S(2), 4-1S			COBALT        1S(2)2S(2), 4-1S		
T.E.= -0.80496479D+03 P.E.= -0.16C99320D+04			T.E.= -0.86964358D+03 P.E.= -0.17392891D+04		
K.E.= 0.80496720D+03 V.T.= -0.19999970D+01			K.E.= 0.86964557D+03 V.T.= -0.19999977D+C1		
S	1S	2S	S	1S	2S
BASIS/ORB E	-312.16108	-70.71199	BASIS/ORB E	-337.63800	-76.78862
1S 25.52450	0.98715	-0.33568	1S 26.51950	0.98759	-0.33764
1S 45.77480	0.01133	-0.00008	1S 47.41310	0.01109	0.00043
2S 11.73700	-0.00008	1.29C72	2S 12.23380	-0.00006	1.29636
2S 20.46870	0.00382	-0.30212	2S 21.19240	0.00351	-0.30703

See page 183 for Explanation of Tables and Notes for Tables 32, 42, and 43

## ROOTHAAN-HARTREE-FOCK ATOMIC WAVEFUNCTIONS

 TABLE 5 (3). HARTREE-FOCK FUNCTIONS FOR Be(<sup>1</sup>S) ISO-ELECTRONIC SERIES.

NICKEL	1S(2)2S(2), 4-1S	COPPER	1S(2)2S(2), 4-1S		
T.E.= -0.93682238D+03	P.E.= -0.18736469D+04	T.E.= -0.10065012D+04	P.E.= -0.20130058D+04		
K.E.= 0.93682455D+03	V.T.= -0.19999977D+01	K.E.= 0.10065046D+04	V.T.= -0.19999966D+01		
S	1S	2S	S		
BASIS/ORB E	-364.11493	-83.11528	BASIS/CRB E	-391.59186	-89.69194
1S 27.51310	0.98789	-0.33875	1S 28.50850	0.98818	-0.33951
1S 48.93450	0.01097	0.00059	1S 50.50170	0.01081	0.00063
2S 12.72440	-0.00004	1.29543	2S 13.21300	-0.00003	1.30158
2S 21.97850	0.00320	-0.30984	2S 22.78620	0.00297	-0.31193
ZINC	1S(2)2S(2), 4-1S	GALLIUM	1S(2)2S(2), 4-1S		
T.E.= -0.10786800D+04	P.E.= -0.21573627D+04	T.E.= -0.11533588D+04	P.E.= -0.23067210D+04		
K.E.= 0.10786827D+04	V.T.= -0.19999975D+01	K.E.= 0.11533622D+04	V.T.= -0.19999971D+01		
S	1S	2S	S		
BASIS/ORB E	-420.06885	-96.51861	BASIS/CRB E	-449.54582	-103.59530
1S 29.50390	0.98852	-0.34689	1S 30.49940	0.98879	-0.34167
1S 52.11430	0.01061	0.00097	1S 53.67720	0.01046	0.00106
2S 13.70730	-0.00001	1.30557	2S 14.19700	0.00000	1.30778
2S 23.53660	0.00273	-0.31545	2S 24.33320	0.00253	-0.31753
GERMANIUM	1S(2)2S(2), 4-1S	ARSENIC	1S(2)2S(2), 4-1S		
T.E.= -0.12305377D+04	P.E.= -0.24610795D+04	T.E.= -0.13102166D+04	P.E.= -0.26204348D+04		
K.E.= 0.12305418D+04	V.T.= -0.19999967D+01	K.E.= 0.13102183D+04	V.T.= -0.19999987D+01		
S	1S	2S	S		
BASIS/ORB E	-480.02281	-110.52199	BASIS/CRB E	-511.49986	-116.49867
1S 31.50430	0.98920	-0.34195	1S 32.50760	0.98974	-0.34388
1S 55.60350	0.00996	0.00101	1S 57.66500	0.00943	0.00168
2S 14.68380	-0.00001	1.3C692	2S 15.18740	-0.00002	1.31526
2S 25.15070	0.00260	-0.31890	2S 25.82810	0.00255	-0.32444
SELENIUM	1S(2)2S(2), 4-1S	BROMINE	1S(2)2S(2), 4-1S		
T.E.= -0.13923954D+04	P.E.= -0.27E47919D+04	T.E.= -0.14770743D+04	P.E.= -0.29541486D+04		
K.E.= 0.13923965D+04	V.T.= -0.19999992D+01	K.E.= 0.1477C743D+04	V.T.= -0.20000000D+01		
S	1S	2S	S		
BASIS/ORB E	-543.97690	-126.32537	BASIS/ORB E	-577.45394	-134.40206
1S 33.51300	0.99017	-0.34458	1S 34.52020	0.99066	-0.34565
1S 59.73310	0.00893	0.00183	1S 62.00040	0.00836	0.00215
2S 15.68000	-0.00004	1.31790	2S 16.17850	-0.00005	1.32215
2S 26.60210	0.00260	-0.32700	2S 27.32510	0.00266	-0.33094
KRYPTON	1S(2)2S(2), 4-1S				
T.E.= -0.15642531D+04	P.E.= -0.31285155D+04				
K.E.= 0.15642623D+04	V.T.= -0.19999941D+01				
S	1S	2S			
BASIS/ORB E	-611.53083	-142.72881			
1S 35.54860	0.99107	-0.34296			
1S 64.93790	0.00737	0.00057			
2S 16.63660	-0.00013	1.31437			
2S 28.42860	0.00336	-0.32526			

See page 183 for Explanation of Tables and Notes for Tables 32, 42, and 43

TABLE 6 (1). HARTREE-FOCK FUNCTIONS FOR B(<sup>2</sup>P) ISO-ELECTRONIC SERIES.

BORON	1S(2)2S(2)2P(1), 5-2P			
T.E.= -0.24529051D+02	P.E.= -0.49557803D+02			
K.E.= 0.24528752D+02	V.T.= -0.20000122D+01			
S	1S	2S	P	2P
BASIS/ORB E	-7.69539	-0.49471	BASIS/ORB E	-0.30985
1S 4.53106	0.91487	-0.18133	2P 1.32678	0.38061
1S 8.05711	0.06996	-0.01571	2P 2.18636	0.14726
2S 1.65698	0.00243	0.53257	2P 0.87466	0.52744
2S 4.10100	0.02729	-0.08214	2P 5.58064	0.00901
2S 1.07980	-0.00078	0.55180		
CARBON	1S(2)2S(2)2P(1), 5-2P			
T.E.= -0.37292215D+02	P.E.= -0.745E4349D+02			
K.E.= 0.37292134D+02	V.T.= -0.20000022D+01			
S	1S	2S	P	2P
BASIS/ORB E	-11.89824	-1.15375	BASIS/ORB E	-0.90476
1S 5.54099	0.92321	-0.20523	2P 1.87782	0.39981
1S 9.68937	0.06002	-0.01473	2P 3.07800	0.12301
2S 2.14468	0.00270	0.48442	2P 1.39268	0.51189
2S 4.96979	0.02758	-0.09915	2P 7.01117	0.00780
2S 1.56842	-0.00102	0.60483		
NITROGEN	1S(2)2S(2)2P(1), 5-2P			
T.E.= -0.52815783D+02	P.E.= -0.105E3128D+03			
K.E.= 0.52815497D+02	V.T.= -0.20000054D+01			
S	1S	2S	P	2P
BASIS/ORB E	-17.11774	-2.07201	BASIS/ORB E	-1.75561
1S 6.48808	0.93609	-0.23331	2P 2.42497	0.42629
1S 11.23530	0.05643	-0.01360	2P 3.96654	0.10051
2S 2.61940	0.00445	0.45235	2P 1.88098	0.49912
2S 5.76887	0.01508	-0.11148	2P 8.45838	0.00673
2S 2.06257	-0.00224	0.64791		
OXYGEN	1S(2)2S(2)2P(1), 5-2P			
T.E.= -0.71094697D+02	P.E.= -0.14218898D+03			
K.E.= 0.71094284D+02	V.T.= -0.20000058D+01			
S	1S	2S	P	2P
BASIS/ORB E	-23.34504	-3.24419	BASIS/ORB E	-2.85977
1S 7.54441	0.94402	-0.25076	2P 2.97232	0.42572
1S 13.24010	0.04291	-0.0C996	2P 4.80708	0.08723
2S 3.05502	0.00367	0.46752	2P 2.37269	0.50781
2S 6.56853	0.02123	-0.12706	2P 9.94087	0.00591
2S 2.54716	-0.00211	0.64497		
FLUORINE	1S(2)2S(2)2P(1), 5-2P			
T.E.= -0.92126759D+02	P.E.= -0.18425304D+03			
K.E.= 0.92126286D+02	V.T.= -0.20000051D+01			
S	1S	2S	P	2P
BASIS/ORB E	-30.57676	-4.66849	BASIS/ORB E	-4.21592
1S 8.54453	0.95057	-0.26594	2P 3.40639	0.52923
1S 14.97100	0.03781	-0.0C766	2P 5.55820	0.08422
2S 3.56178	0.00285	0.41173	2P 2.79994	0.40393
2S 7.28345	0.01920	-0.14254	2P 11.45920	0.00530
2S 3.05480	-0.00171	0.71656		
NEON	1S(2)2S(2)2P(1), 5-2P			
T.E.= -0.11591084D+03	P.E.= -0.23182112D+03			
K.E.= 0.11591027D+03	V.T.= -0.20000049D+01			
S	1S	2S	P	2P
BASIS/ORB E	-38.81124	-6.34406	BASIS/ORB E	-5.82333
1S 9.52524	0.95488	-0.27465	2P 4.02195	0.44762
1S 16.57510	0.03578	-0.0C768	2P 6.49289	0.06947
2S 3.99322	0.00563	0.28761	2P 3.33907	0.49796
2S 8.19267	0.01554	-0.14934	2P 12.92330	0.00455
2S 3.60540	-0.00411	0.84693		

See page 183 for Explanation of Tables and Notes for Tables 32, 42, and 43

## ROOTHAAN-HARTREE-FOCK ATOMIC WAVEFUNCTIONS

 TABLE 6 (2). HARTREE-FOCK FUNCTIONS FOR B(<sup>2</sup>P) ISO-ELECTRONIC SERIES.

SODIUM	1S(2)2S(2)2P(1), 5-2P			
T.E.= -0.14244630D+03	P.E.= -0.28489180D+03			
K.E.= 0.14244550D+03	V.T.= -0.20000C56D+01			
S	1S	2S	P	2P
BASIS/ORB E	-48.04761	-8.27C52	BASIS/ORB E	-7.68168
1S 10.52820	0.95915	-0.28369	2P 4.56420	0.42506
1S 18.32690	0.03216	-0.00637	2P 7.36391	0.06300
2S 4.33866	0.00646	0.54652	2P 3.84660	0.52530
2S 8.95031	0.01455	-0.16233	2P 14.45200	0.00390
2S 4.04446	-0.00524	0.60149		
MAGNESIUM	1S(2)2S(2)2P(1), 5-2P			
T.E.= -0.17173273D+03	P.E.= -0.34346448D+03			
K.E.= 0.17173174D+03	V.T.= -0.200CCC58D+01			
S	1S	2S	P	2P
BASIS/ORB E	-58.28528	-10.44755	BASIS/ORB E	-9.79061
1S 11.51300	0.96257	-0.29147	2P 5.07857	0.43415
1S 19.93510	0.03048	-0.00546	2P 8.19286	0.05806
2S 4.85717	0.00906	0.22462	2P 4.33019	0.51971
2S 9.72144	0.01202	-0.17260	2P 15.89080	0.00355
2S 4.61825	-0.00778	0.93464		
ALUMINUM	1S(2)2S(2)2P(1), 5-2P			
T.E.= -0.20376989D+03	P.E.= -0.40753906D+03			
K.E.= 0.20376917D+03	V.T.= -0.20000035D+01			
S	1S	2S	P	2P
BASIS/ORB E	-69.52388	-12.87501	BASIS/ORB E	-12.15002
1S 12.52350	0.96471	-0.25758	2P 5.60648	0.42704
1S 21.62730	0.02790	-0.00444	2P 9.04080	0.05364
2S 5.21767	0.01521	0.30128	2P 4.82558	0.53015
2S 10.48520	0.01261	-0.18396	2P 17.40180	0.00318
2S 5.12444	-0.01438	0.86951		
SILICON	1S(2)2S(2)2P(1), 5-2P			
T.E.= -0.23855562D+03	P.E.= -0.47680155D+03			
K.E.= 0.23824593D+03	V.T.= -0.20C12999D+01			
S	1S	2S	P	2P
BASIS/ORB E	-81.78268	-15.55687	BASIS/ORB E	-14.77066
1S 13.51000	0.96601	-0.31739	2P 6.01300	0.46740
1S 23.07640	0.02750	0.00361	2P 9.69120	0.05678
2S 5.56264	0.00034	1.16C27	2P 5.31799	0.48550
2S 11.19870	0.01175	-0.16722	2P 18.51250	0.00300
PHOSPHORUS	1S(2)2S(2)2P(1), 5-2P			
T.E.= -0.27609571D+03	P.E.= -0.55219C47D+03			
K.E.= 0.27609476D+03	V.T.= -0.20000034D+01			
S	1S	2S	P	2P
BASIS/ORB E	-95.00306	-18.48C62	BASIS/ORB E	-17.61973
1S 14.54140	0.96992	-0.3C25	2P 6.82689	0.39956
1S 25.34810	0.02270	-0.00232	2P 11.10890	0.03614
2S 6.12609	0.00018	1.19399	2P 5.78445	0.57380
2S 11.96580	0.01265	-0.20619	2P 21.08370	0.00252
SULFUR	1S(2)2S(2)2P(1), 5-2P			
T.E.= -0.31638417D+03	P.E.= -0.63276772D+03			
K.E.= 0.31638355D+03	V.T.= -0.20000019D+01			
S	1S	2S	P	2P
BASIS/ORB E	-109.24335	-21.65903	BASIS/ORB E	-20.72998
1S 15.54580	0.97197	-0.31163	2P 7.39505	0.36862
1S 27.17460	0.02089	-0.00195	2P 12.04200	0.03371
2S 6.61315	0.00012	1.20279	2P 6.30181	0.60656
2S 12.75620	0.01216	-0.21501	2P 22.72380	0.00221

See page 183 for Explanation of Tables and Notes for Tables 32, 42, and 43

TABLE 6 (3). HARTREE-FOCK FUNCTIONS FOR B<sub>\sqrt{2}</sub>P) ISO-ELECTRONIC SERIES.

CHLORINE      1S(2)2S(2)2P(1), 5-2P  
 T.E.= -0.35942290D+03 P.E.= -0.7184541D+03  
 K.E.= 0.35942251D+03 V.T.= -0.20000011D+01

S	1S	2S	P	2P
BASIS/ORB E	-124.48400	-25.08740	BASIS/ORB E	-24.09039
1S 16.54260	0.97347	-0.31475	2P 7.93457	0.36232
1S 28.84370	0.01989	-0.00166	2P 12.89040	0.03170
2S 7.10068	0.00009	1.21090	2P 6.79422	0.61426
2S 13.54340	0.01137	-0.22290	2P 24.26450	0.00208

ARGON      1S(2)2S(2)2P(1), 5-2P  
 T.E.= -0.40521185D+03 P.E.= -0.81042238D+03  
 K.E.= 0.40521054D+03 V.T.= -0.20000032D+01

S	1S	2S	P	2P
BASIS/ORB E	-140.72496	-28.76586	BASIS/ORB E	-27.70091
1S 17.53420	0.97529	-0.31978	2P 8.47809	0.35622
1S 30.56270	0.01894	-0.00043	2P 13.77880	0.02956
2S 7.59659	0.00007	1.22218	2P 7.28663	0.62198
2S 14.21390	0.01020	-0.23258	2P 25.81520	0.00195

POTASSIUM      1S(2)2S(2)2P(1), 5-2P  
 T.E.= -0.45375098D+03 P.E.= -0.9C750C65D+03  
 K.E.= 0.45374967D+03 V.T.= -0.20000029D+01

S	1S	2S	P	2P
BASIS/ORB E	-157.96613	-32.69445	BASIS/ORB E	-31.56157
1S 18.53240	0.97659	-0.32252	2P 9.01762	0.35122
1S 32.28180	0.01800	-0.0004	2P 14.66720	0.02773
2S 8.08644	0.00005	1.22969	2P 7.77904	0.62825
2S 14.98270	0.00962	-0.23576	2P 27.35580	0.00183

CALCIUM      1S(2)2S(2)2P(1), 5-2P  
 T.E.= -0.50504026D+03 P.E.= -0.10100792D+04  
 K.E.= 0.50503896D+03 V.T.= -0.20000026D+01

S	1S	2S	P	2P
BASIS/ORB E	-176.20749	-36.87312	BASIS/ORB E	-35.67232
1S 19.52920	0.97768	-0.32502	2P 9.55714	0.34643
1S 33.95090	0.01727	0.00031	2P 15.55560	0.02609
2S 8.57652	0.00003	1.23662	2P 8.27145	0.63437
2S 15.75210	0.00905	-0.24637	2P 28.90650	0.00173

SCANDIUM      1S(2)2S(2)2P(1), 5-2P  
 T.E.= -0.559G7968D+03 P.E.= -0.11181577D+04  
 K.E.= 0.55907803D+03 V.T.= -0.20000029D+01

S	1S	2S	P	2P
BASIS/ORB E	-195.44903	-41.30185	BASIS/ORB E	-40.03315
1S 20.52620	0.97881	-0.32778	2P 10.09670	0.34157
1S 35.67000	0.01650	0.00086	2P 16.41400	0.02471
2S 9.06933	0.00002	1.24415	2P 8.76385	0.64023
2S 16.49070	0.00849	-0.25329	2P 30.41720	0.00166

TITANIUM      1S(2)2S(2)2P(1), 5-2P  
 T.E.= -0.61586920D+03 P.E.= -0.12317385D+04  
 K.E.= 0.61586929D+03 V.T.= -0.19999999D+01

S	1S	2S	P	2P
BASIS/ORB E	-215.69062	-45.58C61	BASIS/ORB E	-44.64407
1S 21.53560	0.97994	-0.32882	2P 10.69030	0.24599
1S 37.61500	0.01526	0.00C81	2P 17.40280	0.02679
2S 9.55594	-0.00002	1.24845	2P 9.58253	0.73361
2S 17.31520	0.00852	-0.258C4	2P 32.18620	0.00115

See page 183 for Explanation of Tables and Notes for Tables 32, 42, and 43

## ROOTHAAN-HARTREE-FOCK ATOMIC WAVEFUNCTIONS

 TABLE 6 (4). HARTREE-FOCK FUNCTIONS FOR B(<sup>2</sup>P) ISO-ELECTRONIC SERIES.

VANADIUM      1S(2)2S(2)2P(1), 5-2P  
 T.E.= -0.67540883D+03 P.E.= -0.135081750+04  
 K.E.= 0.67540870D+03 V.T.= -0.20000002D+01

S	1S	2S	P	2P
BASIS/ORB E	-236.93242	-50.90546	BASIS/ORB E	-49.50504
1S 22.53370	0.98079	-0.33067	2P 11.24150	0.24072
1S 39.32170	0.01467	0.00108	2P 18.30270	0.02535
2S 10.04640	-0.00003	1.25397	2P 9.87864	0.74003
2S 18.08880	0.00610	-0.26332	2P 33.71250	0.00110

CHROMIUM      1S(2)2S(2)2P(1), 5-2P  
 T.E.= -0.73769853D+03 P.E.= -0.14753571D+04  
 K.E.= 0.73769862D+03 V.T.= -0.19999999D+01

S	1S	2S	P	2P
BASIS/ORB E	-259.17431	-56.08835	BASIS/ORB E	-54.61606
1S 23.53120	0.98153	-0.33240	2P 11.77230	0.23245
1S 40.99750	0.01417	0.00133	2P 19.14090	0.02471
2S 10.53720	-0.00003	1.25520	2P 10.38260	0.74867
2S 18.86080	0.00771	-0.26829	2P 35.27560	0.00103

MANGANESE      1S(2)2S(2)2P(1), 5-2P  
 T.E.= -0.80273830D+03 P.E.= -0.16C54771D+04  
 K.E.= 0.80273882D+03 V.T.= -0.19999994D+01

S	1S	2S	P	2P
BASIS/ORB E	-282.41628	-61.51729	BASIS/ORB E	-59.97712
1S 24.53120	0.98227	-0.33377	2P 12.33030	0.22583
1S 42.74090	0.01360	0.00149	2P 20.05800	0.02343
2S 11.02710	-0.00004	1.24370	2P 10.88100	0.75632
2S 19.64660	0.00742	-0.27270	2P 36.83330	0.00098

IRON      1S(2)2S(2)2P(1), 5-2P  
 T.E.= -0.87052814D+03 P.E.= -0.17410544D+04  
 K.E.= 0.87052626D+03 V.T.= -0.20000022D+01

S	1S	2S	P	2P
BASIS/ORB E	-306.65843	-67.19631	BASIS/ORB E	-65.58822
1S 25.51970	0.98274	-0.33602	2P 12.78930	0.32332
1S 44.16540	0.01359	0.00201	2P 20.78600	0.01915
2S 11.52180	-0.00002	1.26969	2P 11.22390	0.66266
2S 20.37310	0.00677	-0.27793	2P 38.18050	0.00134

COBALT      1S(2)2S(2)2P(1), 5-2P  
 T.E.= -0.94106803D+03 P.E.= -0.18821370D+04  
 K.E.= 0.94106898D+03 V.T.= -0.19999990D+01

S	1S	2S	P	2P
BASIS/ORB E	-331.90046	-73.12525	BASIS/ORB E	-71.44937
1S 26.52880	0.98355	-0.33651	2P 13.40960	0.21162
1S 46.16230	0.01267	0.00190	2P 21.80070	0.02195
2S 12.00880	-0.00005	1.27245	2P 11.88550	0.77137
2S 21.19880	0.00683	-0.28110	2P 39.92480	0.00087

NICKEL      1S(2)2S(2)2P(1), 5-2P  
 T.E.= -0.10143580D+04 P.E.= -0.20287170D+04  
 K.E.= 0.10143590D+04 V.T.= -0.19999989D+01

S	1S	2S	P	2P
BASIS/ORB E	-358.14266	-79.30428	BASIS/ORB E	-77.56054
1S 27.52770	0.98409	-0.33755	2P 13.94940	0.21415
1S 47.85430	0.01227	0.00200	2P 22.69380	0.02084
2S 12.49840	-0.00005	1.27557	2P 12.37380	0.76995
2S 21.99050	0.00658	-0.28455	2P 41.51520	0.00085

See page 183 for Explanation of Tables and Notes for Tables 32, 42, and 43

TABLE 6 (5). HARTREE-FOCK FUNCTIONS FOR B(<sup>2</sup>P) ISO-ELECTRONIC SERIES.

COPPER	1S(2)2S(2)2P(1), 5-2P			
T.E.= -0.10903980D+04	P.E.= -0.21807575D+04			
K.E.= 0.10903995D+04	V.T.= -0.19999986D+01			
S	1S	2S	P	2P
BASIS/ORB E	-385.38489	-85.73333	BASIS/ORB E	-83.92175
1S 28.52890	0.98463	-0.33837	2P 14.50100	0.20576
1S 49.61140	0.01181	0.00205	2P 23.60040	0.02013
2S 12.98730	-0.00005	1.27901	2P 12.87790	0.77888
2S 22.79150	0.00641	-0.28765	2P 43.05380	0.00060
ZINC	1S(2)2S(2)2P(1), 5-2P			
T.E.= -0.11691880D+04	P.E.= -0.23383780D+04			
K.E.= 0.11691900D+04	V.T.= -0.19999983D+01			
S	1S	2S	P	2P
BASIS/ORB E	-413.62718	-92.41240	BASIS/ORB E	-90.53296
1S 29.52770	0.98512	-0.33943	2P 15.03760	0.20622
1S 51.30730	0.01146	0.00221	2P 24.48770	0.01928
2S 13.47830	-0.00006	1.28255	2P 13.36980	0.77909
2S 23.56980	0.00618	-0.29104	2P 44.59730	0.00078
GALLIUM	1S(2)2S(2)2P(1), 5-2P			
T.E.= -0.12507280D+04	P.E.= -0.25C14586D+04			
K.E.= 0.12507305D+04	V.T.= -0.19999980D+01			
S	1S	2S	P	2P
BASIS/ORB E	-442.86951	-99.34149	BASIS/ORB E	-97.39422
1S 30.52780	0.98556	-0.34009	2P 15.58710	0.19721
1S 53.02070	0.01111	0.00222	2P 25.35120	0.01881
2S 13.96660	-0.00006	1.28502	2P 13.87580	0.78842
2S 24.37760	0.00601	-0.29358	2P 46.16620	0.00074
GERMANIUM	1S(2)2S(2)2P(1), 5-2P			
T.E.= -0.13350181D+04	P.E.= -0.26700407D+04			
K.E.= 0.13350226D+04	V.T.= -0.19999966D+01			
S	1S	2S	P	2P
BASIS/ORB E	-473.11178	-106.52C55	BASIS/ORB E	-104.50540
1S 31.53030	0.98613	-0.34122	2P 15.87640	0.04390
1S 54.90990	0.01061	0.00246	2P 25.79640	0.02649
2S 14.46030	-0.00007	1.28899	2P 14.59840	0.92442
2S 25.13160	0.00588	-0.29732		
ARSENIC	1S(2)2S(2)2P(1), 5-2P			
T.E.= -0.14220582D+04	P.E.= -0.28441190D+04			
K.E.= 0.14220608D+04	V.T.= -0.19999982D+01			
S	1S	2S	P	2P
BASIS/ORB E	-504.35424	-113.94980	BASIS/ORB E	-111.86673
1S 32.53340	0.98644	-0.34C88	2P 16.26090	0.14348
1S 56.61900	0.01028	0.00208	2P 26.42480	0.02523
2S 14.94080	-0.00007	1.28879	2P 14.57580	0.83609
2S 26.02210	0.00585	-0.29774		
SELENIUM	1S(2)2S(2)2P(1), 5-2P			
T.E.= -0.15118483D+04	P.E.= -0.30236994D+04			
K.E.= 0.15118511D+04	V.T.= -0.19999982D+01			
S	1S	2S	P	2P
BASIS/ORB E	-536.59669	-121.62854	BASIS/ORB E	-119.47803
1S 33.53330	0.98683	-0.34160	2P 16.78550	0.14989
1S 58.35600	0.00998	0.00216	2P 27.26320	0.02440
2S 15.43080	-0.00007	1.29136	2P 15.46320	0.83036
2S 26.81290	0.00568	-0.30026		

See page 183 for Explanation of Tables and Notes for Tables 32, 42, and 43

ROOCHAAN-HARTREE-FOCK ATOMIC WAVEFUNCTIONS

TABLE 6 (6). HARTREE-FOCK FUNCTIONS FOR B(<sup>2</sup>P) ISO-ELECTRONIC SERIES.

BROMINE      1S(2)2S(2)2P(1), 5-2P				
T.E.= -0.16043885D+04    P.E.= -0.32C87805D+04				
K.E.= 0.16043920D+04    V.T.= -0.19999578D+01				
S	1S	2S	P	
BASIS/ORE E	-569.83916	-129.55813	BASIS/ORB E	-127.33935
1S 34.54240	0.98728	-0.34142	2P 17.56460	0.16729
1S 60.39840	0.00942	0.00190	2P 28.57430	0.02101
2S 15.91430	-0.00009	1.29192	2P 15.90520	0.81627
2S 27.67590	0.00577	-0.30134		
KRYPTON      1S(2)2S(2)2P(1), 5-2P				
T.E.= -0.16996787D+04    P.E.= -0.33993611D+04				
K.E.= 0.16996824D+04    V.T.= -0.19999578D+01				
S	1S	2S	P	
BASIS/ORB E	-604.08166	-137.73730	BASIS/ORB E	-135.45068
1S 35.54170	0.98762	-0.34208	2P 18.14200	0.16944
1S 62.10890	0.00918	0.00198	2P 29.47060	0.02006
2S 16.40420	-0.00009	1.29424	2P 16.38980	0.81496
2S 28.46800	0.00561	-0.30360		

See page 183 for Explanation of Tables and Notes for Tables 32, 42, and 43

TABLE 7 (1). HARTREE-FOCK FUNCTIONS FOR C(<sup>3</sup>P) ISO-ELECTRONIC SERIES.

CARBON            1S(2)2S(2)2P(2), 6-3P T.E.= -0.376885960+02 P.E.= -0.75276550D+02 K.E.= 0.37687954D+02 V.T.= -0.20000170D+01				
S	1S	2S	P	2P
BASIS/ORB E	-11.32563	-0.7C565	BASIS/ORB E	-0.43335
1S 5.53875	0.89523	-0.18C39	2P 1.44C37	0.56470
1S 9.25013	0.07720	-0.02141	2P 2.607E6	0.22955
2S 2.04126	0.00413	0.57726	2P 0.96499	0.26761
2S 5.30567	0.03954	-0.08E43	2P 6.53286	0.01016
2S 1.30552	-0.00123	0.5C92C		
NITROGEN          1S(2)2S(2)2P(2), 6-3P T.E.= -0.53887988D+02 P.E.= -0.10777559D+03 K.E.= 0.53887603D+02 V.T.= -0.20000071D+01				
S	1S	2S	P	2P
BASIS/ORB E	-16.28455	-1.4E247	BASIS/ORB E	-1.11006
1S 6.42321	0.91648	-0.20540	2P 1.97595	0.56289
1S 10.61430	0.07678	-0.02203	2P 3.38577	0.20256
2S 2.53445	0.00539	0.52372	2P 1.47888	0.27610
2S 6.15603	0.01393	-0.09336	2P 8.00193	0.00884
2S 1.79167	-0.00200	0.5E449		
OXYGEN           1S(2)2S(2)2P(2), 6-3P T.E.= -0.73100182D+02 P.E.= -0.14620002D+03 K.E.= 0.73099840D+02 V.T.= -0.20000047D+01				
S	1S	2S	P	2P
BASIS/ORB E	-22.26130	-2.47560	BASIS/ORB E	-2.04382
1S 7.60387	0.91857	-0.22578	2P 2.53573	0.53652
1S 12.68520	0.05180	-0.01438	2P 4.17455	0.17492
2S 3.00188	0.00428	0.50187	2P 1.99335	0.32046
2S 6.94554	0.04030	-0.1C571	2P 9.52379	0.00759
2S 2.27510	-0.00169	0.59314		
FLUORINE         1S(2)2S(2)2P(2), 6-3P T.E.= -0.95319599D+02 P.E.= -0.19C63891D+03 K.E.= 0.95319314D+02 V.T.= -0.20000030D+01				
S	1S	2S	P	2P
BASIS/ORB E	-29.24738	-3.75150	BASIS/ORB E	-3.23145
1S 8.58779	0.93225	-0.24406	2P 3.14091	0.46376
1S 14.48440	0.04421	-0.01140	2P 5.05703	0.14466
2S 3.45944	0.00496	0.48E52	2P 2.54600	0.41810
2S 7.72556	0.03250	-0.11838	2P 11.19290	0.00586
2S 2.76312	-0.00240	0.61508		
NEON             1S(2)2S(2)2P(2), 6-3P T.E.= -0.12054356D+03 P.E.= -0.24108661D+03 K.E.= 0.12054306D+03 V.T.= -0.20000041D+01				
S	1S	2S	P	2P
BASIS/ORB E	-37.23926	-5.27E21	BASIS/ORB E	-4.67155
1S 9.59807	0.93773	-0.25580	2P 3.66994	0.52648
1S 16.14840	0.03952	-0.01002	2P 5.90379	0.12121
2S 3.86603	0.00489	0.52568	2P 2.97531	0.37483
2S 8.56109	0.03131	-0.12769	2P 12.51180	0.00542
2S 3.23673	-0.00270	0.5E567		
SODIUM          1S(2)2S(2)2P(2), 6-3P T.E.= -0.14877057D+03 P.E.= -0.29754088D+03 K.E.= 0.14877031D+03 V.T.= -0.20000018D+01				
S	1S	2S	P	2P
BASIS/ORB E	-46.23485	-7.05262	BASIS/ORB E	-6.36327
1S 10.61260	0.94117	-0.2E255	2P 4.14156	0.56938
1S 17.81550	0.03592	-0.01011	2P 6.68759	0.11367
2S 4.24521	0.00593	0.58257	2P 3.43489	0.33659
2S 9.49319	0.03104	-0.13593	2P 13.99540	0.00469
2S 3.72255	-0.00385	0.53423		

See page 183 for Explanation of Tables and Notes for Tables 32, 42, and 43

## ROOTHAAN-HARTREE-FOCK ATOMIC WAVEFUNCTIONS

 TABLE 7 (2). HARTREE-FOCK FUNCTIONS FOR C(<sup>3</sup>P) ISO-ELECTRONIC SERIES.

MAGNESIUM	1S(2)2S(2)2P(2), 6-3P			
T.E.= -0.17999973D+03	P.E.= -0.35999897D+03			
K.E.= 0.17999923D+03	V.T.= -0.20000028D+01			
S	1S	2S	P	2P
BASIS/ORB E	-56.23306	-9.08C17	BASIS/ORB E	-8.30609
1S 11.60240	0.94803	-0.27326	2P 4.66696	0.56386
1S 19.58160	0.03226	-0.00ECS	2P 7.55004	0.10198
2S 4.70382	0.00726	0.47989	2P 3.93726	0.35174
2S 10.26330	0.02700	-0.14320	2P 15.50580	0.00393
2S 4.28744	-0.00533	0.64551		
ALUMINUM	1S(2)2S(2)2P(2), 6-3P			
T.E.= -0.21423048D+03	P.E.= -0.42846C72D+03			
K.E.= 0.21423024D+03	V.T.= -0.20000011D+01			
S	1S	2S	P	2P
BASIS/ORB E	-67.23325	-11.35862	BASIS/ORB E	-10.49985
1S 12.61970	0.95432	-0.28434	2P 5.20347	0.55198
1S 21.52320	0.02723	-0.00499	2P 8.37266	0.09273
2S 5.27611	0.00271	0.47611	2P 4.43274	0.37115
2S 10.82280	0.02606	-0.15854	2P 17.01780	0.00350
2S 4.73486	-0.00169	0.66706		
SILICON	1S(2)2S(2)2P(2), 6-3P			
T.E.= -0.25146242D+03	P.E.= -0.50292407D+03			
K.E.= 0.25146165D+03	V.T.= -0.20000031D+01			
S	1S	2S	P	2P
BASIS/ORB E	-79.23481	-13.88763	BASIS/ORB E	-12.94413
1S 13.58300	0.95707	-0.28871	2P 5.75256	0.54501
1S 22.95360	0.02767	-0.00563	2P 9.22C61	0.08288
2S 5.67497	0.00873	0.19631	2P 4.91458	0.38655
2S 11.77140	0.02144	-0.16C65	2P 18.44960	0.00322
2S 5.36582	-0.00718	0.94866		
PHOSPHORUS	1S(2)2S(2)2P(2), 6-3P			
T.E.= -0.29169527D+03	P.E.= -0.58339076D+03			
K.E.= 0.29169549D+03	V.T.= -0.19999993D+01			
S	1S	2S	P	2P
BASIS/ORB E	-92.23737	-16.667C5	BASIS/ORB E	-15.63886
1S 14.64340	0.96022	-0.29512	2P 6.52249	0.39452
1S 25.24640	0.02210	-0.00341	2P 10.41590	0.06544
2S 5.90137	0.00048	1.15537	2P 5.52621	0.55391
2S 12.48580	0.02503	-0.17126	2P 20.78170	0.00225
SULFUR	1S(2)2S(2)2P(2), 6-3P			
T.E.= -0.33492886D+03	P.E.= -0.66985814D+03			
K.E.= 0.33492928D+03	V.T.= -0.15999987D+01			
S	1S	2S	P	2P
BASIS/ORB E	-106.24090	-19.65690	BASIS/ORB E	-18.58406
1S 15.62900	0.96352	-0.30C72	2P 7.02073	0.37031
1S 26.95340	0.02092	-0.00259	2P 11.04460	0.06718
2S 6.38761	0.00038	1.16579	2P 6.04330	0.57518
2S 13.20660	0.02237	-0.18043	2P 22.29770	0.00218
CHLORINE	1S(2)2S(2)2P(2), 6-3P			
T.E.= -0.38116302D+03	P.E.= -0.76232621D+03			
K.E.= 0.38116319D+03	V.T.= -0.19999955D+01			
S	1S	2S	P	2P
BASIS/ORB E	-121.24514	-22.97703	BASIS/ORB E	-21.77955
1S 16.61960	0.96630	-0.30553	2P 7.49351	0.47856
1S 28.70160	0.C1971	-0.06184	2P 12.37130	0.05324
2S 6.87474	0.00030	1.17554	2P 6.42165	0.48040
2S 13.93480	0.02038	-0.18919	2P 23.86470	0.00166

See page 183 for Explanation of Tables and Notes for Tables 32, 42, and 43

TABLE 7 (3). HARTREE-FOCK FUNCTIONS FOR C(<sup>3</sup>P) ISO-ELECTRONIC SERIES.

ARGON	1S(2)2S(2)2P(2), 6-3P			
T.E.= -0.43039766D+03	P.E.= -0.86C75525D+03			
K.E.= 0.43039759D+03	V.T.= -0.20C000002D+01			
S	1S	2S	P	2P
BASIS/ORB E	-137.24994	-26.50742	BASIS/ORB E	-25.22532
1S 17.61460	0.96862	-0.30554	2P 8.17707	0.40519
1S 30.48080	0.01852	-0.00124	2P 13.23020	0.04733
2S 7.36214	0.00023	1.18444	2P 6.96049	0.55879
2S 14.67770	0.01891	-0.19742	2P 25.42260	0.00171
POTASSIUM	1S(2)2S(2)2P(2), 6-3P			
T.E.= -0.48263269D+03	P.E.= -0.96526584D+03			
K.E.= 0.48263315D+03	V.T.= -0.19999991D+01			
S	1S	2S	P	2P
BASIS/ORB E	-154.25514	-30.28791	BASIS/ORB E	-28.92124
1S 18.60470	0.97061	-0.31356	2P 8.71348	0.37023
1S 32.17680	0.01773	-0.00057	2P 14.08290	0.04658
2S 7.85137	0.00018	1.19328	2P 7.49944	0.59385
2S 15.40160	0.01735	-0.20531	2P 26.92420	0.00144
CALCIUM	1S(2)2S(2)2P(2), 6-3P			
T.E.= -0.53786806D+03	P.E.= -0.10757363D+04			
K.E.= 0.53786822D+03	V.T.= -0.19999957D+01			
S	1S	2S	P	2P
BASIS/ORB E	-172.26080	-34.31866	BASIS/ORB E	-32.86740
1S 19.58070	0.97126	-0.31610	2P 9.29904	0.35253
1S 33.36440	0.01839	-0.00062	2P 14.69200	0.04474
2S 8.33661	0.00021	1.19977	2P 7.98953	0.61251
2S 16.19960	0.01562	-0.21135	2P 28.02170	0.00171
SCANDIUM	1S(2)2S(2)2P(2), 6-3P			
T.E.= -0.59610370D+03	P.E.= -0.11922073D+04			
K.E.= 0.59610358D+03	V.T.= -0.200000020D+01			
S	1S	2S	P	2P
BASIS/ORB E	-191.26674	-38.59546	BASIS/ORB E	-37.06364
1S 20.59690	0.97376	-0.31952	2P 9.81548	0.37194
1S 35.65750	0.01607	0.00029	2P 15.80430	0.03996
2S 8.82885	0.00009	1.2C835	2P 8.45605	0.59757
2S 16.90550	0.01535	-0.21540	2P 30.02610	0.00140
TITANIUM	1S(2)2S(2)2P(2), 6-3P			
T.E.= -0.65733956D+03	P.E.= -0.13146796D+04			
K.E.= 0.65734007D+03	V.T.= -0.19999992D+01			
S	1S	2S	P	2P
BASIS/ORB E	-211.27299	-43.13C49	BASIS/ORB E	-41.51008
1S 21.59670	0.97433	-0.31997	2P 10.40400	0.39676
1S 37.17480	0.01573	-0.00027	2P 16.90450	0.03352
2S 9.30946	0.00009	1.21189	2P 8.88504	0.57879
2S 17.79400	0.01493	-0.22379	2P 32.02170	0.00138
VANADIUM	1S(2)2S(2)2P(2), 6-3P			
T.E.= -0.72157565D+03	P.E.= -0.14431530D+04			
K.E.= 0.72157735D+03	V.T.= -0.19999976D+01			
S	1S	2S	P	2P
BASIS/ORB E	-232.27934	-47.91138	BASIS/ORB E	-46.20649
1S 22.60080	0.97624	-0.32337	2P 10.85720	0.34793
1S 39.29490	0.01435	0.00064	2P 17.59840	0.03765
2S 9.80395	0.00002	1.22C17	2P 9.48050	0.62308
2S 18.47800	0.01425	-0.23114	2P 33.24250	0.00104

See page 183 for Explanation of Tables and Notes for Tables 32, 42, and 43

## ROOTHAAN-HARTREE-FOCK ATOMIC WAVEFUNCTIONS

 TABLE 7 (4). HARTREE-FOCK FUNCTIONS FOR C(<sup>3</sup>P) ISO-ELECTRONIC SERIES.

**CHROMIUM**      1S(2)2S(2)2P(2), 6-3P  
 T.E.= -0.78881187D+03   P.E.= -0.15776266D+04  
 K.E.= 0.78881470D+03   V.T.= -0.19999964D+01

S	1S	2S	P	2P
BASIS/ORB E	-254.28603	-52.94262	BASIS/ORB E	-51.15317
1S 23.62670	0.97699	-0.32223	2P 11.31000	C.45765
1S 41.43010	0.01295	-0.00C27	2P 18.64150	0.03141
2S 10.27960	-0.00002	1.22118	2P 9.78519	0.51921
2S 19.44760	0.01490	-0.23404	2P 35.10270	C.00120

**MANGANESE**      1S(2)2S(2)2P(2), 6-3P  
 T.E.= -0.85904831D+03   P.E.= -0.17180975D+04  
 K.E.= 0.85904924D+03   V.T.= -0.19999989D+01

S	1S	2S	P	2P
BASIS/ORB E	-277.29285	-58.22368	BASIS/ORB E	-56.34974
1S 24.59310	0.97831	-0.32774	2P 12.06360	0.32126
1S 42.74170	0.01331	0.00135	2P 19.33410	0.03220
2S 10.78510	-0.00003	1.23234	2P 10.46410	0.65436
2S 19.97960	0.01283	-0.24242	2P 36.29310	0.00109

**IRON**      1S(2)2S(2)2P(2), 6-3P  
 T.E.= -0.93228482D+03   P.E.= -0.18645739D+04  
 K.E.= 0.93228910D+03   V.T.= -0.19999954D+01

S	1S	2S	P	2P
BASIS/ORB E	-301.29978	-63.75497	BASIS/ORB E	-61.79653
1S 25.62210	0.97892	-0.32576	2P 12.75110	0.28499
1S 44.97400	0.01196	0.00C17	2P 20.43980	0.02900
2S 11.25670	-0.00005	1.23140	2P 10.99030	0.69357
2S 21.00310	0.01360	-0.24373	2P 38.26370	0.00096

**COBALT**      1S(2)2S(2)2P(2), 6-3P  
 T.E.= -0.10085215D+04   P.E.= -0.20170459D+04  
 K.E.= 0.10085244D+04   V.T.= -0.19999971D+01

S	1S	2S	P	2P
BASIS/ORB E	-326.30692	-69.53623	BASIS/ORB E	-67.49328
1S 26.59910	0.97974	-0.32923	2P 13.17810	0.30154
1S 46.26330	0.01222	0.00111	2P 21.07520	0.02950
2S 11.75550	-0.00006	1.23534	2P 11.46650	0.67615
2S 21.64300	0.01225	-0.25004	2P 39.43010	C.00098

**NICKEL**      1S(2)2S(2)2P(2), 6-3P  
 T.E.= -0.10877583D+04   P.E.= -0.21755188D+04  
 K.E.= 0.10877606D+04   V.T.= -0.19999979D+01

S	1S	2S	P	2P
BASIS/ORB E	-352.31420	-75.56762	BASIS/ORB E	-73.44015
1S 27.60770	0.98060	-0.33018	2P 13.79750	0.31025
1S 48.28750	0.01141	0.00110	2P 22.07500	0.02569
2S 12.24250	-0.00009	1.24303	2P 11.91980	C.67094
2S 22.45560	0.01211	-0.25396	2P 41.20140	0.00106

**COPPER**      1S(2)2S(2)2P(2), 6-3P  
 T.E.= -0.11699950D+04   P.E.= -0.23399988D+04  
 K.E.= 0.11700039D+04   V.T.= -0.19999924D+01

S	1S	2S	P	2P
BASIS/ORB E	-379.22146	-81.84904	BASIS/ORB E	-79.63714
1S 28.63250	0.98044	-0.32667	2P 14.36200	0.30130
1S 50.05530	0.01080	-0.00C71	2P 22.93930	0.02461
2S 12.70300	-0.00007	1.23849	2P 12.41970	0.68070
2S 23.61590	0.01289	-0.25234	2P 42.78080	0.00102

See page 183 for Explanation of Tables and Notes for Tables 32, 42, and 43

TABLE 7 (5). HARTREE-FOCK FUNCTIONS FOR C(<sup>3</sup>P) ISO-ELECTRONIC SERIES.

ZINC	1S(2)2S(2)2P(2), 6-3P			
T.E.= -0.12552320D+04	P.E.= -0.25104678D+04			
K.E.= 0.12552358D+C4	V.T.= -0.19999578D+C1			
S	1S	2S	P	2P
BASIS/ORB E	-407.32882	-88.38C37	BASIS/ORB E	-86.08394
1S 29.61300	0.98205	-0.33240	2P 14.69600	0.28858
1S 52.06870	0.01037	0.00132	2P 24.62410	0.02687
2S 13.22010	-0.00012	1.25C83	2P 12.98660	0.69173
2S 24.03310	0.01149	-0.26167		
GALLIUM	1S(2)2S(2)2P(2), 6-3P			
T.E.= -0.13434690D+04	P.E.= -0.26E9503D+04			
K.E.= 0.13434813D+04	V.T.= -0.199999C8D+01			
S	1S	2S	P	2P
BASIS/ORB E	-436.33617	-95.16170	BASIS/ORB E	-92.78087
1S 30.63500	0.98249	-0.33119	2P 15.36580	0.22111
1S 54.30070	0.00951	0.00057	2P 25.50720	0.02671
2S 13.69470	-0.00015	1.25023	2P 13.58150	0.75901
2S 25.00610	0.01192	-0.2E250		
GERMANIUM	1S(2)2S(2)2P(2), 6-3P			
T.E.= -0.14347060D+04	P.E.= -0.28E94251D+04			
K.E.= 0.14347191D+C4	V.T.= -0.19999909D+01			
S	1S	2S	P	2P
BASIS/ORB E	-466.34376	-102.19E18	BASIS/ORB E	-99.72788
1S 31.63360	0.98305	-0.33227	2P 15.92660	0.20068
1S 56.05500	0.00923	0.00070	2P 26.18660	0.02693
2S 14.18370	-0.00015	1.25372	2P 14.10390	C.77897
2S 25.79250	0.01153	-0.26583		
ARSENIC	1S(2)2S(2)2P(2), 6-3P			
T.E.= -0.15289432D+04	P.E.= -0.30578570D+04			
K.E.= 0.15289538D+04	V.T.= -0.19999930D+01			
S	1S	2S	P	2P
BASIS/ORB E	-497.35149	-109.47480	BASIS/ORB E	-106.92498
1S 32.63580	0.98355	-0.33292	2P 16.16400	0.26952
1S 57.89500	0.00890	0.00068	2P 26.85420	0.02655
2S 14.67040	-0.00016	1.25E38	2P 14.47750	C.69039
2S 26.61050	0.01127	-0.26E57		
SELENIUM	1S(2)2S(2)2P(2), 6-3P			
T.E.= -0.16261804D+04	P.E.= -0.32523680D+04			
K.E.= 0.16261876D+04	V.T.= -0.19999956D+01			
S	1S	2S	P	2P
BASIS/ORB E	-529.35934	-117.00621	BASIS/ORB E	-114.37196
1S 33.61490	0.98421	-0.33600	2P 16.10590	0.53550
1S 59.26230	0.00903	0.00162	2P 27.99160	0.02591
2S 15.17520	-0.00015	1.26380	2P 14.70360	0.44478
2S 27.20610	0.01027	-0.27442		
BROMINE	1S(2)2S(2)2P(2), 6-3P			
T.E.= -0.17264174D+04	P.E.= -0.345284C5D+04			
K.E.= 0.17264231D+04	V.T.= -0.19999967D+01			
S	1S	2S	P	2P
BASIS/ORB E	-562.36702	-124.78787	BASIS/ORB E	-122.06918
1S 34.61090	0.98466	-0.33264	2P 17.56960	0.20149
1S 61.40260	0.00878	-0.00019	2P 28.53950	0.02503
2S 15.62830	0.00005	1.25732	2P 15.56670	0.77953
2S 28.42160	0.00979	-0.27C32		
KRYPTON	1S(2)2S(2)2P(2), 6-3P			
T.E.= -0.18296549D+04	P.E.= -0.36553209D+04			
K.E.= 0.18296659D+04	V.T.= -0.19999940D+01			
S	1S	2S	P	2P
BASIS/ORB E	-596.37484	-132.81929	BASIS/ORB E	-130.01614
1S 35.61650	0.98519	-0.33776	2P 17.73640	0.23808
1S 62.97370	0.00842	0.00186	2P 29.34750	C.02569
2S 16.15590	-0.00017	1.27C08	2P 16.05580	0.74201
2S 28.76360	0.00975	-0.28045		

See page 183 for Explanation of Tables and Notes for Tables 32, 42, and 43

## ROOTHAAN-HARTREE-FOCK ATOMIC WAVEFUNCTIONS

 TABLE 8 (1). HARTREE-FOCK FUNCTIONS FOR C(<sup>1</sup>D) ISO-ELECTRONIC SERIES.

CARBON	1S(2)2S(2)2P(2), 6-1D			
T.E.=	-0.37631319D+02	P.E.=	-0.75262340D+02	
K.E.=	0.37631020D+02	V.T.=	-0.20000C79D+01	
S	1S	2S	P	2P
BASIS/ORB E	-11.35156	-0.71868	BASIS/ORB E	-0.38134
1S 5.50911	0.91804	-0.19243	2P 1.41180	C.50660
1S 9.50932	0.06733	-0.01640	2P 2.56717	0.25026
2S 2.12328	0.00401	0.52416	2P 0.93454	0.31446
2S 5.07048	0.02450	-0.08822	2P 6.55086	0.00994
2S 1.34553	-0.00109	0.57010		
NITROGEN	1S(2)2S(2)2P(2), 6-1D			
T.E.=	-0.538C7393D+02	P.E.=	-0.10761419D+03	
K.E.=	0.53806799D+02	V.T.=	-0.20CCC110D+01	
S	1S	2S	P	2P
BASIS/ORB E	-16.30796	-1.472C3	BASIS/ORB E	-1.03441
1S 6.47807	0.93351	-0.22739	2P 1.98432	C.48641
1S 11.13470	0.05889	-0.00571	2P 3.41861	0.20918
2S 2.72343	0.00384	0.43E64	2P 1.47137	0.35283
2S 5.52701	0.01546	-0.10444	2P 8.29219	0.00736
2S 1.84192	-0.00101	0.67C96		
OXYGEN	1S(2)2S(2)2P(2), 6-1D			
T.E.=	-0.72997266D+02	P.E.=	-0.14599407D+03	
K.E.=	0.72996802D+02	V.T.=	-0.20000C63D+01	
S	1S	2S	P	2P
BASIS/ORB E	-22.28360	-2.48919	BASIS/ORB E	-1.94577
1S 7.48079	0.93457	-0.23989	2P 2.55322	0.51001
1S 12.60770	0.05542	-0.01070	2P 4.31785	C.16803
2S 3.22067	0.00427	0.3E635	2P 1.95310	0.35995
2S 6.52252	0.01728	-0.11346	2P 9.99094	0.00556
2S 2.33291	-0.00136	0.72398		
FLUORINE	1S(2)2S(2)2P(2), 6-1D			
T.E.=	-0.95194781D+02	P.E.=	-0.19038946D+C3	
K.E.=	0.95194682D+02	V.T.=	-0.20000010D+01	
S	1S	2S	P	2P
BASIS/ORB E	-29.26895	-3.76C53	BASIS/ORB E	-3.11138
1S 8.45607	0.94118	-0.25509	2P 3.09724	0.45924
1S 14.17450	0.05165	-0.00536	2P 5.06904	C.15690
2S 3.75354	0.00545	0.31730	2P 2.48415	0.41471
2S 7.35986	0.01280	-0.12143	2P 11.59380	C.00483
2S 2.84406	-0.00212	0.79923		
NEON	1S(2)2S(2)2P(2), 6-1D			
T.E.=	-0.12039707D+03	P.E.=	-0.24079279D+03	
K.E.=	0.12039572D+03	V.T.=	-0.20000112D+01	
S	1S	2S	P	2P
BASIS/ORB E	-37.26053	-5.28499	BASIS/ORB E	-4.52993
1S 9.48279	0.94695	-0.2E290	2P 3.70151	0.39662
1S 15.98250	0.04381	-0.00514	2P 5.87189	C.13927
2S 4.42483	0.00538	0.22655	2P 3.01099	C.49033
2S 8.24901	0.01451	-0.13559	2P 13.43600	0.00402
2S 3.36010	-0.00202	0.89970		
SODIUM	1S(2)2S(2)2P(2), 6-1D			
T.E.=	-0.14860254D+03	P.E.=	-0.29720446D+03	
K.E.=	0.14860192D+03	V.T.=	-0.20000C0420+01	
S	1S	2S	P	2P
BASIS/ORB E	-46.25569	-7.0E1C8	BASIS/ORB E	-6.20001
1S 10.47700	0.95062	-0.27426	2P 4.22104	0.46396
1S 17.55320	0.04086	-0.00728	2P 6.91028	0.11201
2S 4.88604	0.00533	0.2C484	2P 3.46394	0.44761
2S 9.02549	0.01343	-0.14314	2P 15.09550	0.00287
2S 3.85341	-0.00228	0.92933		

See page 183 for Explanation of Tables and Notes for Tables 32, 42, and 43

TABLE 8 (2). HARTREE-FOCK FUNCTIONS FOR C(<sup>1</sup>D) ISO-ELECTRONIC SERIES.

MAGNESIUM      1S(2)2S(2)2P(2), 6-1D  
 T.E.= -0.17981027D+03   P.E.= -0.35962C72D+03  
 K.E.= 0.17981045D+03   V.T.= -0.19959990D+01

S	1S	2S	P	2P
BASIS/ORB E	-56.25356	-9.08843	BASIS/ORB E	-8.12131
1S 11.47320	0.95361	-0.28252	2P 4.76227	0.46289
1S 19.12780	0.03830	-0.00572	2P 7.74820	0.10103
2S 5.25898	0.00580	0.17509	2P 3.94840	0.45707
2S 9.85403	0.01270	-0.14730	2P 16.71610	0.00252
2S 4.36060	-0.00300	0.96342		

ALUMINUM      1S(2)2S(2)2P(2), 6-1D  
 T.E.= -0.21401963D+03   P.E.= -0.42804133D+03  
 K.E.= 0.21402169D+03   V.T.= -0.19959904D+01

S	1S	2S	P	2P
BASIS/ORB E	-67.25342	-11.36667	BASIS/ORB E	-10.29359
1S 12.74710	0.94932	-0.28013	2P 5.26926	0.49956
1S 22.12090	0.02206	-0.00480	2P 8.73902	0.08853
2S 4.93473	0.00039	1.13272	2P 4.40935	0.43132
2S 11.07160	0.03842	-0.15376	2P 19.26050	0.00169

SILICON      1S(2)2S(2)2P(2), 6-1D  
 T.E.= -0.25123025D+03   P.E.= -0.50246131D+03  
 K.E.= 0.25123106D+03   V.T.= -0.19959968D+01

S	1S	2S	P	2P
BASIS/ORB E	-79.25488	-13.89561	BASIS/ORB E	-12.71659
1S 13.65380	0.95608	-0.29221	2P 5.74957	0.54213
1S 23.36380	0.02406	-0.00379	2P 9.59258	0.08213
2S 5.42044	0.00049	1.14562	2P 4.85472	0.39348
2S 11.70830	0.02785	-0.16196	2P 20.97590	0.00145

PHOSPHORUS      1S(2)2S(2)2P(2), 6-1D  
 T.E.= -0.29144184D+03   P.E.= -0.58288486D+03  
 K.E.= 0.29144302D+03   V.T.= -0.19959959D+01

S	1S	2S	P	2P
BASIS/ORB E	-92.25745	-16.67512	BASIS/ORB E	-15.39021
1S 14.69390	0.95980	-0.29253	2P 6.80098	0.27098
1S 25.77800	0.01948	-0.00384	2P 10.45240	0.06866
2S 5.89877	0.00038	1.15263	2P 5.55124	0.67648
2S 12.58770	0.02861	-0.17202	2P 22.90720	0.00151

SULFUR      1S(2)2S(2)2P(2), 6-1D  
 T.E.= -0.33465416D+03   P.E.= -0.66530907D+03  
 K.E.= 0.33465491D+03   V.T.= -0.19999977D+01

S	1S	2S	P	2P
BASIS/ORB E	-106.26087	-19.70488	BASIS/ORB E	-18.31413
1S 15.64640	0.96320	-0.29898	2P 7.42177	0.28474
1S 27.10920	0.02018	-0.00316	2P 11.68940	0.05459
2S 6.38547	0.00038	1.16434	2P 6.02831	0.67582
2S 13.28380	0.02359	-0.18033	2P 24.79180	0.00115

CHLORINE      1S(2)2S(2)2P(2), 6-1D  
 T.E.= -0.38086709D+03   P.E.= -0.76173504D+03  
 K.E.= 0.38086795D+03   V.T.= -0.19959977D+01

S	1S	2S	P	2P
BASIS/ORB E	-121.26498	-22.98495	BASIS/ORB E	-21.48839
1S 16.62960	0.96596	-0.30407	2P 7.65089	0.32669
1S 28.75920	0.01942	-0.00240	2P 11.98810	0.06629
2S 6.87253	0.00032	1.17413	2P 6.49179	0.62091
2S 14.00520	0.02108	-0.18882	2P 26.56550	0.00122

See page 183 for Explanation of Tables and Notes for Tables 32, 42, and 43

## ROOTHAAN-HARTREE-FOCK ATOMIC WAVEFUNCTIONS

 TABLE 8 (3). HARTREE-FOCK FUNCTIONS FOR C(<sup>1</sup>D) ISO-ELECTRONIC SERIES.

ARGON            1S(2)2S(2)2P(2), 6-1D				
T.E.= -0.43008046D+03	P.E.= -0.86016158D+03	K.E.= 0.43008112D+03	V.T.= -0.19999985D+01	
S	1S	2S	P	2P
BASIS/ORB E	-137.26959	-26.51526	BASIS/ORB E	-24.91290
1S 17.63690	0.96871	-0.30804	2P 8.11110	0.44899
1S 30.81580	0.01739	-0.00166	2P 14.01840	0.04726
2S 7.35969	0.00021	1.18299	2P 6.85935	0.51785
2S 14.74990	0.02012	-0.19722		
POTASSIUM        1S(2)2S(2)2P(2), 6-1D				
T.E.= -0.48229429D+03	P.E.= -0.96458912D+03	K.E.= 0.48229483D+03	V.T.= -0.19999989D+01	
S	1S	2S	P	2P
BASIS/ORB E	-154.27475	-30.29575	BASIS/ORB E	-28.58764
1S 18.61990	0.97060	-0.31229	2P 8.96432	0.31335
1S 32.38580	0.01705	-0.00099	2P 15.02890	0.04181
2S 7.84897	0.00016	1.19151	2P 7.47931	0.65802
2S 15.46670	0.01815	-0.20492		
CALCIUM           1S(2)2S(2)2P(2), 6-1D				
T.E.= -0.53750846D+03	P.E.= -0.10750192D+04	K.E.= 0.53751073D+03	V.T.= -0.19999958D+01	
S	1S	2S	P	2P
BASIS/ORB E	-172.28024	-34.32632	BASIS/ORB E	-32.51250
1S 19.60950	0.97211	-0.31545	2P 9.24486	0.37921
1S 33.99290	0.01659	-0.00060	2P 15.77350	0.04327
2S 8.33686	0.00014	1.19950	2P 7.92328	0.58984
2S 16.22230	0.01679	-0.21188		
SCANDIUM          1S(2)2S(2)2P(2), 6-1D				
T.E.= -0.59572291D+03	P.E.= -0.11914481D+04	K.E.= 0.59572518D+03	V.T.= -0.19999962D+01	
S	1S	2S	P	2P
BASIS/ORB E	-191.28615	-38.60724	BASIS/ORB E	-36.68769
1S 20.62590	0.97321	-0.31579	2P 10.03730	0.29363
1S 35.93090	0.01524	-0.00111	2P 16.63910	0.03986
2S 8.81688	0.00009	1.20341	2P 8.48192	0.67822
2S 17.11870	0.01695	-0.21704		
TITANIUM           1S(2)2S(2)2P(2), 6-1D				
T.E.= -0.65693763D+03	P.E.= -0.13138786D+04	K.E.= 0.65694097D+03	V.T.= -0.19999949D+01	
S	1S	2S	P	2P
BASIS/ORB E	-211.29229	-43.13799	BASIS/ORB E	-41.11278
1S 21.60530	0.97483	-0.32031	2P 10.35230	0.37712
1S 37.48500	0.01507	-0.00003	2P 17.84110	0.03634
2S 9.31224	0.00006	1.21265	2P 8.89228	0.59758
2S 17.76850	0.01514	-0.22447		
VANADIUM          1S(2)2S(2)2P(2), 6-1D				
T.E.= -0.72115254D+03	P.E.= -0.14423089D+04	K.E.= 0.72115639D+03	V.T.= -0.19999947D+01	
S	1S	2S	P	2P
BASIS/ORB E	-232.29868	-47.91900	BASIS/ORB E	-45.78811
1S 22.60390	0.97600	-0.32239	2P 10.86460	0.37332
1S 39.24380	0.01439	0.00021	2P 18.61250	0.03584
2S 9.80046	0.00003	1.21862	2P 9.38691	0.60134
2S 18.54390	0.01445	-0.23021		

See page 183 for Explanation of Tables and Notes for Tables 32, 42, and 43

TABLE 8 (4). HARTREE-FOCK FUNCTIONS FOR C(<sup>1</sup>D) ISO-ELECTRONIC SERIES.

CHROMIUM	1S(2)2S(2)2P(2), 6-1D			
T.E.= -0.78836758D+03	P.E.= -0.15767354D+C4			
K.E.= 0.78836783D+03	V.T.= -0.19999997D+01			
S	1S	2S	P	2P
BASIS/ORB E	-254.30535	-52.95023	BASIS/ORB E	-50.71367
1S 23.59390	0.97682	-0.32066	2P 11.44020	0.35766
1S 40.99380	0.01414	-0.00130	2P 19.33280	0.03501
2S 10.27080	0.00024	1.21754	2P 9.87996	0.61741
2S 19.57900	0.01347	-0.23136		
MANGANESE	1S(2)2S(2)2P(2), 6-1D			
T.E.= -0.85858289D+03	P.E.= -0.17171691D+04			
K.E.= 0.85858624D+03	V.T.= -0.19999961D+01			
S	1S	2S	P	2P
BASIS/ORB E	-277.31210	-58.23134	BASIS/ORB E	-55.88911
1S 24.60320	0.97783	-0.32535	2P 11.98930	0.35106
1S 42.68500	0.01328	0.00635	2P 20.25910	0.03324
2S 10.77380	-0.00001	1.22820	2P 10.37480	0.62532
2S 20.14950	0.01340	-0.23981		
IRON	1S(2)2S(2)2P(2), 6-1D			
T.E.= -0.93179820D+03	P.E.= -0.16635963D+04			
K.E.= 0.93179811D+03	V.T.= -0.20000C01D+01			
S	1S	2S	P	2P
BASIS/ORB E	-301.31915	-63.76253	BASIS/ORB E	-61.31471
1S 25.59410	0.97883	-0.32413	2P 11.88170	0.68037
1S 44.62300	0.01286	-0.00682	2P 21.06590	0.03467
2S 11.24640	0.00018	1.22788	2P 10.39630	0.29414
2S 21.14720	0.01244	-0.24688		
COBALT	1S(2)2S(2)2P(2), 6-1D			
T.E.= -0.10080137D+04	P.E.= -0.20160298D+04			
K.E.= 0.10080161D+04	V.T.= -0.19559576D+01			
S	1S	2S	P	2P
BASIS/ORB E	-326.32612	-69.54384	BASIS/ORB E	-66.99039
1S 26.60070	0.97968	-0.32511	2P 13.37050	0.28091
1S 46.54870	0.01211	-0.00080	2P 22.50710	0.02718
2S 11.73200	0.00015	1.23162	2P 11.42380	0.70075
2S 21.97000	0.01224	-0.24483		
NICKEL	1S(2)2S(2)2P(2), 6-1D			
T.E.= -0.10872293D+04	P.E.= -0.21744613D+04			
K.E.= 0.10872319D+04	V.T.= -0.19999976D+01			
S	1S	2S	P	2P
BASIS/ORB E	-352.33335	-75.57510	BASIS/ORB E	-72.91605
1S 27.58480	0.98020	-0.32671	2P 13.24190	0.50233
1S 47.87030	0.01229	-0.00066	2P 23.26650	0.02857
2S 12.22020	0.00017	1.23554	2P 11.63810	0.47758
2S 22.75190	0.01132	-0.24870		
COPPER	1S(2)2S(2)2P(2), 6-1D			
T.E.= -0.11694451D+04	P.E.= -0.23388961D+04			
K.E.= 0.11694510D+04	V.T.= -0.19999550D+01			
S	1S	2S	P	2P
BASIS/ORB E	-379.34065	-81.85644	BASIS/ORB E	-79.09175
1S 28.59910	0.98095	-0.33096	2P 13.77740	0.49586
1S 49.63510	0.01147	0.00097	2P 24.18080	0.02740
2S 12.72790	-0.00007	1.24586	2P 12.12900	0.48491
2S 23.29080	0.01152	-0.25687		

See page 183 for Explanation of Tables and Notes for Tables 32, 42, and 43

## ROOTHAAN-HARTREE-FOCK ATOMIC WAVEFUNCTIONS

 TABLE 8 (5). HARTREE-FOCK FUNCTIONS FOR C(<sup>1</sup>D) ISO-ELECTRONIC SERIES.

ZINC	1S(2)2S(2)2P(2), 6-1D			
T.E.= -0.12546609D+04	P.E.= -0.25053262D+04			
K.E.= 0.12546653D+04	V.T.= -0.19999566D+01			
S	1S	2S	P	2P
BASIS/ORB E	-407.34810	-88.38785	BASIS/ORB E	-85.51755
1S 29.60580	0.98195	-0.33263	2P 14.1770	0.58951
1S 51.80260	0.01065	0.00138	2P 25.35240	0.02523
2S 13.22130	-0.00011	1.25105	2P 12.42010	0.39319
2S 24.02330	0.01127	-0.26169		
GALLIUM	1S(2)2S(2)2P(2), 6-1D			
T.E.= -0.13428768D+04	P.E.= -0.26E57E12D+04			
K.E.= 0.13428844D+04	V.T.= -0.19999944D+01			
S	1S	2S	P	2P
BASIS/ORB E	-436.35553	-95.16925	BASIS/ORB E	-92.19338
1S 30.59760	0.98220	-0.33319	2P 14.82550	0.49215
1S 53.11530	0.01074	0.00122	2P 26.05810	0.02526
2S 13.70570	-0.00008	1.25330	2P 13.10330	0.49018
2S 24.86590	0.01078	-0.26408		
GERMANIUM	1S(2)2S(2)2P(2), 6-1D			
T.E.= -0.14340928D+04	P.E.= -0.28E681898D+04			
K.E.= 0.14340970D+04	V.T.= -0.19999971D+01			
S	1S	2S	P	2P
BASIS/ORB E	-466.36314	-102.20074	BASIS/ORB E	-99.11927
1S 31.59090	0.98305	-0.33564	2P 15.87490	0.31184
1S 54.94390	0.01038	0.00203	2P 27.04950	0.02309
2S 14.20660	-0.00010	1.26017	2P 13.83500	0.67240
2S 25.50810	0.01015	-0.26982		
ARSENIC	1S(2)2S(2)2P(2), 6-1D			
T.E.= -0.15283088D+04	P.E.= -0.3056E229D+04			
K.E.= 0.15283141D+04	V.T.= -0.19999966D+01			
S	1S	2S	P	2P
BASIS/ORB E	-497.37077	-109.48222	BASIS/ORB E	-106.29517
1S 32.59130	0.98357	-0.33669	2P 16.45920	0.29724
1S 56.71630	0.01004	0.00210	2P 27.96950	0.02227
2S 14.69570	-0.00011	1.26334	2P 14.34500	0.68759
2S 26.29990	0.00987	-0.27295		
SELENIUM	1S(2)2S(2)2P(2), 6-1D			
T.E.= -0.16255249D+04	P.E.= -0.32510551D+04			
K.E.= 0.16255302D+04	V.T.= -0.19999967D+01			
S	1S	2S	P	2P
BASIS/ORB E	-529.37849	-117.01374	BASIS/ORB E	-113.72111
1S 33.59090	0.98407	-0.33759	2P 17.01840	0.29075
1S 58.47090	0.00974	0.00221	2P 28.92270	0.02141
2S 15.18550	-0.00012	1.26654	2P 14.84370	0.69472
2S 27.08310	0.00959	-0.27605		
BROMINE	1S(2)2S(2)2P(2), 6-1D			
T.E.= -0.17257410D+04	P.E.= -0.34514881D+04			
K.E.= 0.17257471D+04	V.T.= -0.19999965D+01			
S	1S	2S	P	2P
BASIS/ORB E	-562.38625	-124.79527	BASIS/ORB E	-121.39708
1S 34.59020	0.98451	-0.33841	2P 17.56580	0.28646
1S 60.18900	0.00948	0.00229	2P 29.85890	0.02068
2S 15.67500	-0.00012	1.26548	2P 15.34010	0.69951
2S 27.87130	0.00932	-0.27892		
KRYPTON	1S(2)2S(2)2P(2), 6-1D			
T.E.= -0.18289572D+04	P.E.= -0.36579206D+04			
K.E.= 0.18289634D+04	V.T.= -0.19999960D+01			
S	1S	2S	P	2P
BASIS/ORB E	-596.39407	-132.82682	BASIS/ORB E	-129.32307
1S 35.59030	0.98495	-0.33915	2P 18.12930	0.27974
1S 61.95880	0.00920	0.00236	2P 30.82010	0.01990
2S 16.16450	-0.00013	1.27227	2P 15.83980	0.70681
2S 28.66040	0.00907	-0.28166		

See page 183 for Explanation of Tables and Notes for Tables 32, 42, and 43

TABLE 9 (1). THE HARTREE-FOCK FUNCTIONS FOR C(<sup>1</sup>S) ISO-ELECTRONIC SERIES.

CARBON	1S(2)2S(2)2P(2),6-1S			
T.E.= -0.37549581D+02	P.E.= -0.75C95C22D+02			
K.E.= 0.37549441D+02	V.T.= -0.20000037D+01			
S	1S	2S	P	2P
BASIS/ORB E	-11.39154	-0.73964	BASIS/ORB E	-0.31003
1S 5.52143	0.91853	-0.19435	2P 1.11373	0.62500
1S 9.55291	0.06535	-0.01555	2P 0.64580	0.09122
2S 2.11900	0.00352	0.54294	2P 2.26705	0.36129
2S 5.04667	0.02643	-0.09050	2P 5.16396	0.02139
2S 1.34825	-0.00090	0.55274		
NITROGEN	1S(2)2S(2)2P(2),6-1S			
T.E.= -0.53690146D+02	P.E.= -0.1C738004D+03			
K.E.= 0.53689897D+02	V.T.= -0.20000046D+01			
S	1S	2S	P	2P
BASIS/ORB E	-16.34351	-1.48956	BASIS/ORB E	-0.92662
1S 6.57007	0.93040	-0.22309	2P 1.64533	C.71115
1S 11.42180	0.04955	-0.00960	2P 1.03155	0.04724
2S 2.69026	0.00195	0.45613	2P 3.17489	0.29769
2S 5.66730	0.03091	-0.1C655	2P 7.83155	C.00911
2S 1.83957	-0.00020	0.64572		
OXYGEN	1S(2)2S(2)2P(2),6-1S			
T.E.= -0.72846323D+02	P.E.= -0.14569260D+03			
K.E.= 0.72846278D+02	V.T.= -0.20000006D+01			
S	1S	2S	P	2P
BASIS/ORB E	-22.31724	-2.50396	BASIS/ORB E	-1.80391
1S 7.66428	0.93379	-0.23609	2P 2.17794	0.73082
1S 13.53750	0.03602	-0.00788	2P 1.53850	0.05604
2S 3.21251	0.00121	0.38672	2P 3.98546	0.25662
2S 6.62986	0.04222	-0.12006	2P 9.83809	0.00641
2S 2.33868	0.00007	0.72183		
FLUORINE	1S(2)2S(2)2P(2),6-1S			
T.E.= -0.95010867D+02	P.E.= -0.19002133D+03			
K.E.= 0.95010462D+02	V.T.= -0.20000043D+01			
S	1S	2S	P	2P
BASIS/ORB E	-29.30161	-3.77443	BASIS/ORB E	-2.93646
1S 8.55923	0.94243	-0.25131	2P 2.69304	0.74287
1S 14.76480	0.04063	-0.00867	2P 2.06263	0.06346
2S 3.76871	0.00418	0.30717	2P 4.76631	0.22927
2S 7.47162	0.02473	-0.12553	2P 11.62840	0.00500
2S 2.85159	-0.00151	0.8C791		
NEON	1S(2)2S(2)2P(2),6-1S			
T.E.= -0.12018056D+03	P.E.= -0.24036023D+03			
K.E.= 0.12017967D+03	V.T.= -0.20000074D+01			
S	1S	2S	P	2P
BASIS/ORB E	-37.29233	-5.29E23	BASIS/ORB E	-4.32221
1S 9.54627	0.94785	-0.26458	2P 3.19214	C.76863
1S 16.38290	0.03766	-0.00699	2P 2.54166	0.05416
2S 4.23081	0.00422	0.29859	2P 5.54893	0.20742
2S 8.23260	0.02146	-0.13503	2P 13.21360	0.00405
2S 3.33218	-0.00178	0.82622		
SODIUM	1S(2)2S(2)2P(2),6-1S			
T.E.= -0.14835369D+03	P.E.= -0.2967C656D+03			
K.E.= 0.14835287D+03	V.T.= -0.20000055D+01			
S	1S	2S	P	2P
BASIS/ORB E	-46.28704	-7.07400	BASIS/ORB E	-5.95992
1S 10.57280	0.95250	-0.27395	2P 3.68217	0.77937
1S 18.29440	0.03197	-0.00543	2P 3.06909	0.05112
2S 4.77243	0.00376	0.23669	2P 6.26798	0.19578
2S 9.05121	0.02246	-0.14467	2P 14.98900	0.00350
2S 3.84430	-0.00167	0.89625		

See page 183 for Explanation of Tables and Notes for Tables 32, 42, and 43

## ROOTHAAN-HARTREE-FOCK ATOMIC WAVEFUNCTIONS

 TABLE 9 (2). THE HARTREE-FOCK FUNCTIONS FOR C(<sup>1</sup>S) ISO-ELECTRONIC SERIES.

MAGNESIUM	1S(2)2S(2)2P(2),6-1S			
T.E.= -0.17952921D+03	P.E.= -0.35905752D+03			
K.E.= 0.17952831D+03	V.T.= -0.20000051D+01			
S	1S	2S	P	2P
BASIS/ORB E	-56.28461	-9.10112	BASIS/ORB E	-7.84908
1S 11.62050	0.95646	-0.28105	2P 4.18078	0.78852
1S 20.47820	0.02570	-0.00403	2P 3.61133	0.05292
2S 5.28366	0.00286	0.18573	2P 7.01969	0.18191
2S 9.88552	0.02521	-0.15403	2P 16.70770	0.00298
2S 4.35108	-0.00133	0.95066		
ALUMINUM	1S(2)2S(2)2P(2),6-1S			
T.E.= -0.21370649D+03	P.E.= -0.42741246D+03			
K.E.= 0.21370597D+03	V.T.= -0.20000024D+01			
S	1S	2S	P	2P
BASIS/ORB E	-67.28417	-11.37914	BASIS/ORB E	-9.98921
1S 12.58060	0.95980	-0.28995	2P 4.74637	0.77475
1S 21.84840	0.02625	-0.00304	2P 4.00993	0.08871
2S 5.74327	0.00338	0.16733	2P 7.86407	0.15767
2S 10.61470	0.02024	-0.16143	2P 18.07740	0.00267
2S 4.85079	-0.00180	0.98254		
SILICON	1S(2)2S(2)2P(2),6-1S			
T.E.= -0.25088509D+03	P.E.= -0.50176956D+03			
K.E.= 0.25098447D+03	V.T.= -0.20000025D+01			
S	1S	2S	P	2P
BASIS/ORB E	-79.28532	-13.90790	BASIS/ORB E	-12.38017
1S 13.59360	0.96211	-0.29484	2P 5.25571	0.77881
1S 23.65590	0.02383	-0.00258	2P 4.51269	0.09474
2S 6.19563	0.00321	0.12151	2P 8.65125	0.14573
2S 11.46180	0.02025	-0.168C4	2P 19.74830	0.00228
2S 5.36181	-0.00187	1.03420		
PHOSPHORUS	1S(2)2S(2)2P(2),6-1S			
T.E.= -0.29106470D+03	P.E.= -0.58212757D+03			
K.E.= 0.29106287D+03	V.T.= -0.20000026D+01			
S	1S	2S	P	2P
BASIS/ORB E	-92.28770	-16.68719	BASIS/ORB E	-15.02176
1S 14.59700	0.96560	-0.30120	2P 5.73534	0.77613
1S 25.58700	0.02137	-0.00134	2P 5.03988	0.09565
2S 6.66671	0.00229	0.17954	2P 9.26411	0.14557
2S 12.11290	0.01917	-0.18186	2P 21.55110	0.00226
2S 5.81450	-0.00139	0.99067		
SULFUR	1S(2)2S(2)2P(2),6-1S			
T.E.= -0.33424512D+03	P.E.= -0.66848938D+03			
K.E.= 0.33424426D+03	V.T.= -0.20000026D+01			
S	1S	2S	P	2P
BASIS/ORB E	-106.29083	-19.71678	BASIS/ORB E	-17.91366
1S 15.65580	0.96649	-0.30341	2P 6.42291	0.60225
1S 27.92250	0.01760	-0.00100	2P 5.76808	0.29742
2S 6.39786	0.00024	1.16923	2P 10.40010	0.11712
2S 13.07390	0.02289	-0.18284	2P 24.15650	0.00137
CHLDRINE	1S(2)2S(2)2P(2),6-1S			
T.E.= -0.38042619D+03	P.E.= -0.76085235D+03			
K.E.= 0.38042616D+03	V.T.= -0.20000001D+01			
S	1S	2S	P	2P
BASIS/ORB E	-121.29478	-22.99679	BASIS/ORB E	-21.05607
1S 16.65710	0.96819	-0.30606	2P 6.95296	0.58923
1S 29.67700	0.01662	-0.00113	2P 6.26909	0.31807
2S 6.88025	0.00018	1.17685	2P 11.22910	0.10836
2S 13.89900	0.02186	-0.19088	2P 25.85790	0.00118

See page 183 for Explanation of Tables and Notes for Tables 32, 42, and 43

TABLE 9 (3). THE HARTREE-FOCK FUNCTIONS FOR C(<sup>1</sup>S) ISO-ELECTRONIC SERIES.

ARGON	1S(2)2S(2)2P(2),6-1S			
T.E.= -0.42960775D+03	P.E.= -0.85921463D+03			
K.E.= 0.42960688D+03	V.T.= -0.20000020D+01			
S	1S	2S	P	2P
BASIS/ORB E	-137.29936	-26.52711	BASIS/ORB E	-24.44884
1S 17.66580	0.96940	-0.30493	2P 7.92185	0.39816
1S 31.68800	0.01545	-0.00266	2P 6.83092	0.53874
2S 7.35194	0.00036	1.17924	2P 12.56770	0.07806
2S 14.92470	0.02141	-0.19584	2P 27.77990	0.00086
POTASSIUM	1S(2)2S(2)2P(2),6-1S			
T.E.= -0.48178978D+03	P.E.= -0.96357989D+03			
K.E.= 0.48179011D+03	V.T.= -0.19999993D+01			
S	1S	2S	P	2P
BASIS/ORB E	-154.30437	-30.30743	BASIS/ORB E	-28.09165
1S 18.65470	0.97225	-0.31291	2P 8.23280	0.53371
1S 33.47960	0.01444	-0.00032	2P 7.20102	0.40526
2S 7.85446	0.00004	1.19362	2P 13.46290	0.07519
2S 15.41190	0.01938	-0.20678	2P 29.43700	0.00064
CALCIUM	1S(2)2S(2)2P(2),6-1S			
T.E.= -0.53697210D+03	P.E.= -0.1C739441D+04			
K.E.= 0.53697204D+03	V.T.= -0.20000001D+01			
S	1S	2S	P	2P
BASIS/ORB E	-172.30968	-34.33810	BASIS/ORB E	-31.98484
1S 19.66090	0.97362	-0.31487	2P 8.60674	0.59450
1S 35.41340	0.01343	-0.00031	2P 7.66919	0.34217
2S 8.33903	-0.00001	1.19955	2P 14.25950	0.07717
2S 16.22690	0.01882	-0.21329		
SCANDIUM	1S(2)2S(2)2P(2),6-1S			
T.E.= -0.59515479D+03	P.E.= -0.11903108D+04			
K.E.= 0.59515602D+03	V.T.= -0.19999979D+01			
S	1S	2S	P	2P
BASIS/ORB E	-191.31550	-38.61878	BASIS/ORB E	-36.12808
1S 20.66080	0.97499	-0.31722	2P 9.13478	0.58623
1S 37.28800	0.01269	-0.00011	2P 8.18432	0.35642
2S 8.82597	-0.00005	1.20642	2P 15.25010	0.07033
2S 17.00900	0.01796	-0.21968		
TITANIUM	1S(2)2S(2)2P(2),6-1S			
T.E.= -0.65633770D+03	P.E.= -0.13126801D+04			
K.E.= 0.65634245D+03	V.T.= -0.19999928D+01			
S	1S	2S	P	2P
BASIS/ORB E	-211.32151	-43.14968	BASIS/ORB E	-40.52160
1S 21.69700	0.97548	-0.31591	2P 9.85391	0.43395
1S 39.68150	0.01111	-0.00106	2P 8.81122	0.51370
2S 9.29912	-0.00010	1.2C739	2P 16.14900	0.06467
2S 18.01120	0.01911	-0.22300		
VANADIUM	1S(2)2S(2)2P(2),6-1S			
T.E.= -0.72052087D+03	P.E.= -0.14410462D+04			
K.E.= 0.72052536D+03	V.T.= -0.19999938D+01			
S	1S	2S	P	2P
BASIS/ORB E	-232.32791	-47.93060	BASIS/ORB E	-45.16510
1S 22.68140	0.97684	-0.319C5	2P 10.30410	0.61287
1S 41.28660	0.01098	-0.00054	2P 9.00010	0.34720
2S 9.79075	-0.00012	1.21471	2P 17.59100	0.05174
2S 18.72650	0.01755	-0.22923		

See page 183 for Explanation of Tables and Notes for Tables 32, 42, and 43

## ROOTHAAN-HARTREE-FOCK ATOMIC WAVEFUNCTIONS

 TABLE 9 (4). THE HARTREE-FOCK FUNCTIONS FOR C(<sup>1</sup>S) ISO-ELECTRONIC SERIES.

CHROMIUM	1S(2)2S(2)2P(2),6-1S			
T.E.= -0.78770425D+03	P.E.= -0.15754115D+04			
K.E.= 0.78770725D+03	V.T.= -0.19999962D+01			
S	1S	2S	P	2P
BASIS/ORB E	-254.33443	-52.96160	BASIS/OPB E	-50.05872
1S 23.66190	0.97848	-0.32235	2P 11.14710	0.40474
1S 43.02630	0.01076	0.00051	2P 9.76001	0.55810
2S 10.29040	-0.00015	1.22434	2P 18.45070	0.04838
2S 19.33660	0.01581	-0.23654		
MANGANESE	1S(2)2S(2)2P(2),6-1S			
T.E.= -0.85788774D+03	P.E.= -0.17157819D+04			
K.E.= 0.85789417D+03	V.T.= -0.19999925D+01			
S	1S	2S	P	2P
BASIS/ORB E	-277.34110	-58.24274	BASIS/ORB E	-55.20253
1S 24.68100	0.97887	-0.32263	2P 11.49400	0.45442
1S 45.09070	0.00997	-0.00020	2P 10.22000	0.50590
2S 10.76600	-0.00017	1.22519	2P 19.05240	0.05035
2S 20.29680	0.01617	-0.23927		
IRON	1S(2)2S(2)2P(2),6-1S			
T.E.= -0.93107135D+03	P.E.= -0.18621432D+04			
K.E.= 0.93107189D+03	V.T.= -0.19999994D+01			
S	1S	2S	P	2P
BASIS/ORB E	-301.34810	-63.77396	BASIS/ORB E	-60.59641
1S 25.65020	0.97991	-0.32315	2P 11.84520	0.61937
1S 46.59290	0.01032	-0.00075	2P 10.42980	0.34570
2S 11.24470	0.00007	1.22703	2P 20.18570	0.04520
2S 21.19810	0.01422	-0.24124		
COBALT	1S(2)2S(2)2P(2),6-1S			
T.E.= -0.10072552D+04	P.E.= -0.20145149D+04			
K.E.= 0.10072597D+04	V.T.= -0.19999956D+01			
S	1S	2S	P	2P
BASIS/ORB E	-326.35505	-69.55515	BASIS/ORB E	-66.24027
1S 26.65770	0.98084	-0.32773	2P 12.35520	0.51642
1S 48.40300	0.00967	0.00080	2P 11.15640	0.44259
2S 11.75380	-0.00019	1.23824	2P 20.42790	0.05075
2S 21.71150	0.01404	-0.25045		
NICKEL	1S(2)2S(2)2P(2),6-1S			
T.E.= -0.10864391D+04	P.E.= -0.21728839D+04			
K.E.= 0.10864448D+04	V.T.= -0.19999948D+01			
S	1S	2S	P	2P
BASIS/ORB E	-352.36220	-75.58642	BASIS/ORB E	-72.13424
1S 27.66270	0.98157	-0.32875	2P 12.95680	0.46740
1S 50.43190	0.00913	0.00083	2P 11.69950	0.49447
2S 12.24100	-0.00021	1.24206	2P 21.38130	0.04748
2S 22.51750	0.01374	-0.25435		
COPPER	1S(2)2S(2)2P(2),6-1S			
T.E.= -0.11686230D+04	P.E.= -0.23372475D+04			
K.E.= 0.11686244D+04	V.T.= -0.19999988D+01			
S	1S	2S	P	2P
BASIS/ORB E	-379.36944	-81.86788	BASIS/ORB E	-78.27842
1S 28.64700	0.98212	-0.32697	2P 13.44570	0.57025
1S 52.16700	0.00921	-0.00045	2P 11.94920	0.39633
2S 12.70610	0.00004	1.23903	2P 22.39590	0.04258
2S 23.59710	0.01268	-0.25288		

See page 183 for Explanation of Tables and Notes for Tables 32, 42, and 43

TABLE 9 (5). THE HARTREE-FOCK FUNCTIONS FOR C(<sup>1</sup>S) ISO-ELECTRONIC SERIES.

ZINC	1S(2)2S(2)2P(2),6-1S			
T.E.= -0.12538072D+04	P.E.= -0.25C76206D+04			
K.E.= 0.12538134D+04	V.T.= -0.19999951D+C1			
S	1S	2S	P	2P
BASIS/ORB E	-407.37686	-88.39910	BASIS/ORB E	-84.67235
1S 29.65250	0.98278	-0.33153	2P 13.93120	0.50686
1S 53.77360	0.00880	0.00117	2P 12.63190	0.45813
2S 13.22060	-0.00021	1.25053	2P 23.14340	0.04367
2S 24.06340	0.01255	-0.26222		
GALLIUM	1S(2)2S(2)2P(2),6-1S			
T.E.= -0.13419914D+04	P.E.= -0.26E39898D+04			
K.E.= 0.13419984D+04	V.T.= -0.19999948D+01			
S	1S	2S	P	2P
BASIS/ORB E	-436.38435	-95.18056	BASIS/ORB E	-91.31651
1S 30.66260	0.98326	-0.33161	2P 14.35340	0.67649
1S 55.86390	0.00828	0.00091	2P 12.69350	0.29538
2S 13.70290	-0.00023	1.25220	2P 24.62160	0.03660
2S 24.93540	0.01253	-0.26444		
GERMANIUM	1S(2)2S(2)2P(2),6-1S			
T.E.= -0.14331755D+04	P.E.= -0.26E35360D+04			
K.E.= 0.14331781D+04	V.T.= -0.19999982D+01			
S	1S	2S	P	2P
BASIS/ORB E	-466.39186	-102.21202	BASIS/ORB E	-98.21076
1S 31.64390	0.98385	-0.3309	2P 15.04220	0.56248
1S 57.66200	0.00836	-0.00020	2P 13.41350	0.41075
2S 14.16850	0.00001	1.24520	2P 25.48820	0.03494
2S 25.99830	0.01144	-0.26272		
ARSENIC	1S(2)2S(2)2P(2),6-1S			
T.E.= -0.15273598D+04	P.E.= -0.30547211D+04			
K.E.= 0.15273613D+04	V.T.= -0.19999991D+01			
S	1S	2S	P	2P
BASIS/ORB E	-497.39950	-109.49349	BASIS/ORB E	-105.35496
1S 32.64310	0.98447	-0.33122	2P 15.41250	0.66045
1S 59.64690	0.00804	-0.00003	2P 13.68350	0.31386
2S 14.65810	0.00000	1.25277	2P 26.43770	0.03360
2S 26.77630	0.01104	-0.26605		
SELENIUM	1S(2)2S(2)2P(2),6-1S			
T.E.= -0.16245444D+04	P.E.= -0.32490963D+04			
K.E.= 0.16245519D+04	V.T.= -0.19999953D+01			
S	1S	2S	P	2P
BASIS/ORB E	-529.40713	-117.02507	BASIS/ORB E	-112.74926
1S 33.66420	0.98472	-0.33409	2P 16.46410	0.41453
1S 61.44340	0.00749	0.00104	2P 14.57260	0.56229
2S 15.16680	-0.00024	1.26117	2P 27.27330	0.03091
2S 27.33920	0.01154	-0.27329		
BROMINE	1S(2)2S(2)2P(2),6-1S			
T.E.= -0.17247288D+04	P.E.= -0.34494648D+04			
K.E.= 0.17247360D+04	V.T.= -0.19999958D+01			
S	1S	2S	P	2P
BASIS/ORB E	-562.41493	-124.8C647	BASIS/ORB E	-120.39341
1S 34.66020	0.98539	-0.33589	2P 16.38360	0.69782
1S 63.44910	0.00722	0.00150	2P 14.53750	0.27815
2S 15.66540	-0.00026	1.26661	2P 28.21240	0.03145
2S 28.02240	0.01104	-0.27800		
KRYPTON	1S(2)2S(2)2P(2),6-1S			
T.E.= -0.18279133D+04	P.E.= -0.3655E368D+04			
K.E.= 0.18279235D+04	V.T.= -0.19999944D+01			
S	1S	2S	P	2P
BASIS/ORB E	-596.42265	-132.83801	BASIS/ORB E	-128.26772
1S 35.66310	0.98574	-0.33627	2P 17.27980	0.48445
1S 65.33430	0.00698	0.00142	2P 15.47460	0.49317
2S 16.15110	-0.00026	1.26848	2P 29.13120	0.02957
2S 28.85400	0.01085	-0.28004		

See page 183 for Explanation of Tables and Notes for Tables 32, 42, and 43

## ROOTHAAN-HARTREE-FOCK ATOMIC WAVEFUNCTIONS

 TABLE 10 (1). THE HARTREE-FOCK FUNCTIONS FOR N(<sup>4</sup>S) ISO-ELECTRONIC SERIES.

NITROGEN      1S(2)2S(2)2P(3), 7-4S  
 T.E.= -0.54400921D+02 P.E.= -0.10880134D+03  
 K.E.= 0.54400417D+02 V.T.= -0.20000C93D+01

S	1S	2S	P	2P
BASIS/ORB E	-15.62912	-0.94533	BASIS/ORB E	-0.56759
1S 6.57116	0.92704	-0.2C673	2P 1.72286	0.52180
1S 11.37630	0.05099	-0.00532	2P 3.04792	0.2E 19
2S 2.64739	0.00320	0.49102	2P 1.16023	0.27458
2S 5.70224	0.03275	-0.05630	2P 7.00507	0.01369
2S 1.61177	-0.00039	0.61E55		

CXYGEN      1S(2)2S(2)2P(3), 7-4S  
 T.E.= -0.74372598D+02 P.E.= -0.14E74491D+03  
 K.E.= 0.74372308D+02 V.T.= -0.20000C39D+01

S	1S	2S	P	2P
BASIS/ORB E	-21.34632	-1.80078	BASIS/ORB E	-1.32692
1S 7.63820	0.92666	-0.22180	2P 2.24453	0.55366
1S 13.11140	0.04270	-0.00900	2P 3.84166	0.23309
2S 3.20134	0.00319	0.41880	2P 1.64132	0.25880
2S 6.68310	0.04204	-0.10E43	2P 8.59404	0.01072
2S 2.10186	-0.00041	0.68872		

FLUDRINE      1S(2)2S(2)2P(3), 7-4S  
 T.E.= -0.97608965D+02 P.E.= -0.19521714D+03  
 K.E.= 0.97608175D+02 V.T.= -0.20000C81D+01

S	1S	2S	P	2P
BASIS/ORB E	-28.08160	-2.91706	BASIS/ORB E	-2.34384
1S 8.54671	0.93641	-0.24340	2P 2.80060	0.51916
1S 14.41670	0.04530	-0.00694	2P 4.63591	0.20684
2S 3.75891	0.00391	0.37E57	2P 2.18002	0.31061
2S 7.32399	0.02673	-0.11E37	2P 10.34980	0.00821
2S 2.58632	-0.00082	0.73819		

NEON      1S(2)2S(2)2P(3), 7-4S  
 T.E.= -0.12410421D+03 P.E.= -0.24820723D+03  
 K.E.= 0.12410302D+03 V.T.= -0.20000095D+01

S	1S	2S	P	2P
BASIS/ORB E	-35.82720	-4.28E87	BASIS/ORB E	-3.61517
1S 9.56062	0.94060	-0.25139	2P 3.33327	0.52345
1S 16.15870	0.04029	-0.00762	2P 5.44794	0.18264
2S 4.35368	0.00503	0.30E30	2P 2.67722	0.32451
2S 8.31540	0.02645	-0.12498	2P 11.93450	0.00664
2S 3.09626	-0.00138	0.81273		

SODIUM      1S(2)2S(2)2P(3), 7-4S  
 T.E.= -0.15385528D+03 P.E.= -0.30770897D+03  
 K.E.= 0.15385368D+03 V.T.= -0.20000104D+01

S	1S	2S	P	2P
BASIS/ORB E	-44.57944	-5.91395	BASIS/ORB E	-5.13926
1S 10.57130	0.94474	-0.26162	2P 3.90317	0.54980
1S 17.85520	0.03626	-0.00E50	2P 6.34538	0.15102
2S 4.92192	0.00492	0.26E74	2P 3.13071	0.32612
2S 9.15429	0.02594	-0.13319	2P 13.45390	0.00549
2S 3.59574	-0.00145	0.86422		

MAGNESIUM      1S(2)2S(2)2P(3), 7-4S  
 T.E.= -0.18686043D+03 P.E.= -0.37372085D+03  
 K.E.= 0.18686042D+03 V.T.= -0.20000000D+01

S	1S	2S	P	2P
BASIS/ORB E	-54.33609	-7.79110	BASIS/ORB E	-6.91521
1S 11.69120	0.94398	-0.26922	2P 4.44405	0.52465
1S 19.81840	0.02812	-0.00407	2P 7.10836	0.14014
2S 5.30819	0.00135	0.26E77	2P 3.64321	0.35883
2S 9.99860	0.03786	-0.14165	2P 14.97880	0.00489
2S 4.07241	0.00001	0.86712		

See page 183 for Explanation of Tables and Notes for Tables 32, 42, and 43

TABLE 10 (2). THE HARTREE-FOCK FUNCTIONS FOR N(<sup>4</sup>S) ISO-ELECTRONIC SERIES.

ALUMINUM	1S(2)2S(2)2P(3), 7-4S			
T.E.= -0.22311854D+03	P.E.= -0.44623446D+03			
K.E.= 0.22311592D+C3	V.T.= -0.20000117D+01			
S	1S	2S	P	
BASIS/ORB E	-65.09628	-9.91982	BASIS/ORB E	-8.94268
1S 12.59590	0.95147	-0.27697	2P 4.97203	0.45128
1S 21.31200	0.02972	-0.00484	2P 7.74863	0.14129
2S 5.97480	0.00459	0.19855	2P 4.20793	0.42832
2S 10.85110	0.02528	-0.14694	2P 16.58520	0.00449
2S 4.58601	-0.00163	0.93725		
SILICON	1S(2)2S(2)2P(3), 7-4S			
T.E.= -0.26262886D+03	P.E.= -0.52525721D+03			
K.E.= 0.26262835D+03	V.T.= -0.2000020D+01			
S	1S	2S	P	2P
BASIS/ORB E	-76.85859	-12.29548	BASIS/ORB E	-11.22097
1S 13.69090	0.95053	-0.28CE3	2P 5.7C890	0.44352
1S 23.27600	0.02448	-0.00391	2P 8.96174	0.10041
2S 6.34003	0.00281	0.16176	2P 4.67900	0.47571
2S 11.82660	0.03316	-0.15017	2P 18.3C000	0.00345
2S 5.09759	-0.00097	0.97338		
PHOSPHORUS	1S(2)2S(2)2P(3), 7-4S			
T.E.= -0.30539088D+03	P.E.= -0.61C78164D+03			
K.E.= 0.30539075D+03	V.T.= -0.20C00004D+01			
S	1S	2S	P	2P
BASIS/ORB E	-89.62280	-14.92588	BASIS/ORB E	-13.75003
1S 14.62850	0.95698	-0.29C06	2P 6.03781	0.52714
1S 24.95820	0.02415	-0.00255	2P 9.61915	0.10514
2S 6.71147	0.00470	0.14740	2P 5.10757	0.38546
2S 12.55310	0.02524	-0.15349	2P 19.49210	0.00320
2S 5.59766	-0.00238	0.99404		
SULFUR	1S(2)2S(2)2P(3), 7-4S			
T.E.= -0.35140425D+03	P.E.= -0.7028C737D+03			
K.E.= 0.35140312D+03	V.T.= -0.20000032D+01			
S	1S	2S	P	2P
BASIS/ORB E	-103.38869	-17.81102	BASIS/ORB E	-16.52991
1S 15.63090	0.95942	-0.29E33	2P 6.67108	0.48450
1S 26.59100	0.02266	-0.00138	2P 10.59010	0.08978
2S 7.05116	0.00360	0.19810	2P 5.62582	0.44221
2S 13.23750	0.02453	-0.16315	2P 20.93410	0.00279
2S 6.05344	-0.00197	0.95387		
CHLORINE	1S(2)2S(2)2P(3), 7-4S			
T.E.= -0.40066869D+03	P.E.= -0.80133596D+03			
K.E.= 0.40066727D+03	V.T.= -0.20000036D+01			
S	1S	2S	P	2P
BASIS/ORB E	-118.15567	-20.54260	BASIS/ORB E	-19.56023
1S 16.64030	0.96223	-0.30050	2P 7.26823	0.43702
1S 28.50440	0.02048	-0.00C67	2P 11.50830	0.08171
2S 7.58527	0.00312	0.17817	2P 6.16738	0.49675
2S 14.00910	0.02376	-0.17149	2P 22.62300	0.00231
2S 6.54609	-0.00174	0.98157		
ARGON	1S(2)2S(2)2P(3), 7-4S			
T.E.= -0.45318402D+03	P.E.= -0.90C36870D+03			
K.E.= 0.45318467D+03	V.T.= -0.19999986D+01			
S	1S	2S	P	2P
BASIS/ORB E	-133.92346	-24.32453	BASIS/ORB E	-22.84082
1S 17.74210	0.96059	-0.30146	2P 8.18555	0.27370
1S 30.71300	0.01663	-0.00C57	2P 12.19930	0.07579
2S 7.14871	0.00037	1.15706	2P 6.79195	0.66491
2S 15.03360	0.03041	-0.17185	2P 25.02780	0.00221

See page 183 for Explanation of Tables and Notes for Tables 32, 42, and 43

## ROOTHAAN-HARTREE-FOCK ATOMIC WAVEFUNCTIONS

 TABLE 10 (3). THE HARTREE-FOCK FUNCTIONS FOR N(<sup>4</sup>S) ISO-ELECTRONIC SERIES.

POTASSIUM      1S(2)2S(2)2P(3), 7-4S  
 T.E.= -0.50895007D+03   P.E.= -0.1C179006D+04  
 K.E.= 0.5C895049D+03   V.T.= -0.19999992D+01

S	1S	2S	P	2P
BASIS/ORB E	-150.69213	-27.95681	BASIS/ORB E	-26.37186
1S 18.71640	0.96355	-0.30469	2P 8.38894	0.34884
1S 32.34350	0.01645	-0.00065	2P 12.84800	0.08067
2S 7.63089	0.00042	1.16437	2P 7.23170	0.58400
2S 15.82610	0.02738	-0.17868	2P 26.54210	0.00198

CALCIUM      1S(2)2S(2)2P(3), 7-4S  
 T.E.= -0.56796672D+03   P.E.= -0.11359339D+04  
 K.E.= 0.56796715D+03   V.T.= -0.19999992D+01

S	1S	2S	P	2P
BASIS/ORB E	-168.46150	-21.83941	BASIS/ORB E	-30.15321
1S 19.71710	0.96554	-0.3C726	2P 8.95881	0.35636
1S 34.15950	0.01544	-0.00060	2P 13.70270	0.07343
2S 8.11393	0.00033	1.17129	2P 7.70163	0.58295
2S 16.62280	0.02611	-0.1E568	2P 28.15300	0.00188

SCANDIUM      1S(2)2S(2)2P(3), 7-4S  
 T.E.= -0.63023385D+03   P.E.= -0.12604680D+04  
 K.E.= 0.63023411D+03   V.T.= -0.19999996D+01

S	1S	2S	P	2P
BASIS/ORB E	-187.23136	-35.97213	BASIS/ORB E	-34.18472
1S 20.70110	0.96797	-0.31136	2P 9.53234	0.40664
1S 35.91960	0.01481	0.00009	2P 15.10860	0.05772
2S 8.60244	0.00026	1.17953	2P 8.12365	0.54803
2S 17.32240	0.02391	-0.19273	2P 29.79470	0.00144

TITANIUM      1S(2)2S(2)2P(3), 7-4S  
 T.E.= -0.69575139D+03   P.E.= -0.13915034D+04  
 K.E.= 0.69575206D+03   V.T.= -0.19999990D+01

S	1S	2S	P	2P
BASIS/ORB E	-207.00164	-40.355C8	BASIS/ORB E	-38.46650
1S 21.70520	0.96869	-0.30528	2P 10.05020	0.37477
1S 37.80210	0.01425	-0.00173	2P 15.86260	C.05811
2S 9.07202	0.00046	1.18067	2P 8.66771	0.57887
2S 18.38990	0.02335	-0.19643	2P 31.44250	0.00124

VANADIUM      1S(2)2S(2)2P(3), 7-4S  
 T.E.= -0.76451937D+03   P.E.= -0.15290407D+C4  
 K.E.= 0.76452132D+03   V.T.= -0.19999975D+01

S	1S	2S	P	2P
BASIS/ORB E	-227.77239	-44.98816	BASIS/ORB E	-42.99837
1S 22.70330	0.97063	-0.31480	2P 10.52720	0.40117
1S 39.44960	0.01343	-0.000C7	2P 16.49860	0.05703
2S 9.56918	0.00017	1.19C67	2P 9.11326	C.55285
2S 18.95720	0.02216	-0.20430	2P 32.97050	0.00135

CHROMIUM      1S(2)2S(2)2P(3), 7-4S  
 T.E.= -0.83653761D+03   P.E.= -0.16730797D+04  
 K.E.= 0.83654212D+03   V.T.= -0.19999946D+01

S	1S	2S	P	2P
BASIS/ORB E	-249.54335	-49.87128	BASIS/ORB E	-47.78033
1S 23.70630	0.97218	-0.31690	2P 11.12780	0.38156
1S 41.42670	0.01253	0.00015	2P 17.78510	0.04990
2S 10.05570	0.00010	1.19658	2P 9.63414	0.57931
2S 19.73210	0.02133	-0.21006	2P 34.72180	0.00096

See page 183 for Explanation of Tables and Notes for Tables 32, 42, and 43

TABLE 10 (4). THE HARTREE-FOCK FUNCTIONS FOR N(<sup>4</sup>S) ISO-ELECTRONIC SERIES.

MANGANESE	1S(2)2S(2)2P(3), 7-4S			
T.E.= -0.91180616D+03	P.E.= -0.18236143D+C4			
K.E.= 0.91180811D+03	V.T.= -0.19999979D+01			
S	1S	2S	P	2P
BASIS/ORB E	-272.31479	-55.0C465	BASIS/ORB E	-52.81252
1S 24.68300	0.57350	-0.32017	2P 12.02160	0.30520
1S 42.82830	0.01267	0.00074	2P 18.86430	0.C4182
2S 10.54660	0.00008	1.20349	2P 10.18440	0.66320
2S 20.43220	0.01952	-0.21576	2P 36.06200	0.00104
IRON	1S(2)2S(2)2P(3), 7-4S			
T.E.= -0.99032494D+03	P.E.= -0.19806513D+04			
K.E.= 0.99032635D+03	V.T.= -0.19999986D+01			
S	1S	2S	P	2P
BASIS/ORB E	-296.08640	-60.388C2	BASIS/ORB E	-58.09474
1S 25.66890	0.97499	-0.32342	2P 12.49570	0.31763
1S 44.55270	0.01232	0.00146	2P 19.70440	0.04060
2S 11.04020	0.00004	1.21C77	2P 10.65970	C.65157
2S 21.10650	0.01812	-0.22187	2P 37.58320	0.00097
COBALT	1S(2)2S(2)2P(3), 7-4S			
T.E.= -0.1C720939D+04	P.E.= -0.21441914D+04			
K.E.= 0.1C720974D+04	V.T.= -0.19999967D+01			
S	1S	2S	P	2P
BASIS/ORB E	-320.85821	-66.02155	BASIS/ORB E	-63.62713
1S 26.67880	0.97546	-0.32323	2P 13.06180	0.30856
1S 46.26250	0.01181	0.00C67	2P 20.58550	0.03870
2S 11.51900	0.00003	1.213C8	2P 11.16000	0.66214
2S 22.02070	0.01805	-0.22521	2P 39.19800	C.00091
NICKEL	1S(2)2S(2)2P(3), 7-4S			
T.E.= -0.11571131D+04	P.E.= -0.23142266D+04			
K.E.= 0.11571135D+04	V.T.= -0.19999997D+01			
S	1S	2S	P	2P
BASIS/ORB E	-346.63027	-71.9C505	BASIS/ORB E	-69.40949
1S 27.65400	0.97720	-0.32799	2P 13.61500	0.30289
1S 48.02040	0.01158	0.00230	2P 21.46710	0.C3702
2S 12.02310	-0.00002	1.22276	2P 11.65680	0.66913
2S 22.55210	0.01625	-0.23260	2P 40.74690	0.00086
COPPER	1S(2)2S(2)2P(3), 7-4S			
T.E.= -0.12453825D+04	P.E.= -0.249C7661D+04			
K.E.= 0.12453836D+04	V.T.= -0.19999991D+01			
S	1S	2S	P	2P
BASIS/ORB E	-373.40247	-78.03868	BASIS/ORB E	-75.44200
1S 28.65370	0.97799	-0.32919	2P 14.18170	0.29257
1S 49.77970	0.01116	0.00235	2P 22.30930	0.03570
2S 12.51060	-0.00004	1.227C2	2P 12.16040	0.68042
2S 23.34350	0.01573	-0.23686	2P 42.36400	0.00082
ZINC	1S(2)2S(2)2P(3), 7-4S			
T.E.= -0.13369020D+04	P.E.= -0.26738052D+C4			
K.E.= 0.13369033D+C4	V.T.= -0.19999990D+01			
S	1S	2S	P	2P
BASIS/ORB E	-401.17483	-84.42237	BASIS/ORB E	-81.72457
1S 29.64920	0.97871	-0.33064	2P 14.71890	0.28999
1S 51.43440	0.01091	0.00251	2P 23.16580	0.C3446
2S 12.59970	-0.00006	1.23150	2P 12.65430	0.68392
2S 24.11290	0.01510	-0.24110	2P 43.86590	0.00078

See page 183 for Explanation of Tables and Notes for Tables 32, 42, and 43

## ROOTHAAN-HARTREE-FOCK ATOMIC WAVEFUNCTIONS

 TABLE 10 (5). THE HARTREE-FOCK FUNCTIONS FOR N(<sup>4</sup>S) ISO-ELECTRONIC SERIES.

GALLIUM            1S{2}2S{2}2P{3}, 7-4S					
T.E.= -0.14316715D+04    P.E.= -0.28633445D+04					
K.E.= 0.14316730D+04    V.T.= -0.19999989D+01					
S	1S	2S	P	2P	
BASIS/ORB E	-429.94716	-91.05615	BASIS/ORB E	-88.25721	
1S 30.67050	0.97964	-0.33073	2P 14.89450	0.35738	
1S 53.91660	0.00979	0.00223	2P 24.59960	0.03508	
2S 13.48430	-0.00011	1.23439	2P 13.06660	0.61629	
2S 24.95900	0.01527	-0.24470			
GERMANIUM            1S{2}2S{2}2P{3}, 7-4S					
T.E.= -0.15296913D+04    P.E.= -0.30593842D+04					
K.E.= 0.15296929D+04    V.T.= -0.19999989D+01					
S	1S	2S	P	2P	
BASIS/ORB E	-459.71983	-97.93554	BASIS/ORB E	-95.03990	
1S 31.66920	0.98028	-0.33180	2P 15.74730	0.28131	
1S 55.66720	0.00951	0.00230	2P 25.71280	0.03182	
2S 13.97240	-0.00012	1.23811	2P 13.67060	0.69531	
2S 25.74750	0.01479	-0.24835			
ARSENIC            1S{2}2S{2}2P{3}, 7-4S					
T.E.= -0.16309611D+04    P.E.= -0.32619310D+04					
K.E.= 0.16309699D+04    V.T.= -0.19999946D+01					
S	1S	2S	P	2P	
BASIS/ORB E	-490.49245	-105.07355	BASIS/ORB E	-102.07248	
1S 32.66840	0.98089	-0.33280	2P 15.99870	0.30455	
1S 57.44790	0.00921	0.00236	2P 26.37610	0.03361	
2S 14.46090	-0.00013	1.24172	2P 14.17550	0.66988	
2S 26.53430	0.01435	-0.25188			
SELENIUM            1S{2}2S{2}2P{3}, 7-4S					
T.E.= -0.17354811D+04    P.E.= -0.34709627D+04					
K.E.= 0.17354816D+04    V.T.= -0.19999997D+01					
S	1S	2S	P	2P	
BASIS/ORB E	-522.26546	-112.45760	BASIS/ORB E	-109.35538	
1S 33.65290	0.98162	-0.33522	2P 16.63750	0.31929	
1S 58.97100	0.00921	0.00300	2P 27.43780	0.03026	
2S 14.95950	-0.00014	1.24781	2P 14.60120	0.65836	
2S 27.18870	0.01344	-0.25692			
BROMINE            1S{2}2S{2}2P{3}, 7-4S					
T.E.= -0.18432512D+04    P.E.= -0.36665043D+04					
K.E.= 0.18432531D+04    V.T.= -0.19999989D+01					
S	1S	2S	P	2P	
BASIS/ORB E	-555.03837	-120.09149	BASIS/ORB E	-116.88817	
1S 34.65090	0.98217	-0.33622	2P 17.19300	0.30859	
1S 60.71340	0.00897	0.00311	2P 28.27500	0.02952	
2S 15.44960	-0.00015	1.25137	2P 15.10810	0.66954	
2S 27.96210	0.01302	-0.26035			
KRYPTON            1S{2}2S{2}2P{3}, 7-4S					
T.E.= -0.19542713D+04    P.E.= -0.39085476D+04					
K.E.= 0.19542763D+04    V.T.= -0.19999974D+01					
S	1S	2S	P	2P	
BASIS/ORB E	-588.81140	-127.97525	BASIS/ORB E	-124.67093	
1S 35.65510	0.98276	-0.33696	2P 17.28890	0.40410	
1S 62.73000	0.00854	0.00314	2P 29.02590	0.03068	
2S 15.93910	-0.00017	1.25462	2P 15.50990	0.57255	
2S 28.74540	0.01277	-0.26362			

See page 183 for Explanation of Tables and Notes for Tables 32, 42, and 43

TABLE 11 (1). THE HARTREE-FOCK FUNCTIONS FOR N(<sup>2</sup>D) ISO-ELECTRONIC SERIES.

NITROGEN            1S(2)2S(2)2P(3), 7-2D T.E.=-0.54256154D+C2 P.E.=-0.1CE59161D+03 K.E.= 0.54295456D+02 V.T.=-0.20000128D+01				
S	1S	2S	P	2P
BASIS/ORB E	-15.66648	-0.96368	BASIS/ORB E	-0.50866
1S 6.56715	0.92691	-0.20522	2P 1.65093	0.53253
1S 11.37000	0.05151	-0.00970	2P 3.03124	0.28463
2S 2.62062	0.00342	0.51018	2P 1.08114	0.25470
2S 5.74297	0.03212	-0.09534	2P 7.13881	0.01265
2S 1.60798	-0.00052	0.5579C		
CXYGEN            1S(2)2S(2)2P(3), 7-2D T.E.=-0.74233332D+02 P.E.=-0.14E46603D+03 K.E.= 0.74232694D+02 V.T.=-0.20C0CC86D+01				
S	1S	2S	P	2P
BASIS/ORB E	-21.38091	-1.81440	BASIS/ORB E	-1.24424
1S 7.56431	0.92934	-0.22491	2P 2.21303	0.54485
1S 12.84830	0.04899	-0.00962	2P 3.87813	0.23918
2S 3.18422	0.00399	0.43470	2P 1.58700	0.26836
2S 6.62977	0.03116	-0.10609	2P 8.89754	0.00904
2S 2.09799	-0.00076	0.67400		
FLUORINE            1S(2)2S(2)2P(3), 7-2D T.E.=-0.97436352D+02 P.E.=-0.15487210D+03 K.E.= 0.97435744D+02 V.T.=-0.20000062D+01				
S	1S	2S	P	2P
BASIS/ORB E	-28.11474	-2.93139	BASIS/ORB E	-2.23861
1S 8.53157	0.93628	-0.24405	2P 2.73326	0.52801
1S 14.33200	0.04693	-0.00720	2P 4.64013	0.21968
2S 3.75625	0.00395	0.38357	2P 2.11282	0.29339
2S 7.31469	0.02492	-0.11663	2P 10.40930	0.00748
2S 2.58770	-0.00082	0.73358		
NEON            1S(2)2S(2)2P(3), 7-2D T.E.=-0.12389878D+C3 P.E.=-0.24775658D+03 K.E.= 0.12389781D+C3 V.T.=-0.20000079D+01				
S	1S	2S	P	2P
BASIS/ORB E	-35.85949	-4.30249	BASIS/ORB E	-3.48786
1S 9.52725	0.94035	-0.25321	2P 3.30077	0.53939
1S 15.95290	0.04348	-0.00766	2P 5.48317	0.18665
2S 4.32198	0.00520	0.31717	2P 2.58471	0.30852
2S 8.28469	0.02296	-0.12332	2P 11.93390	0.00618
2S 3.09493	-0.00148	0.80151		
SODIUM            1S(2)2S(2)2P(3), 7-2D T.E.=-0.15361735D+C3 P.E.=-0.30723353D+03 K.E.= 0.15361618D+03 V.T.=-0.20000076D+01				
S	1S	2S	P	2P
BASIS/ORB E	-44.61109	-5.92705	BASIS/ORB E	-4.99020
1S 10.54290	0.94427	-0.26182	2P 3.84334	0.47366
1S 17.64790	0.03889	-0.00713	2P 6.23998	0.17586
2S 4.92606	0.00515	0.26201	2P 3.15432	0.38004
2S 9.15369	0.02325	-0.13255	2P 13.49250	0.00514
2S 3.59795	-0.00152	0.86344		
MAGNESIUM            1S(2)2S(2)2P(3), 7-2D T.E.=-0.18659019D+03 P.E.=-0.37317841D+03 K.E.= 0.18658822D+03 V.T.=-0.20000106D+01				
S	1S	2S	P	2P
BASIS/ORB E	-54.36746	-7.80393	BASIS/ORB E	-6.74463
1S 11.56130	0.94769	-0.26925	2P 4.48604	0.43745
1S 19.37930	0.03481	-0.00648	2P 7.15868	0.14630
2S 5.47090	0.00508	0.22473	2P 3.66522	0.44267
2S 10.03450	0.02371	-0.14016	2P 15.10540	0.00413
2S 4.09410	-0.00164	0.90553		

See page 183 for Explanation of Tables and Notes for Tables 32, 42, and 43

## ROOTHAAN-HARTREE-FOCK ATOMIC WAVEFUNCTIONS

 TABLE 11 (2). THE HARTREE-FOCK FUNCTIONS FOR N(<sup>2</sup>D) ISO-ELECTRONIC SERIES.

**ALUMINUM**      1S(2)2S(2)2P(3), 7-2D  
 T.E.= -0.22281613D+03 P.E.= -0.44562918D+03  
 K.E.= 0.22281305D+03 V.T.= -0.2000C138D+01

S	1S	2S	P	2P
BASIS/ORB E	-65.12722	-9.93239	BASIS/ORB E	-8.75055
1S 12.56690	0.95106	-0.27666	2P 5.04444	0.38433
1S 21.06100	0.03196	-0.00559	2P 7.81805	0.14316
2S 6.01219	0.00496	0.19249	2P 4.19025	0.49583
2S 10.86870	0.02286	-0.14675	2P 16.64170	0.00400
2S 4.59135	-0.00173	0.94349		

**SILICON**      1S(2)2S(2)2P(3), 7-2D  
 T.E.= -0.26229437D+03 P.E.= -0.52458901D+03  
 K.E.= 0.26229464D+03 V.T.= -0.19999990D+01

S	1S	2S	P	2P
BASIS/ORB E	-76.88904	-12.31172	BASIS/ORB E	-11.00723
1S 13.54960	0.95286	-0.28552	2P 5.503C8	0.39434
1S 22.47920	0.03171	-0.00401	2P 8.53770	0.13932
2S 6.23116	0.00569	0.17772	2P 4.68421	0.48730
2S 11.72780	0.02094	-0.14503	2P 17.98950	0.00365
2S 5.09742	-0.00271	0.95755		

**PHOSPHORUS**      1S(2)2S(2)2P(3), 7-2D  
 T.E.= -0.30502439D+03 P.E.= -0.61004819D+03  
 K.E.= 0.30502380D+03 V.T.= -0.20000019D+01

S	1S	2S	P	2P
BASIS/ORB E	-89.65321	-14.94210	BASIS/ORB E	-13.51510
1S 14.59370	0.95667	-0.29239	2P 5.92106	0.50889
1S 24.52250	0.02650	-0.00204	2P 9.36745	0.12763
2S 6.64205	0.00421	0.19544	2P 5.07325	0.38279
2S 12.42060	0.02309	-0.15559	2P 19.46830	0.00319
2S 5.56782	-0.00212	0.94619		

**SULFUR**      1S(2)2S(2)2P(3), 7-2D  
 T.E.= -0.35100581D+03 P.E.= -0.70201061D+03  
 K.E.= 0.35100479D+03 V.T.= -0.2000C029D+01

S	1S	2S	P	2P
BASIS/ORB E	-103.41884	-17.82309	BASIS/ORB E	-16.27362
1S 15.59250	0.95874	-0.29700	2P 6.48987	0.50842
1S 26.11360	0.02523	-0.00166	2P 10.31830	0.11130
2S 7.05018	0.00413	0.20112	2P 5.55769	0.39830
2S 13.22830	0.02210	-0.16237	2P 20.93010	0.00262
2S 6.05323	-0.00228	0.95108		

**CHLORINE**      1S(2)2S(2)2P(3), 7-2D  
 T.E.= -0.40023834D+03 P.E.= -0.80047557D+03  
 K.E.= 0.40023723D+03 V.T.= -0.2000C028D+01

S	1S	2S	P	2P
EASIS/ORB E	-118.18562	-20.95455	BASIS/ORB E	-19.28260
1S 16.59150	0.96159	-0.30239	2P 7.10166	0.51136
1S 27.86340	0.02343	-0.00066	2P 11.38640	0.09274
2S 7.55550	0.00386	0.17023	2P 6.01784	0.41297
2S 13.96810	0.02082	-0.16952	2P 22.52490	0.00211
2S 6.55907	-0.00223	0.98972		

**ARGON**      1S(2)2S(2)2P(3), 7-2D  
 T.E.= -0.45272179D+03 P.E.= -0.90544220D+03  
 K.E.= 0.45272041D+03 V.T.= -0.2000C030D+01

S	1S	2S	P	2P
BASIS/ORB E	-133.95339	-24.33642	BASIS/ORB E	-22.54203
1S 17.58030	0.96364	-0.30673	2P 7.62820	0.48739
1S 29.43460	0.02266	-0.00012	2P 12.18170	0.08900
2S 8.01509	0.00385	0.17C17	2P 6.54430	0.43952
2S 14.71980	0.01922	-0.17685	2P 23.94840	0.00186
2S 7.04532	-0.00235	0.99763		

See page 183 for Explanation of Tables and Notes for Tables 32, 42, and 43

TABLE 11 (3). THE HARTREE-FOCK FUNCTIONS FOR N(<sup>2</sup>D) ISO-ELECTRONIC SERIES.

POTASSIUM	1S(2)2S(2)2P(3), 7-2D			
T.E.= -0.50845602D+03	P.E.= -0.10169149D+04			
K.E.= 0.50845889D+03	V.T.= -0.19999944D+01			
S	1S	2S	P	2P
BASIS/ORB E	-150.72178	-27.96866	BASIS/ORB E	-26.05182
1S 18.74110	0.96113	-0.30038	2P 8.25648	0.25827
1S 32.06580	0.016d9	-0.00241	2P 12.46610	0.10357
2S 7.62257	0.00049	1.160E1	2P 7.26617	0.45287
2S 16.04680	0.02959	-0.17798	2P 26.82410	0.00160
CALCIUM	1S(2)2S(2)2P(3), 7-2D			
T.E.= -0.56744083D+03	P.E.= -0.11348823D+04			
K.E.= 0.56744142D+03	V.T.= -0.19999990D+01			
S	1S	2S	P	2P
BASIS/ORB E	-168.49107	-31.85112	BASIS/ORB E	-25.81186
1S 19.68880	0.96487	-0.30762	2P 8.74680	0.44388
1S 33.52590	0.01712	-0.00078	2P 13.76960	0.07983
2S 8.11504	0.00040	1.17127	2P 7.55499	0.49048
2S 16.62230	0.02488	-0.18508	2P 28.15730	0.00147
SCANDIUM	1S(2)2S(2)2P(3), 7-2D			
T.E.= -0.62967618D+03	P.E.= -0.12593527D+04			
K.E.= 0.62967657D+03	V.T.= -0.19999994D+01			
S	1S	2S	P	2P
BASIS/ORB E	-187.26084	-35.98380	BASIS/ORB E	-33.82216
1S 20.67680	0.96731	-0.31159	2P 9.78666	0.28538
1S 35.31090	0.01625	-0.000C7	2P 14.92370	0.06459
2S 8.60300	0.00032	1.17935	2P 8.19292	0.66353
2S 17.33020	0.02294	-0.19212	2P 29.83040	0.00127
TITANIUM	1S(2)2S(2)2P(3), 7-2D			
T.E.= -0.69516197D+03	P.E.= -0.13903253D+04			
K.E.= 0.69516337D+03	V.T.= -0.19999980D+01			
S	1S	2S	P	2P
BASIS/ORB E	-207.03106	-40.36668	BASIS/ORB E	-38.08270
1S 21.66840	0.96848	-0.31356	2P 10.19280	0.31203
1S 36.81060	0.01601	-0.00017	2P 15.67040	0.06392
2S 9.08631	0.00029	1.18517	2P 8.65746	0.63682
2S 18.14130	0.02172	-0.19797	2P 31.23910	0.00120
VANADIUM	1S(2)2S(2)2P(3), 7-2D			
T.E.= -0.76389814D+03	P.E.= -0.15277977D+04			
K.E.= 0.76389957D+03	V.T.= -0.19999981D+01			
S	1S	2S	P	2P
BASIS/ORB E	-227.80169	-44.95571	BASIS/ORB E	-42.59340
1S 22.65890	0.97008	-0.31637	2P 10.72850	0.29200
1S 38.47040	0.01548	0.00022	2P 16.32460	0.06414
2S 9.57351	0.00024	1.19181	2P 9.17182	0.65592
2S 18.88940	0.02035	-0.20403	2P 32.80750	0.00119
CHROMIUM	1S(2)2S(2)2P(3), 7-2D			
T.E.= -0.83588462D+03	P.E.= -0.161717720D+04			
K.E.= 0.83588738D+03	V.T.= -0.19999967D+01			
S	1S	2S	P	2P
BASIS/ORB E	-249.57264	-49.88286	BASIS/ORB E	-47.35423
1S 23.67140	0.97163	-0.31756	2P 11.44440	0.31197
1S 40.54220	0.01414	0.00012	2P 18.05400	0.04771
2S 10.05720	0.00019	1.15677	2P 9.62618	0.65221
2S 19.71640	0.02001	-0.20550	2P 34.67820	0.00075

See page 183 for Explanation of Tables and Notes for Tables 32, 42, and 43

## ROOTHAAN-HARTREE-FOCK ATOMIC WAVEFUNCTIONS

 TABLE 11 (4). THE HARTREE-FOCK FUNCTIONS FOR N(<sup>2</sup>D) ISO-ELECTRONIC SERIES.

MANGANESE      1S(2)2S(2)2P(3), 7-2D  
 T.E.= -0.91112134D+03   P.E.= -0.18222432D+04  
 K.E.= 0.91112186D+03   V.T.= -0.19999994D+01

S	1S	2S	P	2P
BASIS/ORB E	-272.34377	-55.01614	BASIS/ORB E	-52.36518
1S 24.65970	0.97356	-0.32168	2P 11.77940	0.30173
1S 42.40070	0.01345	0.00123	2P 18.80230	0.05334
2S 10.55270	0.00011	1.20516	2P 10.16400	0.65685
2S 20.34540	0.01853	-0.21632		

IRON      1S(2)2S(2)2P(3), 7-2D  
 T.E.= -0.98960841D+03   P.E.= -0.19792176D+04  
 K.E.= 0.98960918D+03   V.T.= -0.19999992D+01

S	1S	2S	P	2P
BASIS/ORB E	-296.11536	-60.39549	BASIS/ORB E	-57.62626
1S 25.64890	0.97468	-0.32410	2P 12.21030	0.37358
1S 43.99950	0.01319	0.00162	2P 19.99930	0.04685
2S 11.04240	0.00008	1.21121	2P 10.55320	0.59101
2S 21.08130	0.01742	-0.22174		

COBALT      1S(2)2S(2)2P(3), 7-2D  
 T.E.= -0.10713457D+04   P.E.= -0.21426932D+04  
 K.E.= 0.10713475D+04   V.T.= -0.19999983D+01

S	1S	2S	P	2P
BASIS/ORB E	-320.88713	-66.03286	BASIS/ORB E	-63.13738
1S 26.64660	0.97592	-0.32624	2P 12.40020	0.48769
1S 45.86110	0.01255	0.00199	2P 20.66850	0.04869
2S 11.53300	0.00004	1.21713	2P 10.92360	0.47452
2S 21.81510	0.01664	-0.22719		

NICKEL      1S(2)2S(2)2P(3), 7-2D  
 T.E.= -0.11563331D+04   P.E.= -0.23126703D+04  
 K.E.= 0.11563372D+04   V.T.= -0.19999965D+01

S	1S	2S	P	2P
BASIS/ORB E	-346.65905	-71.91637	BASIS/ORB E	-68.89864
1S 27.65650	0.97680	-0.32687	2P 13.19850	0.35251
1S 47.81620	0.01177	0.00161	2P 21.52800	0.04636
2S 12.01720	0.00000	1.22074	2P 11.59000	0.61154
2S 22.65130	0.01646	-0.23129		

COPPER      1S(2)2S(2)2P(3), 7-2D  
 T.E.= -0.12445707D+04   P.E.= -0.24891437D+04  
 K.E.= 0.12445729D+04   V.T.= -0.19999982D+01

S	1S	2S	P	2P
BASIS/ORB E	-373.43120	-78.05011	BASIS/ORB E	-74.91009
1S 28.65670	0.97759	-0.328C1	2P 13.84320	0.29507
1S 49.57390	0.01134	0.00183	2P 21.99410	0.04791
2S 12.50410	-0.00002	1.22488	2P 12.14250	0.66708
2S 23.44980	0.01595	-0.23546		

ZINC      1S(2)2S(2)2P(3), 7-2D  
 T.E.= -0.13360585D+04   P.E.= -0.26721195D+04  
 K.E.= 0.13360609D+04   V.T.= -0.19999982D+01

S	1S	2S	P	2P
BASIS/ORB E	-401.20354	-84.43378	BASIS/ORB E	-81.17154
1S 29.66110	0.97834	-0.32EE2	2P 14.45110	0.28038
1S 51.43620	0.01081	0.00176	2P 22.91170	0.04521
2S 12.98970	-0.00004	1.22E41	2P 12.64730	0.68409
2S 24.26770	0.01561	-0.23920		

See page 183 for Explanation of Tables and Notes for Tables 32, 42, and 43

TABLE 11 (5). THE HARTREE-FOCK FUNCTIONS FOR N(<sup>2</sup>D) ISO-ELECTRONIC SERIES.

<b>CALCIUM</b> 1S(2)2S(2)2P(3), 7-2D				
T.E.= -0.143079650+04    P.E.= -0.286159490+04				
K.E.= 0.143079840+04    V.T.= -0.195999870+01				
S	1S	2S	P	2P
BASIS/ORB E	-429.97608	-91.06746	BASIS/ORB E	-87.68298
1S 30.63730	0.97905	-0.33164	2P 14.70190	0.41908
1S 52.66200	0.01111	0.00247	2P 24.27060	0.03939
2S 13.48580	-0.00004	1.23468	2P 12.93170	0.55092
2S 24.93370	0.01436	-0.24423		
<b>GERMANIUM</b> 1S(2)2S(2)2P(3), 7-2D				
T.E.= -0.152878450+04    P.E.= -0.305757040+04				
K.E.= 0.152878580+04    V.T.= -0.195999920+01				
S	1S	2S	P	2P
BASIS/ORB E	-459.74875	-97.95116	BASIS/ORB E	-94.44447
1S 31.62760	0.97993	-0.33397	2P 15.12620	0.51611
1S 54.36290	0.01086	0.00306	2P 25.84720	0.03329
2S 13.98210	-0.00006	1.24066	2P 13.21780	0.45972
2S 25.61130	0.01357	-0.24535		
<b>ARSENIC</b> 1S(2)2S(2)2P(3), 7-2D				
T.E.= -0.163002270+04    P.E.= -0.326005230+04				
K.E.= 0.163002960+04    V.T.= -0.195995570+01				
S	1S	2S	P	2P
BASIS/ORB E	-490.52129	-105.08480	BASIS/ORB E	-101.45593
1S 32.61730	0.98049	-0.33566	2P 15.87590	0.32986
1S 55.84340	0.01081	0.00341	2P 25.90990	0.03830
2S 14.47460	-0.00006	1.24532	2P 14.07500	0.64048
2S 26.34350	0.01289	-0.25348		
<b>SELENIUM</b> 1S(2)2S(2)2P(3), 7-2D				
T.E.= -0.173451100+04    P.E.= -0.346902340+04				
K.E.= 0.173451240+04    V.T.= -0.195999920+01				
S	1S	2S	P	2P
BASIS/ORB E	-522.29422	-112.46684	BASIS/ORB E	-108.71773
1S 33.62930	0.98124	-0.33599	2P 16.56450	0.32981
1S 58.00640	0.01006	0.00326	2P 26.98240	0.03433
2S 14.96140	-0.00010	1.24819	2P 14.51870	0.64433
2S 27.16180	0.01284	-0.25672		
<b>BROMINE</b> 1S(2)2S(2)2P(3), 7-2D				
T.E.= -0.184224930+04    P.E.= -0.368450020+04				
K.E.= 0.184225080+04    V.T.= -0.195999920+01				
S	1S	2S	P	2P
BASIS/ORB E	-555.06709	-120.10271	BASIS/ORB E	-116.22940
1S 34.61680	0.98163	-0.33744	2P 16.45570	0.47545
1S 59.32260	0.01017	0.00354	2P 26.86690	0.04156
2S 15.45270	-0.00009	1.25211	2P 14.87090	0.49114
2S 27.91160	0.01219	-0.26619		
<b>KRYPTON</b> 1S(2)2S(2)2P(3), 7-2D				
T.E.= -0.195323780+04    P.E.= -0.390647730+04				
K.E.= 0.195323950+04    V.T.= -0.195999910+01				
S	1S	2S	P	2P
BASIS/ORB E	-588.84014	-127.58664	BASIS/ORB E	-123.99114
1S 35.61820	0.98214	-0.33812	2P 17.69810	0.30075
1S 61.08920	0.00984	0.00354	2P 28.59400	0.03291
2S 15.94100	-0.00010	1.25544	2P 15.54510	0.67428
2S 28.70820	0.01192	-0.26318		

See page 183 for Explanation of Tables and Notes for Tables 32, 42, and 43

## ROOTHAAN-HARTREE-FOCK ATOMIC WAVEFUNCTIONS

 TABLE 12 (1). THE HARTREE-FOCK FUNCTIONS FOR N(<sup>2</sup>P) ISO-ELECTRONIC SERIES.

NITROGEN      1S(2)2S(2)2P(3), 7-2P  
 T.E.= -0.54228086D+02   P.E.= -0.1CE45579D+03  
 K.E.= 0.54227707D+02   V.T.= -0.20000G70D+01

S	1S	2S	P	2P
BASIS/ORB E	-15.69167	-0.97635	BASIS/ORB E	-0.47130
1S 6.66734	0.92118	-0.20515	2P 1.63729	0.52016
1S 11.71180	0.04283	-0.00539	2P 3.03952	C.28788
2S 2.59969	0.00262	0.52C47	2P 1.04949	0.27045
2S 5.87155	0.04924	-0.05E57	2P 7.26567	0.01177
2S 1.60687	-0.00022	0.58467		

OXYGEN      1S(2)2S(2)2P(3), 7-2P  
 T.E.= -0.74142083D+02   P.E.= -0.14828309D+03  
 K.E.= 0.74141010D+02   V.T.= -0.20000145D+01

S	1S	2S	P	2P
BASIS/ORB E	-21.40410	-1.82701	BASIS/ORB E	-1.19078
1S 7.51615	0.93510	-0.22888	2P 2.13284	C.56293
1S 12.85750	0.05044	-0.05000	2P 3.81463	0.25983
2S 3.20966	0.00480	0.43284	2P 1.51906	0.23266
2S 6.52747	0.02228	-0.1CE49	2P 8.71122	0.00965
2S 2.10451	-0.00109	0.67951		

FLUORINE      1S(2)2S(2)2P(3), 7-2P  
 T.E.= -0.97322788D+C2   P.E.= -0.19464469D+03  
 K.E.= 0.97321902D+02   V.T.= -0.20000910D+01

S	1S	2S	P	2P
BASIS/ORB E	-28.13697	-2.94110	BASIS/ORB E	-2.17002
1S 8.53541	0.93726	-0.24492	2P 2.67247	0.54971
1S 14.40150	0.04589	-0.0C681	2P 4.62077	0.23094
2S 3.71183	0.00400	0.4C486	2P 2.04733	0.26340
2S 7.31767	0.02499	-0.11554	2P 10.45370	0.00719
2S 2.57703	-0.00091	0.71184		

NEON      1S(2)2S(2)2P(3), 7-2P  
 T.E.= -0.12376329D+03   P.E.= -0.24752623D+03  
 K.E.= 0.1237E294D+03   V.T.= -0.20CCC028D+01

S	1S	2S	P	2P
BASIS/ORB E	-35.88095	-4.31157	BASIS/ORB E	-3.40439
1S 9.50868	0.94133	-0.25777	2P 3.18153	0.56439
1S 15.88760	0.04456	-0.0C557	2P 5.39676	0.21031
2S 4.24066	0.00497	0.35173	2P 2.53334	0.26191
2S 8.17158	0.02078	-0.12120	2P 11.97280	0.00597
2S 3.07875	-0.00150	0.76E26		

SODIUM      1S(2)2S(2)2P(3), 7-2P  
 T.E.= -0.15346016D+03   P.E.= -0.30651997D+03  
 K.E.= 0.15345981D+03   V.T.= -0.2000022D+01

S	1S	2S	P	2P
BASIS/ORB E	-44.63212	-5.93581	BASIS/ORB E	-4.89212
1S 10.52050	0.94518	-0.26800	2P 3.71569	0.56363
1S 17.54830	0.04021	-0.004E8	2P 6.18838	C.18948
2S 4.74310	0.00488	0.31964	2P 3.02448	0.27843
2S 9.00221	0.02107	-0.12901	2P 13.4907C	0.00505
2S 3.57052	-0.00166	0.80585		

MAGNESIUM      1S(2)2S(2)2P(3), 7-2P  
 T.E.= -0.18641145D+03   P.E.= -0.372E2C46D+03  
 K.E.= 0.18640902D+03   V.T.= -0.20000130D+01

S	1S	2S	P	2P
BASIS/ORB E	-54.38837	-7.81255	BASIS/ORB E	-6.63229
1S 11.55670	0.94921	-0.27C57	2P 4.177C7	0.55036
1S 19.45320	0.03419	-0.00577	2P 6.86128	0.18837
2S 5.50359	0.00488	0.22864	2P 3.56015	0.28885
2S 9.95321	0.02272	-0.14233	2P 15.22530	C.0437
2S 4.09344	-0.00152	0.90486		

See page 183 for Explanation of Tables and Notes for Tables 32, 42, and 43

TABLE 12 (2). THE HARTREE-FOCK FUNCTIONS FOR N(<sup>2</sup>P) ISO-ELECTRONIC SERIES.

ALUMINUM		1S(2)2S(2)2P(3), 7-2P			
T.E.=	-0.22261592D+03	P.E.=	-0.44523178D+03	K.E.=	0.22261586D+03 V.T.=
S	1S	2S	P	2P	
BASIS/ORB E	-65.14758	-9.94068	BASIS/ORB E	-8.62366	
1S 12.67530	0.94807	-0.27498	2P 4.64282	0.54284	
1S 21.53900	0.02675	-0.00459	2P 7.55344	0.18393	
2S 5.85963	0.00295	0.19797	2P 4.09406	0.29781	
2S 10.96930	0.03350	-0.14520	2P 16.90040	0.00383	
2S 4.59660	-0.00090	0.93307			
SILICON		1S(2)2S(2)2P(3), 7-2P			
T.E.=	-0.26207275D+03	P.E.=	-0.52414541D+03	K.E.=	0.26207266D+03 V.T.=
S	1S	2S	P	2P	
BASIS/ORB E	-76.90950	-12.32000	BASIS/ORB E	-10.86625	
1S 13.57700	0.95412	-0.28729	2P 5.33236	0.45888	
1S 22.74860	0.02924	-0.00214	2P 8.49827	0.15250	
2S 6.18198	0.00446	0.22799	2P 4.61584	0.41104	
2S 11.59280	0.02290	-0.14530	2P 18.08600	0.00325	
2S 5.06601	-0.00206	0.91217			
PHOSPHORUS		1S(2)2S(2)2P(3), 7-2P			
T.E.=	-0.30478143D+03	P.E.=	-0.60956218D+03	K.E.=	0.30478075D+03 V.T.=
S	1S	2S	P	2P	
BASIS/ORB E	-89.67347	-14.95255	BASIS/ORB E	-13.35983	
1S 14.58120	0.95722	-0.29283	2P 5.86724	0.40763	
1S 24.46720	0.02691	-0.00158	2P 9.17189	0.14868	
2S 6.62741	0.00407	0.22257	2P 5.14657	0.46403	
2S 12.34310	0.02204	-0.15657	2P 19.63940	0.00310	
2S 5.55473	-0.00204	0.92553			
SULFUR		1S(2)2S(2)2P(3), 7-2P			
T.E.=	-0.35074154D+03	P.E.=	-0.70148196D+03	K.E.=	0.35074041D+03 V.T.=
S	1S	2S	P	2P	
BASIS/ORB E	-103.43895	-17.83116	BASIS/ORB E	-16.10410	
1S 15.61940	0.96040	-0.29781	2P 6.25368	0.50752	
1S 26.60950	0.02269	-0.00051	2P 9.89927	0.14408	
2S 7.10438	0.00332	0.20611	2P 5.58326	0.36713	
2S 13.15180	0.02337	-0.16523	2P 21.13790	0.00277	
2S 6.04860	-0.00174	0.94898			
CHLORINE		1S(2)2S(2)2P(3), 7-2P			
T.E.=	-0.39995280D+03	P.E.=	-0.79990427D+03	K.E.=	0.39995147D+03 V.T.=
S	1S	2S	P	2P	
BASIS/ORB E	-118.20563	-20.96257	BASIS/ORB E	-18.09850	
1S 16.61900	0.96257	-0.30219	2P 6.76143	0.50831	
1S 28.30280	0.02139	-0.00042	2P 10.65650	0.13628	
2S 7.58607	0.00315	0.18257	2P 6.07903	0.37279	
2S 13.94000	0.02227	-0.17184	2P 22.63440	0.00251	
2S 6.54933	-0.00175	0.97917			
ARGON		1S(2)2S(2)2P(3), 7-2P			
T.E.=	-0.45241501D+03	P.E.=	-0.90462922D+03	K.E.=	0.45241421D+03 V.T.=
S	1S	2S	P	2P	
BASIS/ORB E	-133.97322	-24.34437	BASIS/ORB E	-22.34408	
1S 17.73300	0.96086	-0.30038	2P 7.38671	0.29862	
1S 30.66450	0.01708	-0.00122	2P 11.26780	0.13794	
2S 7.14814	0.00052	1.15555	2P 6.72736	0.57975	
2S 15.10700	0.02986	-0.17130	2P 25.19440	0.00221	

See page 183 for Explanation of Tables and Notes for Tables 32, 42, and 43

## ROOTHAAN-HARTREE-FOCK ATOMIC WAVEFUNCTIONS

 TABLE 12 (3). THE HARTREE-FOCK FUNCTIONS FOR N(<sup>2</sup>P) ISO-ELECTRONIC SERIES.

POTASSIUM      1S(2)2S(2)2P(3), 7-2P				
T.E.= -0.50812798D+03	P.E.= -0.10162563D+04			
K.E.= 0.50812828D+03	V.T.= -0.19999994D+01			
S	1S	2S	P	2P
BASIS/ORB E	-150.74167	-27.57654	BASIS/ORB E	-25.83972
1S 18.73050	0.96323	-0.30342	2P 8.36899	0.30731
1S 32.47030	0.01603	-0.00112	2P 12.72950	0.09515
2S 7.63046	0.00043	1.16340	2P 7.16296	0.61337
2S 15.89620	0.02821	-0.17869	2P 26.82780	0.00155
CALCIUM      1S(2)2S(2)2P(3), 7-2P				
T.E.= -0.56709158D+03	P.E.= -0.11341833D+04			
K.E.= 0.56709175D+03	V.T.= -0.19959997D+01			
S	1S	2S	P	2P
BASIS/ORB E	-168.51080	-31.85854	BASIS/ORB E	-29.5E561
1S 19.70640	0.96602	-0.3C824	2P 8.90158	0.32698
1S 34.12730	0.01561	-0.00030	2P 13.64520	0.08648
2S 8.11856	0.00034	1.17224	2P 7.63339	0.60152
2S 16.57820	0.02534	-0.18555	2P 28.34550	0.00135
SCANDIUM      1S(2)2S(2)2P(3), 7-2P				
T.E.= -0.62930572D+03	P.E.= -0.125E106D+04			
K.E.= 0.62930489D+03	V.T.= -0.20000013D+01			
S	1S	2S	P	2P
BASIS/ORB E	-187.28058	-35.59170	BASIS/ORB E	-33.58187
1S 20.71240	C.96736	-0.30565	2P 9.37283	0.16792
1S 35.89940	0.01475	-0.00C61	2P 13.48950	0.11604
2S 8.59944	0.00029	1.17779	2P 8.26294	0.72959
2S 17.42790	0.02464	-0.1921E	2P 29.97520	0.00187
TITANIUM      1S(2)2S(2)2P(3), 7-2P				
T.E.= -0.69477032D+03	P.E.= -0.13855409D+04			
K.E.= 0.69477056D+03	V.T.= -0.19999996D+01			
S	1S	2S	P	2P
BASIS/ORB E	-207.05065	-40.37441	BASIS/ORB E	-37.82815
1S 21.68710	0.97010	-0.31497	2P 9.92273	0.26235
1S 37.68130	0.01423	0.0CC65	2P 14.84700	0.09029
2S 9.09347	0.00020	1.18737	2P 8.68862	0.66056
2S 18.03620	0.02199	-0.19559	2P 31.54920	0.00133
VANADIUM      1S(2)2S(2)2P(3), 7-2P				
T.E.= -0.76348530D+03	P.E.= -0.15269711D+04			
K.E.= 0.76348577D+03	V.T.= -0.19999994D+01			
S	1S	2S	P	2P
BASIS/ORB E	-227.82124	-45.0C741	BASIS/ORB E	-42.32472
1S 22.68670	0.97147	-0.31654	2P 10.47550	0.30756
1S 39.47450	0.01354	0.00C72	2P 15.93890	0.07792
2S 9.57852	0.00016	1.19325	2P 9.13011	0.62724
2S 18.82810	0.02108	-0.20545	2P 33.20160	0.00109
CHROMIUM      1S(2)2S(2)2P(3), 7-2P				
T.E.= -0.83545058D+03	P.E.= -0.167C9014D+04			
K.E.= 0.83545086D+03	V.T.= -0.19999997D+01			
S	1S	2S	P	2P
BASIS/ORB E	-249.59216	-49.89062	BASIS/ORB E	-47.07153
1S 23.68590	0.97186	-0.31435	2P 11.03600	0.29796
1S 41.20530	0.01335	-0.00122	2P 16.75610	0.07401
2S 10.04560	0.00038	1.19283	2P 9.63025	0.64016
2S 19.93180	0.02050	-0.20762	2P 34.77430	0.00101

See page 183 for Explanation of Tables and Notes for Tables 32, 42, and 43

TABLE 12 (4). THE HARTREE-FOCK FUNCTIONS FOR N(<sup>2</sup>P) ISO-ELECTRONIC SERIES.

MANGANESE	1S(2)2S(2)2P(3), 7-2P			
T.E.= -0.91066625D+03	P.E.= -0.18213341D+C4			
K.E.= 0.91066784D+C3	V.T.= -0.19999983D+01			
S	1S	2S	P	2P
BASIS/ORB E	-272.36339	-55.02381	BASIS/ORB E	-52.06832
1S 24.68380	0.97372	-0.32034	2P 11.56910	0.29439
1S 42.94080	0.01251	0.00C80	2P 17.55450	0.07100
2S 10.54910	0.00008	1.20380	2P 10.12620	0.64619
2S 20.42330	0.01944	-0.21599	2P 36.37980	0.00094
IRON	1S(2)2S(2)2P(3), 7-2P			
T.E.= -0.98913203D+03	P.E.= -0.19782698D+04			
K.E.= 0.9891378CD+03	V.T.= -0.19999942D+01			
S	1S	2S	P	2P
BASIS/ORB E	-296.13458	-60.4C702	BASIS/ORB E	-57.31516
1S 25.69030	0.97518	-0.22229	2P 12.10850	0.26194
1S 45.10300	0.01150	0.00109	2P 19.06710	0.06363
2S 11.03810	0.00002	1.20562	2P 10.70030	0.68619
2S 21.17630	0.01886	-0.22161		
COBALT	1S(2)2S(2)2P(3), 7-2P			
T.E.= -0.107C8482D+04	P.E.= -0.21416997D+04			
K.E.= 0.10708515D+04	V.T.= -0.19999968D+01			
S	1S	2S	P	2P
BASIS/ORB E	-320.90648	-66.04C63	BASIS/ORB E	-62.81241
1S 26.70560	0.97573	-0.32187	2P 12.58210	0.38943
1S 47.05440	0.01079	0.00045	2P 20.38210	0.05242
2S 11.51560	0.00001	1.21161	2P 10.99200	0.56958
2S 22.10850	0.01892	-0.22481		
NICKEL	1S(2)2S(2)2P(3), 7-2P			
T.E.= -0.11558144D+04	P.E.= -0.23116272D+04			
K.E.= 0.11558128D+04	V.T.= -0.20000C14D+01			
S	1S	2S	P	2P
BASIS/ORB E	-346.67839	-71.92418	BASIS/ORB E	-68.55961
1S 27.67530	0.97683	-0.32221	2P 13.21850	0.28914
1S 48.68650	0.01104	-0.00018	2P 20.76860	0.05656
2S 11.99400	0.00022	1.21273	2P 11.62450	0.66521
2S 23.01410	0.01705	-0.22719		
COPPER	1S(2)2S(2)2P(3), 7-2P			
T.E.= -0.12440310D+04	P.E.= -0.2488C638D+04			
K.E.= 0.12440329D+04	V.T.= -0.19999985D+01			
S	1S	2S	P	2P
BASIS/ORB E	-373.45056	-78.05768	BASIS/ORB E	-74.55676
1S 28.67890	0.97816	-0.32769	2P 13.76210	0.33807
1S 50.48090	0.01032	0.00181	2P 22.04320	0.04858
2S 12.50580	-0.00007	1.22519	2P 12.03450	0.62388
2S 23.44560	0.01652	-0.23613		
ZINC	1S(2)2S(2)2P(3), 7-2P			
T.E.= -0.13354976D+04	P.E.= -0.26709578D+04			
K.E.= 0.13355002D+04	V.T.= -0.19999980D+01			
S	1S	2S	P	2P
BASIS/ORB E	-401.22279	-84.44134	BASIS/ORB E	-80.80409
1S 29.67790	0.97890	-0.32890	2P 14.31850	0.28345
1S 52.25930	0.00997	0.00188	2P 22.48450	0.05164
2S 12.99360	-0.00009	1.22933	2P 12.61050	0.67500
2S 24.23290	0.01598	-0.24019		

See page 183 for Explanation of Tables and Notes for Tables 32, 42, and 43

## ROOTHAAN-HARTREE-FOCK ATOMIC WAVEFUNCTIONS

TABLE 12 (5). THE HARTREE-FOCK FUNCTIONS FOR N(2P) ISO-ELECTRONIC SERIES.

**GALLIUM**       $1S(2)2S(2)2P(3)$ , 7-2P  
 T.E.= -0.14302144D+04 P.E.= -0.28604304D+04  
 K.E.= 0.14302160D+04 V.T.= -0.19999989D+01

S	1S	2S	P	2P
BASIS/ORB E	-429.99525	-91.07502	BASIS/ORB E	-87.30147
1S 30.67160	0.97979	-0.33C86	2P 14.87180	0.27622
1S 54.05750	0.00967	0.00227	2P 23.31400	0.04982
2S 13.48680	-0.00011	1.23474	2P 13.11050	0.68370
2S 24.94760	0.01523	-0.244500		

**GERMANIUM**       $1S(2)2S(2)2P(3)$ , 7-2P  
 T.E.= -0.15281813D+04 P.E.= -0.30563655D+04  
 K.E.= 0.15281842D+04 V.T.= -0.19999982D+01

S	1S	2S	P	2P
BASIS/ORB E	-459.76786	-97.95875	BASIS/ORB E	-94.04890
1S 31.66920	0.98046	-0.33207	2P 15.27220	0.36143
1S 55.81470	0.00940	0.00240	2P 24.59430	0.04363
2S 13.97620	-0.00012	1.23881	2P 13.47140	0.60437
2S 25.72000	0.01470	-0.24888		

**ARSENIC**       $1S(2)2S(2)2P(3)$ , 7-2P  
 T.E.= -0.16293984D+04 P.E.= -0.32587997D+04  
 K.E.= 0.16294013D+04 V.T.= -0.19999982D+01

S	1S	2S	P	2P
BASIS/ORB E	-490.54054	-105.09255	BASIS/ORB E	-101.04640
1S 32.66610	0.98106	-0.33321	2P 15.94340	0.31542
1S 57.52540	0.00917	0.00251	2P 25.43360	0.04201
2S 14.46540	-0.00013	1.24260	2P 14.02240	0.65168
2S 26.49600	0.01420	-0.25251		

**SELENIUM**       $1S(2)2S(2)2P(3)$ , 7-2P  
 T.E.= -0.17338655D+04 P.E.= -0.34677350D+04  
 K.E.= 0.17338695D+04 V.T.= -0.19999977D+01

S	1S	2S	P	2P
BASIS/ORB E	-522.31329	-112.47640	BASIS/ORB E	-108.29396
1S 33.66770	0.98161	-0.33356	2P 16.50580	0.26498
1S 59.35780	0.00885	0.00250	2P 25.82470	0.04484
2S 14.95290	-0.00015	1.24573	2P 14.59880	0.69897
2S 27.29880	0.01386	-0.25570		

**BROMINE**       $1S(2)2S(2)2P(3)$ , 7-2P  
 T.E.= -0.18415827D+04 P.E.= -0.36831666D+04  
 K.E.= 0.18415838D+04 V.T.= -0.19999994D+01

S	1S	2S	P	2P
BASIS/ORB E	-555.08625	-120.11026	BASIS/ORB E	-115.79156
1S 34.65180	0.98215	-0.33598	2P 16.94190	0.29366
1S 60.70440	0.00897	0.00300	2P 26.72060	0.04298
2S 15.44840	-0.00014	1.25081	2P 15.05190	0.67187
2S 27.99180	0.01303	-0.25954		

**KRYPTON**       $1S(2)2S(2)2P(3)$ , 7-2P  
 T.E.= -0.19525501D+04 P.E.= -0.39051020D+04  
 K.E.= 0.19525520D+04 V.T.= -0.19999990D+01

S	1S	2S	P	2P
BASIS/ORB E	-588.85923	-127.99416	BASIS/ORB E	-123.53919
1S 35.65160	0.98265	-0.33677	2P 17.49220	0.28905
1S 62.48010	0.00871	0.00304	2P 27.57660	0.04147
2S 15.93730	-0.00015	1.25252	2P 15.54830	0.67773
2S 28.78020	0.01269	-0.26302		

See page 183 for Explanation of Tables and Notes for Tables 32, 42, and 43

TABLE 13 (1). THE HARTREE-FOCK FUNCTIONS FOR O(<sup>3</sup>P) ISO-ELECTRONIC SERIES.

XYGEN            1S(2)2S(2)2P(4), 8-3P				
T.E.= -0.74809359D+02	P.E.= -0.14561846D+03			
K.E.= 0.74809097D+02	V.T.= -0.20000035D+01			
S	1S	2S	P	2P
BASIS/ORB E	-20.66861	-1.24428	BASIS/ORB E	-0.63186
1S 7.62035	0.93497	-0.21878	2P 1.82324	C.57640
1S 13.38030	0.03922	-0.00602	2P 3.46668	0.32212
2S 3.15190	0.00289	C.49668	2P 1.15634	0.17492
2S 6.45968	0.03681	-0.10532	2P 7.73305	0.01541
2S 1.88150	-0.00008	0.63030		
FLUORINE        1S(2)2S(2)2P(4), 8-3P				
T.E.= -0.98831699D+02	P.E.= -0.15766275D+03			
K.E.= 0.98831054D+02	V.T.= -0.20000065D+01			
S	1S	2S	P	2P
BASIS/ORB E	-27.14132	-2.19484	BASIS/ORB E	-1.44410
1S 8.61501	0.93580	-0.23141	2P 2.33167	0.60326
1S 14.80480	0.03872	-0.00618	2P 4.24798	C.29135
2S 3.74689	0.00360	0.42022	2P 1.64224	0.16094
2S 7.35807	0.03539	-0.11425	2P 9.53227	0.01107
2S 2.36945	-0.00032	0.70036		
NEON            1S(2)2S(2)2P(4), 8-3P				
T.E.= -0.12637210D+03	P.E.= -0.25274400D+03			
K.E.= 0.12637190D+03	V.T.= -0.20000016D+01			
S	1S	2S	P	2P
BASIS/ORB E	-34.63377	-3.40855	BASIS/ORB E	-2.51593
1S 9.65027	0.93636	-0.24099	2P 2.85676	0.62427
1S 16.40750	0.03509	-0.00612	2P 5.05275	0.25933
2S 4.39338	0.00330	0.34753	2P 2.12406	0.16206
2S 8.27019	0.03853	-0.12501	2P 11.29050	0.00825
2S 2.87511	-0.00018	0.77588		
SODIUM          1S(2)2S(2)2P(4), 8-3P				
T.E.= -0.15742371D+03	P.E.= -0.31484596D+03			
K.E.= 0.15742225D+03	V.T.= -0.20000093D+01			
S	1S	2S	P	2P
BASIS/ORB E	-43.13798	-4.87909	BASIS/ORB E	-3.84319
1S 10.58570	0.94333	-0.25712	2P 3.39389	0.62949
1S 17.84610	0.03573	-0.00397	2P 5.85467	0.23244
2S 4.92688	0.00402	0.32782	2P 2.61426	0.17734
2S 8.94172	0.02891	-0.13047	2P 13.19400	0.00630
2S 3.34921	-0.00062	0.80251		
MAGNESIUM       1S(2)2S(2)2P(4), 8-3P				
T.E.= -0.19198292D+03	P.E.= -0.38356588D+03			
K.E.= 0.19198296D+03	V.T.= -0.19999998D+01			
S	1S	2S	P	2P
BASIS/ORB E	-52.64969	-6.60370	BASIS/ORB E	-5.42391
1S 11.70410	0.94067	-0.25986	2P 3.92611	0.61552
1S 19.72340	0.02879	-0.00429	2P 6.65305	0.21185
2S 5.55012	0.00234	0.26506	2P 3.15471	0.20695
2S 10.00590	0.04056	-0.13823	2P 14.90160	0.00500
2S 3.86033	0.00003	0.86443		
ALUMINUM        1S(2)2S(2)2P(4), 8-3P				
T.E.= -0.23004753D+03	P.E.= -0.46005456D+03			
K.E.= 0.23004703D+03	V.T.= -0.20000022D+01			
S	1S	2S	P	2P
BASIS/ORB E	-63.16689	-8.58102	BASIS/ORB E	-7.25703
1S 12.68260	0.94397	-0.26638	2P 4.46572	0.59621
1S 21.35010	0.02822	-0.00466	2P 7.44964	0.19412
2S 6.02169	0.00426	0.23176	2P 3.68366	C.24036
2S 11.00450	0.03596	-0.13753	2P 16.77650	0.00401
2S 4.35386	-0.00093	0.85549		

See page 183 for Explanation of Tables and Notes for Tables 32, 42, and 43

## ROOTHAAN-HARTREE-FOCK ATOMIC WAVEFUNCTIONS

 TABLE 13 (2). THE HARTREE-FOCK FUNCTIONS FOR O(<sup>3</sup>P) ISO-ELECTRONIC SERIES.

SILICON      1S(2)2S(2)2P(4), 8-3P  
 T.E.= -0.271616140+03   P.E.= -0.54323181D+03  
 K.E.= 0.27161566D+03   V.T.= -0.2CCC0C18D+01

S	1S	2S	P	2P
BASIS/ORB E	-74.66808	-10.81025	BASIS/ORB E	-9.34193
1S 13.72880	0.94531	-0.27161	2P 4.99615	0.59124
1S 23.20770	0.02481	-0.0C416	2P 8.24385	0.17870
2S 6.46847	0.00404	0.2CE24	2P 4.18255	0.25778
2S 11.95000	0.03829	-0.14146	2P 18.49200	0.00338
2S 4.84481	-0.00105	0.91576		

PHOSPHORUS      1S(2)2S(2)2P(4), 8-3P  
 T.E.= -0.31668781D+03   P.E.= -0.63337524D+03  
 K.E.= 0.31668743D+03   V.T.= -0.20000012D+01

S	1S	2S	P	2P
BASIS/ORB E	-87.21227	-13.29084	BASIS/ORB E	-11.67813
1S 14.74490	0.96719	-0.27688	2P 5.52885	0.58130
1S 24.88460	0.02315	-0.0C381	2P 9.03669	0.16549
2S 6.92299	0.00399	0.18390	2P 4.68680	0.27851
2S 12.85210	0.03788	-0.14503	2P 20.18230	0.00289
2S 5.34050	-0.00122	0.94635		

SULFUR      1S(2)2S(2)2P(4), 8-3P  
 T.E.= -0.36526186D+03   P.E.= -0.73052260D+03  
 K.E.= 0.36526074D+03   V.T.= -0.200000310+01

S	1S	2S	P	2P
BASIS/ORB E	-100.73887	-16.02248	BASIS/ORB E	-14.26539
1S 15.70700	0.95166	-0.2E534	2P 6.07741	0.58628
1S 26.37840	0.02289	-0.00240	2P 9.89994	0.14890
2S 7.24813	0.00382	0.2C877	2P 5.15924	0.28812
2S 13.54050	0.03307	-0.15015	2P 21.56690	0.00249
2S 5.80252	-0.00143	0.92885		

CHLORINE      1S(2)2S(2)2P(4), 8-3P  
 T.E.= -0.41733781D+03   P.E.= -0.83467509D+03  
 K.E.= 0.41733727D+03   V.T.= -0.200000130+01

S	1S	2S	P	2P
BASIS/ORB E	-115.26727	-19.00491	BASIS/ORB E	-17.10343
1S 16.78560	0.95270	-0.28E29	2P 6.61724	0.57803
1S 28.59450	0.01865	-0.00180	2P 10.72470	0.13766
2S 7.67349	0.00243	C.190C4	2P 5.65562	0.30595
2S 14.43230	0.03725	-0.15604	2P 23.25490	0.00213
2S 6.30009	-0.00081	0.95C97		

ARGON      1S(2)2S(2)2P(4), 8-3P  
 T.E.= -0.47291526D+03   P.E.= -0.94582801D+03  
 K.E.= 0.47291275D+03   V.T.= -0.2000CC53D+01

S	1S	2S	P	2P
BASIS/ORB E	-130.79702	-22.23782	BASIS/ORB E	-20.19184
1S 17.92300	0.94725	-0.28E65	2P 7.07384	0.55373
1S 30.83900	0.01585	-0.00253	2P 11.32720	0.14125
2S 6.93651	0.00117	1.13020	2P 6.21C85	0.32515
2S 15.76050	0.04702	-0.15136	2P 25.89080	0.00188

POTASSIUM      1S(2)2S(2)2P(4), 8-3P  
 T.E.= -0.53199404D+03   P.E.= -0.10629904D+04  
 K.E.= 0.53199635D+03   V.T.= -0.19999957D+01

S	1S	2S	P	2P
BASIS/ORB E	-147.32813	-25.72143	BASIS/ORB E	-23.53112
1S 18.94660	0.95031	-0.29122	2P 7.68945	0.56092
1S 32.55350	0.01399	-0.00170	2P 12.37540	0.12006
2S 7.41828	0.00069	1.13859	2P 6.65007	0.33812
2S 16.46920	0.04582	-0.15931	2P 27.63210	0.00146

See page 183 for Explanation of Tables and Notes for Tables 32, 42, and 43

TABLE 13 (3). THE HARTREE-FOCK FUNCTIONS FOR O(<sup>3</sup>P) ISO-ELECTRONIC SERIES.

CALCIUM	1S(2)2S(2)2P(4), 8-3P			
T.E.= -0.59457384D+03	P.E.= -0.11E51463D+04			
K.E.= 0.59457448D+03	V.T.= -0.1999989D+01			
S	1S	2S	P	2P
BASIS/ORB E	-164.86036	-29.45548	BASIS/ORB E	-27.12080
1S 19.87590	0.95605	-0.29821	2P 8.06009	0.45805
1S 34.11990	0.01415	-0.00058	2P 12.54640	0.14296
2S 7.90426	0.00057	1.14764	2P 7.32852	0.41638
2S 17.08240	0.03887	-0.16508	2P 29.19420	0.00186
SCANDIUM	1S(2)2S(2)2P(4), 8-3P			
T.E.= -0.66065453D+03	P.E.= -0.13213106D+04			
K.E.= 0.66065606D+03	V.T.= -0.1999977D+01			
S	1S	2S	P	2P
BASIS/ORB E	-183.39343	-33.43588	BASIS/ORB E	-30.96088
1S 20.86190	0.95917	-0.30222	2P 8.79225	0.47623
1S 35.90130	0.01337	-0.00008	2P 13.65160	0.11643
2S 8.38808	0.00041	1.15523	2P 7.70881	0.42401
2S 17.80180	0.03611	-0.17173	2P 31.00460	0.00156
TITANIUM	1S(2)2S(2)2P(4), 8-3P			
T.E.= -0.73023597D+03	P.E.= -0.14604729D+04			
K.E.= 0.73023694D+03	V.T.= -0.1999987D+01			
S	1S	2S	P	2P
BASIS/ORB E	-202.92719	-37.67455	BASIS/ORB E	-35.05125
1S 21.84440	0.96098	-0.30330	2P 9.14949	0.39626
1S 37.59170	0.01330	-0.00085	2P 14.04750	0.13019
2S 8.86494	0.00051	1.16C2	2P 8.36278	0.48908
2S 18.69310	0.03383	-0.17709	2P 32.67140	0.00157
VANADIUM	1S(2)2S(2)2P(4), 8-3P			
T.E.= -0.80331804D+03	P.E.= -0.16066390D+04			
K.E.= 0.80332095D+03	V.T.= -0.19999964D+01			
S	1S	2S	P	2P
BASIS/ORB E	-223.46151	-42.15535	BASIS/ORB E	-39.39181
1S 22.82490	0.96364	-0.30688	2P 9.67492	0.51259
1S 39.37700	0.01278	-0.00038	2P 15.23340	0.10977
2S 9.35015	0.00042	1.16691	2P 8.72818	0.39266
2S 19.41540	0.03125	-0.18295	2P 34.45150	0.00111
CHROMIUM	1S(2)2S(2)2P(4), 8-3P			
T.E.= -0.87990063D+03	P.E.= -0.17597987D+04			
K.E.= 0.87989805D+03	V.T.= -0.20000C29D+01			
S	1S	2S	P	2P
BASIS/ORB E	-244.99654	-46.85454	BASIS/ORB E	-43.98272
1S 23.78880	0.96560	-0.3C778	2P 10.20350	0.58044
1S 41.08910	0.01304	-0.00118	2P 16.03680	0.10140
2S 9.82696	0.00063	1.17C80	2P 9.05144	0.33248
2S 20.31670	0.02834	-0.18710	2P 36.18580	0.00114
MANGANESE	1S(2)2S(2)2P(4), 8-3P			
T.E.= -0.95998356D+03	P.E.= -0.19199E49D+04			
K.E.= 0.95998136D+03	V.T.= -0.20000023D+01			
S	1S	2S	P	2P
BASIS/ORB E	-267.53151	-51.87987	BASIS/ORB E	-48.82377
1S 24.79920	0.96713	-0.30920	2P 10.78620	0.68123
1S 43.16050	0.01201	-0.00125	2P 17.92330	0.07637
2S 10.30840	0.00055	1.17567	2P 9.24842	0.25716
2S 21.14590	0.02767	-0.19233		

See page 183 for Explanation of Tables and Notes for Tables 32, 42, and 43

## ROOTHAAN-HARTREE-FOCK ATOMIC WAVEFUNCTIONS

 TABLE 13 (4). THE HARTREE-FOCK FUNCTIONS FOR O(<sup>2</sup>P) ISO-ELECTRONIC SERIES.

IRON	1S(2)2S(2)2P(4), 8-3P			
T.E.= -0.10435671C+04	P.E.= -0.20E71368D+04			
K.E.= C.10435697D+04	V.T.= -0.19999976D+01			
S	1S	2S	P	2P
BASIS/ORB E	-291.06742	-57.11503	BASIS/ORB E	-53.91477
1S 25.79590	0.96982	-0.31543	2P 11.57220	0.51423
1S 45.14690	0.01088	0.00080	2P 19.04410	0.06790
2S 10.80990	0.00019	1.1E5E7	2P 10.08380	0.43180
2S 21.60870	0.02606	-0.19981		
COBALT	1S(2)2S(2)2P(4), 8-3P			
T.E.= -0.11306510D+04	P.E.= -0.22E13043D+04			
K.E.= 0.11306532D+04	V.T.= -0.19999981D+01			
S	1S	2S	P	2P
BASIS/ORB E	-315.60355	-62.60C67	BASIS/ORB E	-59.25618
1S 26.80000	0.97097	-0.31667	2P 11.99560	0.58835
1S 47.07670	0.01029	0.00C71	2P 19.85610	0.06520
2S 11.29310	0.00015	1.19C37	2P 10.41230	0.35987
2S 22.42770	0.02533	-0.20454		
NICKEL	1S(2)2S(2)2P(4), 8-3P			
T.E.= -0.12212352D+04	P.E.= -0.24424709D+04			
K.E.= 0.122123570+04	V.T.= -0.19999996D+01			
S	1S	2S	P	2P
BASIS/ORB E	-341.14002	-68.33E20	BASIS/ORB E	-64.84753
1S 27.74560	0.97286	-0.32176	2P 12.32640	0.61669
1S 48.10130	0.01101	0.00198	2P 20.27810	0.07110
2S 11.79170	0.00011	1.19889	2P 10.94660	0.32494
2S 22.97260	0.02221	-0.21039		
COPPER	1S(2)2S(2)2P(4), 8-3P			
T.E.= -0.13153197D+04	P.E.= -0.26306408D+04			
K.E.= 0.13153211D+04	V.T.= -0.19999990D+01			
S	1S	2S	P	2P
BASIS/ORB E	-367.67679	-74.32197	BASIS/ORB E	-70.68913
1S 28.75390	0.97370	-0.32241	2P 12.86230	0.62999
1S 50.00850	0.01042	0.00174	2P 21.24090	0.06598
2S 12.27430	0.00008	1.20253	2P 11.37430	C.31627
2S 23.81690	0.02185	-0.21452		
ZINC	1S(2)2S(2)2P(4), 8-3P			
T.E.= -0.14129045D+04	P.E.= -0.28258095D+04			
K.E.= 0.14129051D+04	V.T.= -0.19999996D+01			
S	1S	2S	P	2P
BASIS/ORB E	-395.21355	-80.55798	BASIS/ORB E	-76.78091
1S 29.71770	0.97422	-0.32497	2P 13.39730	0.64260
1S 50.70300	0.01132	0.00215	2P 21.89830	0.06433
2S 12.76320	0.00009	1.20767	2P 11.75050	C.30499
2S 24.54500	0.02007	-0.21859		
GALLIUM	1S(2)2S(2)2P(4), 8-3P			
T.E.= -0.15139895D+04	P.E.= -0.3C279802D+04			
K.E.= 0.15139907D+04	V.T.= -0.19999992D+01			
S	1S	2S	P	2P
BASIS/ORB E	-423.75100	-87.04369	BASIS/ORB E	-83.12255
1S 30.73320	0.97587	-0.32E53	2P 13.92890	0.61970
1S 53.41750	0.00997	0.00241	2P 22.99840	C.05983
2S 13.25450	0.00001	1.21306	2P 12.34680	0.33181
2S 25.26960	0.01971	-0.22386		

See page 183 for Explanation of Tables and Notes for Tables 32, 42, and 43

TABLE 13 (5). THE HARTREE-FOCK FUNCTIONS FOR O(<sup>3</sup>P) ISO-ELECTRONIC SERIES.

GERMANIUM		1S(2)2S(2)2P(4), 8-3P			
T.E.=	-0.16185747D+04	P.E.=	-0.32371499D+04		
K.E.=	0.16185752D+04	V.T.=	-0.19999957D+01		
S	1S	2S	P	2P	
BASIS/ORB E	-453.28833	-93.77977	BASIS/ORB E	-89.71446	
1S 31.72230	0.97664	-0.32821	2P 14.68930	0.53318	
1S 54.93170	0.00992	0.00264	2P 24.04950	0.05361	
2S 13.74350	-0.00000	1.21762	2P 12.92680	0.42424	
2S 26.02060	0.01880	-0.22757			
ARSENIC		1S(2)2S(2)2P(4), 8-3P			
T.E.=	-0.17266601D+04	P.E.=	-0.34533236D+04		
K.E.=	0.17266635D+04	V.T.=	-0.1999980D+01		
S	1S	2S	P	2P	
BASIS/ORB E	-483.82588	-100.76587	BASIS/ORB E	-96.55643	
1S 32.73460	0.97700	-0.32785	2P 15.21140	0.52890	
1S 56.72370	0.00950	0.00211	2P 24.86480	0.05205	
2S 14.22220	-0.00002	1.21929	2P 13.42050	0.42970	
2S 26.93680	0.01876	-0.23056			
SELENIUM		1S(2)2S(2)2P(4), 8-3P			
T.E.=	-0.18382456D+04	P.E.=	-0.36764552D+04		
K.E.=	0.18382496D+04	V.T.=	-0.19999978D+01		
S	1S	2S	P	2P	
BASIS/ORB E	-515.36357	-108.00188	BASIS/ORB E	-103.64832	
1S 33.72060	0.97815	-0.33044	2P 15.77050	0.45025	
1S 58.56100	0.00925	0.00278	2P 25.38490	0.05433	
2S 14.71930	-0.00005	1.22540	2P 14.09540	0.50563	
2S 27.57970	0.01769	-0.23559			
BROMINE		1S(2)2S(2)2P(4), 8-3P			
T.E.=	-0.19533313D+04	P.E.=	-0.39066675D+04		
K.E.=	0.19533362D+04	V.T.=	-0.19999975D+01		
S	1S	2S	P	2P	
BASIS/ORB E	-547.90147	-115.48809	BASIS/ORB E	-110.99041	
1S 34.72280	0.97867	-0.33095	2P 16.14600	0.53401	
1S 60.29550	0.00898	0.00263	2P 26.26580	0.05220	
2S 15.20380	-0.00006	1.22815	2P 14.43170	0.42370	
2S 28.41210	0.01732	-0.23858			
KRYPTON		1S(2)2S(2)2P(4), 8-3P			
T.E.=	-0.20719171D+04	P.E.=	-0.41438415D+04		
K.E.=	0.20719243D+04	V.T.=	-0.19999965D+01		
S	1S	2S	P	2P	
BASIS/ORB E	-581.43952	-123.22430	BASIS/ORB E	-118.58255	
1S 35.70390	0.97847	-0.33128	2P 16.51250	0.57114	
1S 60.78000	0.00969	0.00235	2P 26.87940	0.05363	
2S 15.68290	-0.00003	1.22953	2P 14.90790	0.38478	
2S 29.30570	0.01662	-0.24018			

See page 183 for Explanation of Tables and Notes for Tables 32, 42, and 43

## ROOTHAAN-HARTREE-FOCK ATOMIC WAVEFUNCTIONS

 TABLE 14 (1). THE HARTREE-FOCK FUNCTIONS FOR O(<sup>1</sup>D) ISO-ELECTRONIC SERIES.

OXYGEN      1S(2)2S(2)2P(4), 8-1D  
 T.E.= -0.74729220D+02   P.E.= -0.14545803D+03  
 K.E.= 0.74728805D+02   V.T.= -0.20000055D+01

S	1S	2S	P	2P
BASIS/ORB E	-20.69315	-1.25E41	BASIS/ORB E	-0.60063
1S 7.66623	0.93563	-0.21E57	2P 1.81204	0.55686
1S 13.73180	0.03395	-0.00E30	2P 3.46310	0.32757
2S 3.14371	0.00228	0.49E38	2P 1.15290	0.19338
2S 6.48224	0.04247	-0.10689	2P 7.89980	0.01456
2S 1.88230	0.00012	0.62426		

FLUORINE      1S(2)2S(2)2P(4), 8-1D  
 T.E.= -0.98728575D+02   P.E.= -0.19745671D+03  
 K.E.= 0.98728137D+02   V.T.= -0.20000044D+01

S	1S	2S	P	2P
BASIS/ORB E	-27.16421	-2.20534	BASIS/ORB E	-1.40076
1S 8.63635	0.93694	-0.23202	2P 2.30183	0.62348
1S 14.98870	0.03601	-0.00558	2P 4.26553	0.29215
2S 3.74995	0.00309	0.42345	2P 1.56374	0.14307
2S 7.33621	0.03750	-0.11598	2P 9.53712	0.01067
2S 2.37120	-0.00014	0.69841		

NEON      1S(2)2S(2)2P(4), 8-1D  
 T.E.= -0.12624671D+03   P.E.= -0.25249267D+03  
 K.E.= 0.12624597D+03   V.T.= -0.20000059D+01

S	1S	2S	P	2P
BASIS/CRB E	-34.65587	-3.41E24	BASIS/ORB E	-2.46116
1S 9.63191	0.93765	-0.24178	2P 2.84460	0.62034
1S 16.43690	0.03567	-0.00E17	2P 5.08497	0.25991
2S 4.32465	0.00417	0.36378	2P 2.10032	0.16818
2S 8.30502	0.03586	-0.12154	2P 11.59610	0.00731
2S 2.86423	-0.00060	0.75691		

SODIUM      1S(2)2S(2)2P(4), 8-1D  
 T.E.= -0.15727641D+03   P.E.= -0.31455293D+03  
 K.E.= 0.15727651D+03   V.T.= -0.19999994D+01

S	1S	2S	P	2P
BASIS/ORB E	-43.15941	-4.88827	BASIS/ORB E	-3.77727
1S 10.68680	0.93826	-0.25101	2P 3.38854	0.62105
1S 18.08750	0.03122	-0.00516	2P 5.90413	0.23116
2S 4.98476	0.00256	0.30278	2P 2.60472	0.18910
2S 9.14135	0.04078	-0.13295	2P 13.34690	0.00563
2S 3.36986	0.00004	0.82398		

MAGNESIUM      1S(2)2S(2)2P(4), 8-1D  
 T.E.= -0.19181391D+03   P.E.= -0.38362739D+03  
 K.E.= 0.19181348D+03   V.T.= -0.20000022D+01

S	1S	2S	P	2P
BASIS/ORB E	-52.67083	-6.61256	BASIS/ORB E	-5.34702
1S 11.66030	0.94253	-0.25953	2P 3.93701	0.60040
1S 19.70120	0.03047	-0.00520	2P 6.71357	0.20933
2S 5.54929	0.00420	0.25E05	2P 3.14045	0.22648
2S 10.07750	0.03531	-0.13532	2P 15.25410	0.00435
2S 3.86740	-0.00071	0.66898		

ALUMINUM      1S(2)2S(2)2P(4), 8-1D  
 T.E.= -0.22985694D+03   P.E.= -0.45571339D+03  
 K.E.= 0.22985646D+03   V.T.= -0.20000021D+01

S	1S	2S	P	2P
BASIS/ORB E	-63.18775	-8.58564	BASIS/ORB E	-7.16929
1S 12.65100	0.94605	-0.26894	2P 4.48749	0.59544
1S 21.27270	0.02906	-0.00400	2P 7.56236	0.18698
2S 6.05606	0.00409	0.23E37	2P 3.64193	0.24992
2S 10.87720	0.03266	-0.13997	2P 16.94610	0.00344
2S 4.35103	-0.00084	0.893C5		

See page 183 for Explanation of Tables and Notes for Tables 32, 42, and 43

TABLE 14 (2). THE HARTREE-FOCK FUNCTIONS FOR O(<sup>1</sup>D) ISO-ELECTRONIC SERIES.

SILICON      1S(2)2S(2)2P(4), 8-1D  
 T.E.= -0.27140407D+03 P.E.= -0.54280816D+03  
 K.E.= 0.27140409D+C3 V.T.= -0.19999955D+01

S	1S	2S	P	2P
BASIS/ORB E	-74.70865	-10.81866	BASIS/ORB E	-5.24334
1S 13.68100	0.94901	-0.27526	2P 5.04878	0.52011
1S 23.17570	0.02545	-0.00318	2P 8.29842	0.17810
2S 6.63394	0.00383	0.20061	2P 4.23818	0.33085
2S 11.75030	0.03327	-0.14514	2P 18.92730	0.00292
2S 4.85335	-0.00084	0.93405		

PHOSPHORUS    1S(2)2S(2)2P(4), 8-10  
 T.E.= -0.31645433D+03 P.E.= -0.63290878D+03  
 K.E.= 0.31645445D+03 V.T.= -0.19999960D+01

S	1S	2S	P	2P
BASIS/ORB E	-87.23267	-13.29913	BASIS/ORB E	-11.56880
1S 14.69860	0.94983	-0.27974	2P 5.59894	0.50220
1S 24.75590	0.02419	-0.00215	2P 9.10603	0.16409
2S 7.07854	0.00385	0.17672	2P 4.74658	0.36022
2S 12.69430	0.03359	-0.14748	2P 20.66830	0.00246
2S 5.34689	-0.00102	0.95846		

SULFUR        1S(2)2S(2)2P(4), 8-1D  
 T.E.= -0.36500701D+03 P.E.= -0.73001407D+03  
 K.E.= 0.36500707D+03 V.T.= -0.19999980D+01

S	1S	2S	P	2P
BASIS/ORB E	-100.75905	-16.03063	BASIS/ORB E	-14.14531
1S 15.69020	0.95325	-0.28674	2P 6.23158	0.41022
1S 26.43290	0.02281	-0.00198	2P 9.90181	0.15209
2S 7.46007	0.00357	0.18129	2P 5.32660	0.46197
2S 13.44530	0.03128	-0.15257	2P 22.22640	0.00217
2S 5.82207	-0.00114	0.95579		

CHLORINE      1S(2)2S(2)2P(4), 8-1D  
 T.E.= -0.41706163D+03 P.E.= -0.83412306D+03  
 K.E.= 0.41706143D+03 V.T.= -0.20000005D+01

S	1S	2S	P	2P
BASIS/ORB E	-115.28736	-19.01298	BASIS/ORB E	-16.97267
1S 16.67830	0.95557	-0.29205	2P 6.69332	0.47908
1S 27.96020	0.02223	-0.00142	2P 10.76070	0.13971
2S 7.93957	0.00347	0.16615	2P 5.75133	0.40381
2S 14.24170	0.02915	-0.15750	2P 23.90240	0.00178
2S 6.31415	-0.00122	0.98C17		

ARGON          1S(2)2S(2)2P(4), 8-1D  
 T.E.= -0.47261779D+03 P.E.= -0.94523627D+03  
 K.E.= 0.47261847D+03 V.T.= -0.1999986D+01

S	1S	2S	P	2P
BASIS/ORB E	-130.81697	-22.24583	BASIS/ORB E	-20.05044
1S 17.96120	0.94571	-0.28644	2P 7.20149	0.33339
1S 30.67100	0.01527	-0.00224	2P 11.21980	0.15198
2S 6.93879	0.00092	1.13C64	2P 6.40023	0.53550
2S 15.74250	0.04968	-0.15244	2P 26.85210	0.00170

POTASSIUM     1S(2)2S(2)2P(4), 8-1D  
 T.E.= -0.53167530D+03 P.E.= -0.1C93499D+04  
 K.E.= 0.53167463D+03 V.T.= -0.20000013D+01

S	1S	2S	P	2P
BASIS/ORB E	-147.34818	-25.72950	BASIS/ORB E	-23.37914
1S 18.90670	0.95063	-0.29218	2P 7.97892	0.24997
1S 32.02560	0.01556	-0.00173	2P 11.96040	0.14120
2S 7.42010	0.00076	1.13891	2P 6.92465	0.62829
2S 16.43980	0.04356	-0.15654	2P 28.35650	0.00172

See page 183 for Explanation of Tables and Notes for Tables 32, 42, and 43

## ROOTHAAN-HARTREE-FOCK ATOMIC WAVEFUNCTIONS

 TABLE 14 (3). THE HARTREE-FOCK FUNCTIONS FOR O<sup>1</sup>D ISO-ELECTRONIC SERIES.

CALCIUM      1S(2)2S(2)2P(4), 8-1D  
 T.E.= -0.594233890+03 P.E.= -0.118846790+04  
 K.E.= 0.594234020D+03 V.T.= -0.199999980+01

S	1S	2S	P	2P
BASIS/ORB E	-164.88023	-29.46344	BASIS/ORB E	-26.95816
1S 19.87930	0.95516	-0.29598	2P 8.46313	0.37468
1S 34.14000	0.01445	-0.00159	2P 13.11840	0.11610
2S 7.90005	0.00075	1.14597	2P 7.30016	0.52783
2S 17.21210	0.03939	-0.16479	2P 30.27440	0.00124

SCANDIUM      1S(2)2S(2)2P(4), 8-1D  
 T.E.= -0.66029333D+03 P.E.= -0.132059C9D+04  
 K.E.= 0.66029757D+03 V.T.= -0.19999936D+01

S	1S	2S	P	2P
BASIS/ORB E	-183.41310	-33.44767	BASIS/ORB E	-30.78753
1S 20.89990	0.95837	-0.29974	2P 8.80493	0.50619
1S 36.46250	0.01229	-0.00065	2P 14.11090	0.10601
2S 8.38377	0.00046	1.15357	2P 7.65740	0.40552
2S 17.93360	0.03824	-0.17202	2P 32.02090	0.00089

TITANIUM      1S(2)2S(2)2P(4), 8-1D  
 T.E.= -0.72985344D+03 P.E.= -0.14597C74D+04  
 K.E.= 0.72985393D+03 V.T.= -0.19999993D+01

S	1S	2S	P	2P
BASIS/ORB E	-202.94665	-37.6E236	BASIS/ORB E	-34.86730
1S 21.88040	0.96173	-0.30303	2P 9.71425	0.41808
1S 38.67130	0.01143	-0.00062	2P 15.75110	0.07954
2S 8.86638	0.00044	1.16022	2P 8.21262	0.51999
2S 18.69270	0.03517	-0.17790		

VANADIUM      1S(2)2S(2)2P(4), 8-1D  
 T.E.= -0.80291432D+03 P.E.= -0.16C58309D+04  
 K.E.= 0.80291653D+03 V.T.= -0.199999572D+01

S	1S	2S	P	2P
BASIS/ORB E	-223.48104	-42.16720	BASIS/ORB E	-39.19730
1S 22.87460	0.96353	-0.30524	2P 10.22950	0.46195
1S 40.40490	0.01102	-0.00066	2P 16.82640	0.07056
2S 9.34777	0.00037	1.16595	2P 8.62172	0.48422
2S 19.49670	0.03347	-0.18354		

CHROMIUM      1S(2)2S(2)2P(4), 8-1D  
 T.E.= -0.87947575D+03 P.E.= -0.17585530D+04  
 K.E.= 0.87947724D+03 V.T.= -0.19999983D+01

S	1S	2S	P	2P
BASIS/ORB E	-245.01588	-46.90221	BASIS/ORB E	-43.77747
1S 23.82850	0.96657	-0.31016	2P 10.64810	0.48999
1S 41.92050	0.01118	0.00024	2P 17.51070	0.07108
2S 9.83840	0.00030	1.17397	2P 9.07449	0.45481
2S 20.12160	0.02966	-0.18531		

MANGANESE      1S(2)2S(2)2P(4), 8-1D  
 T.E.= -0.95953767D+03 P.E.= -0.19190765D+04  
 K.E.= 0.95553879D+03 V.T.= -0.19999988D+01

S	1S	2S	P	2P
BASIS/ORB E	-267.55122	-51.88741	BASIS/ORB E	-48.60786
1S 24.80210	0.56870	-0.31374	2P 11.17240	0.49142
1S 43.53650	0.01109	0.00062	2P 18.36010	0.06761
2S 10.32720	0.00023	1.18094	2P 9.55432	0.45589
2S 20.80750	0.02722	-0.15495		

See page 183 for Explanation of Tables and Notes for Tables 32, 42, and 43

TABLE 14 (4). THE HARTREE-FOCK FUNCTIONS FOR O(<sup>1</sup>D) ISO-ELECTRONIC SERIES.

IRON	1S(2)2S(2)2P(4), 8-1D			
T.E.= -0.10431000D+04	P.E.= -0.20862011D+04			
K.E.= 0.10431011D+04	V.T.= -0.19599989D+01			
S	1S	2S	P	2P
BASIS/ORB E	-291.08694	-57.12278	BASIS/ORB E	-53.68844
1S 25.78610	0.97029	-0.31641	2P 11.75650	0.45450
1S 45.18390	0.01090	0.00116	2P 19.14050	0.06578
2S 10.81450	0.00018	1.18701	2P 10.09860	0.49415
2S 21.53910	0.02550	-0.20028		
COBALT	1S(2)2S(2)2P(4), 8-1D			
T.E.= -0.11301627D+04	P.E.= -0.22603235D+04			
K.E.= 0.11301608D+04	V.T.= -0.20000016D+01			
S	1S	2S	P	2P
BASIS/ORB E	-315.62309	-62.60839	BASIS/ORB E	-59.01929
1S 26.79050	0.97068	-0.31380	2P 12.22040	0.48222
1S 47.22020	0.01062	-0.00066	2P 19.97620	0.06340
2S 11.27980	0.00043	1.18654	2P 10.54020	0.46819
2S 22.67080	0.02501	-0.20233		
NICKEL	1S(2)2S(2)2P(4), 8-1D			
T.E.= -0.12207258D+04	P.E.= -0.24414533D+04			
K.E.= 0.12207275D+04	V.T.= -0.19999986D+01			
S	1S	2S	P	2P
BASIS/ORB E	-341.15944	-68.34390	BASIS/ORB E	-64.60002
1S 27.76220	0.97309	-0.32120	2P 12.91030	0.41726
1S 48.64280	0.01036	0.00182	2P 20.86300	0.05965
2S 11.79150	0.00009	1.15863	2P 11.12060	0.53631
2S 22.99750	0.02272	-0.21061		
COPPER	1S(2)2S(2)2P(4), 8-1D			
T.E.= -0.13147891D+04	P.E.= -0.26295821D+04			
K.E.= 0.13147930D+04	V.T.= -0.19999970D+01			
S	1S	2S	P	2P
BASIS/ORB E	-367.69610	-74.32570	BASIS/ORB E	-70.43110
1S 28.79010	0.97338	-0.32023	2P 13.27480	0.45244
1S 50.71680	0.00955	0.00100	2P 21.45790	0.06148
2S 12.26640	0.00007	1.20021	2P 11.57100	0.49876
2S 23.97060	0.02322	-0.21380		
ZINC	1S(2)2S(2)2P(4), 8-1D			
T.E.= -0.14123527D+04	P.E.= -0.28247105D+04			
K.E.= 0.14123578D+04	V.T.= -0.19999964D+01			
S	1S	2S	P	2P
BASIS/ORB E	-395.23298	-80.56554	BASIS/ORB E	-76.51221
1S 29.78400	0.97418	-0.32127	2P 13.67390	0.47328
1S 52.32360	0.00943	0.00088	2P 22.03400	0.06339
2S 12.74990	0.00006	1.20392	2P 12.04790	0.47550
2S 24.79580	0.02233	-0.21757		
GALLIUM	1S(2)2S(2)2P(4), 8-1D			
T.E.= -0.15134165D+04	P.E.= -0.30268374D+04			
K.E.= 0.15134209D+04	V.T.= -0.19999971D+01			
S	1S	2S	P	2P
BASIS/ORB E	-423.77020	-87.05141	BASIS/ORB E	-82.84336
1S 30.77240	0.97561	-0.32467	2P 14.42580	0.41175
1S 54.26490	0.00905	0.00154	2P 23.13890	0.05668
2S 13.24430	-0.00000	1.21021	2P 12.60320	0.54331
2S 25.45270	0.02108	-0.22277		

See page 183 for Explanation of Tables and Notes for Tables 32, 42, and 43

## ROOTHAAN-HARTREE-FOCK ATOMIC WAVEFUNCTIONS

 TABLE 14 (5). THE HARTREE-FOCK FUNCTIONS FOR O(<sup>1</sup>D) ISO-ELECTRONIC SERIES.

GERMANIUM	1S(2)2S(2)2P(4), 8-1D			
T.E.= -0.16179806D+04	P.E.= -0.32359641D+04			
K.E.= 0.16179835D+04	V.T.= -0.19599582D+01			
S	1S	2S	P	2P
BASIS/ORB E	-453.30756	-93.78734	BASIS/ORB E	-89.42456
1S 31.73940	0.97693	-0.32769	2P 15.10660	0.37222
1S 55.62400	0.00927	0.00248	2P 24.10590	0.05275
2S 13.74370	-0.00002	1.21748	2P 13.14110	0.58635
2S 26.03980	0.01923	-0.22827		
ARSENIC	1S(2)2S(2)2P(4), 8-1D			
T.E.= -0.17260448D+04	P.E.= -0.34520925D+04			
K.E.= 0.17260477D+04	V.T.= -0.19999984D+01			
S	1S	2S	P	2P
BASIS/ORB E	-483.84514	-100.77340	BASIS/ORB E	-96.25594
1S 32.74200	0.97764	-0.32854	2P 15.44390	0.42452
1S 57.50940	0.00890	0.00243	2P 24.82260	0.05282
2S 14.22960	-0.00005	1.22100	2P 13.55610	0.53360
2S 26.84560	0.01877	-0.23189		
SELENIUM	1S(2)2S(2)2P(4), 8-1D			
T.E.= -0.18376092D+04	P.E.= -0.36752240D+04			
K.E.= 0.18376148D+04	V.T.= -0.19999970D+01			
S	1S	2S	P	2P
BASIS/ORB E	-515.38278	-108.00559	BASIS/ORB E	-103.33742
1S 33.74790	0.97801	-0.32E62	2P 15.65960	0.57429
1S 59.18990	0.00865	0.00209	2P 25.62720	0.05160
2S 14.71050	-0.00006	1.22306	2P 13.73860	0.38475
2S 27.72780	0.01854	-0.23452		
BROMINE	1S(2)2S(2)2P(4), 8-1D			
T.E.= -0.19526738D+04	P.E.= -0.39053529D+04			
K.E.= 0.19526791D+04	V.T.= -0.19999973D+01			
S	1S	2S	P	2P
BASIS/ORB E	-547.92065	-115.49577	BASIS/ORB E	-110.66893
1S 34.74470	0.97866	-0.32569	2P 16.18320	0.57572
1S 60.91260	0.00845	0.00217	2P 26.48150	0.04969
2S 15.19800	0.00008	1.22661	2P 14.21030	0.38491
2S 28.51180	0.01796	-0.23793		
KRYPTON	1S(2)2S(2)2P(4), 8-1D			
T.E.= -0.20712385D+04	P.E.= -0.41424838D+04			
K.E.= 0.20712453D+04	V.T.= -0.19999967D+01			
S	1S	2S	P	2P
BASIS/ORB E	-581.45865	-123.23190	BASIS/ORB E	-118.25041
1S 35.74340	0.97940	-0.33087	2P 17.60920	0.27241
1S 62.83500	0.00814	0.00231	2P 27.41380	0.04609
2S 15.68770	-0.00010	1.23047	2P 15.24850	0.69139
2S 29.27160	0.01741	-0.24157		

See page 183 for Explanation of Tables and Notes for Tables 32, 42, and 43

TABLE 15 (1). THE HARTREE-FOCK FUNCTIONS FOR O(<sup>1</sup>S) ISO-ELECTRONIC SERIES.

CXYGEN	1S(2)2S(2)2P(4), 8-1S			
T.E.= -0.74610969D+02	P.E.= -0.14922187D+03			
K.E.= 0.74610898D+02	V.T.= -0.2000009E+01			
S	1S	2S	P	2P
BASIS/ORB E	-20.73011	-1.27502	BASIS/ORB E	-0.55542
1S 7.68181	0.93654	-0.21939	2P 1.73707	0.55229
1S 13.89960	0.03187	-0.00493	2P 3.37419	0.34916
2S 3.14295	0.00185	0.50278	2P 1.09358	0.17810
2S 6.47042	0.04412	-0.10861	2P 7.35754	0.01854
2S 1.88606	0.00026	0.61889		
FLUORINE	1S(2)2S(2)2P(4), 8-1S			
T.E.= -0.98575680D+02	P.E.= -0.15715062D+03			
K.E.= 0.98574941D+02	V.T.= -0.20000075D+01			
S	1S	2S	P	2P
BASIS/ORB E	-27.19874	-2.22132	BASIS/ORB E	-1.33716
1S 8.61139	0.53719	-0.23277	2P 2.24737	0.60150
1S 14.84940	0.03823	-0.00601	2P 4.19889	0.31039
2S 3.74877	0.00340	0.42744	2P 1.55101	0.14929
2S 7.32919	0.03440	-0.11595	2P 9.33958	0.01168
2S 2.37403	-0.00025	0.69506		
NEON	1S(2)2S(2)2P(4), 8-1S			
T.E.= -0.12606033D+03	P.E.= -0.25212047D+03			
K.E.= 0.12606014D+03	V.T.= -0.20000015D+01			
S	1S	2S	P	2P
BASIS/ORB E	-34.68904	-3.43293	BASIS/ORB E	-2.38032
1S 9.66420	0.93571	-0.24062	2P 2.79723	0.61610
1S 16.45020	0.03437	-0.00631	2P 5.03458	0.27109
2S 4.37175	0.00306	0.35471	2P 2.04335	0.16325
2S 8.30534	0.04022	-0.12538	2P 11.16320	0.00823
2S 2.87646	-0.00010	0.76812		
SODIUM	1S(2)2S(2)2P(4), 8-1S			
T.E.= -0.15705710D+03	P.E.= -0.314113360D+03			
K.E.= 0.15705626D+03	V.T.= -0.20000053D+01			
S	1S	2S	P	2P
BASIS/ORB E	-43.19182	-4.90217	BASIS/ORB E	-3.67969
1S 10.51990	0.93877	-0.25668	2P 3.33507	0.61155
1S 17.20570	0.04414	-0.00579	2P 5.85266	0.24372
2S 4.89536	0.00465	0.33241	2P 2.57142	0.18794
2S 9.00291	0.02398	-0.12719	2P 13.07900	0.00592
2S 3.35064	-0.00082	0.79570		
MAGNESIUM	1S(2)2S(2)2P(4), 8-1S			
T.E.= -0.19156200D+03	P.E.= -0.38312375D+03			
K.E.= 0.19156175D+03	V.T.= -0.200000130D+01			
S	1S	2S	P	2P
BASIS/ORB E	-52.70259	-6.62594	BASIS/ORB E	-5.23293
1S 11.58830	0.94009	-0.25964	2P 3.88815	0.58217
1S 19.04780	0.03737	-0.00666	2P 6.66233	0.22123
2S 5.48617	0.00495	0.26758	2P 3.12376	0.23455
2S 10.10870	0.02969	-0.13191	2P 15.05650	0.00443
2S 3.86252	-0.00102	0.85764		
ALUMINUM	1S(2)2S(2)2P(4), 8-1S			
T.E.= -0.22957264D+03	P.E.= -0.45914533D+03			
K.E.= 0.22957268D+03	V.T.= -0.19999598D+01			
S	1S	2S	P	2P
BASIS/ORB E	-63.21903	-8.60266	BASIS/ORB E	-7.03886
1S 12.61080	0.94272	-0.26714	2P 4.43294	0.55980
1S 20.71430	0.03397	-0.00572	2P 7.46322	0.20284
2S 6.01711	0.00478	0.23375	2P 3.65175	0.27121
2S 10.99590	0.03040	-0.13644	2P 16.93760	0.00350
2S 4.35704	-0.00111	0.89379		

See page 183 for Explanation of Tables and Notes for Tables 32, 42, and 43

## ROOTHAAN-HARTREE-FOCK ATOMIC WAVEFUNCTIONS

 TABLE 15 (2). THE HARTREE-FOCK FUNCTIONS FOR O(<sup>1</sup>S) ISO-ELECTRONIC SERIES.

SILICON	1S(2)2S(2)2P(4), 8-1S			
T.E.= -0.27108753D+03	P.E.= -0.54217516D+03			
K.E.= 0.27108762D+03	V.T.= -0.19999997D+01			
S	1S	2S	P	2P
BASIS/ORB E	-74.73963	-10.83141	BASIS/ORB E	-9.09672
1S 13.64890	0.94666	-0.27427	2P 4.98432	0.52066
1S 22.66320	0.02897	-0.00427	2P 8.24686	0.18842
2S 6.51940	0.00443	0.20551	2P 4.19527	0.32140
2S 11.84360	0.03160	-0.14164	2P 18.70550	0.00290
2S 4.84826	-0.00116	0.92163		
PHOSPHORUS	1S(2)2S(2)2P(4), 8-1S			
T.E.= -0.31610565D+03	P.E.= -0.63221165D+03			
K.E.= 0.31610600D+03	V.T.= -0.19999989D+01			
S	1S	2S	P	2P
BASIS/ORB E	-87.26334	-13.31165	BASIS/ORB E	-11.40602
1S 14.68540	0.94891	-0.27954	2P 5.53290	0.49623
1S 24.52310	0.02555	-0.00351	2P 9.04539	0.17467
2S 6.97125	0.00411	0.18769	2P 4.71391	0.35693
2S 12.73550	0.03297	-0.14565	2P 20.54620	0.00239
2S 5.34141	-0.00122	0.94575		
SULFUR	1S(2)2S(2)2P(4), 8-1S			
T.E.= -0.36462627D+03	P.E.= -0.72925027D+03			
K.E.= 0.36462399D+03	V.T.= -0.20000063D+01			
S	1S	2S	P	2P
BASIS/ORB E	-100.78966	-16.04309	BASIS/ORB E	-13.96653
1S 15.60380	0.95361	-0.28810	2P 6.08915	0.55966
1S 25.79710	0.02723	-0.00258	2P 9.94461	0.15220
2S 7.38898	0.00516	0.19231	2P 5.07768	0.31385
2S 13.43790	0.02498	-0.14584	2P 21.83040	0.00215
2S 5.81606	-0.00199	0.94823		
CHLORINE	1S(2)2S(2)2P(4), 8-1S			
T.E.= -0.41664884D+03	P.E.= -0.83329575D+03			
K.E.= 0.41664691D+03	V.T.= -0.20000046D+01			
S	1S	2S	P	2P
BASIS/ORB E	-115.31748	-19.02505	BASIS/ORB E	-16.77749
1S 16.93660	0.93805	-0.27903	2P 6.61712	0.48768
1S 28.06530	0.02012	-0.00446	2P 10.63600	0.15133
2S 6.45835	0.00143	1.12127	2P 5.68494	0.38482
2S 15.11490	0.05272	-0.14477	2P 24.66790	0.00170
ARGON	1S(2)2S(2)2P(4), 8-1S			
T.E.= -0.47217313D+03	P.E.= -0.94434854D+03			
K.E.= 0.47217542D+03	V.T.= -0.19999951D+01			
S	1S	2S	P	2P
BASIS/ORB E	-130.84703	-22.25793	BASIS/ORB E	-19.83954
1S 17.95790	0.94389	-0.28621	2P 7.01908	0.52101
1S 29.92580	0.01677	-0.00250	2P 11.32440	0.15090
2S 6.94059	0.00082	1.13076	2P 6.18055	0.35017
2S 15.74400	0.05012	-0.15261	2P 26.45320	0.00149
POTASSIUM	1S(2)2S(2)2P(4), 8-1S			
T.E.= -0.53119873D+03	P.E.= -0.1C623970D+04			
K.E.= 0.53119829D+03	V.T.= -0.20000008D+01			
S	1S	2S	P	2P
BASIS/ORB E	-147.37804	-25.74142	BASIS/ORB E	-23.15216
1S 18.85070	0.95105	-0.29288	2P 7.59470	0.53659
1S 31.51240	0.01774	-0.00208	2P 12.21690	0.13551
2S 7.42134	0.00094	1.13890	2P 6.61406	0.34868
2S 16.43510	0.04039	-0.15736	2P 28.23550	0.00126

See page 183 for Explanation of Tables and Notes for Tables 32, 42, and 43

TABLE 15 (3). THE HARTREE-FOCK FUNCTIONS FOR O(<sup>1</sup>S) ISO-ELECTRONIC SERIES.

CALCIUM	1S(2)2S(2)2P(4), 8-1S			
T.E.= -0.59372541D+03	P.E.= -0.11874524D+04			
K.E.= 0.59372702D+03	V.T.= -0.19999973D+01			
S	1S	2S	P	2P
BASIS/ORB E	-164.90995	-29.47526	BASIS/ORB E	-26.71520
1S 19.84220	0.95589	-0.29878	2P 7.94356	0.51025
1S 33.55470	0.01571	-0.00072	2P 12.70060	0.14635
2S 7.90662	0.00065	1.14775	2P 7.23919	0.36263
2S 17.07720	0.03718	-0.16446	2P 29.87800	0.00128
SCANDIUM	1S(2)2S(2)2P(4), 8-1S			
T.E.= -0.65975304D+03	P.E.= -0.13195107D+04			
K.E.= 0.65975769D+03	V.T.= -0.19999953D+01			
S	1S	2S	P	2P
BASIS/ORB E	-183.44277	-33.45557	BASIS/ORB E	-30.52875
1S 20.88090	0.95655	-0.29837	2P 8.87142	0.24158
1S 35.42980	0.01424	-0.00173	2P 13.49800	0.13568
2S 8.38130	0.00055	1.15242	2P 7.90496	0.64089
2S 18.02080	0.03800	-0.17141	2P 31.89870	0.00117
TITANIUM	1S(2)2S(2)2P(4), 8-1S			
T.E.= -0.72928133D+03	P.E.= -0.145E5631D+04			
K.E.= 0.72928178D+03	V.T.= -0.19999994D+01			
S	1S	2S	P	2P
BASIS/ORB E	-202.97626	-37.69411	BASIS/ORB E	-34.59252
1S 21.82690	0.96149	-0.30437	2P 9.73580	0.39118
1S 37.43790	0.01368	-0.00056	2P 15.63420	0.08428
2S 8.86934	0.00051	1.1662	2P 8.19714	0.54287
2S 18.64230	0.03279	-0.17709		
VANADIUM	1S(2)2S(2)2P(4), 8-1S			
T.E.= -0.80231039D+03	P.E.= -0.16C4E214D+04			
K.E.= 0.80231097D+03	V.T.= -0.19999993D+01			
S	1S	2S	P	2P
BASIS/ORB E	-223.51050	-42.17888	BASIS/ORB E	-38.90657
1S 22.79380	0.96375	-0.30809	2P 9.98814	0.49681
1S 38.82020	0.01390	-0.00014	2P 16.31880	0.08548
2S 9.35445	0.00045	1.16771	2P 8.55253	0.43508
2S 19.36160	0.02980	-0.18271		
CHROMIUM	1S(2)2S(2)2P(4), 8-1S			
T.E.= -0.87884003D+03	P.E.= -0.17576812D+04			
K.E.= 0.87884121D+03	V.T.= -0.19999987D+01			
S	1S	2S	P	2P
BASIS/ORB E	-245.04529	-46.913E5	BASIS/ORB E	-43.47084
1S 23.77470	0.96628	-0.31187	2P 10.66360	0.44462
1S 40.64020	0.01330	0.00055	2P 17.27490	0.07778
2S 9.84236	0.00037	1.17490	2P 9.09846	0.49412
2S 20.04910	0.02748	-0.18867		
MANGANESE	1S(2)2S(2)2P(4), 8-1S			
T.E.= -0.95887016D+03	P.E.= -0.19177446D+04			
K.E.= 0.95887447D+03	V.T.= -0.19999955D+01			
S	1S	2S	P	2P
BASIS/ORB E	-267.58051	-51.89610	BASIS/ORB E	-48.28543
1S 24.81340	0.96663	-0.31C61	2P 11.13520	0.45163
1S 42.68520	0.01203	-0.00052	2P 17.99510	0.07704
2S 10.31640	0.00032	1.17750	2P 9.58193	0.48704
2S 21.03570	0.02843	-0.19350		

See page 183 for Explanation of Tables and Notes for Tables 32, 42, and 43

## ROOTHAAN-HARTREE-FOCK ATOMIC WAVEFUNCTIONS

 TABLE 15 (4). THE HARTREE-FOCK FUNCTIONS FOR O<sup>1</sup>S ISO-ELECTRONIC SERIES.

IRON            1S(2)2S(2)2P(4), 8-1S				
T.E.= -0.10424007D+04    P.E.= -0.2C848050D+04				
K.E.= 0.10424042D+04    V.T.= -0.19999967D+01				
S	1S	2S	P	2P
BASIS/ORB E	-291.11618	-57.13442	BASIS/ORB E	-53.35010
1S 25.78860	0.96866	-0.31383	2P 11.67190	0.44267
1S 44.36000	0.01186	-0.00000	2P 18.79890	0.07424
2S 10.80420	0.00028	1.18379	2P 10.08130	0.49807
2S 21.74440	0.02618	-0.19864		
COBALT            1S(2)2S(2)2P(4), 8-1S				
T.E.= -0.11294317D+04    P.E.= -0.22588668D+04				
K.E.= 0.11294351D+04    V.T.= -0.19959970D+01				
S	1S	2S	P	2P
BASIS/ORB E	-315.65222	-62.61587	BASIS/ORB E	-58.66492
1S 26.75210	0.97015	-0.31752	2P 12.15500	0.45978
1S 45.50580	0.01236	0.00072	2P 19.60930	0.07170
2S 11.29480	0.00023	1.19C48	2P 10.54290	0.48286
2S 22.41210	0.02379	-0.20371		
NICKEL            1S(2)2S(2)2P(4), 8-1S				
T.E.= -0.12199630D+04    P.E.= -0.24399294D+04				
K.E.= 0.12195664D+04    V.T.= -0.19999972D+01				
S	1S	2S	P	2P
BASIS/ORB E	-341.18860	-68.35541	BASIS/ORB E	-64.22983
1S 27.73220	0.97208	-0.32116	2P 12.50120	0.56307
1S 47.33030	0.01194	0.00161	2P 20.50710	0.06830
2S 11.78840	0.00017	1.15758	2P 10.84610	C.38241
2S 23.05070	0.02198	-0.20936		
COPPER            1S(2)2S(2)2P(4), 8-1S				
T.E.= -0.13139946D+04    P.E.= -0.2E279907D+04				
K.E.= 0.13139961D+04    V.T.= -0.19999988D+01				
S	1S	2S	P	2P
BASIS/ORB E	-367.72523	-74.34109	BASIS/ORB E	-70.04493
1S 28.70210	0.97345	-0.32480	2P 13.22000	C.45074
1S 48.71210	0.01214	0.00250	2P 21.25190	0.06641
2S 12.28280	0.00014	1.20455	2P 11.52730	C.49605
2S 23.68410	0.02008	-0.21474		
ZINC            1S(2)2S(2)2P(4), 8-1S				
T.E.= -0.14115265D+04    P.E.= -0.2823C531D+04				
K.E.= 0.14115266D+04    V.T.= -0.19999999D+01				
S	1S	2S	P	2P
BASIS/ORB E	-395.26207	-80.57704	BASIS/ORB E	-76.11027
1S 29.70670	0.97414	-0.32E31	2P 13.60060	0.52219
1S 50.41350	0.01171	0.00223	2P 21.91870	0.06593
2S 12.76530	0.00011	1.2C788	2P 11.87160	0.42465
2S 24.53380	0.01970	-0.21854		
GALLIUM            1S(2)2S(2)2P(4), 8-1S				
T.E.= -0.15125586D+04    P.E.= -0.30251194D+04				
K.E.= 0.15125608D+04    V.T.= -0.19999985D+01				
S	1S	2S	P	2P
BASIS/ORB E	-423.79930	-87.06274	BASIS/ORB E	-82.42543
1S 30.69790	0.97552	-0.32789	2P 14.13130	0.54225
1S 52.33200	0.01119	0.00284	2P 23.11970	0.05915
2S 13.25920	0.00007	1.214C2	2P 12.31830	0.41086
2S 25.20450	0.01864	-0.22378		

See page 183 for Explanation of Tables and Notes for Tables 32, 42, and 43

TABLE 15 (5). THE HARTREE-FOCK FUNCTIONS FOR O(<sup>1</sup>S) ISO-ELECTRONIC SERIES.

GERMANIUM      1S(2)2S(2)2P(4), 8-1S				
T.E.= -0.16170909D+04    P.E.= -0.32341840D+04				
K.E.= 0.16170931D+04    V.T.= -0.19999987D+01				
S	1S	2S	P	2P
BASIS/ORB E	-453.33654	-93.75E75	BASIS/ORB E	-88.99089
1S 31.69580	0.97626	-0.329C4	2P 14.42930	0.60781
1S 54.01080	0.01089	0.00268	2P 23.49760	0.06370
2S 13.74600	0.00004	1.2175E	2P 12.70730	0.34029
2S 25.99290	0.01806	-0.22770		
ARSENIC      1S(2)2S(2)2P(4), 8-1S				
T.E.= -0.17251234D+04    P.E.= -0.34502498D+04				
K.E.= 0.17251264D+04    V.T.= -0.19999983D+01				
S	1S	2S	P	2P
BASIS/ORB E	-483.87390	-100.764E2	BASIS/ORB E	-95.80643
1S 32.71090	0.97694	-0.32857	2P 14.68450	0.63610
1S 56.06610	0.01017	0.00249	2P 23.54680	0.07437
2S 14.22780	0.00001	1.22042	2P 13.29170	0.30083
2S 26.86650	0.01804	-0.23C89		
SELENIUM      1S(2)2S(2)2P(4), 8-1S				
T.E.= -0.18366562D+04    P.E.= -0.3673136D+04				
K.E.= 0.18366574D+04    V.T.= -0.19599993D+01				
S	1S	2S	P	2P
BASIS/ORB E	-515.41165	-108.02C66	BASIS/ORB E	-102.87194
1S 33.68340	0.97789	-0.33217	2P 15.31800	0.62987
1S 57.40060	0.01037	0.00339	2P 24.69340	0.06600
2S 14.72660	-0.60001	1.22700	2P 13.69100	0.31511
2S 27.47610	0.01664	-0.23597		
BROMINE      1S(2)2S(2)2P(4), 8-1S				
T.E.= -0.19516890D+04    P.E.= -0.39033818D+04				
K.E.= 0.19516928D+04    V.T.= -0.19599981D+01				
S	1S	2S	P	2P
BASIS/ORB E	-547.94967	-115.5C686	BASIS/ORB E	-110.18745
1S 34.66780	0.97829	-0.33365	2P 15.95690	0.60418
1S 58.59580	0.01060	0.00363	2P 26.06920	0.05740
2S 15.21540	-0.00000	1.23C82	2P 14.20570	0.34901
2S 28.23840	0.01582	-0.23936		
KRYPTON      1S(2)2S(2)2P(4), 8-1S				
T.E.= -0.20702220D+04    P.E.= -0.41404476D+04				
K.E.= 0.20702256D+04    V.T.= -0.19999983D+01				
S	1S	2S	P	2P
BASIS/ORB E	-581.48752	-123.24316	BASIS/ORB E	-117.75321
1S 35.66340	0.97887	-0.33475	2P 16.48390	0.63469
1S 60.19730	0.01042	0.00375	2P 26.93010	0.05424
2S 15.70430	-0.00002	1.23444	2P 14.53660	0.32143
2S 29.01000	0.01531	-0.24282		

See page 183 for Explanation of Tables and Notes for Tables 32, 42, and 43

## ROOTHAAN-HARTREE-FOCK ATOMIC WAVEFUNCTIONS

 TABLE 16 (1). THE HARTREE-FOCK FUNCTIONS FOR F(<sup>2</sup>P) ISO-ELECTRONIC SERIES.

FLUORINE      1S(2)2S(2)2P(5), 9-2P  
 T.E.= -0.99409281D+02   P.E.= -0.19881712D+03  
 K.E.= 0.99407840D+02   V.T.= -0.20000145D+01

	S	1S	2S	P	2P
BASIS/ORB E	-26.38279	-1.57246	BASIS/ORB E	-0.72995	
1S	8.89919	0.90301	2P	0.54597	
1S	15.21420	0.03190	2P	0.33862	
2S	3.34737	0.00494	2P	0.19276	
2S	8.04521	0.08067	2P	0.01784	
2S	2.04776	-0.00094	C.52470		

NEON      1S(2)2S(2)2P(5), 9-2P  
 T.E.= -0.12781777D+03   P.E.= -0.25563410D+03  
 K.E.= 0.12781633D+03   V.T.= -0.20000113D+01

	S	1S	2S	P	2P
BASIS/ORB E	-33.61233	-2.61911	BASIS/ORB E	-1.60658	
1S	9.86116	0.91448	2P	0.58722	
1S	16.78310	0.03022	2P	0.30522	
2S	3.87930	0.00507	2P	0.16718	
2S	8.83998	0.06892	2P	0.01385	
2S	2.52757	-0.00107	0.577E3		

SODIUM      1S(2)2S(2)2P(5), 9-2P  
 T.E.= -0.15999737D+03   P.E.= -0.31999340D+03  
 K.E.= 0.15999603D+03   V.T.= -0.20000084D+01

	S	1S	2S	P	2P
BASIS/ORB E	-41.86284	-3.93051	BASIS/ORB E	-2.74425	
1S	10.84970	0.91080	2P	0.61033	
1S	17.57140	0.03546	2P	0.27983	
2S	4.37799	0.00509	2P	0.15978	
2S	9.78488	0.06675	2P	0.01042	
2S	3.00815	-0.00116	0.61458		

MAGNESIUM      1S(2)2S(2)2P(5), 9-2P  
 T.E.= -0.19594044D+03   P.E.= -0.39187905D+03  
 K.E.= 0.19593862D+03   V.T.= -0.20000093D+01

	S	1S	2S	P	2P
BASIS/ORB E	-51.12597	-5.49982	BASIS/ORB E	-4.13821	
1S	11.86860	0.92149	2P	0.62949	
1S	19.67940	0.02851	2P	0.25803	
2S	4.89691	0.00506	2P	0.15649	
2S	10.59530	0.06216	2P	0.00735	
2S	3.49941	-0.00131	0.65607		

ALUMINUM      1S(2)2S(2)2P(5), 9-2P  
 T.E.= -0.23564282D+03   P.E.= -0.47128407D+03  
 K.E.= 0.23564125D+03   V.T.= -0.20000067D+01

	S	1S	2S	P	2P
BASIS/ORB E	-61.39757	-7.32396	BASIS/ORB E	-5.78626	
1S	12.85980	0.92594	2P	0.59851	
1S	21.15160	0.02763	2P	0.23693	
2S	5.38032	0.00490	2P	0.20299	
2S	11.44010	0.05787	2P	0.00622	
2S	3.98442	-0.00140	0.68279		

SILICON      1S(2)2S(2)2P(5), 9-2P  
 T.E.= -0.27910196D+03   P.E.= -0.55820215D+03  
 K.E.= 0.27910019D+03   V.T.= -0.20000064D+01

	S	1S	2S	P	2P
BASIS/ORB E	-72.67532	-9.40137	BASIS/ORB E	-7.68718	
1S	13.79680	0.93703	2P	0.60316	
1S	22.93210	0.02553	2P	0.21026	
2S	5.97766	0.00446	2P	0.22139	
2S	12.07770	0.04738	2P	0.00492	
2S	4.49500	-0.00127	0.74211		

See page 183 for Explanation of Tables and Notes for Tables 32, 42, and 43

TABLE 16 (2). THE HARTREE-FOCK FUNCTIONS FOR F(2P) ISO-ELECTRONIC SERIES.

PHOSPHORUS      1S(2)2S(2)2P(5), 9-2P  
 T.E.= -0.32631619D+03   P.E.= -0.65263C84D+03  
 K.E.= 0.32631465D+03   V.T.= -0.20000047D+01

S	1S	2S	P	2P
BASIS/ORB E	-84.95764	-11.73106	BASIS/ORB E	-9.84017
1S 14.82490	0.93830	-0.26546	2P 5.22964	0.59937
1S 24.53000	0.02388	-0.00304	2P 8.70593	0.19758
2S 6.39108	0.00429	0.37349	2P 4.24518	0.23452
2S 12.98650	0.04776	-0.13310	2P 18.25650	0.00423
2S 4.97214	-0.00140	0.74686		

SULFUR      1S(2)2S(2)2P(5), 9-2P  
 T.E.= -0.37728436D+03   P.E.= -0.75456770D+03  
 K.E.= 0.37728334D+03   V.T.= -0.20000027D+01

S	1S	2S	P	2P
BASIS/ORB E	-98.24347	-14.31243	BASIS/ORB E	-12.24472
1S 15.86560	0.54270	-0.27566	2P 5.75887	0.59651
1S 26.71790	0.01970	-0.00183	2P 9.49283	0.18429
2S 6.93583	0.00337	0.33005	2P 4.73987	0.24603
2S 13.78000	0.04771	-0.13567	2P 19.80240	0.00365
2S 5.48549	-0.00100	0.75566		

CHLORINE      1S(2)2S(2)2P(5), 9-2P  
 T.E.= -0.43200564D+03   P.E.= -0.864C1095D+03  
 K.E.= 0.43200531D+03   V.T.= -0.20C00008D+01

S	1S	2S	P	2P
BASIS/ORB E	-112.53207	-17.14509	BASIS/ORB E	-14.90052
1S 16.86020	0.94098	-0.27585	2P 6.27029	0.57480
1S 27.77380	0.02169	-0.00397	2P 10.25730	0.17654
2S 7.42288	0.00517	0.26590	2P 5.29304	0.27538
2S 14.91660	0.04641	-0.14132	2P 21.72680	0.00294
2S 6.02175	-0.00216	0.85808		

ARGON      1S(2)2S(2)2P(5), 9-2P  
 T.E.= -0.49047941D+03   P.E.= -0.98C95852D+03  
 K.E.= 0.49047911D+03   V.T.= -0.20000006C+01

S	1S	2S	P	2P
BASIS/ORB E	-127.82301	-20.22877	BASIS/ORB E	-17.80736
1S 17.81860	0.94645	-0.28674	2P 6.77518	0.58263
1S 29.02870	0.02131	-0.001C8	2P 11.00860	0.16781
2S 7.80953	0.00262	0.32343	2P 5.77023	0.27423
2S 15.38610	0.04150	-0.14825	2P 22.98420	0.00274
2S 6.45267	-0.00082	0.81164		

POTASSIUM      1S(2)2S(2)2P(5), 9-2P  
 T.E.= -0.55270522D+03   P.E.= -0.11054088D+04  
 K.E.= 0.5527C355D+03   V.T.= -0.20000030D+01

S	1S	2S	P	2P
BASIS/ORB E	-144.11580	-23.56330	BASIS/ORB E	-20.96500
1S 18.81620	0.94828	-0.28911	2P 7.46258	0.57139
1S 30.66490	0.02068	-0.00163	2P 12.05690	0.14005
2S 8.22000	0.00365	0.30040	2P 6.20509	0.31201
2S 16.34300	0.03962	-0.15098	2P 24.56510	0.00224
2S 6.96223	-0.00164	0.83614		

CALCIUM      1S(2)2S(2)2P(5), 9-2P  
 T.E.= -0.61868274D+03   P.E.= -0.12373637D+04  
 K.E.= 0.61868094D+03   V.T.= -0.20000029D+01

S	1S	2S	P	2P
BASIS/ORB E	-161.41004	-27.14841	BASIS/ORB E	-24.37325
1S 19.81390	0.95077	-0.29296	2P 8.00223	0.56497
1S 32.30100	0.01970	-0.00127	2P 12.86760	0.13169
2S 8.70447	0.00350	0.26617	2P 6.69795	0.32536
2S 17.16530	0.03780	-0.15537	2P 26.11600	0.00198
2S 7.47554	-0.00164	0.87469		

See page 183 for Explanation of Tables and Notes for Tables 32, 42, and 43

## ROOTHAAN-HARTREE-FOCK ATOMIC WAVEFUNCTIONS

TABLE 16 (3). THE HARTREE-FOCK FUNCTIONS FOR F(2P) ISO-ELECTRONIC SERIES.

SCANDIUM	1S(2)2S(2)2P(5), 9-2P			
T.E.= -0.68841169D+03	P.E.= -0.13768223D+04			
K.E.= 0.68841058D+03	V.T.= -0.20000016D+01			
S	1S	2S	P	2P
BASIS/ORB E	-179.70547	-30.9E358	BASIS/ORB E	-28.03199
1S 20.79960	0.95384	-0.29702	2P 8.34968	0.54834
1S 34.04230	0.01874	-0.00080	2P 13.31830	0.14468
2S 9.12154	0.00382	0.25655	2P 7.30151	0.32738
2S 17.96140	0.03520	-0.15940	2P 27.77230	0.00192
2S 7.97427	-0.00204	0.88843		
TITANIUM	1S(2)2S(2)2P(5), 9-2P			
T.E.= -0.76189182D+03	P.E.= -0.15237824D+04			
K.E.= 0.76189061D+03	V.T.= -0.20000016D+01			
S	1S	2S	P	2P
BASIS/ORB E	-199.00199	-35.07003	BASIS/ORB E	-31.94121
1S 21.89230	0.95637	-0.29747	2P 8.81565	0.49879
1S 37.36660	0.01376	-0.00083	2P 13.91420	0.14760
2S 9.66506	0.00382	0.15109	2P 7.90456	0.37275
2S 18.93830	0.03794	-0.16343	2P 29.51460	0.00183
2S 8.54151	-0.00217	0.99553		
VANADIUM	1S(2)2S(2)2P(5), 9-2P			
T.E.= -0.83912298D+03	P.E.= -0.16782477D+04			
K.E.= 0.83912475D+03	V.T.= -0.19959979D+01			
S	1S	2S	P	2P
BASIS/ORB E	-219.29935	-39.4C641	BASIS/ORB E	-36.10073
1S 23.00990	0.95411	-0.29801	2P 9.44531	0.55964
1S 39.44140	0.01149	-0.00061	2P 15.03290	0.12493
2S 9.14045	0.00071	1.14659	2P 8.22418	0.33403
2S 19.92050	0.04396	-0.16617	2P 32.00680	0.00132
CHROMIUM	1S(2)2S(2)2P(5), 9-2P			
T.E.= -0.92010502D+03	P.E.= -0.18402C580+04			
K.E.= 0.92010478D+03	V.T.= -0.20000003D+01			
S	1S	2S	P	2P
BASIS/ORB E	-240.59764	-43.99318	BASIS/ORB E	-40.51070
1S 23.95170	0.95859	-0.30303	2P 9.83446	0.44246
1S 41.28330	0.01134	0.00015	2P 15.23870	0.14360
2S 9.62617	0.00064	1.15381	2P 8.95673	0.43117
2S 20.56710	0.03884	-0.17111	2P 33.70520	0.00162
MANGANESE	1S(2)2S(2)2P(5), 9-2P			
T.E.= -0.10048378D+04	P.E.= -0.20096748D+04			
K.E.= 0.10048370D+04	V.T.= -0.20000009D+01			
S	1S	2S	P	2P
BASIS/ORB E	-262.89667	-48.83C29	BASIS/ORB E	-45.17106
1S 24.94700	0.96064	-0.30517	2P 10.63480	0.45247
1S 43.15310	0.01075	0.00015	2P 16.40930	0.11788
2S 10.10720	0.00055	1.15925	2P 9.32921	0.44635
2S 21.35820	0.03708	-0.17644	2P 35.45800	0.00134
IRON	1S(2)2S(2)2P(5), 9-2P			
T.E.= -0.10933213D+04	P.E.= -0.21866450D+04			
K.E.= 0.10933237D+04	V.T.= -0.19959978D+01			
S	1S	2S	P	2P
BASIS/ORB E	-286.19614	-53.91748	BASIS/ORB E	-50.08156
1S 25.93670	0.96227	-0.30713	2P 10.56620	0.71092
1S 44.74550	0.01055	0.00009	2P 16.78830	0.13432
2S 10.58830	0.00048	1.1C432	2P 9.65676	0.17053
2S 22.15850	0.03532	-0.18134	2P 36.95710	0.00122

See page 183 for Explanation of Tables and Notes for Tables 32, 42, and 43

TABLE 16 (4). THE HARTREE-FOCK FUNCTIONS FOR F(<sup>2</sup>P) ISO-ELECTRONIC SERIES.

COBALT            1S(2)2S(2)2P(5), 9-2P				
T.E.= -0.11855552D+04    P.E.= -0.23711135D+04				
K.E.= 0.11855583D+04    V.T.= -0.19999974D+01				
S	1S	2S	P	2P
BASIS/ORB E	-310.49592	-59.25495	BASIS/ORB E	-55.24229
1S 26.93980	0.96431	-0.30915	2P 11.78950	0.53210
1S 47.01170	0.00962	0.00023	2P 19.17560	0.08465
2S 11.07170	0.00038	1.16558	2P 10.15990	0.39960
2S 22.93130	0.03400	-0.18645		
NICKEL            1S(2)2S(2)2P(5), 9-2P				
T.E.= -0.12815397D+04    P.E.= -0.25630773D+04				
K.E.= 0.12815376D+04    V.T.= -0.20000017D+01				
S	1S	2S	P	2P
BASIS/ORB E	-335.79632	-64.84255	BASIS/ORB E	-60.65318
1S 27.88550	0.96746	-0.31420	2P 12.44030	0.36077
1S 48.67930	0.00969	0.00137	2P 19.46150	0.09328
2S 11.56580	0.00030	1.17730	2P 10.95430	0.56149
2S 23.48670	0.03022	-0.19160		
COPPER            1S(2)2S(2)2P(5), 9-2P				
T.E.= -0.13812748D+04    P.E.= -0.27625511D+04				
K.E.= 0.13812763D+04    V.T.= -0.19999990D+01				
S	1S	2S	P	2P
BASIS/ORB E	-362.05737	-70.6827	BASIS/ORB E	-66.31424
1S 28.87550	0.96896	-0.31623	2P 12.81930	0.52679
1S 50.49550	0.00937	0.00154	2P 20.73660	0.07982
2S 12.05150	0.00024	1.18242	2P 11.14320	0.40839
2S 24.24000	0.02878	-0.19630		
ZINC            1S(2)2S(2)2P(5), 9-2P				
T.E.= -0.14847602D+04    P.E.= -0.29655196D+04				
K.E.= 0.14847594D+04    V.T.= -0.2000006D+01				
S	1S	2S	P	2P
BASIS/ORB E	-389.39856	-76.76820	BASIS/ORB E	-72.22550
1S 29.86760	0.97055	-0.31835	2P 13.38040	0.42177
1S 52.54380	0.00890	0.00180	2P 21.12370	0.08574
2S 12.53900	0.00018	1.19770	2P 11.84720	0.50684
2S 24.96940	0.02743	-0.2016		
GALLIUM            1S(2)2S(2)2P(5), 9-2P				
T.E.= -0.15919961D+04    P.E.= -0.31839947D+04				
K.E.= 0.15919987D+04    V.T.= -0.19999984D+01				
S	1S	2S	P	2P
BASIS/ORB E	-417.70025	-83.10619	BASIS/ORB E	-78.38684
1S 30.86840	0.97167	-0.31566	2P 13.84570	0.51918
1S 54.55440	0.00845	0.00180	2P 22.27250	0.07596
2S 13.02400	0.00013	1.19203	2P 12.13500	0.41872
2S 25.75760	0.02658	-0.20538		
GERMANIUM            1S(2)2S(2)2P(5), 9-2P				
T.E.= -0.17029822D+04    P.E.= -0.34059668D+04				
K.E.= 0.17029846D+04    V.T.= -0.19999986D+01				
S	1S	2S	P	2P
BASIS/ORB E	-447.00216	-89.69430	BASIS/ORB E	-84.79833
1S 31.85010	0.97280	-0.32174	2P 14.29350	0.55228
1S 56.03400	0.00849	0.00268	2P 23.05490	0.07411
2S 13.51210	0.00010	1.15689	2P 12.55900	0.38697
2S 26.48840	0.02516	-0.20557		

See page 183 for Explanation of Tables and Notes for Tables 32, 42, and 43

## ROOCHAAN-HARTREE-FOCK ATOMIC WAVEFUNCTIONS

 TABLE 16 (5). THE HARTREE-FOCK FUNCTIONS FOR F(<sup>2</sup>P) ISO-ELECTRONIC SERIES.

ARSENIC	1S(2)2S(2)2P(5), S-2P			
T.E.= -0.18177186D+04	P.E.= -0.36354399D+04			
K.E.= 0.18177213D+04	V.T.= -0.15559985D+01			
S	1S	2S	P	2P
BASIS/ORB E	-477.3042E	-96.53253	BASIS/ORB E	-91.45994
1S 32.84500	0.97375	-0.32312	2P 14.62740	0.61984
1S 57.82030	0.00825	0.00216	2P 23.63860	0.07605
2S 13.99840	0.00007	1.20105	2P 12.93090	0.31699
2S 27.26270	0.02426	-0.21352		
SELENIUM	1S(2)2S(2)2P(5), 9-2P			
T.E.= -0.19362053D+04	P.E.= -0.38724075D+04			
K.E.= 0.19362022D+04	V.T.= -0.20000C016D+01			
S	1S	2S	P	2P
BASIS/ORB E	-508.60659	-103.62054	BASIS/ORB E	-98.37170
1S 33.81740	0.9748E	-0.32575	2P 15.35200	0.45554
1S 59.13550	0.00845	0.00271	2P 24.09580	0.07854
2S 14.49120	0.00004	1.20E52	2P 13.74870	0.47836
2S 27.92900	0.02266	-0.21786		
BROMINE	1S(2)2S(2)2P(5), 9-2P			
T.E.= -0.20584422D+04	P.E.= -0.41168808D+04			
K.E.= 0.20584386D+C4	V.T.= -0.20000017D+01			
S	1S	2S	P	2P
BASIS/ORB E	-540.90923	-110.95932	BASIS/ORB E	-105.53349
1S 34.81120	0.97571	-0.32710	2P 15.89020	0.44678
1S 60.87240	0.00827	0.00263	2P 24.88920	0.07610
2S 14.97890	0.00001	1.21C54	2P 14.24980	0.48915
2S 28.69140	0.C2185	-0.22163		
KRYPTON	1S(2)2S(2)2P(5), S-2P			
T.E.= -0.21844293D+04	P.E.= -0.43688603D+04			
K.E.= 0.21844310D+04	V.T.= -0.19999992D+01			
S	1S	2S	P	2P
BASIS/ORB E	-574.21193	-118.54770	BASIS/ORB E	-112.94530
1S 35.82290	0.97632	-0.32731	2P 16.36560	0.36026
1S 62.98430	0.00778	0.00256	2P 25.34410	0.08076
2S 15.46160	-0.00002	1.21319	2P 14.93590	0.57055
2S 29.54480	0.C2165	-0.22477		

See page 183 for Explanation of Tables and Notes for Tables 32, 42, and 43

TABLE 17 (1). THE HARTREE-FOCK FUNCTIONS FOR Ne(<sup>1</sup>S) ISO-ELECTRONIC SERIES.

NEON	1S(2)2S(2)2P(6), 1C-1S			
T.E.= -0.12854703G+03	P.E.= -0.25709394D+03			
K.E.= 0.12854691D+03	V.T.= -0.2000G001D+01			
S	1S	2S	P	2P
BASIS/ORB E	-32.77256	-1.93C46	BASIS/ORB E	-0.85045
1S 8.77448	1.02868	-0.22063	2P 2.39255	0.52287
1S 14.73560	0.06436	-0.02452	2P 4.47585	0.33033
2S 3.82552	0.00507	0.54854	2P 1.46748	0.22749
2S 9.34819	-0.10242	-0.07017	2P 9.19774	0.01869
2S 2.32660	-0.00071	0.55550		
SGODIUM	1S(2)2S(2)2P(6), 1C-1S			
T.E.= -0.16167692D+03	P.E.= -0.32335484D+03			
K.E.= 0.16167793D+03	V.T.= -0.19995938D+01			
S	1S	2S	P	2P
BASIS/ORB E	-40.75964	-3.07365	BASIS/ORB E	-1.79715
1S 9.60854	1.04471	-0.23717	2P 2.89481	0.54279
1S 16.19560	0.06184	-0.02342	2P 5.265C9	0.30481
2S 4.38717	0.00584	0.48735	2P 1.95889	0.21629
2S 10.20650	-0.11882	-0.07C38	2P 1C.69400	0.01413
2S 2.81650	-0.00106	0.616C4		
MAGNESIUM	1S(2)2S(2)2P(6), 1C-1S			
T.E.= -0.19883077D+03	P.E.= -0.35766062D+03			
K.E.= 0.19882984D+03	V.T.= -0.20000047D+01			
S	1S	2S	P	2P
BASIS/ORB E	-49.76880	-4.48256	BASIS/ORB E	-3.00617
1S 11.44730	0.89822	-0.22446	2P 3.40554	0.55496
1S 17.00270	0.07634	-0.01556	2P 6.05091	0.28364
2S 4.97455	0.00675	0.43898	2P 2.44651	0.21606
2S 10.70430	0.03263	-0.1C768	2P 12.58860	0.01021
2S 3.30779	-0.00143	0.66551		
ALUMINUM	1S(2)2S(2)2P(6), 1C-1S			
T.E.= -0.24000032D+03	P.E.= -0.48000001D+03			
K.E.= 0.23999968D+03	V.T.= -0.20000027D+01			
S	1S	2S	P	2P
BASIS/ORB E	-59.79114	-6.15105	BASIS/ORB E	-4.47222
1S 12.81930	0.90480	-0.23417	2P 3.92330	0.56284
1S 19.46880	0.04457	-0.01226	2P 6.83553	0.26314
2S 5.50851	0.00547	0.35E68	2P 2.93879	0.22166
2S 11.65060	0.06224	-0.12065	2P 14.24410	0.00803
2S 3.79920	-0.00102	0.71041		
SILICON	1S(2)2S(2)2P(6), 10-1S			
T.E.= -0.28518091D+03	P.E.= -0.57C36096D+03			
K.E.= 0.28518005D+03	V.T.= -0.20000030D+01			
S	1S	2S	P	2P
BASIS/ORB E	-70.82276	-8.07468	BASIS/ORB E	-6.19291
1S 13.81770	0.91333	-0.24408	2P 4.44563	0.56567
1S 21.22170	0.03966	-0.01032	2P 7.61787	0.24500
2S 6.00648	0.00596	0.37121	2P 3.43541	0.23169
2S 12.53060	0.05759	-0.12339	2P 15.87970	0.00649
2S 4.28480	-0.00144	C.73512		
PHOSPHORUS	1S(2)2S(2)2P(6), 10-1S			
T.E.= -0.33436963D+03	P.E.= -0.66873746D+03			
K.E.= 0.33436783D+03	V.T.= -0.20000054D+01			
S	1S	2S	P	2P
BASIS/ORB E	-82.86118	-10.25211	BASIS/ORB E	-8.16689
1S 14.73800	0.92880	-0.26258	2P 4.93758	0.58581
1S 22.87610	0.03534	-0.00445	2P 8.37781	0.23192
2S 6.66055	0.00423	0.33341	2P 3.88898	0.22070
2S 12.94030	0.04535	-0.12839	2P 17.79440	0.00522
2S 4.78517	-0.00067	0.78751		

See page 183 for Explanation of Tables and Notes for Tables 32, 42, and 43

## ROOTHAAN-HARTREE-FOCK ATOMIC WAVEFUNCTIONS

 TABLE 17 (2). THE HARTREE-FOCK FUNCTIONS FOR Ne(<sup>1</sup>S) ISO-ELECTRONIC SERIES.

**SULFUR**      **1S(2)2S(2)2P(6), 1C-1S**  
 T.E.= -0.387564598D+03 P.E.= -0.77512807D+03  
 K.E.= 0.38756349D+03 V.T.= -0.20000C28D+01

	S	1S	2S	P	2P
BASIS/ORB E	-95.90459	-12.68216	BASIS/ORB E	-10.39324	
1S 15.77510	0.93182	-0.26E55	2P 5.51211	0.54918	
1S 24.56060	0.03174	-0.00366	2P 9.18537	0.21473	
2S 7.16162	0.00399	0.30546	2P 4.45918	0.27116	
2S 13.82900	0.04596	-0.13272	2P 19.41840	0.00428	
2S 5.27562	-0.00071	0.81391			

**CHLORINE**      **1S(2)2S(2)2P(6), 10-1S**  
 T.E.= -0.44476439D+03 P.E.= -0.88552811D+03  
 K.E.= 0.44476372D+03 V.T.= -0.20000C15D+01

	S	1S	2S	P	2P
BASIS/ORB E	-109.95204	-15.34426	BASIS/ORB E	-12.87144	
1S 16.85690	0.93143	-0.27C21	2P 6.04280	0.54109	
1S 26.21510	0.02831	-0.00412	2P 9.96001	0.20234	
2S 7.65369	0.00373	0.27863	2P 4.96587	0.28879	
2S 14.84770	0.05031	-0.13726	2P 21.01180	0.00367	
2S 5.77652	-0.00070	0.84493			

**ARGON**      **1S(2)2S(2)2P(6), 10-1S**  
 T.E.= -0.50596808D+03 P.E.= -0.10119360D+04  
 K.E.= 0.50596790D+03 V.T.= -0.20000030D+01

	S	1S	2S	P	2P
BASIS/ORB E	-125.00269	-18.25788	BASIS/ORB E	-15.60110	
1S 17.95820	0.93002	-0.27C45	2P 6.57298	0.53243	
1S 27.89950	0.02504	-0.00453	2P 10.73330	0.19139	
2S 8.15476	0.00347	0.24113	2P 5.47203	0.30602	
2S 15.90640	0.05566	-0.14187	2P 22.63460	0.00317	
2S 6.28713	-0.00066	0.88230			

**POTASSIUM**      **1S(2)2S(2)2P(6), 10-1S**  
 T.E.= -0.57117491D+03 P.E.= -0.11423488D+04  
 K.E.= 0.57117387D+03 V.T.= -0.20000C018D+01

	S	1S	2S	P	2P
BASIS/ORB E	-141.05597	-21.48268	BASIS/ORB E	-18.58189	
1S 18.82300	0.94158	-0.28465	2P 7.10142	0.52413	
1S 29.58400	0.02459	-0.00107	2P 11.50370	0.18170	
2S 8.55782	0.0314	0.265E5	2P 5.97657	0.32197	
2S 16.33510	0.04294	-0.14439	2P 24.25680	0.00276	
2S 6.73983	-0.00072	0.86694			

**CALCIUM**      **1S(2)2S(2)2P(6), 10-1S**  
 T.E.= -0.64038435D+03 P.E.= -0.12807678D+04  
 K.E.= 0.64038343D+03 V.T.= -0.20000014D+01

	S	1S	2S	P	2P
BASIS/ORB E	-158.11140	-24.91852	BASIS/ORB E	-21.81368	
1S 20.01890	0.93407	-0.27700	2P 7.68935	0.53558	
1S 31.23850	0.02142	-0.00461	2P 12.39460	0.16389	
2S 9.06389	0.00336	0.19282	2P 6.41531	0.32675	
2S 17.75370	0.05495	-0.14813	2P 25.84840	0.00235	
2S 7.29121	-0.00088	0.93421			

**SCANDIUM**      **1S(2)2S(2)2P(6), 10-1S**  
 T.E.= -0.71359594D+03 P.E.= -0.14271904D+04  
 K.E.= 0.71359444D+03 V.T.= -0.20000021D+01

	S	1S	2S	P	2P
BASIS/ORB E	-176.16859	-28.60506	BASIS/ORB E	-25.29619	
1S 20.89600	0.94417	-0.28945	2P 8.21852	0.53072	
1S 32.92300	0.02088	-0.00109	2P 13.17820	0.15588	
2S 9.46396	0.00263	0.22392	2P 6.91134	0.33806	
2S 18.17240	0.04421	-0.15149	2P 27.46930	0.00207	
2S 7.74265	-0.00067	0.91276			

See page 183 for Explanation of Tables and Notes for Tables 32, 42, and 43

TABLE 17 (3). THE HARTREE-FOCK FUNCTIONS FOR Ne(<sup>1</sup>S) ISO-ELECTRONIC SERIES.

TITANIUM      1S(2)2S(2)2P(6), 10-1S  
 T.E.= -0.790809370+03   P.E.= -0.15216181D+04  
 K.E.= 0.790808750+03   V.T.= -0.200000080D+01

S	1S	2S	P	2P
BASIS/ORB E	-195.22715	-32.54218	BASIS/ORB E	-29.02924
1S 21.83860	0.94655	-0.29C55	2P 8.71338	0.51895
1S 34.46940	0.02189	-0.00235	2P 13.90350	0.15238
2S 9.91729	0.00522	0.16132	2P 7.43780	0.35187
2S 19.23400	0.03916	-0.15043	2P 28.94610	0.00187
2S 8.29184	-0.00239	0.97365		

VANADIUM      1S(2)2S(2)2P(6), 10-1S  
 T.E.= -0.87202429D+03   P.E.= -0.17440504D+04  
 K.E.= 0.87202606D+03   V.T.= -0.19999980D+01

S	1S	2S	P	2P
BASIS/ORB E	-215.28688	-36.72971	BASIS/ORB E	-33.01272
1S 23.27050	0.93470	-0.28433	2P 9.28081	0.49193
1S 36.98190	0.01399	-0.00276	2P 14.74090	0.14418
2S 8.93416	0.00118	1.12773	2P 7.97359	0.38612
2S 20.64240	0.06350	-0.15407	2P 31.91940	0.00139

CHROMIUM      1S(2)2S(2)2P(6), 10-1S  
 T.E.= -0.95724065D+03   P.E.= -0.19144833D+04  
 K.E.= 0.95724260D+03   V.T.= -0.19999980D+01

S	1S	2S	P	2P
BASIS/ORB E	-236.34798	-41.16798	BASIS/ORB E	-37.24699
1S 24.18320	0.94037	-0.28811	2P 9.79447	0.48500
1S 38.70640	0.01436	-0.00256	2P 15.48350	0.13967
2S 9.41091	0.00121	1.13323	2P 8.47655	0.39639
2S 21.41760	0.05632	-0.15785	2P 33.54850	0.00127

MANGANESE      1S(2)2S(2)2P(6), 10-1S  
 T.E.= -0.10464581D+04   P.E.= -0.20525208D+04  
 K.E.= 0.10464626D+04   V.T.= -0.19999957D+01

S	1S	2S	P	2P
BASIS/ORB E	-258.40999	-45.65659	BASIS/ORB E	-41.73165
1S 25.17160	0.94434	-0.29193	2P 10.33870	0.47775
1S 40.40080	0.01320	-0.00232	2P 16.28740	0.13291
2S 9.89093	0.00096	1.13911	2P 8.97294	0.40943
2S 22.14240	0.05311	-0.16271	2P 35.24700	0.00113

IRON      1S(2)2S(2)2P(6), 10-1S  
 T.E.= -0.11396766D+04   P.E.= -0.22793542D+04  
 K.E.= 0.11396776D+04   V.T.= -0.19999991D+01

S	1S	2S	P	2P
BASIS/ORB E	-281.47288	-50.79547	BASIS/ORB E	-46.46656
1S 26.03750	0.95190	-0.30068	2P 10.64670	0.50865
1S 42.10530	0.01355	-0.00017	2P 16.72340	0.14169
2S 10.38010	0.00084	1.14688	2P 9.46485	0.36858
2S 22.61850	0.04394	-0.16539	2P 36.87490	0.00125

COBALT      1S(2)2S(2)2P(6), 10-1S  
 T.E.= -0.12368959D+04   P.E.= -0.24737888D+04  
 K.E.= 0.12368929D+04   V.T.= -0.20000025D+01

S	1S	2S	P	2P
BASIS/ORB E	-305.53657	-55.65480	BASIS/ORB E	-51.45192
1S 26.98110	0.95399	-0.30031	2P 11.39250	0.49675
1S 43.82980	0.01431	-0.00180	2P 17.83780	0.12144
2S 10.85260	0.00109	1.15006	2P 9.88752	0.40013
2S 23.58450	0.04026	-0.16926	2P 36.57220	0.00102

See page 183 for Explanation of Tables and Notes for Tables 32, 42, and 43

## ROOTHAAN-HARTREE-FOCK ATOMIC WAVEFUNCTIONS

 TABLE 17 (4). THE HARTREE-FOCK FUNCTIONS FOR Ne(<sup>1</sup>S) ISO-ELECTRONIC SERIES.

NICKEL            1S(2)2S(2)2P(6), 1C-1S T.E.= -0.13381161D+04 P.E.= -0.267E2326D+04 K.E.= 0.13381166D+04 V.T.= -0.15599956D+01				
S	1S	2S	P	2P
BASIS/ORB E	-330.60068	-61.42419	BASIS/ORB E	-56.68744
1S 27.98280	0.95568	-0.30151	2P 11.92670	0.33890
1S 45.52420	0.01366	-0.00208	2P 18.22080	0.13252
2S 11.33090	0.00101	1.15437	2P 10.66820	0.54589
2S 24.42250	0.03898	-0.17391	2P 40.26880	0.00104
COPPER            1S(2)2S(2)2P(6), 1C-1S T.E.= -0.14433368D+04 P.E.= -0.28866773D+04 K.E.= 0.14433405D+04 V.T.= -0.19999574D+01				
S	1S	2S	P	2P
BASIS/ORB E	-356.66508	-67.11360	BASIS/ORB E	-62.17316
1S 29.00140	0.95904	-0.30676	2P 12.62150	0.48701
1S 47.68870	0.01160	-0.00015	2P 20.23420	0.09632
2S 11.82220	0.00063	1.16140	2P 10.87710	0.43429
2S 24.97490	0.03769	-0.17511		
ZINC            1S(2)2S(2)2P(6), 1C-1S T.E.= -0.15525582D+04 P.E.= -0.31051148D+04 K.E.= 0.15525566D+04 V.T.= -0.20000010D+01				
S	1S	2S	P	2P
BASIS/ORB E	-383.73044	-73.05367	BASIS/ORB E	-67.90914
1S 29.93510	0.96142	-0.30798	2P 13.16770	0.47630
1S 49.43320	0.01222	-0.00082	2P 21.03230	0.09291
2S 12.29990	0.00083	1.16494	2P 11.38040	0.44769
2S 25.83570	0.05391	-0.18221		
GALLIUM            1S(2)2S(2)2P(6), 10-1S T.E.= -0.16657801D+04 P.E.= -0.33315586D+04 K.E.= 0.16657784D+04 V.T.= -0.20000010D+01				
S	1S	2S	P	2P
BASIS/ORB E	-411.79613	-79.24367	BASIS/ORB E	-73.89529
1S 30.91520	0.96336	-0.31037	2P 13.61780	0.48432
1S 51.14760	0.01190	-0.00050	2P 21.70400	0.09296
2S 12.78400	0.00076	1.16567	2P 11.86660	0.43897
2S 26.57750	0.03199	-0.18623		
GERMANIUM            1S(2)2S(2)2P(6), 1C-1S T.E.= -0.178300260D+04 P.E.= -0.35659586D+04 K.E.= 0.17829960D+04 V.T.= -0.20000037D+01				
S	1S	2S	P	2P
BASIS/ORB E	-440.86214	-85.68393	BASIS/ORB E	-80.13165
1S 31.89840	0.96633	-0.31726	2P 14.18330	0.40966
1S 52.86210	0.01095	0.00207	2P 22.13330	0.09758
2S 13.28720	0.00039	1.17E47	2P 12.49270	0.50840
2S 26.94220	0.02987	-0.19175		
ARSENIC            1S(2)2S(2)2P(6), 10-1S T.E.= -0.190422550D+04 P.E.= -0.380E4535D+04 K.E.= 0.19042279D+04 V.T.= -0.19999987D+01				
S	1S	2S	P	2P
BASIS/ORB E	-470.92853	-92.37404	BASIS/ORB E	-86.61795
1S 32.89630	0.96767	-0.31E62	2P 14.79900	0.35042
1S 54.75320	0.01043	0.00210	2P 22.91700	0.09524
2S 13.77160	0.00034	1.182E5	2P 13.09320	0.56936
2S 27.72120	0.02887	-0.19584		

See page 183 for Explanation of Tables and Notes for Tables 32, 42, and 43

TABLE 17 (5). THE HARTREE-FOCK FUNCTIONS FOR Ne(<sup>1</sup>S) ISO-ELECTRONIC SERIES.

SELENIUM	1S(2)2S(2)2P(6), 1C-1S			
T.E.= -0.20294487D+04	P.E.= -0.40589064D+04			
K.E.= 0.20254577D+04	V.T.= -0.19959556D+01			
S	1S	2S	P	2P
BASIS/ORB E	-501.99527	-99.31427	BASIS/ORB E	-93.35443
1S 33.86310	0.96793	-0.31593	2P 15.34830	0.30097
1S 56.50970	0.01070	0.00014	2P 23.67910	0.09411
2S 14.23710	0.00059	1.18250	2P 13.68750	0.61931
2S 28.85930	0.02793	-0.15778		
EROMINE	1S(2)2S(2)2P(6), 10-1S			
T.E.= -0.21586725D+04	P.E.= -0.43173573D+04			
K.E.= 0.21586848D+04	V.T.= -0.19959543D+01			
S	1S	2S	P	2P
BASIS/ORB E	-534.06250	-106.50480	BASIS/ORB E	-100.34113
1S 34.88260	0.96974	-0.32121	2P 15.78280	0.40163
1S 58.05920	0.00997	0.00215	2P 24.72190	0.08554
2S 14.74030	0.00026	1.19035	2P 13.99490	0.52683
2S 29.29150	0.02688	-0.20326		
KRYPTON	1S(2)2S(2)2P(6), 1C-1S			
T.E.= -0.22918964D+04	P.E.= -0.45837967D+04			
K.E.= 0.22919003D+04	V.T.= -0.19959563D+01			
S	1S	2S	P	2P
BASIS/ORB E	-567.12995	-113.94541	BASIS/ORB E	-107.57797
1S 35.82840	0.97080	-0.32110	2P 16.04260	0.45099
1S 59.60100	0.01067	0.00125	2P 25.27310	0.08863
2S 15.21590	0.00050	1.19206	2P 14.45950	0.47388
2S 30.22830	0.02454	-0.20520		

TABLE 18 NUMBER OF ATOMS 26

See page 183 for Explanation of Tables and Notes for Tables 32, 42, and 43

## ROOTHAAN-HARTREE-FOCK ATOMIC WAVEFUNCTIONS

 TABLE 18 (1). THE HARTREE-FOCK FUNCTIONS FOR  $\text{Na}({}^2\text{S})$  ISO-ELECTRONIC SERIES.

SODIUM K(2)L(8)3S(1) - 2S					
T.E.= -0.16185859D+03 P.E.= -0.32371655D+03					
K.E.= 0.16185797D+03 V.T.= -0.20000038D+01					
S	1S	2S	3S	P	2P
BASIS/ORB E	-40.47837	-2.75700	-0.18197	BASIS/ORB E	-1.51815
1S 11.15330	0.89487	-0.218C2	0.03260	2P 2.29454	0.55155
1S 18.70360	0.02251	-0.00573	0.00092	2P 4.26424	0.46248
2S 4.06872	0.00449	0.81820	-0.13256	2P 7.94307	0.06390
2S 9.99041	0.10061	-0.11111	0.01795		
3S 1.18620	0.00029	0.00C19	0.34870		
3S 0.72354	-0.00015	0.00C44	0.71188		
3S 3.08130	-0.00086	0.31060	-0.05734		
MAGNESIUM K(2)L(8)3S(1) - 2S					
T.E.= -0.19937151D+03 P.E.= -0.39874194D+03					
K.E.= 0.19937042D+03 V.T.= -0.20000055D+01					
S	1S	2S	3S	P	2P
BASIS/ORB E	-49.35642	-4.CE567	-0.54128	BASIS/CRB E	-2.60258
1S 12.16010	0.89679	-0.22539	0.05115	2P 2.83019	0.60377
1S 19.88220	0.02391	-0.00661	0.00160	2P 5.12522	0.42107
2S 4.52530	0.00483	0.83069	-0.20582	2P 9.56577	0.04058
2S 10.93280	0.09625	-0.11655	0.02873		
3S 1.41355	0.00054	-0.00077	0.65000		
3S 1.06321	-0.00035	0.00129	0.40655		
3S 3.55363	-0.00115	0.29691	-0.09583		
ALUMINUM K(2)L(8)3S(1) - 2S					
T.E.= -0.24103044D+03 P.E.= -0.48206074D+03					
K.E.= 0.241C3030D+03 V.T.= -0.20000060D+01					
S	1S	2S	3S	P	2P
BASIS/ORB E	-59.26470	-5.65249	-1.03088	BASIS/CRB E	-3.96395
1S 13.16350	0.89974	-0.23339	0.06575	2P 3.34979	0.63835
1S 21.20500	0.02450	-0.00665	0.00141	2P 5.90995	0.38807
2S 4.90029	0.00511	0.87218	-0.26274	2P 11.02820	0.03000
2S 11.88950	0.09175	-0.11944	0.03479		
3S 1.72058	0.00091	-0.00607	0.82888		
3S 1.38268	-0.00062	0.0C466	0.25014		
3S 3.93106	-0.00156	0.25303	-0.12792		
SILICON K(2)L(8)3S(1) - 2S					
T.E.= -0.28682122D+03 P.E.= -0.57364426D+03					
K.E.= 0.28682304D+03 V.T.= -0.19999936D+01					
S	1S	2S	3S	P	2P
BASIS/ORB E	-70.18814	-7.48208	-1.64124	BASIS/ORB E	-5.58653
1S 14.05720	0.91580	-0.24872	0.C7968	2P 3.85948	0.66276
1S 22.78600	0.02319	-0.00388	0.00043	2P 6.63588	0.36099
2S 5.41618	0.00405	0.869C5	-0.29458	2P 12.16410	0.02591
2S 12.50920	0.07503	-0.12090	0.03919		
3S 1.97882	0.00011	0.00127	1.09556		
3S 4.49554	-0.00093	0.25948	-0.16221		
PHOSPHORUS K(2)L(8)3S(1) - 2S					
T.E.= -0.33673713D+03 P.E.= -0.67348402D+03					
K.E.= 0.33674690D+03 V.T.= -0.19999710D+01					
S	1S	2S	3S	P	2P
BASIS/ORB E	-82.12144	-9.56945	-2.36850	BASIS/ORB E	-7.46631
1S 15.35830	0.89640	-0.24C52	0.08391	2P 4.36220	0.67970
1S 24.26260	0.02062	-0.00745	0.00154	2P 7.32010	0.34128
2S 5.69789	0.00454	0.93127	-0.34389	2P 13.32740	0.02334
2S 13.86130	C.0987	-0.12148	0.04612		
3S 2.32056	0.00019	-0.00025	1.13267		
3S 4.78544	-0.00136	0.18E55	-0.17903		

See page 183 for Explanation of Tables and Notes for Tables 32, 42, and 43

TABLE 18 (2). THE HARTREE-FOCK FUNCTIONS FOR Na(<sup>2</sup>S) ISO-ELECTRONIC SERIES.

SULFUR K(2)L(8)3S(1) - 2S							
T.E.=-0.39077424D+03 P.E.=-0.78155C82D+03				K.E.= 0.39077658D+03 V.T.=-0.19999940D+01			
S	1S	2S	3S		P		2P
BASIS/ORB E	-95.06338	-11.91286	-3.21093	BASIS/CRB E	-9.60168		
1S 16.49640	0.89417	-0.24232	0.09091	2P 4.85700	0.69415		
1S 25.54150	0.01801	-0.00803	0.00123	2P 8.00112	0.32404		
2S 6.11693	0.00338	0.95595	-0.37304	2P 14.21410	0.02207		
2S 14.81100	0.10587	-0.13948	0.05085				
3S 2.65778	0.00007	-0.00045	1.16657				
3S 5.20861	-0.00079	0.16496	-0.20921				
 CHLORINE K(2)L(8)3S(1) - 2S							
T.E.=-0.44893008D+03 P.E.=-0.89787105D+03				K.E.= 0.44894098D+03 V.T.=-0.19999757D+01			
S	1S	2S	3S		P		2P
BASIS/ORB E	-109.00882	-14.5C854	-4.16702	BASIS/ORB E	-11.98919		
1S 17.28670	0.90905	-0.25288	-0.09950	2P 5.35157	0.70417		
1S 26.99510	0.02077	-0.0C764	-0.00102	2P 8.64429	0.31174		
2S 6.52247	0.00401	0.98640	0.40352	2P 15.32430	0.02083		
2S 15.58080	0.08493	-0.13862	-0.05286				
3S 2.99425	0.00019	-0.00087	-1.20212				
3S 5.58273	-0.00131	0.13654	0.23539				
 ARGON K(2)L(8)3S(1) - 2S							
T.E.=-0.51120296D+03 P.E.=-0.10224141D+04				K.E.= 0.51121119D+03 V.T.=-0.19999839D+01			
S	1S	2S	3S		P		2P
BASIS/ORB E	-123.95933	-17.35750	-5.23636	BASIS/CRB E	-14.62962		
1S 18.14840	0.91995	-0.26368	-0.10609	2P 5.84181	0.71224		
1S 28.22350	0.02227	-0.0C605	-0.00117	2P 9.27105	0.30102		
2S 6.89720	0.00361	1.02689	0.44232	2P 16.20960	0.02062		
2S 16.27520	0.07063	-0.13864	-0.05714				
3S 3.33725	0.00021	-0.00158	-1.24724				
3S 5.82644	-0.00123	0.09806	0.26029				
 POTASSIUM K(2)L(8)3S(1) - 2S							
T.E.=-0.57759166D+03 P.E.=-0.11551933D+04				K.E.= 0.57760163D+03 V.T.=-0.19999827D+01			
S	1S	2S	3S		P		2P
BASIS/ORB E	-139.91277	-20.45625	-6.41832	BASIS/ORB E	-17.52188		
1S 19.22060	0.51839	-0.26368	-0.10853	2P 6.33360	0.71973		
1S 29.59180	0.02146	-0.0C743	-0.00216	2P 9.88230	0.29043		
2S 7.29139	0.00343	1.05170	0.46997	2P 16.94510	0.02124		
2S 17.29320	0.07325	-0.14405	-0.06229				
3S 3.67745	0.00022	-0.00118	-1.28810				
3S 6.15711	-0.00121	0.07247	0.28815				
 CALCIUM K(2)L(8)3S(1) - 2S							
T.E.=-0.64809526D+03 P.E.=-0.12961751D+04				K.E.= 0.64807979D+03 V.T.=-0.2000C239D+01			
S	1S	2S	3S		P		2P
BASIS/ORB E	-156.87058	-23.81177	-7.71271	BASIS/CRB E	-20.66682		
1S 20.27160	0.91817	-0.26495	-0.11050	2P 6.81966	0.72593		
1S 31.08090	0.02076	-0.0C817	-0.00320	2P 10.49770	0.28180		
2S 7.67444	0.00354	1.07516	0.49560	2P 17.61880	0.02166		
2S 18.31310	0.07406	-0.14722	-0.06669				
3S 4.00498	0.00026	0.00095	-1.31619				
3S 6.55662	-0.00137	0.04569	0.30228				
 SCANDIUM K(2)L(8)3S(1) - 2S							
T.E.=-0.72271309D+03 P.E.=-0.14454282D+04				K.E.= 0.72271510D+03 V.T.=-0.19999572D+01			
S	1S	2S	3S		P		2P
BASIS/ORB E	-174.82791	-27.41480	-9.11898	BASIS/ORB E	-24.06120		
1S 21.13780	0.92801	-0.27245	-0.11652	2P 7.30909	0.73031		
1S 32.36540	0.02138	-0.0C745	-0.00269	2P 11.09470	0.27645		
2S 8.18767	0.00294	1.07779	0.50660	2P 18.76240	0.02071		
2S 18.93570	0.06211	-0.15176	-0.06992				
3S 4.34086	0.00019	-0.00129	-1.35053				
3S 6.96153	-0.00105	0.05393	0.34003				

See page 183 for Explanation of Tables and Notes for Tables 32, 42, and 43

## ROOTHAAN-HARTREE-FOCK ATOMIC WAVEFUNCTIONS

 TABLE 18 (3). THE HARTREE-FOCK FUNCTIONS FOR  $\text{Na}({}^2\text{S})$  ISO-ELECTRONIC SERIES.

TITANIUM K(2)L(8)3S(1) - 2S					
T.E.= -0.80144468D+03 P.E.= -0.16028884D+04			K.E.= 0.80144371D+03 V.T.= -0.20000012D+01		
S	1S	2S	3S	P	2P
BASIS/ORB E	-193.78809	-31.26539	-10.63721	BASIS/ORB E	-27.70717
1S 22.14210	0.93016	-0.21536	-0.11983	2P 7.80141	0.73676
1S 33.78900	0.02087	-0.00748	-0.00278	2P 11.71250	0.26667
2S 8.60715	0.00278	1.09342	0.52300	2P 19.65430	0.02042
2S 19.83470	0.06013	-0.15473	-0.07262		
3S 4.67074	0.00018	-0.00001	-1.37616		
3S 7.39289	-0.00101	0.03845	0.35904		
 VANADIUM K(2)L(8)3S(1) - 2S					
T.E.= -0.88428958D+03 P.E.= -0.17685756D+04			K.E.= 0.88428598D+03 V.T.= -0.2000041D+01		
S	1S	2S	3S	P	2P
BASIS/ORB E	-213.74972	-35.37476	-12.26719	BASIS/ORB E	-31.60392
1S 23.12470	0.93413	-0.28172	-0.12552	2P 8.29361	0.74232
1S 35.09080	0.02012	-0.00575	-0.00259	2P 12.31360	0.26145
2S 9.04147	0.00195	1.10502	0.54262	2P 20.45120	0.02063
2S 20.55540	0.05670	-0.15741	-0.07662		
3S 5.00985	0.00006	0.00079	-1.41320		
3S 7.73543	-0.00053	0.02568	0.38705		
 CHROMIUM K(2)L(8)3S(1) - 2S					
T.E.= -0.97124746D+03 P.E.= -0.15424915D+04			K.E.= 0.97124401D+03 V.T.= -0.20000036D+01		
S	1S	2S	3S	P	2P
BASIS/ORB E	-234.71255	-39.73083	-14.00682	BASIS/ORB E	-35.75134
1S 24.09040	0.93801	-0.28649	-0.12724	2P 8.78771	0.74828
1S 36.46830	0.01978	-0.00488	-0.00229	2P 12.92220	0.25411
2S 9.50340	0.00152	1.11821	0.55499	2P 21.26180	0.02070
2S 21.29930	0.05269	-0.16097	-0.07969		
3S 5.34308	-0.00001	0.0CC62	-1.44123		
3S 8.13997	-0.00030	0.02107	0.41229		
 MANGANESE K(2)L(8)3S(1) - 2S					
T.E.= -0.10623181D+04 P.E.= -0.21246455D+04			K.E.= 0.10623274D+04 V.T.= -0.19955912D+01		
S	1S	2S	3S	P	2P
BASIS/ORB E	-256.67595	-44.33655	-15.86204	BASIS/ORB E	-40.14876
1S 24.98810	0.94147	-0.28542	-0.13072	2P 9.28174	0.75418
1S 37.69100	0.02177	-0.00557	-0.00228	2P 13.54480	0.24759
2S 9.95718	0.00206	1.12688	0.56520	2P 22.19380	0.02016
2S 22.13360	0.04595	-0.1E333	-0.08130		
3S 5.69378	0.00013	0.00076	-1.48390		
3S 8.49986	-0.00072	0.01570	0.45310		
 IRON K(2)L(8)3S(1) - 2S					
T.E.= -0.11575012D+04 P.E.= -0.23150064D+04			K.E.= 0.11575052D+04 V.T.= -0.15599956D+01		
S	1S	2S	3S	P	2P
BASIS/ORB E	-279.64119	-49.19421	-17.82678	BASIS/ORB E	-44.79740
1S 26.09430	0.94177	-0.29271	-0.13325	2P 9.76812	0.75775
1S 39.02390	0.01890	-0.00393	-0.00176	2P 14.17990	0.24505
2S 10.40220	0.00056	1.13785	0.57778	2P 23.52870	0.01813
2S 22.90880	0.04962	-0.16808	-0.08504		
3S 6.02701	-0.00017	0.00169	-1.50965		
3S 8.90262	0.00027	0.00727	0.47405		
 COBALT K(2)L(8)3S(1) - 2S					
T.E.= -0.12567966D+04 P.E.= -0.25135948D+04			K.E.= 0.12567981D+04 V.T.= -0.19955988D+01		
S	1S	2S	3S	P	2P
BASIS/ORB E	-303.60706	-54.30177	-19.90291	BASIS/ORB E	-49.69634
1S 27.04290	0.94441	-0.29607	-0.13593	2P 10.26510	0.76410
1S 40.39930	0.01945	-0.00364	-0.00172	2P 14.81560	0.23825
2S 10.83760	0.00074	1.14E45	0.58874	2P 24.47120	0.01761
2S 23.73090	0.04569	-0.16986	-0.08698		
3S 6.35795	-0.00012	0.00212	-1.53105		
3S 9.32379	0.00010	-0.00208	0.49095		

See page 183 for Explanation of Tables and Notes for Tables 32, 42, and 43

TABLE 18 (4). THE HARTREE-FOCK FUNCTIONS FOR  $\text{Na}({}^2\text{S})$  ISO-ELECTRONIC SERIES.

NICKEL      K(2)L(8)3S(1) - 2S					
T.E.= -0.13602042D+04    P.E.= -0.27203893D+04					
K.E.= 0.13601852D+04    V.T.= -0.20000140D+01					
S	1S	2S	3S	P	2P
BASIS/ORB E	-328.57453	-55.66038	-22.09047	BASIS/ORB E	-54.84635
1S 28.05500	0.94570	-0.29755	-0.13590	2P 10.75670	0.76942
1S 41.82480	0.01880	-0.00372	-0.00282	2P 15.49130	0.23429
2S 11.27580	0.00055	1.15744	0.60341	2P 25.96430	0.01541
2S 24.61010	0.04492	-0.17279	-0.09160		
3S 6.68151	-0.00015	0.00348	-1.55009		
3S 9.70813	0.00020	-0.00588	0.50182		
COPPER      K(2)L(8)3S(1) - 2S					
T.E.= -0.14677239D+04    P.E.= -0.29254260D+04					
K.E.= 0.14677021D+04    V.T.= -0.20000148D+01					
S	1S	2S	3S	P	2P
BASIS/ORB E	-354.54178	-65.26E63	-24.38936	BASIS/ORB E	-60.24596
1S 28.74610	0.95427	-0.31087	-0.14543	2P 11.25410	0.77511
1S 43.05590	0.02304	-0.00000	0.00017	2P 16.12430	0.22811
2S 11.88230	0.00147	1.15320	0.59814	2P 26.88980	0.01509
2S 24.75630	0.02954	-0.176E4	-0.09191		
3S 6.99089	0.00009	0.00C39	-1.54416		
3S 10.28510	-0.00051	0.01216	0.51173		
ZINC      K(2)L(8)3S(1) - 2S					
T.E.= -0.15793554D+04    P.E.= -0.315E6761D+04					
K.E.= 0.15793206D+04    V.T.= -0.20000220D+01					
S	1S	2S	3S	P	2P
BASIS/ORB E	-381.50992	-71.12724	-26.79962	BASIS/ORB E	-65.89599
1S 29.69180	0.95825	-0.31810	-0.14906	2P 11.75180	0.78256
1S 44.84750	0.02212	0.00271	0.00101	2P 16.86380	0.22254
2S 12.35350	0.00143	1.16368	0.61191	2P 28.72110	0.01251
2S 25.27090	0.02591	-0.18005	-0.09603		
3S 7.32871	0.00012	0.00122	-1.57273		
3S 10.63870	-0.00056	0.00C7C5	0.53482		
GALLIUM      K(2)L(8)3S(1) - 2S					
T.E.= -0.16950989D+04    P.E.= -0.339C1892D+04					
K.E.= 0.16950902D+04    V.T.= -0.20000051D+01					
S	1S	2S	3S	P	2P
BASIS/ORB E	-409.47732	-77.23540	-29.32118	BASIS/ORB E	-71.79550
1S 30.76590	0.95536	-0.51215	-0.14859	2P 12.24480	0.78551
1S 45.75820	0.02221	-0.00068	0.00019	2P 17.44380	0.21852
2S 12.75110	0.00124	1.17019	0.61316	2P 29.42050	0.01289
2S 26.56980	0.02914	-0.18168	-0.09477		
3S 7.67391	0.00006	0.00186	-1.59851		
3S 11.07560	-0.00040	-0.004C8	0.56004		
GERMANIUM      K(2)L(8)3S(1) - 2S					
T.E.= -0.18149554D+04    P.E.= -0.3E298994D+04					
K.E.= 0.18149452D+04    V.T.= -0.20000050D+01					
S	1S	2S	3S	P	2P
BASIS/ORB E	-438.44608	-83.59438	-31.95399	BASIS/CRB E	-77.94589
1S 31.74660	0.95659	-0.31451	-0.15070	2P 12.74280	0.79053
1S 47.08760	0.02217	-0.00C23	0.00047	2P 18.08050	0.21314
2S 13.21760	0.00114	1.17604	0.61883	2P 30.36640	0.01262
2S 27.34510	0.02771	-0.18471	-0.09670		
3S 8.00227	0.00005	0.00196	-1.61283		
3S 11.51270	-0.00036	-0.00663	0.57380		
ARSENIC      K(2)L(8)3S(1) - 2S					
T.E.= -0.19389211D+04    P.E.= -0.3877E360D+04					
K.E.= 0.19389149D+04    V.T.= -0.20000032D+01					
S	1S	2S	3S	P	2P
BASIS/ORB E	-468.41519	-90.20352	-34.69806	BASIS/ORB E	-84.34645
1S 32.71530	0.95811	-0.31744	-0.15302	2P 13.23930	0.79462
1S 48.42140	0.02222	0.00C50	0.00088	2P 18.69840	0.20855
2S 13.72150	0.00103	1.17846	0.62299	2P 31.24590	0.01253
2S 28.03830	0.02586	-0.18889	-0.09936		
3S 8.33551	0.00004	0.00122	-1.63195		
3S 11.92740	-0.00032	-0.00284	0.59483		

See page 183 for Explanation of Tables and Notes for Tables 32, 42, and 43

## ROOCHAAN-HARTREE-FOCK ATOMIC WAVEFUNCTIONS

 TABLE 18 (5). THE HARTREE-FOCK FUNCTIONS FOR Na(<sup>2</sup>S) ISO-ELECTRONIC SERIES.

SELENIUM K(2)L(8)3S(1) - 2S					
T.E.=-0.20669998D+04 P.E.=-0.41339954D+04			K.E.= 0.20669957D+04 V.T.=-0.20000020D+01		
S	1S	2S	3S	P	2P
BASIS/ORB E	-499.38468	-57.06283	-37.55338	BASIS/ORB E	-90.99715
1S 33.69860	0.95936	-0.31997	-0.15510	2P 13.73570	0.79821
1S 49.78160	0.02201	0.00117	0.00126	2P 19.29730	0.20420
2S 14.21360	0.00087	1.18201	0.62725	2P 31.57940	0.01274
2S 28.75950	0.02466	-0.19272	-0.10174		
3S 8.66629	0.00002	0.00082	-1.64764		
3S 12.35310	-0.00024	-0.00135	0.61162		
 BROMINE K(2)L(8)3S(1) - 2S					
T.E.=-0.21991899D+04 P.E.=-0.43583809D+04			K.E.= 0.21991910D+04 V.T.=-0.19599995D+01		
S	1S	2S	3S	P	2P
BASIS/ORB E	-531.35447	-104.17228	-40.51995	BASIS/ORB E	-97.89806
1S 34.79540	0.96169	-0.31649	-0.15379	2P 14.23630	0.80468
1S 52.32280	0.01791	0.00048	0.00019	2P 20.01630	0.19824
2S 14.65860	0.00050	1.18686	0.63859	2P 33.37610	0.01152
2S 29.73710	0.02683	-0.19593	-0.10605		
3S 9.02723	-0.00004	0.00121	-1.69638		
3S 12.61810	-0.00002	-0.00599	0.65351		
 KRYPTON K(2)L(8)3S(1) - 2S					
T.E.=-0.23354916D+04 P.E.=-0.46705535D+04			K.E.= 0.23354619D+04 V.T.=-0.20000127D+01		
S	1S	2S	3S	P	2P
BASIS/ORB E	-564.32552	-111.53253	-43.59764	BASIS/ORB E	-105.04968
1S 35.52780	0.56358	0.33485	0.16407	2P 14.73170	0.80491
1S 52.33620	0.02379	-0.00715	-0.00440	2P 20.44430	0.19504
2S 15.43260	0.00080	-1.18096	-0.62836	2P 32.58240	0.01416
2S 29.31710	0.01763	0.20561	0.11110		
3S 9.28162	0.00005	0.00282	1.63845		
3S 13.36890	-0.00029	-0.03028	-0.62010		

See page 183 for Explanation of Tables and Notes for Tables 32, 42, and 43

TABLE 19 (1). THE HARTREE-FOCK FUNCTIONS FOR Mg(<sup>1</sup>S) ISO-ELECTRONIC SERIES.

MAGNESIUM K(2)L(8)3S(2) - 1S					
T.E.= -0.19961432D+03		P.E.= -0.35522762D+03			
K.E.= 0.19961330D+03		V.T.= -0.20000051D+01			
S	1S	2S	3S	P	2P
BASIS/ORB E	-49.03146	-3.76753	-0.25297	BASIS/CRB E	-2.28204
1S 12.32250	0.87725	-0.21729	0.04158	2P 2.71869	0.52773
1S 19.54750	0.02545	-0.0CE66	0.00180	2P 4.70007	0.46516
2S 4.43909	0.00534	0.85563	-0.17900	2P 8.50518	0.07407
2S 11.16630	0.11674	-0.11922	0.02476		
3S 1.48671	0.00047	-0.00195	0.46353		
3S 0.89667	-0.00022	0.00054	0.61982		
3S 3.47562	-0.00147	0.26593	-0.07589		
ALUMINUM K(2)L(8)3S(2) - 1S					
T.E.= -0.24167433D+03		P.E.= -0.48334741D+03			
K.E.= 0.24167309D+03		V.T.= -0.20000051D+01			
S	1S	2S	3S	P	2P
BASIS/ORB E	-58.81218	-5.21754	-0.65209	BASIS/ORB E	-3.52263
1S 13.41920	0.87459	-0.22161	0.05386	2P 3.28098	0.60412
1S 20.82510	0.02490	-0.00557	0.00304	2P 5.69821	0.41354
2S 4.83620	0.00538	0.88725	-0.24286	2P 10.42940	0.04012
2S 12.17030	0.12018	-0.12545	0.03467		
3S 1.77513	0.00069	-0.00308	0.55460		
3S 1.25381	-0.00038	0.00148	0.52628		
3S 3.88799	-0.00171	0.23144	-0.09809		
SILICON K(2)L(8)3S(2) - 1S					
T.E.= -0.28799551D+03		P.E.= -0.57559398D+03			
K.E.= 0.28799847D+03		V.T.= -0.19999898D+01			
S	1S	2S	3S	P	2P
BASIS/ORB E	-69.62149	-6.94585	-1.18169	BASIS/ORB E	-5.04009
1S 14.14120	0.90483	0.24318	-0.06980	2P 3.81690	0.65065
1S 22.17320	0.02553	0.00582	-0.00184	2P 6.58364	0.37494
2S 5.32639	0.00403	-0.89873	0.28457	2P 12.31740	0.02515
2S 12.66550	0.08504	0.12295	-0.03885		
3S 2.10450	0.00045	0.00412	-0.56966		
3S 1.61958	-0.00026	-0.00214	-0.52711		
3S 4.36783	-0.00107	-0.22742	0.13116		
PHOSPHORUS K(2)L(8)3S(2) - 1S					
T.E.= -0.33856300D+03		P.E.= -0.67713231D+03			
K.E.= 0.33856931D+03		V.T.= -0.19999814D+01			
S	1S	2S	3S	P	2P
BASIS/ORB E	-81.44684	-8.93898	-1.83286	BASIS/ORB E	-6.82149
1S 15.14370	0.90434	0.24606	-0.07788	2P 4.33624	0.68139
1S 23.53210	0.02737	0.0C158	-0.00264	2P 7.38978	0.34529
2S 5.69559	0.00539	-0.93374	0.32748	2P 13.92920	0.01859
2S 13.73440	0.08251	0.12575	-0.04397		
3S 2.37278	0.00127	0.00143	-0.69125		
3S 1.93440	-0.00081	-0.00053	-0.42547		
3S 4.78053	-0.00215	-0.18698	0.14734		
SULFUR K(2)L(8)3S(2) - 1S					
T.E.= -0.39336916D+03		P.E.= -0.78674677D+03			
K.E.= 0.39337760D+03		V.T.= -0.19999786D+01			
S	1S	2S	3S	P	2P
BASIS/ORB E	-94.28278	-11.19124	-2.60170	BASIS/CRB E	-8.86148
1S 15.99500	0.91752	-0.25E28	-0.08886	2P 4.84314	0.70283
1S 24.70330	0.02891	-0.00E67	-0.00176	2P 8.15623	0.32360
2S 6.16896	0.00465	0.94920	0.35606	2P 15.58410	0.01435
2S 14.36510	0.06567	-0.12E17	-0.04728		
3S 2.67610	0.00115	-0.00531	-0.77477		
3S 2.25077	-0.00076	0.00303	-0.36770		
3S 5.22215	-0.00180	0.17918	0.17693		

See page 183 for Explanation of Tables and Notes for Tables 32, 42, and 43

## ROOTHAAN-HARTREE-FOCK ATOMIC WAVEFUNCTIONS

 TABLE 19 (2). THE HARTREE-FOCK FUNCTIONS FOR Mg(<sup>1</sup>S) ISO-ELECTRONIC SERIES.

**CHLORINE**      K(2)L(8)3S(2) - 1S  
 T.E.=-0.45240949D+03 P.E.=-0.90483550D+03  
 K.E.= 0.45242601D+03 V.T.=-0.19999635D+01

	S	1S	2S	3S	P	2P
BASIS/ORB E	-108.12532	-13.695C1	-3.48598	BASIS/ORB E	-11.15664	
1S	16.98050	0.91796	-0.25E24	0.09370	2P 5.34041	0.71581
1S	26.12920	0.03021	-0.008E5	0.00290	2P 8.85071	0.30909
2S	6.53673	0.00605	0.98382	-0.39054	2P 17.03000	0.01254
2S	15.45830	0.06272	-0.13202	0.05150		
3S	3.00435	0.00251	-0.00E75	0.80264		
3S	2.59025	-0.00171	0.00403	0.36989		
3S	5.58060	-0.00306	0.14202	-0.19565		

**ARGON**      K(2)L(8)3S(2) - 1S  
 T.E.=-0.51568106D+03 P.E.=-0.10313677D+04  
 K.E.= 0.51568668D+03 V.T.=-0.19999891D+01

	S	1S	2S	3S	P	2P
BASIS/ORB E	-122.97496	-16.46207	-4.48466	BASIS/ORB E	-13.70689	
1S	18.03890	0.92300	-0.26714	0.10144	2P 5.82931	0.72529
1S	27.62640	0.02577	-0.0C569	0.00167	2P 9.51854	0.29726
2S	7.01799	0.00369	0.99324	-0.41067	2P 17.93840	0.01206
2S	16.11380	0.06305	-0.13799	0.05592		
3S	3.25862	0.00113	-0.00605	0.93965		
3S	2.93417	-0.00083	0.00408	0.24928		
3S	6.08568	-0.00140	0.13830	-0.21451		

**POTASSIUM**      K(2)L(8)3S(2) - 1S  
 T.E.=-0.58318185D+03 P.E.=-0.11663673D+04  
 K.E.= 0.58318548D+03 V.T.=-0.19999938D+01

	S	1S	2S	3S	P	2P
BASIS/ORB E	-138.82792	-19.47773	-5.59672	BASIS/ORB E	-16.50956	
1S	18.93130	0.93069	-0.27590	0.10785	2P 6.31648	0.73182
1S	28.87040	0.02693	-0.00441	0.00153	2P 10.15240	0.28832
2S	7.46483	0.00321	1.01684	-0.43858	2P 18.84760	0.01201
2S	16.75570	0.05288	-0.14183	0.06073		
3S	3.58077	0.00115	-0.01913	1.01599		
3S	3.25889	-0.00085	0.01364	0.20732		
3S	6.38948	-0.00122	0.12398	-0.24046		

**CALCIUM**      K(2)L(8)3S(2) - 1S  
 T.E.=-0.654910430D+03 P.E.=-0.13C98206D+04  
 K.E.= 0.65491012D+03 V.T.=-0.20C00005D+01

	S	1S	2S	3S	P	2P
BASIS/ORB E	-155.68432	-22.74598	-6.82183	BASIS/CRB E	-19.56474	
1S	20.07030	0.92727	-0.27162	-0.10863	2P 6.79997	0.73526
1S	30.73670	0.02360	-0.0C692	-0.00290	2P 10.75620	0.28303
2S	7.81884	0.00347	1.04423	0.46377	2P 20.03760	0.01171
2S	17.98750	0.06031	-0.14659	-0.0C6479		
3S	3.84038	0.00020	-0.00103	-1.23903		
3S	6.85450	-0.00125	0.08729	0.24281		

**SCANDIUM**      K(2)L(8)3S(2) - 1S  
 T.E.=-0.73086578D+03 P.E.=-0.14617556D+C4  
 K.E.= 0.73088986D+03 V.T.=-0.19999671D+01

	S	1S	2S	3S	P	2P
BASIS/ORB E	-173.54126	-26.26422	-8.15889	BASIS/ORB E	-22.86973	
1S	21.16340	0.92730	-0.27509	-0.11437	2P 7.28550	0.73918
1S	32.01890	0.02114	-0.00586	-0.00163	2P 11.34860	0.27651
2S	8.23284	0.00210	1.06487	0.48038	2P 20.67890	0.01243
2S	18.83060	0.06369	-0.15145	-0.06658		
3S	4.17816	0.00003	-0.00025	-1.26883		
3S	7.28002	-0.00048	0.06779	0.26852		

See page 183 for Explanation of Tables and Notes for Tables 32, 42, and 43

TABLE 19 (3). THE HARTREE-FOCK FUNCTIONS FOR Mg(<sup>1</sup>S) ISO-ELECTRONIC SERIES.

TITANIUM K(2)L(8)3S(2) - 1S					
T.E.= -0.811047080+03 P.E.= -0.162210450+04			K.E.= 0.81105743D+03 V.T.= -0.19999E72D+01		
S	1S	2S	3S	P	2P
BASIS/ORB E	-192.40319	-30.03609	-9.60872	BASIS/ORB E	-26.42837
1S 22.02430	0.93429	-0.28065	-0.11946	2P 7.76437	0.74158
1S 33.47830	0.02292	-0.00593	-0.00148	2P 11.94270	0.27229
2S 8.68438	0.00278	1.07775	0.49533	2P 21.41000	0.01269
2S 19.60670	0.05301	-0.15241	-0.06852		
3S 4.50947	0.00015	-0.00056	-1.29592		
3S 7.68845	-0.00097	0.05915	0.29264		
 VANADIUM K(2)L(8)3S(2) - 1S					
T.E.= -0.895453720+03 P.E.= -0.17909015D+04			K.E.= 0.89544782D+03 V.T.= -0.20000066D+01		
S	1S	2S	3S	P	2P
BASIS/ORB E	-212.26700	-34.05443	-11.17073	BASIS/ORB E	-30.23852
1S 23.10270	0.93561	-0.28457	-0.12195	2P 8.25009	0.74480
1S 34.82420	0.02022	-0.00449	-0.00159	2P 12.52670	0.26701
2S 9.13162	0.00121	1.09282	0.51550	2P 22.09800	0.01329
2S 20.35830	0.05529	-0.15921	-0.07422		
3S 4.83809	-0.00005	-0.00077	-1.32336		
3S 8.03793	-0.00005	0.04867	0.31155		
 CHROMIUM K(2)L(8)3S(2) - 1S					
T.E.= -0.98408522D+03 P.E.= -0.19681534D+04			K.E.= 0.98406823D+03 V.T.= -0.20000173D+01		
S	1S	2S	3S	P	2P
BASIS/ORB E	-233.13179	-38.33326	-12.84450	BASIS/ORB E	-34.29911
1S 23.90640	0.94190	-0.29115	-0.12460	2P 8.73922	0.74833
1S 36.17000	0.02379	-0.00421	-0.00261	2P 13.12320	0.26249
2S 9.53051	0.00261	1.11374	0.54058	2P 23.28540	0.01291
2S 21.13990	0.04299	-0.15778	-0.07778		
3S 5.16831	0.00020	0.00023	-1.35230		
3S 8.34929	-0.00101	0.02785	0.32512		
 MANGANESE K(2)L(8)3S(2) - 1S					
T.E.= -0.10769412D+04 P.E.= -0.21538891D+04			K.E.= 0.10769479D+04 V.T.= -0.19999937D+01		
S	1S	2S	3S	P	2P
BASIS/ORB E	-254.99625	-42.65665	-14.62962	BASIS/ORB E	-38.60916
1S 25.04840	0.94077	-0.29116	-0.12782	2P 9.23146	0.75344
1S 37.56580	0.02035	-0.00407	-0.00178	2P 13.73310	0.25598
2S 9.99241	0.00109	1.12123	0.54689	2P 24.06800	0.01311
2S 22.02170	0.04895	-0.16472	-0.08010		
3S 5.50322	-0.00004	0.00008	-1.37690		
3S 8.80115	-0.00007	0.02415	0.35183		
 IRON K(2)L(8)3S(2) - 1S					
T.E.= -0.11740213D+04 P.E.= -0.23480471D+04			K.E.= 0.11740258D+04 V.T.= -0.19999961D+01		
S	1S	2S	3S	P	2P
BASIS/ORB E	-277.86323	-47.63173	-16.52668	BASIS/ORB E	-43.17092
1S 26.01320	0.94372	-0.29533	-0.13136	2P 9.71742	0.75698
1S 38.87080	0.02033	-0.00328	-0.00137	2P 14.36050	0.25248
2S 10.46830	0.00073	1.12826	0.55673	2P 25.43670	0.01204
2S 22.74680	0.04562	-0.16864	-0.08296		
3S 5.83488	-0.00008	-0.00025	-1.40116		
3S 9.20788	0.00011	0.02255	0.37529		
 COBALT K(2)L(8)3S(2) - 1S					
T.E.= -0.12753253D+04 P.E.= -0.25506542D+04			K.E.= 0.12753289D+04 V.T.= -0.19999972D+01		
S	1S	2S	3S	P	2P
BASIS/ORB E	-301.73108	-52.65736	-18.52528	BASIS/ORB E	-47.98322
1S 26.84450	0.94832	-0.30013	-0.13544	2P 10.21340	0.76315
1S 40.17090	0.02323	-0.00327	-0.00110	2P 15.00100	0.24562
2S 10.94960	0.00179	1.13363	0.56351	2P 26.41310	0.01173
2S 23.46480	0.03625	-0.17043	-0.08420		
3S 6.16239	0.00011	-0.00065	-1.42024		
3S 9.65301	-0.00062	0.02248	0.39562		

See page 183 for Explanation of Tables and Notes for Tables 32, 42, and 43

## ROOTHAAN-HARTREE-FOCK ATOMIC WAVEFUNCTIONS

 TABLE 19 (4). THE HARTREE-FOCK FUNCTIONS FOR Mg(<sup>1</sup>S) ISO-ELECTRONIC SERIES.

NICKEL K(2)L(8)3S(2) - 1S						
T.E.= -0.13808530D+04 P.E.= -0.27617681D+04			K.E.= 0.13808551D+04 V.T.= -0.19999985D+01			
S	1S	2S	3S	P	2P	
BASIS/ORB E	-326.59984	-57.93356	-20.65541	BASIS/ORB E	-53.04614	
1S 27.96600	0.94837	-0.30197	-0.13749	2P 10.71280	0.77051	
1S 41.65330	0.01991	-0.00210	-0.00063	2P 15.67380	0.23805	
2S 11.39240	0.00034	1.14421	0.57401	2P 27.56510	0.01104	
2S 24.28670	0.04070	-0.17528	-0.08743			
3S 6.48986	-0.00011	-0.00008	-1.43885			
3S 10.07960	0.00028	0.01413	0.41048			
COPPER K(2)L(8)3S(2) - 1S						
T.E.= -0.14906043D+04 P.E.= -0.29812104D+04			K.E.= 0.14906061D+04 V.T.= -0.19999986D+01			
S	1S	2S	3S	P	2P	
BASIS/ORB E	-352.46932	-63.46017	-22.88699	BASIS/ORB E	-58.35944	
1S 28.95140	0.95030	-0.30513	-0.14043	2P 11.21340	0.77787	
1S 42.99920	0.01960	-0.00138	-0.00014	2P 16.35440	0.23053	
2S 11.87050	0.00000	1.14953	0.58052	2P 28.73440	0.01057	
2S 25.02830	0.03891	-0.17913	-0.08973			
3S 6.81709	-0.00015	-0.00027	-1.45620			
3S 10.51930	0.00046	0.01319	0.42831			
ZINC K(2)L(8)3S(2) - 1S						
T.E.= -0.16045789D+04 P.E.= -0.32051499D+04			K.E.= 0.16045711D+04 V.T.= -0.20000049D+01			
S	1S	2S	3S	P	2P	
BASIS/ORB E	-379.33968	-69.23722	-25.22999	BASIS/ORB E	-63.92318	
1S 29.68620	0.95553	-0.31493	-0.14623	2P 11.71500	0.78506	
1S 44.17240	0.02424	0.00C92	0.00101	2P 17.03690	0.22313	
2S 12.37450	0.00160	1.15637	0.58813	2P 29.85910	0.00981	
2S 25.45140	0.02652	-0.18006	-0.09118			
3S 7.14273	0.00013	-0.00031	-1.47202			
3S 10.95410	-0.00062	0.01462	0.44501			
GALLIUM K(2)L(8)3S(2) - 1S						
T.E.= -0.17227767D+04 P.E.= -0.34455559D+04			K.E.= 0.17227793D+04 V.T.= -0.19999985D+01			
S	1S	2S	3S	P	2P	
BASIS/ORB E	-407.21011	-75.26435	-27.68425	BASIS/ORB E	-69.73696	
1S 30.81640	0.95601	-0.31053	-0.14415	2P 12.21850	0.79329	
1S 46.27520	0.02018	-0.00115	-0.00057	2P 17.77790	0.21554	
2S 12.77680	0.00114	1.16554	0.60158	2P 31.57470	0.00848	
2S 26.62530	0.03080	-0.18316	-0.09492			
3S 7.49136	0.00007	0.00016	-1.50779			
3S 11.24580	-0.00034	0.00265	0.47139			
GERMANIUM K(2)L(8)3S(2) - 1S						
T.E.= -0.18451976D+04 P.E.= -0.36903986D+04			K.E.= 0.18452010D+04 V.T.= -0.19999982D+01			
S	1S	2S	3S	P	2P	
BASIS/ORB E	-436.08141	-81.54204	-30.25001	BASIS/ORB E	-75.80135	
1S 31.68990	0.95792	-0.31818	-0.15055	2P 12.71660	0.79791	
1S 46.95040	0.02292	0.00132	0.00165	2P 18.40560	0.21007	
2S 13.41100	0.00091	1.15777	0.59365	2P 32.26150	0.00867	
2S 26.93760	0.02545	-0.19107	-0.09682			
3S 7.80359	0.00004	-0.00235	-1.50843			
3S 11.81270	-0.00024	0.02702	0.48941			
ARSENIC K(2)L(8)3S(2) - 1S						
T.E.= -0.19718416D+04 P.E.= -0.39436876D+04			K.E.= 0.19718460D+04 V.T.= -0.19999977D+01			
S	1S	2S	3S	P	2P	
BASIS/ORB E	-465.95313	-88.06590	-32.92702	BASIS/ORB E	-82.11590	
1S 32.66680	0.95893	-0.32C86	-0.15248	2P 13.21240	0.80189	
1S 48.23810	0.02305	0.00200	0.00184	2P 19.03860	0.20560	
2S 13.88530	0.00083	1.16421	0.60176	2P 33.21190	0.00856	
2S 27.67510	0.02408	-0.19436	-0.09965			
3S 8.13722	0.00004	-0.00235	-1.52900			
3S 12.20160	-0.00022	0.02447	0.50781			

See page 183 for Explanation of Tables and Notes for Tables 32, 42, and 43

TABLE 19 (5). THE HARTREE-FOCK FUNCTIONS FOR Mg(<sup>1</sup>S) ISO-ELECTRONIC SERIES.

SELENIUM K(2)L(8)3S(2) - 1S					
T.E.= -0.21027084D+04 P.E.= -0.42054094D+04			K.E.= 0.21027009D+04 V.T.= -0.20000036D+01		
S	1S	2S	3S	P	2P
BASIS/ORB E	-496.82570	-94.84826	-35.71543	BASIS/ORB E	-88.68100
1S 33.60120	0.96111	0.32658	0.15719	2P 13.70340	0.80361
1S 49.65290	0.02343	-0.00409	-0.00349	2P 19.61860	0.20287
2S 14.43940	0.00091	-1.16519	-0.59894	2P 33.92680	0.00823
2S 28.15320	0.02101	0.20012	0.10095		
3S 8.44516	0.00007	0.00281	1.52581		
3S 12.75920	-0.00030	-0.03321	-0.51406		
 BROMINE K(2)L(8)3S(2) - 1S					
T.E.= -0.22377982D+04 P.E.= -0.44755878D+04			K.E.= 0.22377896D+04 V.T.= -0.20000039D+01		
S	1S	2S	3S	P	2P
BASIS/ORB E	-528.69833	-101.87662	-38.61503	BASIS/ORB E	-95.49607
1S 34.59860	0.96231	0.32805	0.15856	2P 14.18520	0.80222
1S 51.17730	0.02272	-0.00433	-0.00354	2P 20.10640	0.20315
2S 14.90290	0.00088	-1.17160	-0.60538	2P 34.35710	0.00963
2S 28.95000	0.02038	0.20295	0.10308		
3S 8.77379	0.00007	0.00263	1.54060		
3S 13.18940	-0.00031	-0.02921	-0.52697		
 KRYPTON K(2)L(8)3S(2) - 1S					
T.E.= -0.23771109D+04 P.E.= -0.47542269D+04			K.E.= 0.23771160D+04 V.T.= -0.19999578D+01		
S	1S	2S	3S	P	2P
BASIS/ORB E	-561.57090	-109.15453	-41.62579	BASIS/ORB E	-102.56105
1S 35.72960	0.96130	-0.32087	-0.15417	2P 14.65630	0.79606
1S 52.85930	0.02013	0.00076	0.00086	2P 20.45690	0.20692
2S 15.15380	0.00063	1.18895	0.62482	2P 34.24440	0.01155
2S 30.47880	0.02457	-0.19873	-0.10413		
3S 9.12661	0.00002	-0.00023	-1.57535		
3S 13.44570	-0.00013	-0.00268	0.54069		

See page 183 for Explanation of Tables and Notes for Tables 32, 42, and 43

## ROOTHAAN-HARTREE-FOCK ATOMIC WAVEFUNCTIONS

 TABLE 20 (1). THE HARTREE-FOCK FUNCTIONS FOR AI(<sup>2</sup>P) ISO-ELECTRONIC SERIES.

ALUMINUM K(2)L(8)3S(2)3P(1) - 2P  
 T.E.= -0.24187639D+03 P.E.= -0.48374606D+03 K.E.= 0.24186967D+03 V.T.= -0.20300278D+01

	S	1S	2S	3S	P	2P	3P
BASIS/ORB E	-58.50050	-4.90573	-0.39296	BASIS/CRB E	-3.21744	-0.20997	
1S 13.77300	0.85319	-0.218C8	0.04986	2P 5.30423	0.65002	-0.11753	
1S 22.00060	0.01700	-0.00619	0.00166	2P 10.10690	0.04855	-0.00865	
2S 4.58921	0.00588	0.97122	-0.24597	3P 1.49706	0.01139	0.39123	
2S 12.43820	0.15383	-0.12496	0.03127	3P 0.86152	-0.00291	0.68377	
2S 1.91150	0.00123	-0.01230	0.48492	3P 3.82661	0.38666	-0.07258	
3S 1.14459	-0.00045	0.00324	0.63833				
3S 3.40973	-0.00254	0.13841	-0.09405				

SILICON K(2)L(8)3S(2)3P(1) - 2P  
 T.E.= -0.28857286D+03 P.E.= -0.57713930D+03 K.E.= 0.28856642D+03 V.T.= -0.20000224D+01

	S	1S	2S	3S	P	2P	3P
BASIS/ORB E	-69.17485	-6.51253	-0.83853	BASIS/CRB E	-4.60963	-0.58590	
1S 14.37600	0.88733	-0.23583	0.06283	2P 5.78133	0.67042	-0.16576	
1S 22.84810	0.02220	-0.00611	0.00225	2P 11.00520	0.04869	-0.01132	
2S 5.03531	0.00541	0.99217	-0.29911	3P 1.70780	0.00819	0.61271	
2S 13.04660	0.10842	-0.12132	0.03699	3P 1.14775	-0.00222	0.44999	
2S 2.34292	0.00171	-0.02360	0.47721	3P 4.27372	0.35965	-0.08952	
3S 1.51148	-0.00057	0.00590	0.68147				
3S 3.68465	-0.00279	0.13132	-0.14132				

PHOSPHORUS K(2)L(8)3S(2)3P(1) - 2P  
 T.E.= -0.339644750D+03 P.E.= -0.675281350D+03 K.E.= 0.33963660D+03 V.T.= -0.200002400D+01

	S	1S	2S	3S	P	2P	3P
BASIS/ORB E	-80.87626	-8.39347	-1.41460	BASIS/ORB E	-6.27851	-1.09052	
1S 15.17990	0.90556	-0.24861	0.07354	2P 6.25073	0.66755	-0.20180	
1S 24.12390	0.02417	-0.00535	0.00254	2P 11.79560	0.05018	-0.01378	
2S 5.48746	0.00538	1.00494	-0.34122	3P 2.02027	0.00528	0.66793	
2S 13.75740	0.08487	-0.12135	0.04238	3P 1.50205	-0.00098	0.39426	
3S 2.63943	0.00192	-0.01772	0.50563	3P 4.72385	0.33509	-0.10448	
3S 1.84128	-0.00073	0.00494	0.66571				
3S 4.15133	-0.00295	0.11751	-0.15875				

SULFUR K(2)L(8)3S(2)3P(1) - 2P  
 T.E.= -0.39507696D+03 P.E.= -0.79C14759D+03 K.E.= 0.39507063D+03 V.T.= -0.20000150D+01

	S	1S	2S	3S	P	2P	3P
BASIS/ORB E	-93.59331	-10.54C39	-2.11265	BASIS/ORB E	-8.21235	-1.71672	
1S 16.08200	0.91397	-0.25510	0.08163	2P 6.71240	0.70477	-0.23176	
1S 25.37790	0.02585	-0.00614	0.00308	2P 12.56590	0.05158	-0.01582	
2S 5.94603	0.00571	1.01462	-0.37435	3P 2.31348	0.00164	0.75044	
2S 14.59290	0.07282	-0.12519	0.04765	3P 1.82980	0.00091	0.31686	
3S 2.97678	0.00238	-0.01458	0.49825	3P 5.16166	0.31183	-0.11574	
3S 2.18696	-0.00098	0.00446	0.69215				
3S 4.63005	-0.00344	0.10570	-0.18096				

CHLORINE K(2)L(8)3S(2)3P(1) - 2P  
 T.E.= -0.45486138D+03 P.E.= -0.90571748E+03 K.E.= 0.45485610D+03 V.T.= -0.20000116D+01

	S	1S	2S	3S	P	2P	3P
BASIS/ORB E	-107.32075	-12.94142	-2.92867	BASIS/ORB E	-10.40564	-2.46102	
1S 16.94700	0.92478	-0.26455	0.09002	2P 7.16751	0.72059	-0.25705	
1S 26.65830	0.02724	-0.00545	0.00303	2P 13.28620	0.05344	-0.01779	
2S 6.40596	0.00566	1.02737	-0.40409	3P 2.61061	-0.00206	0.82405	
2S 15.29610	0.05854	-0.12770	0.05204	3P 2.15964	0.00301	0.25584	
3S 3.31580	0.00274	-0.01566	0.51395	3P 5.59570	0.29007	-0.12538	
3S 2.51954	-0.00117	0.00511	0.70712				
3S 5.03742	-0.00368	0.10273	-0.21123				

See page 183 for Explanation of Tables and Notes for Tables 32, 42, and 43

TABLE 20 (2). THE HARTREE-FOCK FUNCTIONS FOR AI(<sup>2</sup>P) ISO-ELECTRONIC SERIES.

ARGON K(2)L(8)3S(2)3P(1) - 2P T.E.= -0.51899304D+03 P.E.= -0.10379815D+04 K.E.= 0.51898851D+03 V.T.= -0.20300087D+01						
S	1S	2S	3S	P	2P	3P
BASIS/ORB E	-122.05552	-15.61130	-3.86046	BASIS/CRB E	-12.85528	-3.52127
1S 17.83930	0.93272	-0.27307	0.09761	2P 7.61475	0.73599	-0.27908
1S 27.94850	0.02836	-0.04454	0.00276	2P 13.57870	0.05552	-0.01971
2S 6.87099	0.00576	1.03786	-0.42864	3P 2.91344	-0.00605	0.89022
2S 15.99840	0.04784	-0.13062	0.05600	3P 2.49089	0.00553	0.20240
3S 3.71796	0.00318	-0.01389	0.44526	3P 6.02131	0.26903	-0.13413
3S 2.88859	-0.00137	0.00449	0.79944			
3S 5.49920	-0.00407	0.09650	-0.23498			
POTASSIUM K(2)L(8)3S(2)3P(1) - 2P T.E.= -0.58746861D+03 P.E.= -0.11749331D+04 K.E.= 0.58746448D+03 V.T.= -0.20300070D+01						
S	1S	2S	3S	P	2P	3P
BASIS/ORB E	-137.79585	-18.53023	-4.90677	BASIS/ORB E	-15.55961	-4.29624
1S 18.74490	0.93877	-0.28091	0.10460	2P 8.05348	0.75117	-0.29885
1S 29.21840	0.02951	-0.00352	0.00239	2P 14.64910	0.05777	-0.02159
2S 7.34109	0.05080	1.04776	-0.44987	3P 3.21969	-0.01022	0.95467
2S 16.68320	0.03931	-0.13410	0.05976	3P 2.82043	0.00835	0.15177
3S 4.03623	0.00349	-0.01255	0.43651	3P 6.43701	0.24838	-0.14199
3S 3.22557	-0.00161	0.00446	0.82671			
3S 5.96490	-0.00425	0.09111	-0.25316			
CALCIUM K(2)L(8)3S(2)3P(1) - 2P T.E.= -0.66028581D+03 P.E.= -0.13205694D+04 K.E.= 0.66028362D+03 V.T.= -0.20300033D+01						
S	1S	2S	3S	P	2P	3P
BASIS/ORB E	-154.54045	-21.70254	-6.06673	BASIS/CRB E	-18.51742	-5.38507
1S 19.67780	0.94265	-0.28701	0.11026	2P 8.48281	0.76665	-0.31698
1S 30.45900	0.03045	-0.00265	0.00225	2P 15.30760	0.06007	-0.02344
2S 7.81813	0.00546	1.05889	-0.47113	3P 3.53691	-0.01458	1.00159
2S 17.36450	0.03371	-0.13550	0.06462	3P 3.14710	0.01136	0.12005
3S 4.35044	0.00375	-0.02154	0.54539	3P 6.83739	0.22774	-0.14978
3S 3.51433	-0.00172	0.00828	0.77055			
3S 6.26574	-0.00425	0.09226	-0.30312			
SCANDIUM K(2)L(8)3S(2)3P(1) - 2P T.E.= -0.73744302D+03 P.E.= -0.14748844D+04 K.E.= 0.73744140D+03 V.T.= -0.20300022D+01						
S	1S	2S	3S	P	2P	3P
BASIS/DRB E	-172.28848	-25.12E51	-7.33974	BASIS/ORB E	-21.72790	-6.58709
1S 20.61920	0.94567	-0.29311	-0.11593	2P 8.50520	0.78133	-0.33360
1S 31.70290	0.03128	-0.00183	-0.00176	2P 15.53780	0.06271	-0.02533
2S 8.30047	0.00535	1.06673	0.48712	3P 3.85964	-0.01826	1.03684
2S 18.04740	0.02913	-0.14424	-0.06844	3P 3.47392	0.01392	0.10040
3S 4.66496	0.00389	-0.02252	-0.55146	3P 7.22991	0.20767	-0.15720
3S 3.84334	-0.00188	0.00519	-0.78345			
3S 6.72368	-0.00422	0.09043	0.32239			
TITANIUM K(2)L(8)3S(2)3P(1) - 2P T.E.= -0.81853899D+03 P.E.= -0.16378770D+04 K.E.= 0.81893799D+03 V.T.= -0.20300012D+01						
S	1S	2S	3S	P	2P	3P
BASIS/DRB E	-191.03930	-28.80635	-8.72542	BASIS/ORB E	-25.19048	-7.90190
1S 21.58170	0.94772	-0.29867	-0.12118	2P 9.32125	0.79055	-0.34602
1S 32.94550	0.03170	-0.00066	-0.00115	2P 16.45320	0.06768	-0.02840
2S 8.78892	0.00501	1.073E5	0.50087	3P 4.19195	-0.01262	1.04077
2S 18.72220	0.02629	-0.14556	-0.07225	3P 3.80021	0.00969	0.11C23
3S 4.97737	0.00376	-0.02361	-0.55939	3P 7.68563	0.18874	-0.16415
3S 4.17053	-0.00192	0.01032	-0.79349			
3S 7.18455	-0.00393	0.08989	0.34124			

See page 183 for Explanation of Tables and Notes for Tables 32, 42, and 43

## ROOTHAAN-HARTREE-FOCK ATOMIC WAVEFUNCTIONS

 TABLE 20 (3). THE HARTREE-FOCK FUNCTIONS FOR A1(<sup>2</sup>P) ISO-ELECTRONIC SERIES.

VANADIUM K(2)L(8)3S(2)3P(1) - 2P						
T.E.= -0.90477276D+03 P.E.= -0.18095441D+04 K.E.= 0.90477131D+03 V.T.= -0.20000016D+01						
S	1S	2S	3S	P	2P	3P
BASIS/ORB E	-210.79240	-32.73605	-10.22348	BASIS/ORB E	-28.90482	-9.32917
1S 22.48120	0.95049	-0.30508	-0.12658	2P 9.73388	0.80362	-0.35858
1S 34.14510	0.03384	0.90044	-0.00052	2P 17.03350	0.07084	-0.03091
2S 9.27292	0.00569	1.08208	0.51391	3P 4.58882	-0.01448	0.93772
2S 19.36860	0.02009	-0.15332	-0.07529	3P 4.12131	0.01035	0.23425
3S 5.28486	0.00474	-0.02330	-0.57305	3P 8.05951	0.17044	-0.17716
3S 4.49459	-0.00253	0.0176	-0.79695			
3S 7.64192	-0.00469	0.08724	0.35848			
CHROMIUM K(2)L(8)3S(2)3P(1) - 2P						
T.E.= -0.99494367D+03 P.E.= -0.19898863D+04 K.E.= 0.99494264D+03 V.T.= -0.20000010D+01						
S	1S	2S	3S	P	2P	3P
BASIS/ORB E	-231.54751	-36.91740	-11.83365	BASIS/ORB E	-32.87061	-10.86871
1S 23.51020	0.95082	-0.30855	-0.13065	2P 10.13910	0.81989	-0.37675
1S 35.43130	0.03263	0.00152	0.00017	2P 17.70400	0.07242	-0.03114
2S 9.78115	0.00455	1.08576	0.52270	3P 4.83698	-0.02114	1.11982
2S 20.07450	0.02156	-0.16045	-0.07933	3P 4.45269	0.01582	0.06318
3S 5.60546	0.00371	-0.02705	-0.56306	3P 8.38472	0.15054	-0.17620
3S 4.82858	-0.00206	0.01327	-0.82136			
3S 8.12008	-0.00358	0.09191	0.37631			
MANGANESE K(2)L(8)3S(2)3P(1) - 2P						
T.E.= -0.10894511D+04 P.E.= -0.21789010D+04 K.E.= 0.10894499D+04 V.T.= -0.20000010D+01						
S	1S	2S	3S	P	2P	3P
BASIS/ORB E	-253.30424	-41.34953	-13.55580	BASIS/ORB E	-37.08755	-12.52027
1S 24.48510	0.95187	-0.31279	-0.13488	2P 10.54260	0.83060	-0.38901
1S 36.67500	0.03289	0.00255	0.00086	2P 18.26290	0.07617	-0.03320
2S 10.28550	0.00426	1.09059	0.53115	3P 5.16261	-0.01793	1.14511
2S 20.75630	0.02005	-0.16618	-0.08271	3P 4.77883	0.01339	0.05182
3S 5.92053	0.00359	-0.02959	-0.56382	3P 8.77850	0.13251	-0.18125
3S 5.15697	-0.00207	0.01522	-0.83515			
3S 8.59143	-0.00333	0.09447	0.39353			
IRON K(2)L(8)3S(2)3P(1) - 2P						
T.E.= -0.11882945D+04 P.E.= -0.23765879D+04 K.E.= 0.11882934D+04 V.T.= -0.20000010D+C1						
S	1S	2S	3S	P	2P	3P
BASIS/ORB E	-276.06237	-46.03351	-15.38977	BASIS/ORB E	-41.55547	-14.28372
1S 25.46030	0.95290	-0.31686	-0.13889	2P 10.54280	0.84057	-0.39326
1S 37.93520	0.03308	0.00360	0.00159	2P 18.81460	0.08005	-0.03562
2S 10.79540	0.00402	1.09495	0.53839	3P 5.53798	-0.01194	1.05681
2S 21.43150	0.01863	-0.17199	-0.08599	3P 5.10673	0.00853	0.15378
3S 6.23546	0.00352	-0.03244	-0.56209	3P 9.17599	0.11495	-0.18978
3S 5.48616	-0.00210	0.01740	-0.85033			
3S 9.06486	-0.00313	0.09772	0.41010			
COBALT K(2)L(8)3S(2)3P(1) - 2P						
T.E.= -0.12914737D+04 P.E.= -0.25829440D+04 K.E.= 0.12914703D+04 V.T.= -0.20000026D+01						
S	1S	2S	3S	P	2P	3P
BASIS/ORB E	-299.82172	-50.96802	-17.33547	BASIS/ORB E	-46.27424	-16.15896
1S 26.34740	0.95426	-0.31961	-0.14199	2P 11.34950	0.84902	-0.40936
1S 39.14860	0.03577	0.00313	0.00154	2P 19.35970	0.08374	-0.03769
2S 11.21680	0.00584	1.1C7C3	0.54913	3P 5.88458	-0.00869	1.04163
2S 22.29670	0.01286	-0.17176	-0.08645	3P 5.42849	0.00607	0.18668
3S 6.54430	0.00581	-0.02525	-0.56721	3P 9.56791	0.09970	-0.19663
3S 5.81088	-0.00358	0.01410	-0.85694			
3S 9.52815	-0.00493	0.08179	0.41743			

See page 183 for Explanation of Tables and Notes for Tables 32, 42, and 43

TABLE 20 (4). THE HARTREE-FOCK FUNCTIONS FOR AI(<sup>2</sup>P) ISO-ELECTRONIC SERIES.

NICKEL K(2)L(8)3S(2)3P(1) - 2P						
T.E.= -0.13989882D+04 P.E.= -0.27975726D+04 K.E.= 0.13985843D+04 V.T.= -0.20300028D+01						
S	1S	2S	3S	P	2P	3P
BASIS/ORB E	-324.58215	-56.15332	-19.39278	BASIS/ORB E	-51.24376	-18.14591
1S 27.33420	0.95485	-0.32256	-0.14526	2P 11.74600	0.86472	-0.42797
1S 40.41600	0.03568	0.00387	0.00215	2P 20.04470	0.08436	-0.03659
2S 11.73050	0.00558	1.10572	0.55398	3P 6.19785	-0.01631	1.13670
2S 23.00830	0.01229	-0.17739	-0.08937	3P 5.75761	0.01131	0.11653
3S 6.86202	0.00573	-0.02951	-0.05907	3P 9.69689	0.08317	-0.20742
3S 6.14250	-0.00363	0.01712	-0.87716			
3S 10.00400	-0.00467	0.08665	0.43336			
COPPER K(2)L(8)3S(2)3P(1) - 2P						
T.E.= -0.15108379D+04 P.E.= -0.30216719D+04 K.E.= 0.15108340D+04 V.T.= -0.20300026D+01						
S	1S	2S	3S	P	2P	3P
BASIS/ORB E	-350.34349	-61.58526	-21.56166	BASIS/CRB E	-56.46388	-20.24444
1S 28.34060	0.95520	-0.32548	-0.14836	2P 12.14830	0.87178	-0.43736
1S 41.67140	0.03516	0.00486	0.00285	2P 20.59160	0.08811	-0.03637
2S 12.26570	0.00487	1.11080	0.55775	3P 6.51480	-0.00710	1.17591
2S 23.68740	0.01274	-0.18414	-0.09289	3P 6.08508	0.00466	0.08831
3S 7.17775	0.00514	-0.03650	-0.55799	3P 10.10280	0.06762	-0.21054
3S 6.47235	-0.00334	0.02186	-0.89137			
3S 10.47090	-0.00401	0.09533	0.45156			
ZINC K(2)L(8)3S(2)3P(1) - 2P						
T.E.= -0.16270224D+04 P.E.= -0.32540416D+04 K.E.= 0.16270192D+04 V.T.= -0.20300020D+01						
S	1S	2S	3S	P	2P	3P
BASIS/ORB E	-377.10567	-67.27577	-23.84205	BASIS/ORB E	-61.93455	-22.45451
1S 29.38530	0.95537	-0.32768	-0.15107	2P 12.54950	0.87962	-0.44604
1S 42.95320	0.03366	0.00586	0.00358	2P 21.17360	0.09113	-0.04006
2S 12.79540	0.00355	1.11226	0.56081	3P 6.89444	0.00342	1.08923
2S 24.43420	0.01487	-0.19C87	-0.09618	2P 6.41601	-0.00316	0.19097
3S 7.49641	0.00370	-0.04221	-0.54651	3P 10.48960	0.05232	-0.21902
3S 6.80484	-0.00246	0.02662	-0.91385			
3S 10.94730	-0.00279	0.10211	0.46738			
GALLIUM K(2)L(8)3S(2)3P(1) - 2P						
T.E.= -0.17475417D+04 P.E.= -0.34950813D+04 K.E.= 0.17475396D+04 V.T.= -0.20300012D+01						
S	1S	2S	3S	P	2P	3P
BASIS/ORB E	-404.86856	-73.21277	-26.23390	BASIS/ORB E	-67.65568	-24.77606
1S 30.39000	0.95577	-0.33001	-0.15362	2P 12.96900	0.88481	-0.45117
1S 44.19810	0.03323	0.00660	0.00412	2P 21.76460	0.09369	-0.04210
2S 13.35260	0.00289	1.11147	0.56316	3P 7.22323	0.01524	1.07513
2S 25.09070	0.01515	-0.19757	-0.09995	3P 6.74196	-0.01168	0.20878
3S 7.81036	0.00307	-0.05332	-0.55186	3P 11.02330	0.03971	-0.21841
3S 7.13404	-0.00210	0.03381	-0.92238			
3S 11.40290	-0.00221	0.11417	0.48726			
GERMANIUM K(2)L(8)3S(2)3P(1) - 2P						
T.E.= -0.18723955D+04 P.E.= -0.37447878D+04 K.E.= 0.18723922D+04 V.T.= -0.20300018D+01						
S	1S	2S	3S	P	2P	3P
BASIS/ORB E	-433.63204	-79.40022	-28.73715	BASIS/ORB E	-73.62723	-27.20907
1S 31.33650	0.95670	-0.33641	-0.15806	2P 13.40520	0.88906	-0.45610
1S 45.42800	0.03406	0.00922	0.00559	2P 22.36620	0.09539	-0.04354
2S 13.91500	0.00297	1.11779	0.56894	3P 7.62803	0.01701	0.96971
2S 25.51420	0.01296	-0.20652	-0.10458	3P 7.06551	-0.01228	0.32918
3S 8.12160	0.00349	-0.05577	-0.55915	3P 11.45180	0.03129	-0.22960
3S 7.45974	-0.00243	0.03580	-0.92683			
3S 11.85870	-0.00235	0.12004	0.50320			

See page 183 for Explanation of Tables and Notes for Tables 32, 42, and 43

## ROOTHAAN-HARTREE-FOCK ATOMIC WAVEFUNCTIONS

 TABLE 20 (5). THE HARTREE-FOCK FUNCTIONS FOR AI(<sup>2</sup>P) ISO-ELECTRONIC SERIES.

ARSEVIC      K(2)L(8)3S(2)3P(1) - 2P  
 T.E.= -0.20015838D+04    P.E.= -0.40031646D+04    K.E.= 0.20015808D+04    V.T.= -0.20000015D+01

S	1S	2S	3S	P	2P	3P
BASIS/ORB E	-463.39617	-85.83807	-31.35180	BASIS/ORB E	-79.84914	-29.75345
1S 32.29230	0.95705	-0.33693	-0.15942	2P 13.84730	0.89354	-0.45727
1S 46.68240	0.03490	0.00658	0.00538	2P 23.02170	0.09614	-0.04561
2S 14.34440	0.00379	1.12514	0.57532	3P 7.95514	0.02581	0.93390
2S 26.43770	0.01105	-0.20614	-0.10475	3P 7.39275	-0.01854	0.36117
3S 8.43801	0.00476	-0.05343	-0.055725	3P 12.11120	0.02232	-0.22513
3S 7.78937	-0.00357	0.03519	-0.93990			
3S 12.30520	-0.00309	0.10963	0.51112			

SELENIUM      K(2)L(8)3S(2)3P(1) - 2P  
 T.E.= -0.21351064D+04    P.E.= -0.42702101D+04    K.E.= 0.21351037D+04    V.T.= -0.20000013D+01

S	1S	2S	3S	P	2P	3P
BASIS/ORB E	-494.16075	-92.52626	-34.07778	BASIS/ORB E	-86.32140	-32.40924
1S 33.28260	0.95758	-0.34201	-0.16298	2P 14.31530	0.89648	-0.45173
1S 47.91950	0.03472	0.01097	0.00667	2P 23.69350	0.09583	-0.04580
2S 14.94670	0.00314	1.12809	0.57940	3P 8.29145	0.02565	0.93152
2S 26.87400	0.01089	-0.21682	-0.11062	3P 7.71670	-0.01850	0.37243
3S 8.74874	0.00419	-0.06304	-0.57497	3P 12.55710	0.01871	-0.23170
3S 8.11461	-0.00303	0.04205	-0.93582			
3S 12.74630	-0.00256	0.12264	0.53104			

BROMINE      K(2)L(8)3S(2)3P(1) - 2P  
 T.E.= -0.22729632D+04    P.E.= -0.45459267D+04    K.E.= 0.22729635D+04    V.T.= -0.19999599D+01

S	1S	2S	3S	P	2P	3P
BASIS/ORB E	-525.92593	-99.46478	-36.91510	BASIS/ORB E	-93.04398	-35.17635
1S 34.39370	0.95795	-0.34356	-0.16467	2P 14.74710	0.90551	-0.46752
1S 49.20950	0.03159	0.01238	0.00741	2P 24.44710	0.09468	-0.04606
2S 15.50330	0.00039	1.13011	0.58287	3P 8.68578	0.03332	0.84341
2S 27.57230	0.01555	-0.22528	-0.11533	3P 8.04971	-0.02332	0.46844
3S 9.07075	0.00035	-0.07306	-0.56428	3P 13.03990	0.00683	-0.23547
3S 8.45116	-0.00030	0.04974	-0.95924			
3S 13.18670	-0.00020	0.13075	0.54765			

KRYPTON      K(2)L(8)3S(2)3P(1) - 2P  
 T.E.= -0.24151542D+04    P.E.= -0.48303C75D+04    K.E.= 0.24151533D+04    V.T.= -0.20000004D+01

S	1S	2S	3S	P	2P	3P
BASIS/ORB E	-558.69104	-106.65363	-39.86369	BASIS/ORB E	-100.01679	-38.05482
1S 35.28730	0.95882	-0.34482	-0.16620	2P 15.17660	0.89974	-0.46620
1S 50.54700	0.03351	0.01172	0.00717	2P 24.72650	0.10193	-0.05033
2S 16.05960	0.00243	1.12932	0.58456	3P 8.00045	0.02336	0.84703
2S 28.30630	0.01108	-0.22964	-0.11794	3P 8.39080	-0.01599	0.47028
3S 9.40173	0.00367	-0.08843	-0.53360	3P 13.53940	0.00732	-0.24014
3S 8.79517	-0.00274	0.06155	-1.00244			
3S 13.62970	-0.00199	0.141C1	0.56464			

See page 183 for Explanation of Tables and Notes for Tables 32, 42, and 43

TABLE 21 (1). THE HARTREE-FOCK FUNCTIONS FOR Si(<sup>3</sup>P) ISO-ELECTRONIC SERIES.

SILICON K(2)L(8)3S(2)3P(2) -3P T.E.= -0.28885420D+03 P.E.= -0.57770936D+03 K.E.= 0.28885516D+03 V.T.= -0.19999967D+01						
S	1S	2S	3S	P	2P	3P
BASIS/ORB E	-68.81221	-6.15637	-0.53977	BASIS/ORB E	-4.25588	-0.29706
1S 14.55420	0.88029	-0.22801	-0.05809	2P 5.54870	0.64679	-0.13990
1S 23.41790	0.01683	-0.00765	-0.00211	2P 11.24470	0.04123	-0.00861
2S 5.29058	0.00503	0.89657	0.25097	3P 1.73837	0.01107	0.50090
2S 13.11440	0.12287	-0.13217	-0.03652	3P 1.01984	-0.00275	0.58188
3S 2.09030	0.00045	0.000C8	-0.57872	3P 4.37588	0.39134	-0.08744
3S 1.30291	-0.00020	0.00C55	-0.53370			
3S 4.37285	-0.00160	0.22197	0.11315			
PHOSPHORUS K(2)L(8)3S(2)3P(2) -3P T.E.= -0.34034959D+03 P.E.= -0.68C69365D+03 K.E.= 0.34034406D+03 V.T.= -0.20000153D+01						
S	1S	2S	3S	P	2P	3P
BASIS/ORB E	-80.38155	-7.91509	-1.03401	BASIS/ORB E	-5.80262	-0.72003
1S 15.29030	0.90282	-0.24446	0.06967	2P 6.46199	0.66290	-0.17746
1S 24.54860	0.02003	-0.00585	0.00208	2P 12.31770	0.03898	-0.00971
2S 5.68698	0.00496	0.93148	-0.29598	3P 2.02237	0.00931	0.58676
2S 13.77400	0.09302	-0.12784	0.04078	3P 1.34371	-0.00224	0.48308
3S 2.40272	0.00062	0.00160	0.60037	3P 4.84290	0.37205	-0.10439
3S 1.62738	-0.00029	-0.00011	0.51897			
3S 4.76941	-0.00182	0.18734	-0.12664			
SULFUR K(2)L(8)3S(2)3P(2) -3P T.E.= -0.39633244D+03 P.E.= -0.79265691D+03 K.E.= 0.39632447D+03 V.T.= -0.20000201D+01						
S	1S	2S	3S	P	2P	3P
BASIS/ORB E	-92.97576	-9.55099	-1.65782	BASIS/CRB E	-7.62500	-1.27039
1S 16.18010	0.91397	0.25490	0.07915	2P 6.98324	0.67904	-0.20750
1S 25.79640	0.02103	0.00475	0.00200	2P 13.52140	0.03544	-0.01009
2S 6.10928	0.00451	-0.95708	-0.33351	3P 2.33664	0.00621	0.62586
2S 14.50410	0.07904	0.12909	0.04548	3P 1.68363	-0.00062	0.44713
3S 2.69961	0.00063	-0.00273	0.63849	3P 5.30067	0.35547	-0.12005
3S 1.94216	-0.00031	0.00667	0.49376			
3S 5.18471	-0.00172	-0.16361	-0.14196			
CHLORINE K(2)L(8)3S(2)3P(2) -3P T.E.= -0.45678867D+03 P.E.= -0.91256567D+03 K.E.= 0.456781000D+03 V.T.= -0.20000168D+01						
S	1S	2S	3S	P	2P	3P
BASIS/ORB E	-106.58472	-12.25317	-2.40336	BASIS/ORB E	-9.71259	-1.94188
1S 17.02110	0.92398	-0.26337	0.08736	2P 7.42212	0.69198	-0.23279
1S 27.09110	0.02395	-0.00482	0.00220	2P 13.90850	0.04097	-0.01273
2S 6.53221	0.00578	0.57655	-0.36453	3P 2.62970	0.00445	0.67378
2S 15.32660	0.06325	-0.12884	0.04885	3P 2.01535	-0.00012	0.40397
3S 3.00960	0.00128	0.00663	0.63823	3P 5.75140	0.33242	-0.12897
3S 2.28671	-0.00069	-0.00260	0.50654			
3S 5.65603	-0.00280	0.14344	-0.15515			
ARGON K(2)L(8)3S(2)3P(2) -3P T.E.= -0.5217C978D+03 P.E.= -0.10434121D+04 K.E.= 0.5217C229D+03 V.T.= -0.20000144D+01						
S	1S	2S	3S	P	2P	3P
BASIS/ORB E	-121.20429	-14.81615	-3.26704	BASIS/ORB E	-12.06013	-2.73142
1S 17.89750	0.93255	-0.27136	0.09471	2P 7.52639	0.70790	-0.25537
1S 28.36610	0.02551	-0.00439	0.00224	2P 15.01920	0.03804	-0.01267
2S 6.97032	0.00578	1.00C37	-0.39548	3P 2.93081	-0.00020	0.71444
2S 16.03160	0.05133	-0.13203	0.05338	3P 2.34642	0.00241	0.37236
3S 3.27080	0.00155	0.00257	0.75755	3P 6.18855	0.31707	-0.13965
3S 2.54130	-0.00085	-0.00C71	0.41001			
3S 5.99418	-0.00297	0.12681	-0.17329			

See page 183 for Explanation of Tables and Notes for Tables 32, 42, and 43

## ROOTHAAN-HARTREE-FOCK ATOMIC WAVEFUNCTIONS

 TABLE 21 (2). THE HARTREE-FOCK FUNCTIONS FOR Si(<sup>3</sup>P) ISO-ELECTRONIC SERIES.

POTASSIUM K(2)L(8)3S(2)3P(2) -3P						
T.E.= -0.59109091D+03 P.E.= -0.11821748D+04 K.E.= 0.59108384D+03 V.T.= -0.20000120D+01						
S	1S	2S	3S	P	2P	3P
BASIS/ORB E	-136.83092	-17.63659	-4.24661	BASIS/ORB E	-14.66458	-3.63685
1S 18.80350	0.93878	-0.27959	0.10171	2P 8.30698	0.72469	-0.27645
1S 29.61690	0.02666	-0.00297	0.00195	2P 15.27640	0.04541	-0.01604
2S 7.42400	0.00581	1.01419	-0.41926	3P 3.23100	-0.00219	0.75558
2S 16.71180	0.04265	-0.13420	0.05720	3P 2.67593	0.00342	0.34141
2S 3.58035	0.00192	0.00664	0.71392	3P 6.60278	0.28869	-0.14380
3S 2.93548	-0.00116	-0.00307	0.46424			
3S 6.48917	-0.00317	0.115E2	-0.18339			
CALCIUM K(2)L(8)3S(2)3P(2) -3P						
T.E.= -0.66492828D+03 P.E.= -0.13298514D+04 K.E.= 0.66492310D+03 V.T.= -0.20000780D+01						
S	1S	2S	3S	P	2P	3P
BASIS/ORB E	-153.46332	-20.71245	-5.34088	BASIS/ORB E	-17.52393	-4.65711
1S 19.74010	0.94271	-0.26640	0.10813	2P 8.72300	0.74051	-0.29535
1S 30.83640	0.02753	-0.00209	0.00149	2P 15.63380	0.04869	-0.01800
2S 7.89436	0.00544	1.02737	-0.43935	3P 3.54855	0.00019	0.74394
2S 17.39030	0.03710	-0.13905	0.06105	3P 3.04448	0.00156	0.36306
3S 3.89791	0.00204	0.00406	0.73996	3P 7.04445	0.26467	-0.14784
2S 3.25579	-0.00126	-0.00170	0.46099			
3S 6.89342	-0.00305	0.10593	-0.20561			
SCANDIUM K(2)L(8)3S(2)3P(2) -3P						
T.E.= -0.74321957D+03 P.E.= -0.14E64334D+04 K.E.= 0.74321388D+03 V.T.= -0.2000077D+01						
S	1S	2S	3S	P	2P	3P
BASIS/ORB E	-171.10006	-24.04295	-6.54893	BASIS/ORB E	-20.63754	-5.79125
1S 20.67230	0.94616	-0.29237	0.11402	2P 9.13083	0.75862	-0.31471
1S 32.08970	0.02854	-0.00127	0.00101	2P 16.48670	0.05177	-0.01960
2S 8.36554	0.00543	1.03912	-0.45686	3P 3.81309	-0.00833	0.87254
2S 18.08170	0.03178	-0.14344	0.06451	3P 3.33250	0.00721	0.24608
3S 4.21168	0.00234	0.00254	0.76457	3P 7.40563	0.24219	-0.15062
3S 3.57816	-0.00148	-0.00088	0.45745			
3S 7.31790	-0.00319	0.10458	-0.22618			
TITANIUM K(2)L(8)3S(2)3P(2) -3P						
T.E.= -0.82596284D+03 P.E.= -0.16519214D+04 K.E.= 0.82595852D+03 V.T.= -0.2000052D+01						
S	1S	2S	3S	P	2P	3P
BASIS/ORB E	-189.74039	-27.62643	-7.87020	BASIS/ORB E	-24.00383	-7.03870
1S 21.63880	0.94801	-0.29755	0.11936	2P 9.52717	0.77907	-0.33313
1S 33.29180	0.02904	-0.00029	0.00042	2P 17.23720	0.05335	-0.02087
2S 8.85407	0.00485	1.04845	-0.47172	3P 4.13767	-0.00916	0.89263
2S 18.75300	0.02918	-0.14933	0.06838	3P 3.65698	0.00737	0.23597
3S 4.54143	0.00225	-0.00122	0.78404	3P 7.77630	0.21675	-0.15464
3S 3.89623	-0.00143	0.00130	0.46192			
3S 7.72343	-0.00287	0.10366	-0.25078			
VANADIUM K(2)L(8)3S(2)3P(2) -3P						
T.E.= -0.91315685D+03 P.E.= -0.18263107D+04 K.E.= 0.91315386D+03 V.T.= -0.2000033D+01						
S	1S	2S	3S	P	2P	3P
BASIS/ORB E	-209.38345	-31.4E271	-9.30422	BASIS/ORB E	-27.62268	-8.39901
1S 22.58850	0.95002	-0.30223	0.12408	2P 9.91861	0.79551	-0.34965
1S 34.52370	0.02988	0.00040	0.00001	2P 17.78540	0.05693	-0.02276
2S 9.34008	0.00469	1.05945	-0.48729	3P 4.45266	-0.01235	0.92812
2S 19.42960	0.02580	-0.15519	0.07253	3P 3.98447	0.00948	0.21819
3S 4.92129	0.00243	-0.0C784	0.77348	3P 8.13598	0.19417	-0.15827
2S 4.21874	-0.00150	0.00497	0.50544			
3S 8.05894	-0.00293	0.10235	-0.28229			

See page 183 for Explanation of Tables and Notes for Tables 32, 42, and 43

TABLE 21 (3). THE HARTREE-FOCK FUNCTIONS FOR Si(<sup>3</sup>P) ISO-ELECTRONIC SERIES.

CHROMIUM K(2)L(8)3S(2)3P{2} -3P						
T.E.= -0.100480050D+04 P.E.= -0.20C95966D+04 K.E.= 0.10047981D+04 V.T.= -0.20000023D+01						
S	1S	2S	3S	P	2P	3P
BASIS/ORB E	-230.02877	-35.55112	-10.85071	BASIS/OPB E	-31.49345	-9.87186
1S 23.43140	0.95348	-0.30804	-0.12911	2P 10.30340	0.81029	-0.36327
1S 35.70800	0.03339	0.00074	0.00029	2P 18.25670	0.06140	-0.02549
2S 9.82882	0.00649	1.06713	0.49980	3P 4.84981	-0.01536	0.85385
2S 20.09240	0.01663	-0.15824	-0.07521	3P 4.30733	0.01090	0.31276
3S 5.25435	0.00405	-0.01127	-0.79382	3P 8.47207	0.17313	-0.16904
3S 4.53388	-0.00251	0.00652	-0.50877			
3S 8.46657	-0.00449	0.10168	0.30610			
MANGANESE K(2)L(8)3S(2)3P{2} -3P						
T.E.= -0.110C8930D+04 P.E.= -0.22017847D+04 K.E.= 0.11008917D+04 V.T.= -0.20000011D+01						
S	1S	2S	3S	P	2P	3P
BASIS/ORB E	-251.67614	-39.89136	-12.50937	BASIS/CRB E	-35.61588	-11.45697
1S 24.42430	0.95345	-0.30809	-0.13078	2P 10.68440	0.82261	-0.37720
1S 36.95220	0.03358	0.00017	-0.00041	2P 18.69550	0.06667	-0.02796
2S 10.24790	0.00631	1.08333	0.51870	3P 5.16821	-0.01649	0.88133
2S 21.01350	0.01640	-0.16118	-0.07916	3P 4.63469	0.01170	0.29903
3S 5.57525	0.00442	-0.01231	-0.82723	3P 8.82714	0.15277	-0.17255
3S 4.85503	-0.00277	0.00763	-0.50106			
3S 8.80472	-0.00456	0.08696	0.32283			
IRON K(2)L(8)3S(2)3P{2} -3P						
T.E.= -0.12014336D+04 P.E.= -0.24C28658D+04 K.E.= 0.12014322D+04 V.T.= -0.20000012D+01						
S	1S	2S	3S	P	2P	3P
BASIS/ORB E	-274.32534	-44.48306	-14.28006	BASIS/GRB E	-39.98963	-13.15420
1S 25.43020	0.95370	-0.31312	-0.13468	2P 11.06200	0.83941	-0.39411
1S 38.17980	0.03322	0.00155	0.00032	2P 19.29980	0.06943	-0.02888
2S 10.73900	0.00548	1.09090	0.52916	3P 5.48589	-0.02042	0.92277
2S 21.68700	0.01682	-0.16692	-0.08283	3P 4.96131	0.01419	0.27456
3S 5.89795	0.00398	-0.01366	-0.84528	3P 9.08535	0.13152	-0.17688
3S 5.17542	-0.00253	0.00846	-0.50219			
3S 9.23495	-0.00396	0.08609	0.34236			
COBALT K(2)L(8)3S(2)3P{2} -3P						
T.E.= -0.13064219D+04 P.E.= -0.26128424D+04 K.E.= 0.13064205D+04 V.T.= -0.20000011D+01						
S	1S	2S	3S	P	2P	3P
BASIS/ORB E	-297.97600	-49.32602	-16.16269	BASIS/ORB E	-44.61453	-14.96339
1S 26.45650	0.95379	-0.31585	-0.13773	2P 11.43430	0.85049	-0.40715
1S 39.43750	0.03232	0.00245	0.00079	2P 19.77620	0.07466	-0.03113
2S 11.23940	0.00446	1.05586	0.53767	3P 5.79310	-0.01499	0.96509
2S 22.41630	0.01817	-0.17297	-0.08665	3P 5.29189	0.01053	0.24413
3S 6.20872	0.00333	-0.01693	-0.86764	3P 9.44683	0.11069	-0.17808
3S 5.49994	-0.00217	0.01065	-0.49646			
3S 9.67485	-0.00316	0.08805	0.36044			
NICKEL K(2)L(8)3S(2)3P{2} -3P						
T.E.= -0.14158574D+04 P.E.= -0.28317125D+04 K.E.= 0.14158552D+04 V.T.= -0.20000016D+01						
S	1S	2S	3S	P	2P	3P
BASIS/ORB E	-322.62776	-54.42007	-18.15708	BASIS/ORB E	-49.49040	-16.88440
1S 27.42660	0.95454	-0.31935	-0.14105	2P 11.74510	0.85965	-0.41917
1S 40.66990	0.03277	0.00330	0.00129	2P 19.59000	0.08555	-0.03594
2S 11.73570	0.00436	1.10181	0.54602	3P 6.11178	-0.00561	0.99278
2S 23.11730	0.01670	-0.17779	-0.08979	3P 5.62032	0.00421	0.22842
3S 6.52983	0.00347	-0.01934	-0.88505	3P 9.80850	0.08478	-0.17705
3S 5.82215	-0.00229	0.01226	-0.49655			
3S 10.10780	-0.00315	0.08654	0.37878			

See page 183 for Explanation of Tables and Notes for Tables 32, 42, and 43

## ROOTHAAN-HARTREE-FOCK ATOMIC WAVEFUNCTIONS

 TABLE 21 (4). THE HARTREE-FOCK FUNCTIONS FOR Si(<sup>3</sup>P) ISO-ELECTRONIC SERIES.

COPPER K(2)L(8)3S(2)3P(2) -3P						
T.E.= -0.15297397D+04 P.E.= -0.30594771D+04 K.E.= 0.15297374D+04 V.T.= -0.20000015D+01						
S	1S	2S	3S	P	2P	3P
BASIS/ORB E	-348.28099	-59.76502	-20.26315	BASIS/ORB E	-54.61712	-18.91716
1S 28.47410	0.95437	-0.323C9	-0.14445	2P 12.19340	0.87384	-0.43498
1S 41.84820	0.03154	0.00513	0.00227	2P 20.88200	0.08198	-0.03351
2S 12.27000	0.00264	1.10566	0.55266	3P 6.45362	-0.0084	1.02748
2S 23.73440	0.01913	-0.18573	-0.09439	3P 5.52981	0.00565	0.21833
3S 6.86944	0.00195	-0.02444	-0.90135	3P 9.96333	0.07378	-0.19196
3S 6.13518	-0.00128	0.01517	-0.50154			
3S 10.52220	-0.00178	0.09538	0.40328			
ZINC K(2)L(8)3S(2)3P(2) -3P						
T.E.= -0.16480686D+04 P.E.= -0.325E1350D+04 K.E.= 0.16480664D+04 V.T.= -0.20000013D+01						
S	1S	2S	3S	P	2P	3P
BASIS/ORB E	-374.53496	-65.36C76	-22.48084	BASIS/CRB E	-59.99452	-21.06156
1S 29.45390	0.95503	-0.32586	-0.14725	2P 12.57680	0.88059	-0.44364
1S 43.08950	0.03173	0.00580	0.00272	2P 21.35970	0.08706	-0.03667
2S 12.79570	0.00245	1.1C830	0.55837	3P 6.84304	0.00119	0.95804
2S 24.43180	0.01814	-0.19152	-0.09787	3P 6.26672	-0.00139	0.30456
3S 7.19127	0.00190	-0.03011	-0.92030	3P 1C.33800	0.05690	-0.20116
3S 6.45588	-0.00127	0.01889	-0.49931			
3S 10.95800	-0.00167	0.10136	0.42313			
GALLIUM K(2)L(8)3S(2)3P(2) -3P						
T.E.= -0.17708437D+04 P.E.= -0.35416865D+04 K.E.= 0.17708427D+04 V.T.= -0.20000006D+01						
S	1S	2S	3S	P	2P	3P
BASIS/ORB E	-402.58981	-71.20716	-24.81009	BASIS/CRB E	-65.62254	-23.31755
1S 30.46780	0.95533	-0.32891	-0.15052	2P 12.57680	0.88497	-0.44826
1S 44.29970	0.03120	0.00703	0.00367	2P 21.86890	0.09153	-0.03913
2S 13.31750	0.00156	1.11273	0.56287	3P 7.17258	0.01536	0.93696
2S 25.10420	0.01880	-0.19779	-0.10083	3P 6.59049	-0.01088	0.32697
3S 7.59114	0.00106	-0.03275	-0.88565	3P 10.52710	0.04166	-0.19754
3S 6.77336	-0.00069	0.01557	-0.55871			
3S 11.37590	-0.00099	0.10569	0.45113			
GERMANIUM K(2)L(8)3S(2)3P(2) -3P						
T.E.= -0.18980650D+04 P.E.= -0.379E1287D+04 K.E.= 0.18980637D+04 V.T.= -0.20000007D+01						
S	1S	2S	3S	P	2P	3P
BASIS/ORB E	-431.24541	-77.30423	-27.25081	BASIS/CRB E	-71.50115	-25.685C5
1S 31.43780	0.95596	-0.33172	-0.15308	2P 13.38340	0.89071	-0.45644
1S 45.53930	0.03163	0.CC776	0.00410	2P 22.42370	0.09467	-0.04055
2S 13.84240	0.00159	1.11626	0.56844	3P 7.49245	0.02247	0.95623
2S 25.78920	0.01745	-0.20322	-0.10425	3P 6.91952	-0.01592	0.31766
3S 7.91429	0.00121	-0.03750	-0.90105	3P 11.32850	0.02910	-0.20064
3S 7.09527	-0.00079	0.02265	-0.55886			
3S 11.80710	-0.00106	0.11025	0.46899			
ARSENIC K(2)L(8)3S(2)3P(2) -3P						
T.E.= -0.20297322D+04 P.E.= -0.4C594633D+04 K.E.= 0.20297311D+04 V.T.= -0.20000006D+01						
S	1S	2S	3S	P	2P	3P
BASIS/ORB E	-460.50169	-83.65182	-29.80298	BASIS/ORB E	-77.63024	-28.16403
1S 32.41450	0.95647	-0.33439	-0.15534	2P 13.81130	0.89576	-0.46212
1S 46.77610	0.03192	0.00653	0.00446	2P 23.03610	0.09628	-0.04184
2S 14.35170	0.00155	1.12152	0.57533	3P 7.88872	0.02632	0.88462
2S 26.48870	0.01646	-0.208C7	-0.10765	3P 7.24720	-0.01789	0.40276
3S 8.23792	0.00128	-0.04095	-0.91918	3P 11.75460	0.01922	-0.20997
3S 7.41676	-0.00085	0.02454	-0.55693			
3S 12.22320	-0.00108	0.11165	0.48557			

See page 183 for Explanation of Tables and Notes for Tables 32, 42, and 43

TABLE 21 (5). THE HARTREE-FOCK FUNCTIONS FOR Si(<sup>3</sup>P) ISO-ELECTRONIC SERIES.

SELENIUM K(2)L(8)3S(2)3P(2) -3P T.E.= -0.21658452D+04 P.E.= -0.4331688CD+04 K.E.= 0.21658428D+04 V.T.= -0.20000011D+01						
S	1S	2S	3S	P	2P	3P
BASIS/ORB E	-491.55864	-90.24992	-32.46657	BASIS/ORB E	-84.00979	-30.75447
1S 33.37620	0.95706	-0.33677	-0.15793	2P 14.26250	0.89989	-0.46805
1S 48.03180	0.03249	0.00505	0.00500	2P 23.70150	0.09445	-0.04207
2S 14.87580	0.00189	1.12432	0.57831	3P 8.21146	0.03039	0.89392
2S 27.19680	0.01483	-0.21272	-0.10989	3P 7.57636	-0.02066	0.40176
3S 8.73113	0.00172	-0.04502	-0.74935	3P 12.19170	0.01276	-0.21442
3S 7.81740	-0.00109	0.02596	-0.75039			
3S 12.64580	-0.00145	0.11748	0.51252			

  

BROMINE K(2)L(8)3S(2)3P(2) -3P T.E.= -0.23064038D+04 P.E.= -0.46128061D+04 K.E.= 0.23064023D+04 V.T.= -0.20000007D+01						
S	1S	2S	3S	P	2P	3P
BASIS/ORB E	-523.21594	-97.09841	-35.24151	BASIS/ORB E	-90.63968	-33.45629
1S 34.34620	0.95754	-0.33946	-0.16062	2P 14.68170	0.90224	-0.47252
1S 49.27560	0.03289	0.00588	0.00571	2P 24.21110	0.09988	-0.04400
2S 15.38210	0.00200	1.13056	0.58317	3P 8.53453	0.03301	0.69661
2S 27.88020	0.01367	-0.21741	-0.11218	3P 7.90522	-0.02268	0.40342
3S 9.06434	0.00182	-0.04428	-0.84435	3P 12.65840	0.00499	-0.21662
3S 8.06345	-0.00112	0.02454	-0.67892			
3S 13.05120	-0.00159	0.11731	0.53715			

  

KRYPTON K(2)L(8)3S(2)3P(2) -3P T.E.= -0.24514079D+04 P.E.= -0.49028142D+04 K.E.= 0.24514063D+04 V.T.= -0.20000007D+01						
S	1S	2S	3S	P	2P	3P
BASIS/ORB E	-555.67407	-104.19725	-38.12782	BASIS/ORB E	-97.51995	-36.26948
1S 35.35860	0.95808	-0.34560	-0.16419	2P 15.26780	0.90419	-0.47520
1S 50.48840	0.03222	0.01218	0.00717	2P 25.24420	0.09141	-0.04042
2S 15.92860	0.00881	1.14192	0.59406	3P 8.86306	0.03016	0.91395
2S 28.27350	0.01443	-0.22720	-0.11876	2P 8.22912	-0.02117	0.40578
3S 9.39085	0.00080	-0.04359	-0.86568	3P 13.12940	0.01292	-0.22795
3S 8.38108	-0.00051	0.02380	-0.67466			
3S 13.44070	-0.00065	0.11775	0.55356			

TABLE 22 NUMBER OF ATOMS 23

See page 183 for Explanation of Tables and Notes for Tables 32, 42, and 43

## ROOTHAAN-HARTREE-FOCK ATOMIC WAVEFUNCTIONS

 TABLE 22 (1). THE HARTREE-FOCK FUNCTIONS FOR S1(<sup>1</sup>D) ISO-ELECTRONIC SERIES.

SILICON K(2)L(8)3S(2)3P(2) -1D						
T.E.= -0.28881499D+03 P.E.= -0.577E2829D+03 K.E.= 0.28881339D+03 V.T.= -0.20000055D+01						
S	1S	2S	3S	P	2P	3P
BASIS/ORB E	-68.82657	-6.16535	-0.54761	BASIS/CRB E	-4.26870	-0.26101
1S 14.54290	0.88282	-0.23120	-0.05873	2P 5.82303	0.66328	-0.14182
1S 23.60200	0.01590	-0.0C609	-0.00192	2P 11.09240	0.04688	-0.00963
2S 5.22173	0.00473	0.92C09	0.26015	3P 1.74114	0.00955	0.512E0
2S 13.07360	0.12124	-0.12522	-0.03646	3P 0.96795	-0.00160	0.58172
3S 2.07084	0.00043	-0.00C34	-0.60861	3P 4.31097	0.36601	-0.08140
3S 1.28696	-0.00C19	0.00C51	-0.50540			
3S 4.28564	-0.00149	0.19544	0.1053E			
PHOSPHORUS K(2)L(8)3S(2)3P(2) -1D						
T.E.= -0.34029793D+03 P.E.= -0.68C58761D+03 K.E.= 0.34028968D+C3 V.T.= -0.20000242D+C1						
S	1S	2S	3S	P	2P	3P
BASIS/ORB E	-80.39323	-7.92529	-1.03922	BASIS/CRB E	-5.81272	-0.67056
1S 15.20110	0.90848	-0.24793	0.06994	2P 6.27074	0.68314	-0.18304
1S 24.63370	0.02108	-0.00516	0.00231	2P 11.79320	0.04974	-0.01202
2S 5.67605	0.00553	0.93414	-0.29988	3P 2.03525	0.00647	0.58030
2S 13.72040	0.08498	-0.12436	0.04099	3P 1.30656	-0.00061	0.49701
3S 2.36321	0.00079	0.00311	0.62561	3P 4.73959	0.33971	-0.09285
3S 1.61985	-0.00039	-0.00C88	0.48798			
3S 4.77597	-0.00221	0.18328	-0.11854			
SULFUR K(2)L(8)3S(2)3P(2) -1D						
T.E.= -0.39626985D+03 P.E.= -0.79253251D+03 K.E.= 0.39626266D+03 V.T.= -0.20000181D+01						
S	1S	2S	3S	P	2P	3P
BASIS/ORB E	-92.98623	-9.960C7	-1.66216	BASIS/ORB E	-7.63403	-1.20971
1S 16.08910	0.91886	0.25669	-0.07903	2P 6.70507	0.70332	-0.21625
1S 25.88270	0.02238	0.00493	-0.00244	2P 12.50560	0.05254	-0.01450
2S 6.12754	0.0053E	-0.95223	0.33438	3P 2.34562	0.00356	0.625C3
2S 14.46760	0.07137	0.12740	-0.04605	3P 1.63703	0.00063	0.45164
3S 2.64453	0.00091	-0.00219	-0.68724	3P 5.15969	0.31171	-0.1029E
3S 1.91812	-0.00047	0.00043	-0.43914			
3S 5.20245	-0.00227	-0.17C04	0.13676			
CHLORINE K(2)L(8)3S(2)3P(2) -1D						
T.E.= -0.45671572D+03 P.E.= -0.91342546D+03 K.E.= 0.45670974D+03 V.T.= -0.20000131D+01						
S	1S	2S	3S	P	2P	3P
BASIS/DRB E	-106.59477	-12.26147	-2.40730	BASIS/CRB E	-9.72066	-1.87093
1S 17.00760	0.92488	0.26362	0.08724	2P 7.12184	0.72391	-0.24523
1S 27.05280	0.02410	0.00488	0.00235	2P 13.17690	0.05592	-0.01695
2S 6.54145	0.00547	-0.97807	-0.36653	3P 2.65389	0.00072	0.66242
2S 15.28160	0.06217	0.12979	0.04969	3P 1.96489	0.00184	0.41963
3S 2.94785	0.00113	-0.00279	0.74503	3P 5.56494	0.28322	-0.10979
3S 2.20856	-0.00060	0.00075	0.40162			
3S 5.60290	-0.00254	-0.14569	-0.15532			
ARGON K(2)L(8)3S(2)3P(2) -1D						
T.E.= -0.52162710D+03 P.E.= -0.10432490D+04 K.E.= 0.52162194D+03 V.T.= -0.20000099D+01						
S	1S	2S	3S	P	2P	3P
BASIS/DRB E	-121.21365	-14.82383	-3.27061	BASIS/CRB E	-12.06785	-2.65044
1S 17.91800	0.93192	-0.27200	0.09479	2P 7.54073	0.74196	-0.26975
1S 28.28370	0.02511	-0.00385	0.00215	2P 13.81060	0.05938	-0.01946
2S 7.00144	0.00520	0.99185	-0.39232	3P 2.97634	-0.00205	0.68327
2S 15.98110	0.05282	-0.13278	0.05389	3P 2.29559	0.00311	0.40876
3S 3.26516	0.00128	0.00404	0.72590	3P 5.96740	0.25781	-0.11721
3S 2.57829	-0.00073	-0.00145	0.43501			
3S 6.06678	-0.00252	0.13E31	-0.17123			

See page 183 for Explanation of Tables and Notes for Tables 32, 42, and 43

TABLE 22 (2). THE HARTREE-FOCK FUNCTIONS FOR Si(<sup>1</sup>D) ISO-ELECTRONIC SERIES.

POTASSIUM K(2)L(8)3S(2)3P(2) -1D						
T.E.= -0.59099859D+03 P.E.= -0.11819928D+04 K.E.= 0.59099424D+C3 V.T.= -0.20300074D+01						
S	1S	2S	3S	P	2P	3P
BASIS/ORB E	-136.84015	-17.64353	-4.24999	BASIS/ORB E	-14.67193	-3.54631
1S 18.81640	0.93830	-0.27555	0.10239	2P 7.55959	0.75820	-0.29170
1S 29.55450	0.02648	-0.00307	0.00156	2P 14.42860	0.06282	-0.02173
2S 7.48146	0.00539	1.00024	-0.41057	3P 3.29231	-0.00434	0.70273
2S 16.67870	0.04359	-0.13608	0.05674	3P 2.62875	0.00422	0.39992
3S 3.57055	0.00155	0.00454	0.74795	3P 6.36829	0.23455	-0.12275
3S 2.90359	-0.00093	-0.00175	0.43013			
3S 6.55431	-0.00277	0.13352	-0.19245			
CALCIUM K(2)L(8)3S(2)3P(2) -1D						
T.E.= -0.66482661D+03 P.E.= -0.13296493D+04 K.E.= 0.66482271D+03 V.T.= -0.20000059D+01						
S	1S	2S	3S	P	2P	3P
BASIS/ORB E	-153.47228	-20.71568	-5.34406	BASIS/ORB E	-17.53121	-4.55709
1S 19.74240	0.94259	-0.28618	0.10870	2P 8.37405	0.77182	-0.31092
1S 30.80790	0.02754	-0.00219	0.00119	2P 14.99240	0.06713	-0.02422
2S 7.93243	0.00534	1.01774	-0.43271	3P 3.60526	-0.00524	0.72283
2S 17.37830	0.03727	-0.13989	0.06040	3P 2.96073	0.00463	0.39083
3S 3.88163	0.00183	0.00351	0.77338	3P 6.77821	0.21285	-0.12736
3S 3.22797	-0.00113	-0.00128	0.42552			
3S 6.96056	-0.00290	0.12138	-0.21033			
SCANDIUM K(2)L(8)3S(2)3P(2) -1D						
T.E.= -0.74310859D+03 P.E.= -0.14862147D+04 K.E.= 0.74310609D+03 V.T.= -0.20000034D+01						
S	1S	2S	3S	P	2P	3P
BASIS/ORB E	-171.10890	-24.04972	-6.55195	BASIS/ORB E	-20.64439	-5.68192
1S 20.73490	0.94427	-0.29169	0.11423	2P 8.78751	0.78595	-0.32940
1S 31.99250	0.02738	-0.00094	0.00064	2P 15.62540	0.07033	-0.02607
2S 8.40635	0.00406	1.03302	-0.45286	3P 3.89813	-0.00395	0.76344
2S 18.03230	0.03595	-0.14663	0.06520	3P 3.28581	0.00371	0.35981
3S 4.22201	0.00140	-0.00176	0.79291	3P 7.19234	0.19123	-0.12917
3S 3.54399	-0.00086	0.00162	0.43411			
3S 7.30706	-0.00212	0.11533	-0.23591			
TITANIUM K(2)L(8)3S(2)3P(2) -1D						
T.E.= -0.82584274D+03 P.E.= -0.16516826D+04 K.E.= 0.82583989D+03 V.T.= -0.20300035D+01						
S	1S	2S	3S	P	2P	3P
BASIS/ORB E	-189.74901	-27.63313	-7.87310	BASIS/ORB E	-24.01063	-6.92016
1S 21.65870	0.94748	-0.29743	0.11924	2P 9.20224	0.79840	-0.34445
1S 33.27500	0.02865	-0.00014	0.00040	2P 16.21530	0.07377	-0.02845
2S 8.85640	0.00446	1.04833	-0.47204	3P 4.24743	-0.00406	0.74544
2S 18.74830	0.03046	-0.14985	0.06874	3P 3.62093	0.00361	0.38859
3S 4.52078	0.00194	-0.00137	0.82378	3P 7.59323	0.17206	-0.13674
3S 3.87235	-0.00124	0.00138	0.42160			
3S 7.72317	-0.00255	0.10408	-0.25010			
VANADIUM K(2)L(8)3S(2)3P(2) -1D						
T.E.= -0.91302763D+03 P.E.= -0.18260536D+04 K.E.= 0.91302601D+03 V.T.= -0.20000018D+01						
S	1S	2S	3S	P	2P	3P
BASIS/ORB E	-209.39201	-31.46529	-9.30699	BASIS/ORB E	-27.62935	-8.27132
1S 22.64440	0.94871	-0.30206	0.12353	2P 9.62193	0.81722	-0.36440
1S 34.47010	0.02875	0.00091	0.00007	2P 16.97830	0.07324	-0.02815
2S 9.33630	0.00351	1.06263	-0.49125	3P 4.52820	-0.01123	0.81380
2S 19.40310	0.02924	-0.15681	0.07414	3P 3.94658	0.00796	0.33693
3S 4.91142	0.00160	-0.00579	0.81850	3P 7.87582	0.15314	-0.13855
3S 4.19095	-0.00097	0.00588	0.46614			
3S 7.98942	-0.00201	0.10082	-0.28487			

See page 183 for Explanation of Tables and Notes for Tables 32, 42, and 43

## ROOTHAAN-HARTREE-FOCK ATOMIC WAVEFUNCTIONS

 TABLE 22 (3). THE HARTREE-FOCK FUNCTIONS FOR Si(<sup>1</sup>D) ISO-ELECTRONIC SERIES.

CHROMIUM K(2)L(8)3S(2)3P(2) -1D						
T.E.= -0.10046622D+04 P.E.= -0.20093222D+04 K.E.= 0.10046599D+04 V.T.= -0.20000023D+01						
S	1S	2S	3S	P	2P	3P
BASIS/ORB E	-230.03746	-35.55756	-10.85340	BASIS/CRB E	-31.50000	-9.73513
1S 23.58660	0.95073	-0.30695	-0.12759	2P 10.03900	0.82895	-0.37784
1S 35.74100	0.02972	0.00179	0.00014	2P 17.60990	0.07556	-0.02982
2S 9.79487	0.00376	1.07562	0.50811	3P 4.89060	-0.01047	0.78742
2S 20.11220	0.02551	-0.16052	-0.07800	3P 4.28088	0.00717	0.37953
3S 5.22292	0.00208	-0.01001	-0.84195	3P 8.24591	0.13614	-0.14740
3S 4.52005	-0.00130	0.006C9	-0.46330			
3S 8.38371	-0.00234	0.09236	0.30115			
MANGANESE K(2)L(8)3S(2)3P(2) -1D						
T.E.= -0.11007457D+04 P.E.= -0.22014895D+04 K.E.= 0.11007438D+04 V.T.= -0.20000018D+01						
S	1S	2S	3S	P	2P	3P
BASIS/ORB E	-251.68486	-39.89768	-12.51202	BASIS/ORB E	-35.62230	-11.31126
1S 24.56730	0.95098	-0.30814	-0.12948	2P 10.46330	0.83927	-0.39094
1S 36.96630	0.03034	0.00118	-0.00051	2P 18.24460	0.07751	-0.03094
2S 10.20790	0.00390	1.09250	0.52772	3P 5.21816	-0.01019	0.79978
2S 21.02820	0.02427	-0.16312	-0.08167	3P 4.60957	0.00690	0.38155
3S 5.61415	0.00247	-0.01138	-0.84118	3P 8.61289	0.12131	-0.15363
3S 4.84097	-0.00147	0.00653	-0.50414			
3S 8.65549	-0.00266	0.07683	0.23124			
IRON K(2)L(8)3S(2)3P(2) -1D						
T.E.= -0.12012774D+04 P.E.= -0.24025524D+04 K.E.= 0.12012750D+04 V.T.= -0.20000020D+01						
S	1S	2S	3S	P	2P	3P
BASIS/ORB E	-274.33401	-44.48527	-14.28269	BASIS/ORB E	-39.99596	-12.99954
1S 25.54280	0.95205	-0.31274	-0.13305	2P 10.88970	0.84844	-0.40310
1S 38.19240	0.03062	0.00249	-0.00011	2P 18.87800	0.07938	-0.03193
2S 10.68780	0.00348	1.10197	0.54169	3P 5.53988	-0.00896	0.81714
2S 21.69610	0.02279	-0.16806	-0.08601	3P 4.93851	0.00606	0.37737
3S 5.94126	0.00238	-0.01303	-0.86556	3P 8.98458	0.10753	-0.15933
3S 5.16349	-0.00143	0.00739	-0.50438			
3S 9.03115	-0.00242	0.07396	0.35315			
COBALT K(2)L(8)3S(2)3P(2) -1D						
T.E.= -0.13062568D+04 P.E.= -0.26125113D+04 K.E.= 0.13062545D+04 V.T.= -0.20000017D+01						
S	1S	2S	3S	P	2P	3P
BASIS/ORB E	-297.98447	-49.33216	-16.16527	BASIS/CRB E	-44.62077	-14.79585
1S 26.51810	0.95526	-0.31620	-0.13736	2P 11.25570	0.85640	-0.41468
1S 39.42090	0.03094	0.00326	0.00085	2P 19.26810	0.08667	-0.03520
2S 11.19410	0.00322	1.1C668	0.54742	3P 5.86328	-0.00415	0.83080
2S 22.38900	0.02138	-0.17374	-0.08836	3P 5.26770	0.00304	0.37595
3S 6.40677	0.00220	-0.01763	-0.81652	3P 9.36011	0.08784	-0.16145
3S 5.48628	-0.00122	0.00857	-0.59583			
3S 9.41430	-0.00235	0.07882	0.39916			
NICKEL K(2)L(8)3S(2)3P(2) -1D						
T.E.= -0.14156834D+04 P.E.= -0.28213639D+04 K.E.= 0.14156806D+04 V.T.= -0.20000020D+01						
S	1S	2S	3S	P	2P	3P
BASIS/ORB E	-322.63634	-54.42611	-18.15962	BASIS/CRB E	-49.49656	-16.71198
1S 27.49040	0.95380	-0.31981	-0.14032	2P 11.67820	0.86358	-0.42504
1S 40.65720	0.03133	0.00419	0.00115	2P 19.86960	0.08901	-0.03631
2S 11.67930	0.00307	1.11421	0.55854	3P 6.18426	-0.00117	0.84782
2S 23.09090	0.01992	-0.17E35	-0.09221	3P 5.59792	0.00105	0.37114
3S 6.74073	0.00227	-0.01538	-0.83211	3P 9.74121	0.07535	-0.16661
3S 5.81012	-0.00127	0.00588	-0.60310			
3S 9.80710	-0.00232	0.07744	0.42043			

See page 183 for Explanation of Tables and Notes for Tables 32, 42, and 43

TABLE 22 (4). THE HARTREE-FOCK FUNCTIONS FOR Si(<sup>1</sup>D) ISO-ELECTRONIC SERIES.

COPPER K(2)L(8)3S(2)3P(2) -1D T.E.= -0.152955680+04 P.E.= -0.3C591101D+04 K.E.= 0.152955330+04 V.T.= -0.20000023D+01						
S	1S	2S	3S	P	2P	3P
BASIS/ORB E	-348.28928	-59.77056	-20.26568	BASIS/ORB E	-54.62318	-18.73588
1S 28.48000	0.95487	-0.32129	-0.14514	2P 12.11870	0.86878	-0.43248
1S 41.87200	0.03106	0.0C758	0.0026E	2P 20.48220	0.09064	-0.03755
2S 12.20500	0.00198	1.12364	0.57046	3P 6.58102	-0.00022	0.79429
2S 23.50270	0.01948	-0.18630	-0.0978E	3P 5.92616	0.00044	0.44250
3S 7.06990	0.00144	-0.01558	-0.84963	3P 10.12440	0.06657	-0.17977
3S 6.13177	-0.00082	0.00965	-0.60661			
3S 10.20320	-0.00143	C.07914	0.44141			
ZINC K(2)L(8)3S(2)3P(2) -1D T.E.= -0.164787690+04 P.E.= -0.32557499D+04 K.E.= 0.16478730D+04 V.T.= -0.20000024D+01						
S	1S	2S	3S	P	2P	3P
BASIS/ORB E	-374.94325	-65.36665	-22.48334	BASIS/ORB E	-60.00055	-20.87144
1S 29.46260	0.95547	-0.33C50	-0.14798	2P 12.54580	0.87502	-0.44148
1S 43.10870	0.03121	0.00855	0.00316	2P 21.09950	0.09245	-0.03839
2S 12.70870	0.00173	1.12926	0.57862	3P 6.90738	0.00380	0.80466
2S 24.18640	0.01864	-0.19168	-0.10162	3P 6.25486	-0.00219	0.44372
3S 7.40097	0.00132	-0.02186	-0.86295	3P 10.51390	0.05544	-0.18507
3S 6.45378	-0.00076	0.01C87	-0.61209			
3S 10.62110	-0.00126	0.08068	0.46075			
GALLIUM K(2)L(8)3S(2)3P(2) -1D T.E.= -0.17706432D+04 P.E.= -0.35412843D+04 K.E.= 0.17706411D+04 V.T.= -0.20000012D+01						
S	1S	2S	3S	P	2P	3P
BASIS/ORB E	-402.59802	-71.21306	-24.81257	BASIS/ORB E	-65.62854	-23.11860
1S 30.42990	0.95570	-0.32933	-0.14861	2P 12.97830	0.87971	-0.44637
1S 44.35360	0.03197	0.0C691	0.00239	2P 21.69700	0.09443	-0.04026
2S 13.20720	0.00236	1.12817	0.58206	3P 7.38647	0.00643	0.70074
2S 25.14710	0.01704	-0.19451	-0.10364	3P 6.58627	-0.00345	0.56259
3S 7.73628	0.00202	-0.03063	-0.87450	3P 10.52770	0.04595	-0.20247
3S 6.77835	-0.00117	0.01597	-0.61990			
3S 11.04660	-0.00186	0.0E731	0.48252			
GERMANIUM K(2)L(8)3S(2)3P(2) -1D T.E.= -0.18978557D+04 P.E.= -0.37557094D+04 K.E.= 0.18578536D+04 V.T.= -0.20000011D+01						
S	1S	2S	3S	P	2P	3P
BASIS/ORB E	-431.25356	-77.310C5	-27.25325	BASIS/ORB E	-71.50706	-25.47730
1S 31.36360	0.95626	-0.336C4	-0.15302	2P 13.44460	0.88321	-0.45347
1S 45.45620	0.03351	0.00961	0.00375	2P 22.36720	0.09426	-0.04006
2S 13.82540	0.00228	1.13035	0.58845	3P 7.69578	0.00612	0.74070
2S 25.48470	0.01455	-0.20587	-0.11081	3P 6.89626	-0.00330	0.54081
3S 8.04532	0.00214	-0.04198	-0.92482	3P 11.30680	0.04167	-0.21086
3S 7.08058	-0.00126	0.02189	-0.59005			
3S 11.45280	-0.00186	0.10609	0.50968			
ARSENIC K(2)L(8)3S(2)3P(2) -1D T.E.= -0.20295142D+04 P.E.= -0.4C590260D+04 K.E.= 0.20295118D+04 V.T.= -0.20000012D+01						
S	1S	2S	3S	P	2P	3P
BASIS/ORB E	-460.90982	-83.65760	-29.80540	BASIS/ORB E	-77.63614	-27.94750
1S 32.35820	0.95667	-0.33E78	-0.15581	2P 13.87750	0.88760	-0.45596
1S 46.69910	0.03333	0.01061	0.00449	2P 22.97470	0.09594	-0.04098
2S 14.33840	0.00154	1.13488	0.59268	3P 8.02926	0.01022	0.73615
2S 26.17660	0.01436	-0.21109	-0.11346	3P 7.22785	-0.00575	0.55375
3S 8.37900	0.00185	-0.04239	-0.92145	3P 11.74100	0.03265	-0.21456
3S 7.40390	-0.00111	0.02233	-0.60397			
3S 11.91930	-0.00159	0.1C730	0.52283			

See page 183 for Explanation of Tables and Notes for Tables 32, 42, and 43

## ROOTHAAN-HARTREE-FOCK ATOMIC WAVEFUNCTIONS

 TABLE 22 (5). THE HARTREE-FOCK FUNCTIONS FOR Si(<sup>1</sup>D) ISO-ELECTRONIC SERIES.

SELENIUM K(2)L(8)3S(2)3P(2) -1D  
 T.E.= -0.216561840+04 P.E.= -0.432123470+04 K.E.= 0.216561630+04 V.T.= -0.20000009D+01

S	1S	2S	3S	P	2P	3P
BASIS/ORB E	-491.56667	-90.25563	-32.46896	BASIS/ORB E	-84.01563	-30.52915
1S 33.35490	0.95711	-0.34101	-0.15841	2P 14.31000	0.89158	-0.46588
1S 47.95240	0.03307	0.01138	0.00520	2P 23.57330	0.09770	-0.04196
2S 14.87640	0.00159	1.13689	0.59465	3P 8.36238	0.01397	0.73118
2S 26.86970	0.01428	-0.21711	-0.11621	3P 7.55907	-0.00801	0.56649
3S 8.71308	0.00154	-0.04574	-0.91534	3P 12.18140	0.02421	-0.21792
3S 7.72806	-0.00093	0.02444	-0.61934			
3S 12.39780	-0.00129	0.11127	0.53691			

BROMINE K(2)L(8)3S(2)3P(2) -1D  
 T.E.= -0.23061683D+04 P.E.= -0.46123388D+04 K.E.= 0.23061655D+04 V.T.= -0.20000012D+01

S	1S	2S	3S	P	2P	3P
BASIS/ORB E	-523.22447	-97.10408	-35.24392	BASIS/CRB E	-90.64554	-33.22224
1S 34.36100	0.95750	-0.34354	-0.16135	2P 14.82290	0.90002	-0.47258
1S 49.19430	0.03262	0.01244	0.00620	2P 24.59090	0.09084	-0.03912
2S 15.40710	0.00104	1.13975	0.59541	3P 8.69498	0.02142	0.72172
2S 27.55270	0.01458	-0.22276	-0.11813	3P 7.88983	-0.01323	0.58192
3S 9.04750	0.00101	-0.04554	-0.90089	3P 12.64460	0.01962	-0.22254
3S 8.05047	-0.00063	0.02460	-0.63847			
3S 12.90510	-0.00083	0.11620	0.54674			

KRYPTON K(2)L(8)3S(2)3P(2) -1D  
 T.E.= -0.24511636D+04 P.E.= -0.49023252D+04 K.E.= 0.24511616D+04 V.T.= -0.20000008D+01

S	1S	2S	3S	P	2P	3P
BASIS/ORB E	-555.88242	-104.20294	-38.13021	BASIS/ORB E	-97.52579	-36.02669
1S 35.38510	0.95801	-0.34557	-0.16413	2P 15.25950	0.90472	-0.47761
1S 50.46830	0.03164	0.01340	0.00725	2P 25.23420	0.09166	-0.03986
2S 15.94150	0.00022	1.14144	0.59409	3P 9.03336	0.02653	0.70163
2S 28.26230	0.01552	-0.22824	-0.11941	3P 8.22587	-0.01653	0.60685
3S 9.38711	0.00020	-0.04495	-0.87308	3P 13.12420	0.01119	-0.22372
3S 8.37774	-0.00015	0.02456	-0.66811			
3S 13.43550	-0.00015	0.11975	0.55491			

TABLE 23 NUMBER OF ATOMS 23

See page 183 for Explanation of Tables and Notes for Tables 32, 42, and 43

TABLE 23 (1). THE HARTREE-FOCK FUNCTIONS FOR Si(<sup>1</sup>S) ISO-ELECTRONIC SERIES.

SILICON K(2)L(8)3S(2)3P(2) -1S T.E.= -0.28875862D+03 P.E.= -0.57751214D+03 K.E.= 0.28675352D+03 V.T.= -0.20000177D+01						
S	1S	2S	3S	P	2P	3P
BASIS/ORB E	-68.84693	-6.18860	-0.55904	BASIS/CRB E	-4.28767	-0.21022
1S 14.93760	0.85030	-0.21891	0.05609	2P 5.27173	0.71135	-0.14785
1S 23.92080	0.01454	-0.0C755	C.00221	2P 9.63932	0.09491	-0.01988
2S 5.13952	0.00596	0.93045	-C.26322	3P 1.80473	0.00287	0.48237
2S 13.50740	0.15921	-C.13429	0.03739	3P 0.93239	0.00102	0.63072
3S 2.10660	0.00092	C.00861	0.57282	3P 4.01296	0.26728	-0.06458
3S 1.31983	-0.00041	-C.00319	0.53954			
2S 4.34999	-0.00297	C.17C24	-0.10120			

  

PHOSPHORUS K(2)L(8)3S(2)3P(2) -1S T.E.= -0.34022251D+03 P.E.= -0.68C44361D+03 K.E.= 0.34022110D+03 V.T.= -0.20000042D+01						
S	1S	2S	3S	P	2P	3P
BASIS/ORB E	-80.41106	-7.94166	-1.04831	BASIS/ORB E	-5.82854	-0.60015
1S 15.27900	0.90437	0.24325	0.07187	2P 6.17367	0.68566	-0.18175
1S 24.63420	0.01966	0.00662	0.00116	2P 11.33530	0.05969	-0.01448
2S 5.72846	0.00498	-C.92364	-0.28781	3P 2.07030	0.00680	0.57412
2S 13.75080	0.09164	0.13054	0.03877	3P 1.23710	-0.00013	0.51758
3S 2.69718	0.00073	0.00296	0.41298	3P 4.71190	0.32572	-0.09005
3S 1.75090	-0.00028	-0.00209	0.72705			
2S 4.75257	-0.00195	-0.20172	-0.15922			

  

SULFUR K(2)L(8)3S(2)3P(2) -1S T.E.= -0.39617737D+03 P.E.= -0.79235195D+03 K.E.= 0.39617458D+03 V.T.= -0.20000071D+01						
S	1S	2S	3S	P	2P	3P
BASIS/ORB E	-93.00230	-9.57400	-1.66923	BASIS/ORB E	-7.64786	-1.12124
1S 16.09270	0.92118	-0.25675	0.08281	2P 6.65625	0.70528	-0.21951
1S 25.88190	0.02105	-0.00491	0.00057	2P 12.31300	0.05682	-0.01440
2S 6.22892	0.00429	0.93177	-0.31542	3P 2.26258	0.00495	0.73902
2S 14.32240	0.07079	-0.13240	0.04261	3P 1.45803	0.00016	0.34077
3S 3.26253	0.00069	-0.0C6E5	0.31550	3P 5.14694	0.30440	-0.08981
3S 2.13855	-0.00022	0.00290	0.84806			
3S 5.21203	-0.00173	0.20381	-0.19600			

  

CHLORINE K(2)L(8)3S(2)3P(2) -1S T.E.= -0.45660759D+03 P.E.= -0.9121130D+03 K.E.= 0.4566C371D+03 V.T.= -0.2CJ00085D+01						
S	1S	2S	3S	P	2P	3P
BASIS/ORB E	-106.60995	-12.27403	-2.41323	BASIS/ORB E	-9.73335	-1.76E30
1S 16.96190	0.93095	-0.26704	0.09165	2P 7.11755	0.72475	-0.24992
1S 27.11880	0.02282	-0.00373	0.00032	2P 13.20710	0.05575	-0.01514
2S 6.68228	0.00438	0.95151	-0.34525	3P 2.53367	0.00282	0.82581
2S 14.98490	0.05723	-0.13460	0.04685	3P 1.72057	0.00087	0.25253
3S 3.87056	0.00102	-0.01042	0.25337	3P 5.56695	0.28180	-0.09375
2S 2.50807	-0.00026	0.00318	0.94119			
3S 5.61452	-0.00220	0.19230	-0.22931			

  

ARGON K(2)L(8)3S(2)3P(2) -1S T.E.= -0.52150401D+03 P.E.= -0.10430022D+04 K.E.= 0.52149820D+03 V.T.= -0.20000112D+01						
S	1S	2S	3S	P	2P	3P
BASIS/ORB E	-121.22860	-14.83562	-3.27604	BASIS/ORB E	-12.07957	-2.53086
1S 17.86550	0.93757	-0.27646	-0.09973	2P 7.60227	0.74263	-0.27437
1S 28.35200	0.02423	-0.00221	0.00015	2P 14.22050	0.05243	-0.01543
2S 7.14277	0.00438	0.96628	0.36991	3P 2.84010	0.00004	0.87748
2S 15.64950	0.04779	-0.13695	-0.05059	3P 1.99526	0.00198	0.20630
3S 4.32713	0.00119	-0.0C615	-0.21474	3P 5.98230	0.26423	-0.10314
3S 2.85199	-0.00029	0.00219	-0.99286			
3S 6.10016	-0.00246	0.17909	0.24367			

See page 183 for Explanation of Tables and Notes for Tables 32, 42, and 43

## ROOTHAAN-HARTREE-FOCK ATOMIC WAVEFUNCTIONS

 TABLE 23 (2). THE HARTREE-FOCK FUNCTIONS FOR Si(<sup>1</sup>S) ISO-ELECTRONIC SERIES.

K(2)L(8)3S(2)3P(2) -1S						
T.E.= -0.59086113D+03 P.E.= -0.11817157D+04 K.E.= 0.59085459D+03 V.T.= -0.20300111D+01						
S	1S	2S	3S	P	2P	3P
BASIS/ORB E	-136.85475	-17.65527	-4.25510	BASIS/ORB E	-14.68326	-3.41227
1S 18.77530	0.94047	-0.27884	0.10454	2P 8.00823	0.75925	-0.29674
1S 29.60330	0.02689	-0.00393	0.00063	2P 14.75550	0.05706	-0.01799
2S 7.54929	0.00653	0.98562	-0.39529	3P 3.15334	-0.00145	0.91407
2S 16.65880	0.04010	-0.13786	0.05375	3P 2.28262	0.00248	0.18118
3S 4.50268	0.00233	-0.00268	0.21492	3P 6.38025	0.23891	-0.10802
3S 3.16798	-0.00073	0.00188	0.99696			
3S 6.56219	-0.00443	0.15533	-0.24200			
CALCIUM K(2)L(8)3S(2)3P(2) -1S						
T.E.= -0.66467501D+03 P.E.= -0.13293425D+04 K.E.= 0.66466754D+03 V.T.= -0.20300112D+01						
S	1S	2S	3S	P	2P	3P
BASIS/ORB E	-153.48667	-20.73062	-5.34896	BASIS/ORB E	-17.54215	-4.40896
1S 19.69420	0.94487	-0.28688	0.11132	2P 8.44633	0.77385	-0.31557
1S 30.86920	0.02808	-0.00280	0.00003	2P 15.43810	0.05678	-0.01968
2S 8.02479	0.00668	0.994C3	-0.41155	3P 3.47984	-0.00327	0.93608
2S 17.36110	0.03338	-0.14C62	0.05640	3P 2.58490	0.00318	0.17155
3S 4.56918	0.00235	0.00172	0.24097	3P 6.78157	0.21971	-0.11610
3S 3.47030	-0.00095	0.00C62	0.97134			
3S 7.09927	-0.00434	0.14870	-0.24452			
SCANDIUM K(2)L(8)3S(2)3P(2) -1S						
T.E.= -0.74294309D+03 P.E.= -0.14E58816D+04 K.E.= 0.74293852D+03 V.T.= -0.20000062D+01						
S	1S	2S	3S	P	2P	3P
BASIS/ORB E	-171.12281	-24.06C20	-6.55661	BASIS/ORB E	-20.65488	-5.51974
1S 20.63400	0.94780	-0.29121	-0.11623	2P 8.87860	0.78745	-0.33261
1S 32.11110	0.02903	-0.00233	-0.00003	2P 16.08840	0.06086	-0.02138
2S 8.51235	0.00652	1.00576	0.43099	3P 3.81091	-0.00492	0.95129
2S 18.05680	0.02877	-0.14639	-0.06134	3P 2.89713	0.00384	0.16962
3S 4.88752	0.00263	-0.00522	-0.24245	3P 7.17529	0.20128	-0.12390
3S 3.79843	-0.00115	0.00316	-0.99256			
3S 7.47049	-0.00441	0.14800	0.26559			
TITANIUM K(2)L(8)3S(2)3P(2) -1S						
T.E.= -0.82566347D+03 P.E.= -0.16513237D+04 K.E.= 0.82566C23D+03 V.T.= -0.20000039D+01						
S	1S	2S	3S	P	2P	3P
BASIS/ORB E	-189.76272	-27.64331	-7.87757	BASIS/ORB E	-24.02086	-6.74415
1S 21.65250	0.94795	-0.25638	-0.12094	2P 9.29699	0.80222	-0.34959
1S 33.26150	0.02862	-0.00079	0.00048	2P 16.73770	0.06303	-0.02286
2S 8.98377	0.00466	1.02319	0.45180	3P 4.14620	-0.00677	0.95412
2S 18.70020	0.02984	-0.15362	-0.06680	3P 3.24554	0.00465	0.18028
3S 5.17680	0.00192	-0.01106	-0.27800	3P 7.54436	0.18177	-0.12978
3S 4.11021	-0.00087	0.00532	-0.98554			
3S 7.80296	-0.00301	0.14104	0.28925			
VANADIUM K(2)L(8)3S(2)3P(2) -1S						
T.E.= -0.91283476D+03 P.E.= -0.18256679D+04 K.E.= 0.91283315D+03 V.T.= -0.20000018D+01						
S	1S	2S	3S	P	2P	3P
BASIS/ORB E	-209.40537	-31.47E55	-9.31124	BASIS/CRB E	-27.63911	-8.08144
1S 22.59270	0.95157	-0.30767	-0.12649	2P 9.71921	0.80844	-0.36222
1S 34.52380	0.02890	0.00337	0.00128	2P 17.21920	0.06815	-0.02538
2S 9.49265	0.00336	1.04142	0.47841	3P 4.47007	-0.00347	0.94948
2S 18.99420	0.02589	-0.16175	-0.07558	3P 3.61936	0.00304	0.19354
3S 5.47090	0.00156	-0.01420	-0.20868	3P 8.01836	0.16582	-0.13275
3S 4.48314	-0.00077	0.00649	-1.06539			
3S 8.15043	-0.00214	0.13726	0.29254			

See page 183 for Explanation of Tables and Notes for Tables 32, 42, and 43

TABLE 23 (3). THE HARTREE-FOCK FUNCTIONS FOR Si(<sup>1</sup>s) ISO-ELECTRONIC SERIES.

CHROMIUM K(2)L(8)3S(2)3P(2) -1S T.E.= -0.100445580D+04 P.E.= -0.20C89080D+04 K.E.= 0.10044522D+04 V.T.= -0.20000036D+01						
S	1S	2S	3S	P	2P	3P
BASIS/ORB E	-230.05085	-35.56720	-10.85758	BASIS/ORB E	-31.50973	-9.53174
1S 23.61620	0.94966	-0.3C496	-0.12780	2P 10.12760	0.62251	-0.37782
1S 35.68930	0.02938	0.00102	0.00038	2P 17.86350	0.07054	-0.02657
2S 9.80772	0.00378	1.065C8	0.49960	3P 4.80365	-0.00393	0.94091
2S 20.22410	0.02715	-0.16C43	-0.07585	3P 3.99327	0.00317	0.21436
3S 5.74015	0.00195	-0.01C02	-0.31990	3P 8.37948	0.14673	-0.13599
3S 4.75596	-0.00097	0.00459	-0.99157			
3S 8.46630	-0.00258	0.09858	0.31434			
MANGANESE K(2)L(8)3S(2)3P(2) -1S T.E.= -0.11005259D+04 P.E.= -0.22010495D+04 K.E.= 0.11005236D+04 V.T.= -0.20000020D+01						
S	1S	2S	3S	P	2P	3P
BASIS/ORB E	-251.69795	-39.9C713	-12.51609	BASIS/CRB E	-35.63187	-11.09432
1S 24.55040	0.95164	-0.3C827	-0.13100	2P 10.53190	0.83358	-0.39144
1S 36.98070	0.03050	0.00106	0.00025	2P 18.38130	0.07413	-0.02840
2S 10.29990	0.00440	1.07440	0.51138	3P 5.16182	-0.00719	0.90514
2S 20.98220	0.02309	-0.16468	-0.07966	3P 4.38681	0.00506	C.26550
3S 6.02154	0.00272	-0.01433	-0.30801	3P 8.70782	0.13039	-0.14256
3S 5.09397	-0.00145	0.0C747	-1.01768			
3S 8.89595	-0.00323	0.10C67	0.32844			
IRON K(2)L(8)3S(2)3P(2) -1S T.E.= -0.12010441D+04 P.E.= -0.24C20857D+04 K.E.= 0.12010415D+04 V.T.= -0.20000021D+01						
S	1S	2S	3S	P	2P	3P
BASIS/ORB E	-274.34696	-44.49E59	-14.28668	BASIS/CRB E	-40.00541	-12.76915
1S 25.55130	0.95273	-0.31539	-0.13542	2P 10.92700	0.84309	-0.40448
1S 38.18750	0.02999	0.00404	0.00124	2P 18.89260	0.07867	-0.03032
2S 10.80980	0.00272	1.08E35	0.53029	3P 5.49102	-0.00545	0.88081
2S 21.43140	0.C2318	-0.17329	-0.08672	3P 4.77687	0.00417	0.29987
2S 6.28605	0.00171	-0.02237	-0.44948	3P 5.09096	0.11284	-0.14547
3S 5.36591	-0.00093	0.01C94	-0.92169			
3S 9.12991	-0.00189	0.10181	0.36895			
COBALT K(2)L(8)3S(2)3P(2) -1S T.E.= -0.13060101D+04 P.E.= -0.26120160D+04 K.E.= 0.13060059D+04 V.T.= -0.20000032D+01						
S	1S	2S	3S	P	2P	3P
BASIS/ORB E	-297.99731	-49.34137	-16.16917	BASIS/ORB E	-44.63012	-14.55602
1S 26.49750	0.95349	-0.31658	-0.13718	2P 11.25420	0.85074	-0.41620
1S 39.46490	0.03122	0.00327	0.00064	2P 19.13540	0.08955	-0.03509
2S 11.19410	0.00375	1.10560	0.54747	3P 5.84699	-0.00026	0.81517
2S 22.38800	0.02019	-0.17294	-0.08844	3P 5.17692	0.00120	0.37584
3S 6.56228	0.00289	-0.01689	-0.53684	3P 9.49183	0.08911	-0.14204
3S 5.65489	-0.00160	0.00860	-0.86186			
3S 9.47668	-0.00295	0.07922	0.38581			
NICKEL K(2)L(8)3S(2)3P(2) -1S T.E.= -0.14154233D+04 P.E.= -0.283C8453D+04 K.E.= 0.14154220D+04 V.T.= -0.20000010D+01						
S	1S	2S	3S	P	2P	3P
BASIS/ORB E	-322.64933	-54.43517	-18.16350	BASIS/ORB E	-49.50579	-16.45487
1S 27.56710	0.95309	-0.32002	-0.14056	2P 11.70500	0.86310	-0.42728
1S 40.60110	0.02954	0.00506	0.00161	2P 19.99590	0.08658	-0.03438
2S 11.75150	0.00137	1.1C762	0.55509	3P 6.26338	0.00462	0.71145
2S 22.98040	0.02374	-0.18304	-0.09436	3P 5.55611	-0.00220	0.49567
3S 6.81673	0.00064	-0.02841	-0.75860	3P 9.86006	0.07623	-0.15233
3S 5.85685	-0.00035	0.01399	-0.68412			
3S 9.79817	-0.00074	0.09367	0.43381			

See page 183 for Explanation of Tables and Notes for Tables 32, 42, and 43

## ROOTHAAN-HARTREE-FOCK ATOMIC WAVEFUNCTIONS

 TABLE 23 (4). THE HARTREE-FOCK FUNCTIONS FOR Si(<sup>1</sup>S) ISO-ELECTRONIC SERIES.

COPPER K(2)L(8)3S(2)3P(2) -1S						
T.E.= -0.152928350+04 P.E.= -0.30585649D+04 K.E.= 0.15292814D+04 V.T.= -0.20000014D+01						
S	1S	2S	3S	P	2P	3P
BASIS/ORB E	-348.30225	-59.77595	-20.26950	BASIS/CRB E	-54.63234	-18.46546
1S 28.54680	0.95439	-0.32614	-0.14441	2P 12.08250	0.87185	-0.43757
1S 41.84550	0.02945	0.00757	0.00254	2P 20.49850	0.09150	-0.03681
2S 12.27790	0.00058	1.11664	0.56811	3P 6.68460	0.01093	0.59442
2S 23.46830	0.02268	-0.19086	-0.10055	3P 5.54435	-0.00596	0.62525
3S 7.09311	0.00004	-0.03197	-0.85093	3P 10.25480	0.05771	-0.15598
3S 6.13825	-0.00003	0.01579	-0.61632			
3S 10.15980	-0.00013	0.09666	0.45723			
ZINC K(2)L(8)3S(2)3P(2) -1S						
T.E.= -0.164759030+04 P.E.= -0.32951747D+04 K.E.= 0.16475844D+04 V.T.= -0.20000036D+01						
S	1S	2S	3S	P	2P	3P
BASIS/ORB E	-374.55616	-65.37558	-22.48711	BASIS/ORB E	-60.00965	-20.58775
1S 29.47150	0.95563	-0.32585	-0.14710	2P 12.36080	0.88476	-0.45101
1S 43.15900	0.03082	0.00824	0.00268	2P 20.81740	0.10190	-0.04143
2S 12.72020	0.00162	1.12851	0.58116	3P 7.25481	0.02385	0.32591
2S 24.19770	0.01897	-0.19258	-0.10323	3P 6.40162	-0.01241	0.90052
3S 7.38810	0.00123	-0.02669	-0.90829	3P 10.67540	0.02476	-0.14761
3S 6.43444	-0.00071	0.01329	-0.57701			
3S 10.55110	-0.00117	0.08448	0.46956			
GALLIUM K(2)L(8)3S(2)3P(2) -1S						
T.E.= -0.17703435D+04 P.E.= -0.35406790D+04 K.E.= 0.17703355D+04 V.T.= -0.20000045D+01						
S	1S	2S	3S	P	2P	3P
BASIS/ORB E	-402.61097	-71.22190	-24.81625	BASIS/ORB E	-65.63756	-22.82164
1S 30.32760	0.95623	-0.33135	-0.14850	2P 12.85610	0.88840	-0.45847
1S 44.32420	0.03446	0.00713	0.00189	2P 21.58720	0.09907	-0.04004
2S 13.15580	0.00400	1.13611	0.59161	3P 7.60108	0.02341	0.29451
2S 25.08530	0.01262	-0.19175	-0.10456	3P 6.75105	-0.01245	0.94196
3S 7.66987	0.00388	-0.02515	-0.98645	3P 11.05450	0.02353	-0.15565
3S 6.71793	-0.00224	0.01296	-0.51645			
3S 10.94220	-0.00345	0.07538	0.48214			
GERMANIUM K(2)L(8)3S(2)3P(2) -1S						
T.E.= -0.18975428D+04 P.E.= -0.37950768D+04 K.E.= 0.18975340D+04 V.T.= -0.20000046D+01						
S	1S	2S	3S	P	2P	3P
BASIS/ORB E	-431.26649	-77.31880	-27.25690	BASIS/ORB E	-71.51604	-25.16712
1S 31.33550	0.95672	-0.33741	-0.15262	2P 13.27360	0.89459	-0.46750
1S 45.54600	0.03389	0.01013	0.00338	2P 22.19100	0.10099	-0.04071
2S 13.69730	0.00296	1.14375	0.60071	3P 7.93959	0.02828	0.25352
2S 25.52350	0.01320	-0.20050	-0.11030	3P 7.10397	-0.01549	0.99066
3S 7.97440	0.00292	-0.02590	-1.02827	3P 11.45250	0.01203	-0.15618
3S 7.01995	-0.00172	0.01321	-0.48929			
3S 11.36410	-0.00252	0.07914	0.49839			
ARSENIC K(2)L(8)3S(2)3P(2) -1S						
T.E.= -0.20291880D+04 P.E.= -0.40583676D+04 K.E.= 0.20291796D+04 V.T.= -0.20000041D+01						
S	1S	2S	3S	P	2P	3P
BASIS/ORB E	-460.92281	-83.66635	-29.80906	BASIS/ORB E	-77.64508	-27.62416
1S 32.31070	0.95690	-0.33652	-0.15354	2P 13.70670	0.90089	-0.47333
1S 46.79100	0.03434	0.00884	0.00295	2P 22.85940	0.10134	-0.04157
2S 14.18970	0.00336	1.14309	0.60186	3P 8.25924	0.03178	0.34530
2S 26.47190	0.01214	-0.20270	-0.11118	3P 7.37354	-0.01730	0.91412
3S 8.29903	0.00338	-0.03128	-1.03842	3P 11.87040	0.00233	-0.16744
3S 7.33793	-0.00201	0.01670	-0.49036			
3S 11.83270	-0.00288	0.08297	0.51279			

See page 183 for Explanation of Tables and Notes for Tables 32, 42, and 43

TABLE 23 (5). THE HARTREE-FOCK FUNCTIONS FOR Si(<sup>1</sup>S) ISO-ELECTRONIC SERIES.

SELENIUM K(2)L(8)3S(2)3P(2) -1S T.E.= -0.21652790D+04 P.E.= -0.43305495D+04 K.E.= 0.21652705D+04 V.T.= -0.20000040D+01						
S	1S	2S	3S	P	2P	3P
BASIS/ORB E	-491.57957	-90.26432	-32.47258	BASIS/ORB E	-84.02451	-30.19263
1S 33.28120	0.95739	-0.33870	-0.15632	2P 14.10610	0.90553	-0.48035
1S 48.04860	0.03468	0.00534	0.00365	2P 23.38120	0.10503	-0.04329
2S 14.70940	0.00355	1.14509	0.60288	3P 8.55352	0.03575	0.37438
2S 27.19110	0.01098	-0.20728	-0.11276	3P 7.68751	-0.01992	0.89363
3S 8.64405	0.00363	-0.03330	-1.01433	3P 12.28520	-0.00881	-0.16985
3S 7.67090	-0.00219	0.01804	-0.52223			
3S 12.32850	-0.00307	0.08701	0.52541			

  

BROMINE K(2)L(8)3S(2)3P(2) -1S T.E.= -0.23058158D+04 P.E.= -0.46116247D+04 K.E.= 0.23058089D+04 V.T.= -0.20000030D+01						
S	1S	2S	3S	P	2P	3P
BASIS/ORB E	-523.23707	-97.11270	-35.24751	BASIS/ORB E	-90.65434	-32.87256
1S 34.32350	0.95747	-0.34170	-0.15981	2P 14.69840	0.90525	-0.48233
1S 49.24510	0.03351	0.01101	0.00513	2P 24.36100	0.09683	-0.03962
2S 15.24900	0.00227	1.14739	0.60199	3P 8.80790	0.03163	0.46931
2S 27.83320	0.01287	-0.21397	-0.11467	3P 7.96885	-0.01850	0.81121
3S 9.00049	0.00225	-0.03339	-0.96512	3P 12.70270	0.00257	-0.18672
3S 8.01233	-0.00137	0.01817	-0.57445			
3S 12.86110	-0.00190	0.09194	0.53539			

  

KRYPTON K(2)L(8)3S(2)3P(2) -1S T.E.= -0.245079800D+04 P.E.= -0.49015928D+04 K.E.= 0.24507948D+04 V.T.= -0.20000013D+01						
S	1S	2S	3S	P	2P	3P
BASIS/ORB E	-555.89454	-104.21148	-38.13375	BASIS/CRB E	-97.53449	-35.66386
1S 35.36590	0.95806	-0.34561	-0.16416	2P 15.15510	0.90035	-0.48372
1S 50.48290	0.03206	0.01324	0.00718	2P 24.75850	0.10154	-0.04198
2S 15.93210	0.00064	1.14185	0.59423	3P 9.03596	0.02359	0.60493
2S 28.27040	0.01472	-0.22749	-0.11900	3P 8.22823	-0.01359	0.68587
3S 9.38982	0.00063	-0.04404	-0.86821	3P 13.12800	0.00534	-0.19587
3S 8.38016	-0.00041	0.02406	-0.67236			
3S 13.43930	-0.00051	0.11830	0.55381			

TABLE 24 NUMBER OF ATOMS 22

See page 183 for Explanation of Tables and Notes for Tables 32, 42, and 43

## ROOTHAAN-HARTREE-FOCK ATOMIC WAVEFUNCTIONS

TABLE 24 (1). THE HARTREE-FOCK FUNCTIONS FOR P(4S) ISO-ELECTRONIC SERIES.

PHOSPHORUS K(2)L(8)3S(2)3P(3) -4S						
T.E.= -0.34071859D+03 P.E.= -0.68143731D+03 K.E.= 0.34071872D+03 V.T.= -0.19999996D+01						
S	1S	2S	3S	P	2P	3P
BASIS/ORB E	-79.96982	-7.51113	-0.69638	BASIS/CRB E	-5.40099	-0.39175
1S 16.14890	0.83880	-0.20761	0.05581	2P 6.51465	0.65521	-0.15797
1S 23.28360	0.01750	-0.01657	0.00526	2P 12.37150	0.03726	-0.00854
2S 5.60322	0.00527	0.94566	-0.28576	3P 2.02705	0.00941	0.53363
2S 14.52140	0.16964	-0.15C79	0.04495	3P 1.19796	-0.00211	0.55506
3S 2.39990	0.00049	0.00125	0.60632	3P 4.87455	0.38190	-0.097E2
3S 1.48370	-0.00020	0.00035	0.52533			
3S 4.69535	-0.00188	0.16439	-0.11713			
SULFUR K(2)L(8)3S(2)3P(3) -4S						
T.E.= -0.39717296D+03 P.E.= -0.79434200D+03 K.E.= 0.39716904D+03 V.T.= -0.20000099D+C1						
S	1S	2S	3S	P	2P	3P
BASIS/ORB E	-92.43411	-9.42767	-1.24006	BASIS/ORB E	-7.10393	-0.86169
1S 16.61110	0.87854	-0.23309	0.06764	2P 6.87921	0.68387	-0.19398
1S 24.51550	0.02262	-0.01175	0.00501	2P 12.94140	0.04532	-0.01134
2S 6.02289	0.00411	0.975E5	-0.32790	3P 2.33228	0.00627	0.57242
2S 15.00660	0.11829	-0.14C80	0.04816	3P 1.53607	-0.00094	0.50786
3S 2.72748	0.00037	0.00085	0.60312	3P 5.2638E	0.34162	-0.10538
3S 1.82072	-0.00015	0.00051	0.53665			
3S 5.04320	-0.00137	0.13E54	-0.12860			
CHLORINE K(2)L(8)3S(2)3P(3) -4S						
T.E.= -0.458226200D+03 P.E.= -0.916446200D+03 K.E.= 0.45822001D+03 V.T.= -0.20000135D+01						
S	1S	2S	3S	P	2P	3P
BASIS/ORB E	-105.92140	-11.62018	-1.91232	BASIS/ORB E	-9.08126	-1.45809
1S 17.23500	0.90279	0.25171	0.07869	2P 7.26197	0.70801	-0.22428
1S 25.84570	0.02778	0.00871	0.00438	2P 13.50700	0.04862	-0.01416
2S 6.45977	0.00472	-0.99197	-0.35934	3P 2.62240	0.00345	0.63110
2S 15.62160	0.08386	0.13380	0.05005	3P 1.84240	0.00014	0.45126
3S 3.04149	0.00068	-0.00700	0.59149	3P 5.65575	0.30743	-0.11155
3S 2.16224	-0.00031	0.00196	0.55425			
3S 5.55714	-0.00199	-0.12263	-0.13877			
ARGON K(2)L(8)3S(2)3P(3) -4S						
T.E.= -0.52386495D+03 P.E.= -0.10477255D+04 K.E.= 0.52386054D+03 V.T.= -0.20000084D+01						
S	1S	2S	3S	P	2P	3P
BASIS/ORB E	-120.42300	-14.07890	-2.70594	BASIS/ORB E	-11.32365	-2.17530
1S 18.09050	0.90884	-0.25419	0.08408	2P 7.65630	0.72963	-0.25070
1S 27.15320	0.03197	-0.01152	0.00562	2P 14.10220	0.05297	-0.01674
2S 6.86861	0.00641	1.01265	-0.38874	3P 2.93571	0.00066	0.65645
2S 16.60660	0.07098	-0.13539	0.05370	3P 2.17066	0.00135	0.43235
3S 3.32929	0.00147	0.00E72	0.63415	3P 6.04428	0.27741	-0.11713
3S 2.46095	-0.00072	-0.00273	0.52686			
3S 5.98428	-0.00339	0.10131	-0.15145			
POTASSIUM K(2)L(8)3S(2)3P(3) -4S						
T.E.= -0.59408118D+03 P.E.= -0.118E1589D+04 K.E.= 0.59407772D+03 V.T.= -0.20000058D+C1						
S	1S	2S	3S	P	2P	3P
BASIS/ORB E	-135.93445	-16.75E47	-3.61745	BASIS/CRB E	-13.82600	-3.01014
1S 18.95270	0.92001	-0.26450	0.09244	2P 8.05818	0.74922	-0.27448
1S 28.44590	0.03242	-0.00540	0.00480	2P 14.71710	0.05660	-0.01893
2S 7.34423	0.00598	1.02018	-0.40929	3P 3.25977	-0.00210	0.65599
2S 17.25650	0.05760	-0.13658	0.05648	3P 2.52052	0.00264	0.44117
3S 3.64856	0.00146	0.01024	0.61659	3P 6.42828	0.25065	-0.12145
3S 2.80827	-0.00075	-0.00352	0.55634			
3S 6.49033	-0.00321	0.09902	-0.16773			

See page 183 for Explanation of Tables and Notes for Tables 32, 42, and 43

TABLE 24 (2). THE HARTREE-FOCK FUNCTIONS FOR P(<sup>4</sup>S) ISO-ELECTRONIC SERIES.

CALCIUM K(2)L(8)3S(2)3P(3) -4S						
T.E.= -0.66886956D+03 P.E.= -0.13377350D+04 K.E.= 0.66886547D+03 V.T.= -0.20000061D+01						
S	1S	2S	3S	P	2P	3P
BASIS/ORB E	-152.45337	-19.77611	-4.64510	BASIS/GRB E	-16.58572	-3.96108
1S 19.78700	0.93340	-0.28237	0.10384	2P 8.46616	0.76648	-0.29561
1S 29.75270	0.03217	-0.00303	0.00208	2P 15.32940	0.05993	-0.02098
2S 7.84589	0.00429	1.03254	-0.43072	3P 3.56983	-0.00441	0.677E6
2S 17.51310	0.04311	-0.13808	0.05935	3P 2.84866	0.00376	0.42943
3S 3.91596	0.00096	0.0C813	0.71436	3P 6.81158	0.22684	-0.125E2
2S 3.06226	-0.00051	-0.C0289	0.48035			
3S 6.87020	-0.00211	C.09899	-0.19085			
SCANDIUM K(2)L(8)3S(2)3P(3) -4S						
T.E.= -0.748226550D+03 P.E.= -0.14564506D+04 K.E.= 0.74822408D+03 V.T.= -0.20000033D+01						
S	1S	2S	3S	P	2P	3P
BASIS/ORB E	-169.97774	-23.0C569	-5.78743	BASIS/GRB E	-19.60078	-5.02663
1S 20.66030	0.93674	-0.28276	0.10742	2P 8.87785	0.78022	-0.31380
1S 31.06670	0.03545	-0.0C646	0.00319	2P 15.88950	0.06386	-0.02323
2S 8.32469	0.00660	1.02571	-0.43973	3P 3.88306	-0.00567	0.69677
2S 18.56110	0.03412	-0.14035	0.06112	3P 3.17652	0.00439	0.42149
3S 4.22819	0.00208	0.01037	0.65078	3P 7.20740	0.20593	-0.13017
3S 3.45451	-0.00122	-0.0C0402	0.54787			
3S 7.49054	-0.00386	0.10258	-0.20269			
TITANIUM K(2)L(8)3S(2)3P(3) -4S						
T.E.= -0.832149440D+03 P.E.= -0.16642962D+04 K.E.= 0.83214672D+03 V.T.= -0.20300033D+01						
S	1S	2S	3S	P	2P	3P
BASIS/ORB E	-188.50670	-26.49783	-7.04370	BASIS/ORB E	-22.86998	-6.20620
1S 21.61450	0.93996	-0.29C57	0.11286	2P 9.28936	0.79321	-0.32992
1S 32.32070	0.03558	-0.00413	0.00267	2P 16.49630	0.06725	-0.02542
2S 8.75889	0.00591	1.051C4	-0.46407	3P 4.20688	-0.00401	0.708C1
2S 19.18960	0.03046	-0.14380	0.06547	3P 3.56027	0.00326	0.42221
3S 4.51461	0.00212	0.01090	0.68804	3P 7.62021	0.18549	-0.13536
3S 3.77188	-0.00128	-0.00472	0.52836			
3S 7.85707	-0.00351	0.086C3	-0.21263			
VANADIUM K(2)L(8)3S(2)3P(3) -4S						
T.E.= -0.92063636D+03 P.E.= -0.18412701D+04 K.E.= 0.92063369D+03 V.T.= -0.20000029D+01						
S	1S	2S	3S	P	2P	3P
BASIS/ORB E	-208.03911	-30.23970	-8.41324	BASIS/ORB E	-26.39250	-7.49913
1S 22.51320	0.94407	-0.25673	0.11886	2P 9.70619	0.80540	-0.34564
1S 33.62520	0.03691	-0.00314	0.00184	2P 17.0C8700	0.07023	-0.02709
2S 9.26646	0.00641	1.05349	-0.47353	3P 4.51755	-0.00537	0.73019
2S 19.84790	0.02374	-0.14771	0.06782	3P 3.82820	0.00401	0.41137
3S 4.82203	0.00262	0.CC888	0.70107	3P 8.00231	0.16776	-0.13918
3S 4.09592	-0.00164	-0.00372	0.53115			
3S 8.33442	-0.00396	0.09154	-0.23370			
CHROMIUM K(2)L(8)3S(2)3P(3) -4S						
T.E.= -0.10136858D+04 P.E.= -0.20273703D+04 K.E.= 0.10136845D+04 V.T.= -0.20000013D+01						
S	1S	2S	3S	P	2P	3P
BASIS/ORB E	-228.57456	-34.23447	-9.89560	BASIS/ORB E	-30.16764	-8.90495
1S 23.64560	0.94324	-0.30C32	0.12286	2P 10.12360	0.82016	-0.36267
1S 34.90930	0.03288	-0.00092	0.00089	2P 17.81550	0.07105	-0.02750
2S 9.80173	0.00333	1.05573	-0.48468	3P 4.79243	-0.00451	0.78356
2S 20.47840	0.03076	-0.15786	0.07384	3P 4.15261	0.00334	0.36684
3S 5.14404	0.00108	0.00208	0.72210	3P 8.37201	0.14892	-0.13901
2S 4.41516	-0.00068	0.00011	0.53196			
3S 8.71525	-0.00174	0.10156	-0.25940			

See page 183 for Explanation of Tables and Notes for Tables 32, 42, and 43

## ROOTHAAN-HARTREE-FOCK ATOMIC WAVEFUNCTIONS

TABLE 24 (3). THE HARTREE-FOCK FUNCTIONS FOR P(4S) ISO-ELECTRONIC SERIES.

MANGANESE K(2)L(8)3S(2)3P(3) -4S						
T.E.= -0.11112967D+04 P.E.= -0.22225914D+04 K.E.= 0.11112947D+04 V.T.= -C.20000018D+01						
S	1S	2S	3S	P	2P	3P
BASIS/ORB E	-250.11228	-38.48170	-11.49054	BASIS/ORB E	-34.19494	-10.42339
1S 24.54370	0.94668	-0.303582	0.12760	2P 10.54440	0.83195	-0.37680
1S 36.28080	0.03430	-0.00001	0.00038	2P 18.42510	0.07302	-0.02862
2S 10.27580	0.00431	1.06406	-0.49600	3P 5.13172	-0.00928	0.78300
2S 21.17580	0.02453	-0.16033	0.07607	3P 4.48873	0.00624	0.38313
3S 5.40900	0.00194	0.00281	0.75482	3P 8.68672	0.13436	-0.14664
3S 4.74695	-0.00131	-0.001C7	0.50880			
3S 9.20781	-0.00255	0.09728	-0.26930			
IRON K(2)L(8)3S(2)3P(3) -4S						
T.E.= -0.12134681D+04 P.E.= -0.24269334D+04 K.E.= 0.12134653D+04 V.T.= -0.20000023D+01						
S	1S	2S	3S	P	2P	3P
BASIS/ORB E	-272.65218	-42.98C89	-13.19779	BASIS/ORB E	-38.47401	-12.05419
1S 25.50080	0.94862	-0.31075	-0.13282	2P 10.96400	0.84168	-0.38950
1S 37.58870	0.03453	0.0C133	0.00084	2P 19.04390	0.07530	-0.02980
2S 10.81540	0.00432	1.060C7	0.49647	3P 5.44368	-0.00773	0.80490
2S 21.83720	0.02186	-0.16498	-0.07758	3P 4.81869	0.00524	0.37278
3S 5.64068	0.00219	0.00537	-0.82658	3P 9.06583	0.11936	-0.15061
3S 5.07081	-0.00159	-0.00231	-0.44107			
3S 9.80086	-0.00255	0.1C810	0.28384			
COBALT K(2)L(8)3S(2)3P(3) -4S						
T.E.= -0.13201993D+04 P.E.= -0.26403558D+04 K.E.= 0.13201966D+04 V.T.= -0.20000020D+01						
S	1S	2S	3S	P	2P	3P
BASIS/ORB E	-296.19383	-47.73181	-15.01712	BASIS/ORB E	-43.60460	-13.79714
1S 26.47320	0.95004	-0.31451	-0.13593	2P 11.3E490	0.85068	-0.40127
1S 38.87790	0.03454	0.00226	0.00105	2P 19.66210	0.07743	-0.03089
2S 11.34710	0.00392	1.06477	0.50786	3P 5.76123	-0.00584	0.82605
2S 22.47570	0.02028	-0.17207	-0.08288	3P 5.14507	0.00395	0.36378
3S 5.95447	0.00226	-0.003E3	-0.86298	3P 9.43933	0.10539	-0.15541
3S 5.39218	-0.00166	0.00392	-0.42551			
3S 10.15520	-0.00235	0.11466	0.30545			
NICKEL K(2)L(8)3S(2)3P(3) -4S						
T.E.= -0.14314896D+04 P.E.= -0.28E29761D+04 K.E.= 0.14314864D+04 V.T.= -0.20000022D+01						
S	1S	2S	3S	P	2P	3P
BASIS/ORB E	-320.73702	-52.73414	-16.94842	BASIS/ORB E	-47.78645	-15.65211
1S 27.43290	0.95157	-0.31E20	-0.13988	2P 11.80560	0.65896	-0.41237
1S 40.19760	0.03477	0.00311	0.00182	2P 20.27860	0.07955	-0.03189
2S 11.89480	0.00400	1.064C6	0.51098	3P 6.07305	-0.00278	0.85144
2S 23.13700	0.018C7	-0.17802	-0.08571	3P 5.47393	0.001E7	0.34962
3S 6.24692	0.00263	-0.00892	-0.90501	3P 9.81867	0.09195	-0.15541
3S 5.71613	-0.00199	0.0C764	-0.39652			
3S 10.63450	-0.00244	0.12450	0.32550			
COPPER K(2)L(8)3S(2)3P(3) -4S						
T.E.= -0.15473387D+04 P.E.= -0.30546750D+04 K.E.= 0.15473363D+04 V.T.= -0.20000016D+01						
S	1S	2S	3S	P	2P	3P
BASIS/ORB E	-346.28168	-57.98766	-18.99158	BASIS/ORB E	-52.81938	-17.61897
1S 28.47250	0.95181	-0.32160	-0.14399	2P 12.23510	0.86978	-0.42376
1S 41.41240	0.03348	0.00467	0.00315	2P 21.04450	0.07913	-0.03190
2S 12.47950	0.00238	1.06231	0.51199	3P 6.41427	0.00306	0.85743
2S 23.74400	0.02003	-0.18719	-0.08940	3P 5.78993	-0.00237	0.35756
3S 6.62446	0.00130	-0.01693	-0.86279	3P 10.17430	C.07794	-0.16E21
3S 6.02775	-0.00097	0.01291	-0.45916			
3S 11.07210	-0.00133	0.13929	0.35515			

See page 183 for Explanation of Tables and Notes for Tables 32, 42, and 43

TABLE 24 (4). THE HARTREE-FOCK FUNCTIONS FOR P(<sup>4</sup>S) ISO-ELECTRONIC SERIES.

ZINC K(2)L(8)3S(2)3P(3) -4S						
T.E.= -0.166774620+04 P.E.= -0.33354894D+04 K.E.= 0.166774330+04 V.T.= -0.20300017D+01						
S	1S	2S	3S	P	2P	3P
BASIS/ORB E	-372.82729	-63.49230	-21.14643	BASIS/CRB E	-58.10327	-19.69756
1S 29.44060	0.95299	-0.32495	-0.14733	2P 12.65930	0.87634	-0.43346
1S 42.71770	0.03362	0.00558	0.00382	2P 21.64460	0.08123	-0.03276
2S 13.03100	0.00236	1.06396	0.51613	3P 6.72522	0.00675	0.88555
2S 24.39290	0.01840	-0.19365	-0.09276	3P 6.11925	-0.00497	0.34043
3S 6.92585	0.00149	-0.02202	-0.89488	3P 10.54920	0.06646	-0.17056
3S 6.35114	-0.00113	0.01746	-0.44053			
3S 11.52840	-0.00137	0.14712	0.37379			
 GALLIUM K(2)L(8)3S(2)3P(3) -4S						
T.E.= -0.17927116D+04 P.E.= -0.35854197D+04 K.E.= 0.17927082D+04 V.T.= -0.26000019D+01						
S	1S	2S	3S	P	2P	3P
BASIS/ORB E	-400.37349	-69.24787	-23.41293	BASIS/CRB E	-63.63794	-21.88787
1S 30.22750	0.95505	-0.32891	-0.15100	2P 13.C1450	0.87752	-0.43940
1S 44.00320	0.03818	0.00518	0.00399	2P 21.80790	0.09165	-0.03772
2S 13.58090	0.00593	1.06523	0.51907	3P 7.11865	0.00673	0.83617
2S 25.03440	0.00862	-0.157C7	-0.09437	3P 6.44324	-0.00427	0.40635
3S 7.25316	0.00484	-0.02988	-0.90299	3P 10.92700	0.05247	-0.17951
3S 6.67006	-0.00364	0.02242	-0.44744			
3S 11.97900	-0.00392	0.15488	0.39414			
 GERMANIUM K(2)L(8)3S(2)3P(3) -4S						
T.E.= -0.19222347D+04 P.E.= -0.38444660D+04 K.E.= 0.19222313D+04 V.T.= -0.20300018D+01						
S	1S	2S	3S	P	2P	3P
BASIS/ORB E	-428.92099	-75.25424	-25.79100	BASIS/CRB E	-69.42336	-24.18977
1S 31.22190	0.95567	-0.33176	-0.15368	2P 13.43840	0.88234	-0.44778
1S 45.30360	0.03772	0.00619	0.00457	2P 22.39090	0.09395	-0.03862
2S 14.13390	0.00554	1.06870	0.52433	3P 7.43703	0.01010	0.85663
2S 25.68010	0.00853	-0.20427	-0.09844	3P 6.77082	-0.00653	0.39702
3S 7.55396	0.00491	-0.03741	-0.94284	3P 11.30130	0.04257	-0.18455
3S 6.99270	-0.00377	0.02828	-0.42112			
3S 12.41670	-0.00367	0.16112	0.41121			
 ARSENIC K(2)L(8)3S(2)3P(3) -4S						
T.E.= -0.20563153D+04 P.E.= -0.41126285D+04 K.E.= 0.20563132D+04 V.T.= -0.20000010D+01						
S	1S	2S	3S	P	2P	3P
BASIS/ORB E	-458.46926	-81.51128	-28.28064	BASIS/ORB E	-75.45938	-26.60324
1S 32.23780	-0.95611	-0.33462	-0.15632	2P 13.87410	0.88629	-0.45251
1S 46.59360	-0.03683	0.00745	0.00529	2P 22.98890	0.09566	-0.04019
2S 14.67140	-0.00474	1.07439	0.53026	3P 7.91002	0.01112	0.75871
2S 26.32940	-0.00940	-0.21126	-0.10232	3P 7.09685	-0.00653	0.51649
3S 7.86898	-0.00445	-0.04265	-0.96701	3P 11.68330	0.03451	-0.20274
3S 7.31372	0.00345	0.03233	-0.41C79			
3S 12.85020	0.00315	0.16404	0.42721			
 SELENIUM K(2)L(8)3S(2)3P(3) -4S						
T.E.= -0.21949532D+04 P.E.= -0.43895035D+04 K.E.= 0.21949503D+04 V.T.= -0.20000013D+01						
S	1S	2S	3S	P	2P	3P
BASIS/ORB E	-489.01858	-88.01899	-30.88174	BASIS/CRB E	-81.74602	-29.12823
1S 33.25870	-0.95659	-0.33733	-0.15910	2P 14.30770	0.89547	-0.46216
1S 47.88430	-0.03582	0.00871	0.00617	2P 23.76480	0.09436	-0.03945
2S 15.20510	-0.00386	1.08118	0.53560	3P 8.23522	0.02033	0.76832
2S 26.97870	-0.01043	-0.21833	-0.10574	3P 7.42392	-0.01255	0.51703
3S 8.26691	-0.00349	-0.04432	-0.89166	3P 12.C5600	0.02212	-0.20657
3S 7.63579	0.00264	0.03226	-0.50507			
3S 13.26140	0.00261	0.16E30	C.44815			

See page 183 for Explanation of Tables and Notes for Tables 32, 42, and 43

## ROOTHAAN-HARTREE-FOCK ATOMIC WAVEFUNCTIONS

 TABLE 24 (5). THE HARTREE-FOCK FUNCTIONS FOR P(<sup>4</sup>S) ISO-ELECTRONIC SERIES.

BROMINE      K{2}L{8}3S{2}3P{3} -4S  
 T.E.= -0.23381482D+04    P.E.= -0.46762941D+04    K.E.= 0.233814590D+04    V.T.= -0.20000010D+01

S	1S	2S	3S	P	2P	3P
BASIS/ORB E	-520.56797	-94.77727	-33.59423	BASIS/ORB E	-88.28310	-31.76464
1S 34.24070	-0.95736	-0.3393	-0.16110	2P 14.71980	0.89516	-0.46737
1S 49.21550	-0.03558	0.00558	0.00648	2P 24.15930	0.09993	-0.04177
2S 15.73340	-0.00383	1.08811	0.54341	3P 8.56481	0.01942	0.77685
2S 27.63490	-0.00972	-0.22451	-0.11000	3P 7.75485	-0.01169	0.51984
3S 8.56104	-0.00387	-0.05131	-0.53704	3P 12.43690	0.01580	-0.21286
2S 7.96187	0.00298	0.03803	-0.47253			
3S 13.67670	0.00264	0.16735	0.46094			

KRYPTON      K{2}L{8}3S{2}3P{3} -4S  
 T.E.= -0.24859001D+04    P.E.= -0.49717979D+04    K.E.= 0.24858977D+04    V.T.= -0.20000010D+01

S	1S	2S	3S	P	2P	3P
BASIS/ORB E	-553.11822	-101.78605	-36.41815	BASIS/ORB E	-95.07065	-34.51251
1S 35.27790	-0.95807	-0.34251	-0.16326	2P 15.13070	0.89935	-0.47410
1S 50.56430	-0.03404	0.01095	0.00716	2P 24.71790	0.10270	-0.04293
2S 16.21630	-0.00276	1.09502	0.55226	3P 8.89931	0.02502	0.77221
2S 28.31600	-0.01125	-0.22975	-0.11336	3P 8.09028	-0.01521	0.53359
3S 8.93852	-0.00285	-0.04558	-0.88346	3P 12.83580	0.00550	-0.21626
3S 8.29254	0.00217	0.03587	-0.54301			
3S 14.07360	0.00196	0.16165	0.47518			

See page 183 for Explanation of Tables and Notes for Tables 32, 42, and 43

TABLE 25 (1). THE HARTREE-FOCK FUNCTIONS FOR P(2D) ISO-ELECTRONIC SERIES.

PHOSPHORUS		K(2)L(8)3S(2)3P(3) -2D					
T.E.= -0.340648620+03		P.E.= -0.681301770+03			K.E.= 0.340653150+03	V.T.= -0.199996670+01	
S		1S	2S	3S	P	2P	3P
BASIS/ORB E	-79.98901	-7.52676	-0.70659	BASIS/ORB E	-5.41843	-0.35065	
1S 15.66470	0.85303	-0.21324	0.05818	2P 6.50747	0.65614	-0.15567	
1S 23.28260	0.02228	-0.01658	0.00491	2P 12.36020	0.03751	-0.00905	
2S 5.66662	0.00567	0.92E42	-0.28026	3P 2.09007	0.00941	0.50686	
2S 14.38640	0.14746	-0.14661	0.04345	3P 1.17236	-0.00111	0.59439	
3S 2.41959	0.00060	-0.00001	0.58998	3P 4.87078	0.38031	-0.10213	
3S 1.50467	-0.00025	0.0CC96	0.54107				
3S 4.75452	-0.00212	0.1E649	-0.12543				
SULFUR		K(2)L(8)3S(2)3P(3) -2D			V.T.= -0.200000430+01		
T.E.= -0.39708539D+03		P.E.= -0.79416909D+03			K.E.= 0.39708370D+03		
S		1S	2S	3S	P	2P	3P
BASIS/ORB E	-92.45101	-9.44270	-1.24784	BASIS/ORB E	-7.11664	-0.80793	
1S 16.52000	0.87955	-0.23C92	0.06806	2P 6.96741	0.67010	-0.18888	
1S 24.55520	0.02609	-0.01405	0.00515	2P 12.96970	0.04117	-0.01091	
2S 6.07393	0.00542	0.95806	-0.31995	3P 2.39154	0.00831	0.53769	
2S 15.06040	0.11239	-0.14C85	0.04720	3P 1.51523	-0.00076	0.55011	
3S 2.71463	0.00071	0.00110	0.61891	3P 5.32758	0.35746	-0.11212	
3S 1.80692	-0.00031	0.00060	0.51953				
3S 5.14492	-0.00221	C.15827	-0.13546				
CHLORINE		K(2)L(8)3S(2)3P(3) -2D			V.T.= -0.20000087D+01		
T.E.= -0.45812250D+03		P.E.= -0.91624102D+03			K.E.= 0.45811853D+03		
S		1S	2S	3S	P	2P	3P
BASIS/ORB E	-105.93673	-11.63311	-1.91876	BASIS/ORB E	-9.09415	-1.39290	
1S 17.12700	0.90752	0.25418	0.08017	2P 7.38050	0.68884	-0.21738	
1S 25.86680	0.02984	0.00866	0.00402	2P 13.55340	0.04661	-0.01347	
2S 6.49800	0.00554	-0.97E52	-0.35293	3P 2.68299	0.00948	0.57725	
2S 15.58220	0.07559	0.13127	0.04859	3P 1.83531	-0.00168	0.50845	
3S 3.03752	0.00089	-0.00909	0.58295	3P 5.78059	0.32913	-0.11836	
3S 2.16964	-0.00043	0.00280	0.55827				
3S 5.66995	-0.00253	-0.13E30	-0.14149				
ARGON		K(2)L(8)3S(2)3P(3) -2D			V.T.= -0.20000110D+C1		
T.E.= -0.523746020+03		P.E.= -0.10474863D+04			K.E.= 0.52374024D+03		
S		1S	2S	3S	P	2P	3P
BASIS/ORB E	-120.43784	-14.09114	-2.71172	BASIS/CRB E	-11.33586	-2.09968	
1S 17.99270	0.91849	-0.26464	0.08878	2P 7.75752	0.71375	-0.24540	
1S 27.14570	0.03074	-0.0C695	0.00346	2P 14.14940	0.05060	-0.01583	
2S 6.94671	0.00505	0.99651	-0.38082	3P 2.99656	0.00356	0.60203	
2S 16.24500	0.06194	-0.13286	0.05209	3P 2.16065	0.00093	0.48959	
3S 3.32253	0.00089	0.00886	0.63140	3P 6.13675	0.29551	-0.12262	
3S 2.46289	-0.00044	-0.00285	0.52580				
3S 6.08550	-0.00234	0.12259	-0.15791				
POTASSIUM		K(2)L(8)3S(2)3P(3) -2D			V.T.= -0.20000083D+01		
T.E.= -0.59394750D+03		P.E.= -0.11878901D+04			K.E.= 0.59394255D+03		
S		1S	2S	3S	P	2P	3P
BASIS/ORB E	-135.94890	-16.81007	-3.62286	BASIS/ORB E	-13.83761	-2.92462	
1S 18.86100	0.92757	-0.27469	0.09688	2P 8.12484	0.73856	-0.271C0	
1S 28.44560	0.03195	-0.00510	0.00277	2P 14.74470	0.05514	-0.01828	
2S 7.40511	0.00486	1.01158	-0.40504	3P 3.30828	0.00039	0.62351	
2S 16.88280	0.04997	-0.13473	0.05536	3P 2.48540	0.00219	0.47603	
3S 3.60073	0.00097	0.00891	0.68627	3P 6.49865	0.26246	-0.12486	
3S 2.75280	-0.00050	-0.00307	0.48680				
3S 6.51557	-0.00235	0.11422	-0.17391				

See page 183 for Explanation of Tables and Notes for Tables 32, 42, and 43

## ROOTHAAAN-HARTREE-FOCK ATOMIC WAVEFUNCTIONS

TABLE 25 (2). THE HARTREE-FOCK FUNCTIONS FOR P(2D) ISO-ELECTRONIC SERIES.

CALCIUM K(2)L(8)3S(2)3P(3) -2D						
T.E.= -0.66872155D+03 P.E.= -0.13374398D+04 K.E.= 0.66871828D+03 V.T.= -0.20000049D+01						
S	1S	2S	3S	P	2P	3P
BASIS/ORB E	-152.46736	-19.78707	-4.65009	BASIS/CRB E	-16.59670	-3.86570
1S 19.78280	0.93299	-0.28219	0.10288	2P 8.48415	0.76416	-0.29552
1S 29.70740	0.03263	-0.00375	0.00266	2P 15.35930	0.05919	-0.02056
2S 7.88230	0.00448	1.02230	-0.42718	3P 3.62937	-0.00519	0.64104
2S 17.54130	0.04294	-0.13885	0.06017	3P 2.80865	0.00367	0.46555
3S 3.93061	0.00104	0.00798	0.64163	3P 6.82832	0.22962	-0.12665
3S 3.13151	-0.00058	-0.00280	0.54500			
3S 6.94702	-0.00222	C.11052	-0.18786			
SCANDIUM K(2)L(8)3S(2)3P(3) -2D						
T.E.= -0.74806442D+03 P.E.= -0.14961265D+04 K.E.= 0.74806205D+03 V.T.= -0.20000032D+01						
S	1S	2S	3S	P	2P	3P
BASIS/ORB E	-169.99157	-23.02225	-5.79223	BASIS/ORB E	-19.61139	-4.92186
1S 20.68610	0.93617	-0.28235	0.10775	2P 8.85421	0.78546	-0.31703
1S 31.09690	0.03475	-0.00639	0.00291	2P 15.93250	0.06345	-0.02262
2S 8.35084	0.00651	1.02272	-0.43375	3P 3.92048	-0.00565	0.69960
2S 18.58220	0.03564	-0.14057	0.06046	3P 3.09538	0.00460	0.42266
3S 4.20829	0.00192	0.01250	0.64619	3P 7.15944	0.20096	-0.12831
3S 3.46232	-0.00115	-0.00525	0.54634			
3S 7.59283	-0.00371	C.11112	-0.20258			
TITANIUM K(2)L(8)3S(2)3P(3) -2D						
T.E.= -0.83197345D+03 P.E.= -0.16639450D+04 K.E.= 0.83197152D+03 V.T.= -0.20000023D+01						
S	1S	2S	3S	P	2P	3P
BASIS/ORB E	-188.52028	-26.50808	-7.04820	BASIS/CRB E	-22.88029	-6.09204
1S 21.65270	0.93929	-0.28805	0.11302	2P 9.22764	0.80225	-0.33656
1S 32.36990	0.03449	-0.00511	0.00242	2P 16.47020	0.06852	-0.02515
2S 8.84953	0.00560	1.02574	-0.45046	3P 4.28939	-0.00503	0.62646
2S 19.22370	0.03260	-0.14680	0.06503	3P 3.49853	0.00414	0.50580
3S 4.53346	0.00183	0.00652	0.66352	3P 7.52540	0.17484	-0.12852
3S 3.78177	-0.00111	-0.00203	0.55154			
3S 7.95098	-0.00319	0.11244	-0.22555			
VANADIUM K(2)L(8)3S(2)3P(3) -2D						
T.E.= -0.92044663D+03 P.E.= -0.18408904D+04 K.E.= 0.92044376D+03 V.T.= -0.20000031D+01						
S	1S	2S	3S	P	2P	3P
BASIS/ORB E	-208.05252	-30.24966	-8.41756	BASIS/ORB E	-26.40254	-7.37572
1S 22.54570	0.94362	-0.29574	0.11969	2P 9.61253	0.82017	-0.35598
1S 33.65970	0.03598	-0.00334	0.00124	2P 17.06920	0.07160	-0.02658
2S 9.33564	0.00620	1.03515	-0.45991	3P 4.60338	-0.00914	0.64608
2S 19.87330	0.02545	-0.14877	0.06629	3P 3.82556	0.00615	0.49975
3S 4.79502	0.00230	C.01005	0.69547	3P 7.80795	0.15220	-0.13106
3S 4.10411	-0.00149	-0.00442	0.52777			
3S 8.50241	-0.00367	0.11128	-0.23826			
CHROMIUM K(2)L(8)3S(2)3P(3) -2D						
T.E.= -0.10134825D+04 P.E.= -0.20269625D+04 K.E.= 0.10134800D+04 V.T.= -0.20000024D+01						
S	1S	2S	3S	P	2P	3P
BASIS/ORB E	-228.58772	-34.24426	-9.89986	BASIS/ORB E	-30.17750	-8.77245
1S 23.46100	0.94677	-0.30121	0.12430	2P 10.00840	0.83467	-0.37196
1S 34.95750	0.03708	-0.00240	0.00090	2P 17.65850	0.07465	-0.02832
2S 9.84077	0.00644	1.04294	-0.47395	3P 5.03053	-0.01269	0.57256
2S 20.50870	0.02023	-0.15401	0.07042	3P 4.19738	0.00750	0.59375
3S 5.11307	0.00284	0.00414	0.71671	3P 8.08420	0.13360	-0.14213
3S 4.42482	-0.00187	-0.00097	0.52745			
3S 8.87191	-0.00397	0.11336	-0.25936			

See page 183 for Explanation of Tables and Notes for Tables 32, 42, and 43

TABLE 25 (3). THE HARTREE-FOCK FUNCTIONS FOR P(<sup>2</sup>D) ISO-ELECTRICAL SERIES.

MANGANESE K(2)L(8)3S(2)3P(3) -2D T.E.=-0.11110798D+04 P.E.=-0.22221566D+04 K.E.= 0.11110768D+04 V.T.=-0.20000027D+01						
S	1S	2S	3S	P	2P	3P
BASIS/ORB E	-250.12554	-38.49127	-11.49474	BASIS/ORB E	-34.20462	-10.28186
1S 24.39780	0.94891	-0.30643	0.12950	2P 10.41380	0.85163	-0.38949
1S 36.23670	0.03787	-0.00121	-0.00005	2P 18.39960	0.07490	-0.02851
2S 10.36200	0.00663	1.04577	-0.48098	3P 5.34997	-0.01696	0.64360
2S 21.15000	0.01658	-0.15914	0.07297	3P 4.47773	0.00893	0.54652
3S 5.43183	0.00320	0.00102	0.72855	3P 8.27266	0.11618	-0.15522
2S 4.74448	-0.00213	0.00089	0.53242			
3S 9.33019	-0.00417	0.11914	-0.28142			
IRON K(2)L(8)3S(2)3P(3) -2D T.E.=-0.12132377D+04 P.E.=-0.24264725D+04 K.E.= 0.12132348D+04 V.T.=-0.20000024D+01						
S	1S	2S	3S	P	2P	3P
BASIS/ORB E	-272.66530	-42.95032	-13.20184	BASIS/ORB E	-38.48354	-11.90361
1S 25.36200	0.95017	-0.31065	-0.13319	2P 10.82610	0.86182	-0.40409
1S 37.50470	0.03817	-0.00018	0.00043	2P 19.01430	0.07730	-0.02931
2S 10.88350	0.00634	1.05224	0.49289	3P 5.66758	-0.01716	0.66728
2S 21.78380	0.01476	-0.16591	-0.07775	3P 4.80270	0.00863	0.53944
3S 5.76276	0.00340	-0.00650	-0.74726	3P 8.55118	0.10136	-0.16278
3S 5.06247	-0.00227	0.0C547	-0.53600			
3S 9.69126	-0.00407	0.12362	0.30435			
COBALT K(2)L(8)3S(2)3P(3) -2D T.E.=-0.13199555D+04 P.E.=-0.26399075D+04 K.E.= 0.13199520D+04 V.T.=-0.20000026D+01						
S	1S	2S	3S	P	2P	3P
BASIS/ORB E	-296.20682	-47.74108	-15.02106	BASIS/ORB E	-43.01399	-13.63755
1S 26.41870	0.95074	-0.31444	-0.13599	2P 11.25310	0.86904	-0.41638
1S 38.88510	0.03580	0.00166	0.00084	2P 19.62200	0.07950	-0.03008
2S 11.37780	0.00488	1.05533	0.50479	3P 6.00242	-0.01626	0.66964
2S 22.47260	0.01748	-0.17187	-0.08264	3P 5.14146	0.00827	0.55319
2S 5.94428	0.00306	-0.0C649	-0.27112	3P 8.86626	0.08951	-0.17153
3S 5.39589	-0.00227	0.0C589	-0.41613			
3S 10.17580	-0.00302	0.12177	0.30769			
NICKEL K(2)L(8)3S(2)3P(3) -2D T.E.=-0.14312325D+04 P.E.=-0.28624608D+04 K.E.= 0.14312283D+04 V.T.=-0.20000030D+01						
S	1S	2S	3S	P	2P	3P
BASIS/ORB E	-320.74989	-52.74330	-16.95228	BASIS/ORB E	-47.79573	-15.48357
1S 27.36170	0.95247	-0.31E37	-0.13993	2P 11.68530	0.87524	-0.42765
1S 40.22180	0.03634	0.00249	0.00153	2P 20.23560	0.08144	-0.03069
2S 11.90760	0.00533	1.06124	0.50960	3P 6.33018	-0.01474	0.68271
2S 23.13980	0.01449	-0.17698	-0.08527	3P 5.47312	0.00740	0.55646
3S 6.22928	0.00390	-0.01042	-0.92202	3P 9.18402	0.07864	-0.18105
3S 5.72318	-0.00299	0.0C891	-0.37772			
3S 10.65140	-0.00338	0.12767	0.32521			
COPPER K(2)L(8)3S(2)3P(3) -2D T.E.=-0.15470683D+04 P.E.=-0.30941325D+04 K.E.= 0.15470641D+04 V.T.=-0.20000027D+01						
S	1S	2S	3S	P	2P	3P
BASIS/ORB E	-346.29433	-57.95E74	-18.99537	BASIS/ORB E	-52.82855	-17.44152
1S 28.31270	0.95385	-0.32226	-0.14351	2P 12.20960	0.87946	-0.43498
1S 41.54610	0.03676	0.00348	0.00216	2P 21.14700	0.07677	-0.02902
2S 12.43150	0.00568	1.06523	0.51577	3P 6.74479	-0.02005	0.66620
2S 23.79430	0.01208	-0.18223	-0.08830	3P 5.80495	0.00940	0.60041
3S 6.50703	0.00486	-0.01478	-0.99891	3P 9.52233	0.08168	-0.20772
3S 6.04942	-0.00385	0.01244	-0.31326			
3S 11.11090	-0.00367	0.1E129	0.34090			

See page 183 for Explanation of Tables and Notes for Tables 32, 42, and 43

## ROOTHAAN-HARTREE-FOCK ATOMIC WAVEFUNCTIONS

TABLE 25 (4). THE HARTREE-FOCK FUNCTIONS FOR P(2D) ISO-ELECTRICAL SERIES.

ZINC K(2)L(8)3S(2)3P(3) -2D T.E.= -0.166746250+04 P.E.= -0.33349200D+04 K.E.= 0.166745750+C4 V.T.= -0.200000300+01						
S	1S	2S	3S	P	2P	3P
BASIS/ORB E	-372.83989	-63.50128	-21.15016	BASIS/ORB E	-58.11236	-19.51125
1S 29.26810	0.95499	-0.32541	-0.14671	2P 12.64440	0.88391	-0.44405
1S 42.86320	0.03714	0.00416	0.00269	2P 21.73420	0.07898	-0.02979
2S 12.97760	0.00600	1.06669	0.52005	3P 7.07744	-0.01594	0.67175
2S 24.45850	0.01002	-0.1823	-0.09153	3P 6.13733	0.00739	0.60883
3S 6.79662	0.00591	-0.02308	-1.07320	3P 5.88593	0.07134	-0.21591
3S 6.37476	-0.00479	0.01521	-0.25245			
3S 11.56320	-0.00391	0.13882	0.35924			
 GALLIUM K(2)L(8)3S(2)3P(3) -2D T.E.= -0.17924147D+04 P.E.= -0.35848236D+04 K.E.= 0.17924090D+04 V.T.= -0.200000320+C1						
S	1S	2S	3S	P	2P	3P
BASIS/ORB E	-400.38648	-69.25674	-23.41662	BASIS/ORB E	-63.64658	-21.69269
1S 30.22630	0.95606	-0.32853	-0.14985	2P 13.10220	0.88764	-0.45181
1S 44.19170	0.03740	0.00492	0.00330	2P 22.39640	0.07958	-0.02998
2S 13.51710	0.00635	1.06533	0.52409	3P 7.40941	-0.01264	0.67675
2S 25.12240	0.00815	-0.19393	-0.09442	3P 6.46811	0.00578	0.61630
3S 7.08802	0.00714	-0.03C72	-1.15434	3P 10.27670	0.06406	-0.22422
3S 6.69984	-0.00592	0.02575	-0.18394			
3S 12.02250	-0.00418	0.14429	0.37621			
 GERMANIUM K(2)L(8)3S(2)3P(3) -2D T.E.= -0.19219245D+04 P.E.= -0.38428405D+04 K.E.= 0.19219160D+04 V.T.= -0.20000044D+01						
S	1S	2S	3S	P	2P	3P
BASIS/ORB E	-428.93405	-75.26306	-25.79468	BASIS/ORB E	-69.43236	-23.98579
1S 31.14020	0.95624	-0.33211	-0.15370	2P 13.42480	0.89357	-0.46224
1S 45.31660	0.03955	0.00563	0.00422	2P 22.67910	0.08884	-0.03365
2S 14.13620	0.00716	1.06841	0.52493	3P 7.67829	0.00604	0.72321
2S 25.66780	0.00482	-0.20221	-0.09827	3P 6.77073	-0.00385	0.57330
3S 7.54564	0.00659	-0.03947	-0.95426	3P 10.66790	0.03754	-0.21633
3S 6.99589	-0.00508	0.03001	-0.40977			
3S 12.40930	-0.00480	0.16176	0.41093			
 ARSENIC K(2)L(8)3S(2)3P(3) -2D T.E.= -0.20559919D+04 P.E.= -0.41115733D+04 K.E.= 0.20555814D+04 V.T.= -0.20000051D+01						
S	1S	2S	3S	P	2P	3P
BASIS/ORB E	-458.48265	-81.52009	-28.28426	BASIS/ORB E	-75.46840	-26.39047
1S 32.19470	0.95628	-0.33456	-0.15676	2P 13.86680	0.90031	-0.47110
1S 46.58210	-0.03786	0.00702	0.00536	2P 23.43400	0.08825	-0.03322
2S 14.70690	-0.00557	1.07153	0.52722	3P 7.91833	0.01872	0.76814
2S 26.30480	-0.00752	-0.21213	-0.10192	3P 7.09358	-0.01170	0.52615
3S 7.95718	-0.00477	-0.04307	-0.86892	3P 11.12110	0.02521	-0.20869
3S 7.31283	0.00354	0.03110	-0.51505			
3S 12.83540	0.00375	0.17C24	0.43664			
 SELENIUM K(2)L(8)3S(2)3P(3) -2D T.E.= -0.21946167D+04 P.E.= -0.43852228D+04 K.E.= 0.21946061D+04 V.T.= -0.20000048D+01						
S	1S	2S	3S	P	2P	3P
BASIS/ORB E	-489.03162	-88.02772	-30.88532	BASIS/ORB E	-81.75494	-28.90665
1S 33.20750	0.95677	-0.33655	-0.15951	2P 14.31550	0.90269	-0.47575
1S 47.88630	0.03700	0.00897	0.00619	2P 24.04320	0.08959	-0.03418
2S 15.13530	0.00491	1.08817	0.53994	3P 8.24241	0.02427	0.75944
2S 26.96510	0.00826	-0.21542	-0.10472	3P 7.42321	-0.01503	0.53729
3S 8.26449	0.00454	-0.03751	-0.89174	3P 11.63860	0.01822	-0.20840
3S 7.63672	-0.00342	0.02137	-0.50430			
3S 13.25170	-0.00338	0.15471	0.44207			

See page 183 for Explanation of Tables and Notes for Tables 32, 42, and 43

TABLE 25 (5). THE HARTREE-FOCK FUNCTIONS FOR P(<sup>2</sup>D) ISO-ELECTRICAL SERIES.

BROMINE K(2)L(8)3S(2)3P(3) -2D T.E.= -0.233779850+04 P.E.= -0.46755888D+04 K.E.= 0.23377902D+04 V.T.= -0.20000035D+01						
S	1S	2S	3S	P	2P	3P
BASIS/ORB E	-520.58117	-94.78591	-33.59783	BASIS/ORB E	-88.29198	-31.53431
1S 34.24180	-0.95728	-0.34067	-0.16140	2P 14.76570	0.90457	-0.47923
1S 49.19460	-0.03563	0.01003	0.00666	2P 24.64000	0.09101	-0.03538
2S 15.69710	-0.00376	1.09237	0.54598	3P 8.56459	0.02842	0.74823
2S 27.61460	-0.00982	-0.22366	-0.10976	3P 7.75105	-0.01760	0.54863
3S 8.57582	-0.00373	-0.04626	-0.92308	3P 12.19530	0.01239	-0.20675
3S 7.95879	0.00285	0.03393	-0.48745			
3S 13.66420	0.00260	0.16114	0.45895			

  

KRYPTON K(2)L(6)3S(2)3P(3) -2D T.E.= -0.248553730+04 P.E.= -0.4971C692D+04 K.E.= 0.24855319D+04 V.T.= -0.20000022D+01						
S	1S	2S	3S	P	2P	3P
BASIS/ORB E	-553.13115	-101.75462	-36.42175	BASIS/ORB E	-95.07946	-34.27341
1S 35.28510	-0.95804	-0.34250	-0.16325	2P 15.13240	0.90671	-0.48207
1S 50.55870	-0.03389	0.01101	0.00718	2P 24.97860	0.09811	-0.03951
2S 16.22010	-0.00259	1.09893	0.55229	3P 8.89633	0.03551	0.70577
2S 28.31290	-0.01155	-0.23055	-0.11354	3P 8.08939	-0.02181	0.58651
3S 8.94159	-0.00267	-0.04581	-0.88227	3P 12.83440	-0.00120	-0.19719
3S 8.29163	0.00203	0.03596	-0.54455			
3S 14.07200	0.00184	0.16212	0.47564			

See page 183 for Explanation of Tables and Notes for Tables 32, 42, and 43

## ROOTHAAN-HARTREE-FOCK ATOMIC WAVEFUNCTIONS

 TABLE 26 (1). THE HARTREE-FOCK FUNCTIONS FOR P(<sup>2</sup>P) ISO-ELECTRICAL SERIES.

**PHOSPHORUS**    K(2)L(8)3S(2)3P(3) -2P  
 T.E.= -0.34060290D+03   P.E.= -0.68121420D+03   K.E.= 0.34061130D+03   V.T.= -0.19999753D+01

S	1S	2S	3S	P	2P	3P
BASIS/ORB E	-80.00038	-7.53523	-0.71236	BASIS/CRB E	-5.42879	-0.32366
1S 15.79590	0.85947	-0.21616	0.06030	2P 6.57423	0.64572	-0.15112
1S 23.21000	0.02187	-0.01579	0.00402	2P 12.38130	0.03587	-0.00910
2S 5.84735	0.00504	0.86732	-0.25901	3P 2.16833	0.01109	0.46287
2S 14.29120	0.14074	-0.14629	0.04219	3P 1.18350	-0.00086	0.64406
2S 2.38552	0.00030	0.00538	0.60320	3P 4.91685	0.39197	-0.10940
3S 1.49314	-0.00013	-0.00090	0.51937			
3S 5.01647	-0.00151	0.25205	-0.14054			

**SULFUR**    K(2)L(8)3S(2)3P(3) -2P  
 T.E.= -0.39702779D+03   P.E.= -0.79405418D+03   K.E.= 0.39702639D+03   V.T.= -0.20300035D+01

S	1S	2S	3S	P	2P	3P
BASIS/ORB E	-92.46269	-9.45289	-1.25345	BASIS/ORB E	-7.12695	-0.77312
1S 16.35710	0.88965	-0.23532	0.07052	2P 6.91552	0.67794	-0.18913
1S 24.52920	0.02781	-0.01356	0.00441	2P 12.94950	0.04245	-0.01175
2S 6.24546	0.00554	0.90478	-0.29927	3P 2.46180	0.00740	0.50819
2S 14.92220	0.09860	-0.13521	0.04563	3P 1.50535	0.00030	0.58873
3S 2.69551	0.00059	0.00414	0.60804	3P 5.29191	0.34781	-0.11496
3S 1.81853	-0.00028	-0.00035	0.52019			
3S 5.39514	-0.00210	0.21763	-0.14940			

**CHLORINE**    K(2)L(8)3S(2)3P(3) -2P  
 T.E.= -0.45805408D+03   P.E.= -0.91610465D+03   K.E.= 0.45805077D+03   V.T.= -0.20000072D+01

S	1S	2S	3S	P	2P	3P
BASIS/ORB E	-105.94744	-11.64228	-1.92321	BASIS/CRB E	-9.10324	-1.35033
1S 17.12310	0.90859	0.25152	0.08056	2P 7.28018	0.70395	-0.22170
1S 25.88200	0.02940	0.00997	0.00385	2P 13.49220	0.04856	-0.01435
2S 6.67876	0.00533	-0.92604	-0.33072	3P 2.77958	0.00490	0.51716
2S 15.55080	0.07487	0.13534	0.04866	3P 1.85027	0.00111	0.57646
3S 2.97301	0.00066	-0.00733	0.63387	3P 5.67890	0.31062	-0.11757
3S 2.13252	-0.00033	0.00189	0.50045			
3S 5.86764	-0.00216	-0.15755	-0.15905			

**ARGON**    K(2)L(8)3S(2)3P(3) -2P  
 T.E.= -0.52366733D+03   P.E.= -0.10473329D+04   K.E.= 0.52366558D+03   V.T.= -0.20000033D+01

S	1S	2S	3S	P	2P	3P
BASIS/ORB E	-120.44771	-14.09921	-2.71553	BASIS/CRB E	-11.34391	-2.04991
1S 18.00690	0.91775	0.26032	0.08839	2P 7.66501	0.72885	-0.25062
1S 27.11000	0.03061	0.00521	0.00366	2P 14.13290	0.05233	-0.01639
2S 7.11633	0.00488	-0.95082	-0.35982	3P 3.09819	0.00103	0.52449
2S 16.25440	0.06294	0.13838	0.05266	3P 2.18912	0.00257	0.57266
3S 3.27573	0.00069	-0.00422	0.67061	3P 6.04681	0.27844	-0.11993
3S 2.43416	-0.00036	0.00047	0.48123			
3S 6.24502	-0.00203	-0.17545	-0.17590			

**POTASSIUM**    K(2)L(8)3S(2)3P(3) -2P  
 T.E.= -0.59385899D+03   P.E.= -0.11877155D+04   K.E.= 0.59385649D+03   V.T.= -0.20000042D+01

S	1S	2S	3S	P	2P	3P
BASIS/ORB E	-135.95844	-16.81765	-3.62634	BASIS/CRB E	-13.84515	-2.86810
1S 18.88070	0.92284	-0.26491	0.09480	2P 8.05922	0.74911	-0.27547
1S 28.42460	0.03380	-0.01026	0.00384	2P 14.73160	0.05636	-0.01854
2S 7.51625	0.00671	0.96962	-0.38146	3P 3.40873	-0.00121	0.53871
2S 17.23250	0.05232	-0.13700	0.05378	3P 2.51764	0.00359	0.56508
3S 3.58620	0.00137	0.01103	0.65583	3P 6.42712	0.25050	-0.12219
3S 2.77909	-0.00076	-0.00387	0.50530			
3S 6.79014	-0.00344	0.15612	-0.18514			

See page 183 for Explanation of Tables and Notes for Tables 32, 42, and 43

TABLE 26 (2). THE HARTREE-FOCK FUNCTIONS FOR P(2P) ISO-ELECTRICAL SERIES.

CALCIUM K(2)L(8)3S(2)3P(3) -2P						
T.E.= -0.66862346D+03 P.E.= -0.13372454D+04 K.E.= 0.66862192D+03 V.T.= -0.20000023D+01						
S	1S	2S	3S	P	2P	3P
BASIS/ORB E	-152.47670	-19.79439	-4.65338	BASIS/CRB E	-16.60400	-3.80276
1S 19.80050	0.92946	-0.27301	0.10166	2P 8.46210	0.76706	-0.29762
1S 29.73170	0.03386	-0.0C861	0.00325	2P 15.34200	0.05982	-0.02046
2S 7.97934	0.00613	0.984E1	-0.40281	3P 3.72005	-0.00338	0.55126
2S 17.90240	0.04471	-0.14034	0.05724	3P 2.84573	0.00416	0.56095
3S 3.85724	0.00135	C.0C930	0.72131	3P 6.80549	0.22583	-0.12451
3S 3.06482	-0.00078	-0.00321	0.45578			
3S 7.21121	-0.00317	C.146E3	-0.20058			
SCANDIUM K(2)L(8)3S(2)3P(3) -2P						
T.E.= -0.74795694D+03 P.E.= -0.14959117D+04 K.E.= 0.74795479D+03 V.T.= -0.20000029D+01						
S	1S	2S	3S	P	2P	3P
BASIS/ORB E	-170.00082	-23.02724	-5.79534	BASIS/ORB E	-19.61841	-4.85254
1S 20.77210	0.93369	-C.28118	0.10804	2P 8.86953	0.77990	-0.31572
1S 31.02450	0.03302	-0.00610	0.00240	2P 15.51130	0.06421	-0.02285
2S 8.45826	0.00513	0.99454	-0.41989	3P 4.03737	-0.00071	0.55936
2S 18.54290	0.04116	-0.14410	0.06081	3P 3.17145	0.00262	0.56151
3S 4.17497	0.00120	0.01079	0.67121	3P 7.23818	0.20353	-0.12722
3S 3.45060	-0.00074	-0.00435	0.51673			
3S 7.69801	-0.00260	0.14219	-0.21332			
TITANIUM K(2)L(8)3S(2)3P(3) -2P						
T.E.= -0.83185668D+03 P.E.= -0.16637103D+04 K.E.= 0.83185363D+03 V.T.= -0.20000037D+01						
S	1S	2S	3S	P	2P	3P
BASIS/ORB E	-188.52933	-26.51492	-7.05126	BASIS/ORB E	-22.88715	-6.01655
1S 21.53620	0.94217	-C.29019	0.11588	2P 9.28185	0.79351	-0.23343
1S 32.32720	0.03718	-0.00523	0.00136	2P 16.49290	0.06751	-0.02461
2S 8.93773	0.00730	1.00287	-0.43059	3P 4.34827	-0.00220	0.56975
2S 19.20230	0.02531	-0.14365	0.06072	3P 3.50019	0.00322	0.56090
3S 4.48544	0.00232	0.01193	0.67807	3P 7.62076	0.18392	-0.12966
3S 3.77350	-0.00148	-0.00518	0.52451			
3S 8.20165	-0.00423	0.13854	-0.23229			
VANADIUM K(2)L(8)3S(2)3P(3) -2P						
T.E.= -0.92032069D+03 P.E.= -0.184C6382D+04 K.E.= 0.92031752D+03 V.T.= -0.20000035D+01						
S	1S	2S	3S	P	2P	3P
BASIS/ORB E	-208.06145	-30.25632	-8.42051	BASIS/ORB E	-26.40925	-7.29402
1S 22.56490	0.94296	-0.25E30	0.11975	2P 9.69635	0.80656	-0.34978
1S 33.60760	0.03575	-0.00282	0.00114	2P 17.09610	0.07028	-0.02615
2S 9.34087	0.00576	1.03410	-0.45985	3P 4.66219	-0.00371	0.58276
2S 19.84540	0.02669	-0.14898	0.66661	3P 3.82544	0.00386	0.55886
3S 4.76037	0.00206	0.01134	0.72760	3P 7.59217	0.16570	-0.13291
3S 4.09455	-0.00136	-0.0C536	0.49250			
3S 8.52683	-0.0C332	0.11236	-0.23559			
CHROMIUM K(2)L(8)3S(2)3P(3) -2P						
T.E.= -0.10133474D+04 P.E.= -0.20266923D+04 K.E.= 0.10133449D+04 V.T.= -0.20000025D+01						
S	1S	2S	3S	P	2P	3P
BASIS/ORB E	-228.59657	-34.25C72	-9.90265	BASIS/ORB E	-30.18402	-8.68459
1S 23.59100	0.94432	-0.30152	0.12441	2P 10.11390	0.82257	-0.36746
1S 34.94310	0.03408	-0.00C82	0.00027	2P 17.81470	0.07077	-0.02642
2S 9.81692	0.00444	1.04600	-0.47455	3P 4.96923	-0.00741	0.59828
2S 20.50280	0.02758	-0.15481	0.07061	3P 4.15588	0.00563	0.55534
3S 5.04946	0.00163	0.01096	0.75958	3P 8.29781	0.14798	-0.13556
3S 4.41998	-0.00112	-0.00551	0.47582			
3S 8.95580	-0.00247	0.1C653	-0.24961			

See page 183 for Explanation of Tables and Notes for Tables 32, 42, and 43

## ROOTHAAN-HARTREE-FOCK ATOMIC WAVEFUNCTIONS

TABLE 26 (3). THE HARTREE-FOCK FUNCTIONS FOR P(2P) ISO-ELECTRICAL SERIES.

MANGANESE K(2)L(8)3S(2)3P(3) -2P						
T.E.= -0.11109357D+04 P.E.= -0.22218692D+04 K.E.= 0.11105335D+04 V.T.= -0.200000200+01						
S	1S	2S	3S	P	2P	3P
BASIS/ORB E	-250.13422	-36.49763	-11.49743	BASIS/ORB E	-34.21103	-10.18793
1S 24.50970	0.94643	-0.30220	0.12770	2P 10.53150	0.83298	-0.38142
1S 36.26500	0.03557	-0.00241	0.00047	2P 18.43010	0.07328	-0.02765
2S 10.29060	0.00560	1.05210	-0.48292	3P 5.27614	-0.00586	0.60927
2S 21.40450	0.02268	-0.15822	0.07221	3P 4.48617	0.00470	0.55409
3S 5.39908	0.00250	0.00606	0.74518	3P 8.68555	0.13173	-0.13761
3S 4.74510	-0.00171	-0.00221	0.51038			
3S 9.38361	-0.00341	0.10539	-0.27147			
IRON K(2)L(8)3S(2)3P(3) -2P						
T.E.= -0.12130846D+04 P.E.= -0.24261667D+04 K.E.= 0.12130821D+04 V.T.= -0.20000021D+01						
S	1S	2S	3S	P	2P	3P
BASIS/ORB E	-272.67393	-42.99658	-13.20452	BASIS/CRB E	-38.48987	-11.80371
1S 25.43480	0.94910	-0.31095	-0.13302	2P 10.55440	0.84261	-0.39407
1S 37.49890	0.03647	0.00075	0.00065	2P 19.44810	0.07539	-0.02876
2S 10.84630	0.00508	1.05926	0.49743	3P 5.59599	-0.00562	0.62638
2S 21.77750	0.01063	-0.16623	-0.07839	3P 4.80648	0.00445	0.54933
3S 5.75310	0.00259	-0.00333	-0.75918	3P 9.04975	0.11757	-0.14266
3S 5.05844	-0.00174	0.00342	+0.52374			
3S 9.67470	-0.00317	0.11435	0.29925			
COBALT K(2)L(8)3S(2)3P(3) -2P						
T.E.= -0.13197935D+04 P.E.= -0.26355838D+04 K.E.= 0.13197903D+04 V.T.= -0.20000024D+01						
S	1S	2S	3S	P	2P	3P
BASIS/ORB E	-296.21544	-47.74724	-15.02373	BASIS/ORB E	-43.02024	-13.53171
1S 26.43130	0.95025	-0.31546	-0.13681	2P 11.37500	0.85139	-0.40615
1S 38.81430	0.03579	0.00236	0.00136	2P 19.66330	0.07762	-0.02577
2S 11.33950	0.00444	1.06842	0.50897	3P 5.90251	-0.00336	0.64031
2S 22.42570	0.01831	-0.17189	-0.08233	3P 5.13602	0.00307	0.54529
3S 6.05488	0.00246	-0.00518	-0.78502	3P 9.43287	0.10342	-0.14516
3S 5.38257	-0.00169	0.00454	-0.51382			
3S 10.09310	-0.00278	0.11226	0.31451			
NICKEL K(2)L(8)3S(2)3P(3) -2P						
T.E.= -0.14310616D+04 P.E.= -0.28621195D+04 K.E.= 0.14310580D+04 V.T.= -0.20000025D+01						
S	1S	2S	3S	P	2P	3P
BASIS/ORB E	-320.75846	-52.74939	-16.95492	BASIS/CRB E	-47.80192	-15.37177
1S 27.44720	0.95119	-0.31901	-0.14005	2P 11.72500	0.86136	-0.41691
1S 40.13800	0.03463	0.00371	0.00197	2P 20.07420	0.08461	-0.03273
2S 11.86100	0.00350	1.07348	0.51793	3P 6.21020	0.00403	0.65162
2S 23.08260	0.01894	-0.17872	-0.08676	3P 5.46543	-0.00142	0.54271
3S 6.35757	0.00203	-0.00588	-0.81441	3P 9.81664	0.08079	-0.14285
3S 5.70655	-0.00143	0.00762	-0.50070			
3S 10.50970	-0.00215	0.11617	0.33251			
COPPER K(2)L(8)3S(2)3P(3) -2P						
T.E.= -0.15468885D+04 P.E.= -0.30937729D+04 K.E.= 0.15468845D+04 V.T.= -0.2000026D+01						
S	1S	2S	3S	P	2P	3P
BASIS/ORB E	-346.30271	-58.00281	-18.99801	BASIS/ORB E	-52.83472	-17.32382
1S 28.38430	0.95271	-0.32322	-0.14356	2P 12.15910	0.86512	-0.42510
1S 41.45100	0.03547	0.00474	0.00250	2P 20.60230	0.08774	-0.03452
2S 12.36800	0.00403	1.08019	0.52674	3P 6.66319	0.00272	0.59466
2S 23.72910	0.01580	-0.18355	-0.09010	3P 5.79490	-0.00038	0.61591
3S 6.65581	0.00277	-0.01271	-0.84592	3P 10.19910	0.07254	-0.15923
3S 6.03173	-0.00200	0.00562	-0.48364			
3S 10.94080	-0.00261	0.11670	0.34771			

See page 183 for Explanation of Tables and Notes for Tables 32, 42, and 43

TABLE 26 (4). THE HARTREE-FOCK FUNCTIONS FOR P(2P) ISO-ELECTRICAL SERIES.

ZINC K(2)L(8)3S(2)3P(3) -2P T.E.= -0.16672738D+04 P.E.= -0.33345459D+04 K.E.= 0.16672701D+04 V.T.= -0.20300022D+C1						
S	1S	2S	3S	P	2P	3P
BASIS/ORB E	-372.84863	-63.5C723	-21.15279	BASIS/CRB E	-58.11846	-19.38766
1S 29.46960	0.95279	-0.32600	-0.14659	2P 12.64700	0.67692	-0.43666
1S 42.69880	0.03294	0.00645	0.00350	2P 21.63520	0.08161	-0.03226
2S 12.94370	0.00166	1.08073	0.53123	3P 6.97236	0.00810	0.61463
2S 24.35050	0.01982	-0.19352	-0.09538	3P 6.11617	-0.00409	0.61073
3S 7.00322	0.00086	-0.02155	-0.84876	3P 10.56230	0.06370	-0.16530
3S 6.34628	-0.00064	0.01534	-0.50085			
3S 11.34870	-0.00091	0.12542	0.37383			
GALLIUM K(2)L(8)3S(2)3P(3) -2P T.E.= -0.17922171D+04 P.E.= -0.35844301D+04 K.E.= 0.17922130D+04 V.T.= -0.20300023D+01						
S	1S	2S	3S	P	2P	3P
BASIS/ORB E	-400.39517	-69.26264	-23.41921	BASIS/CRB E	-63.65303	-21.56319
1S 30.44580	0.95385	-0.32534	-0.14966	2P 13.07130	0.88315	-0.44580
1S 44.00680	0.03290	0.00748	0.00414	2P 22.24150	0.08354	-0.03305
2S 13.47420	0.00154	1.0E533	0.53736	3P 7.29001	0.01195	0.62442
2S 25.00180	0.01861	-0.19962	-0.09893	3P 6.44347	-0.00648	0.61091
3S 7.31620	0.0094	-0.02591	-0.86980	3P 10.54670	0.05244	-0.16898
2S 6.66833	-0.00069	0.01844	-0.49438			
3S 11.78560	-0.00088	0.13327	C.39101			
GERMANIUM K(2)L(8)3S(2)3P(3) -2P T.E.= -0.19217182D+04 P.E.= -0.38434323D+04 K.E.= C.19217141D+04 V.T.= -0.20300021D+01						
S	1S	2S	3S	P	2P	3P
BASIS/ORB E	-428.94264	-75.26888	-25.79723	BASIS/CRB E	-69.43834	-23.85039
1S 31.42270	0.95478	-0.33229	-C.15299	2P 13.49610	0.86902	-0.45466
1S 45.30560	0.03289	0.00351	0.00501	2P 22.84830	0.08528	-0.03372
2S 14.03020	0.01143	1.08760	0.53989	3P 7.60827	0.01592	0.63548
2S 25.64580	0.01750	-0.20E58	-6.10189	3P 6.77089	-0.00900	0.61017
3S 7.70741	0.00092	-0.03C73	-0.82075	3P 11.32060	0.04176	-0.17309
3S 6.99067	-0.00067	0.02C98	-0.56287			
3S 12.21950	-0.00086	0.14148	0.41610			
ARSENIC K(2)L(8)3S(2)3P(3) -2P T.E.= -0.20557769D+04 P.E.= -0.41115492D+04 K.E.= 0.20557723D+04 V.T.= -0.20300022D+C1						
S	1S	2S	3S	P	2P	3P
BASIS/ORB E	-458.49089	-81.52584	-28.28677	BASIS/CRB E	-75.47428	-26.24916
1S 32.39620	0.95563	-0.33518	-0.15575	2P 13.52140	0.89420	-0.46267
1S 46.60630	0.03299	0.00521	0.00561	2P 23.44600	0.08729	-0.03444
2S 14.57110	0.00147	1.09123	0.54426	3P 7.52749	C.02022	0.64545
2S 26.30380	0.01629	-0.21267	-0.10516	3P 7.09861	-0.01176	0.61001
3S 8.01934	0.00109	-0.03502	-0.83685	3P 11.70390	0.03170	-0.17709
3S 7.31353	-0.00080	0.02413	-0.55918			
3S 12.67130	-0.00054	0.14615	0.43199			
SELENIUM K(2)L(8)3S(2)3P(3) -2P T.E.= -0.21943928D+04 P.E.= -0.43887808D+04 K.E.= 0.21943880D+04 V.T.= -0.20000022D+01						
S	1S	2S	3S	P	2P	3P
BASIS/ORB E	-489.03983	-88.03345	-30.88779	BASIS/CRB E	-81.76080	-28.75945
1S 33.33150	0.95636	-C.33758	-0.15831	2P 14.35570	0.89610	-0.47011
1S 47.87350	0.03412	0.00550	0.00600	2P 24.03670	0.08905	-0.03498
2S 15.15940	0.00225	1.09100	0.54622	3P 8.24263	0.02295	0.66576
2S 26.94590	0.01359	-0.21999	-0.10887	3P 7.42210	-0.01358	0.60063
3S 8.35261	0.00192	-0.04425	-0.84445	3P 12.66710	0.02391	-0.18280
3S 7.63228	-0.00139	0.03036	-0.56664			
3S 13.11220	-0.00154	0.15E48	0.45353			

See page 183 for Explanation of Tables and Notes for Tables 32, 42, and 43

## ROOTHAAN-HARTREE-FOCK ATOMIC WAVEFUNCTIONS

 TABLE 26 (5). THE HARTREE-FOCK FUNCTIONS FOR P(<sup>2</sup>P) ISO-ELECTRICAL SERIES.

BROMINE      K(2)L(8)3S(2)3P(3) -2P  
 T.E.= -0.23375658D+04    P.E.= -0.46751264D+04    K.E.= 0.23375605D+04    V.T.= -0.20000023D+01

S	1S	2S	3S	P	2P	3P
EASIS/ORB E	-520.58939	-94.79163	-33.60025	EASIS/ORB E	-86.29781	-31.38123
1S 34.26010	-0.95700	-0.34017	-0.16697	2P 14.79190	0.90117	-0.47700
1S 49.14040	-0.03539	0.00590	0.00649	2P 24.61350	0.09096	-0.03552
2S 15.74060	-0.00322	1.09229	0.54819	3P 8.55594	0.02526	0.69148
2S 27.57770	-0.01071	-0.22700	-0.11220	3P 7.74299	-0.01515	0.58606
3S 8.69121	-0.00289	-0.05122	-0.84738	3P 12.42670	0.01706	-0.18904
3S 7.94870	0.00209	0.03453	-0.57789			
3S 13.56040	0.00227	0.16840	0.47357			

KRYPTON      K(2)L(8)3S(2)3P(3) -2P  
 T.E.= -0.24852958D+04    P.E.= -0.49705853D+04    K.E.= 0.24852895D+04    V.T.= -0.20000026D+01

S	1S	2S	3S	P	2P	3P
BASIS/ORB E	-553.13957	-101.80033	-36.42413	BASIS/ORB E	-95.08529	-34.11446
1S 35.27540	-0.95809	-0.34252	-0.16324	2P 15.13010	0.90736	-0.48546
1S 50.56630	-0.03408	0.01093	0.00714	2P 24.99890	0.09781	-0.03846
2S 16.21490	-0.00281	1.09515	0.55247	3P 8.89967	0.03688	0.66123
2S 28.31710	-0.01114	-0.22966	-0.11339	3P 8.09061	-0.02237	0.62282
3S 8.93741	-0.00291	-0.04563	-0.88495	3P 12.83630	-0.00222	-0.18606
3S 8.29287	0.00221	0.03594	-0.54140			
3S 14.07420	0.00200	0.16141	0.47487			

See page 183 for Explanation of Tables and Notes for Tables 32, 42, and 43

TABLE 27 (1). THE HARTREE-FOCK FUNCTIONS FOR S(<sup>3</sup>P) ISO-ELECTRICAL SERIES.

SULFUR K(2)L(8)3S(2)3P(4) - 3P T.E.= -0.39750468D+03 P.E.= -0.79501020D+03 K.E.= 0.39750552D+03 V.T.= -0.19999979D+01						
S	1S	2S	3S	P	2P	3P
BASIS/ORB E	-92.00424	-9.00412	-0.87937	BASIS/CRB E	-6.68233	-0.43725
1S 15.33760	0.91013	-0.25340	-0.07560	2P 7.17550	0.64512	-0.16698
1S 22.22000	0.07223	-0.01667	-0.00415	2P 13.37000	0.03328	-0.00601
2S 6.74842	0.00733	0.78310	0.24294	3P 2.32896	0.01108	0.55448
2S 14.20930	0.02222	-0.12493	-0.03702	3P 1.31985	-0.00183	0.54885
3S 2.61633	0.00056	0.00646	-0.64667	3P 5.44695	0.39159	-0.11007
3S 1.64378	-0.00026	-0.00159	-0.47814			
3S 5.75104	-0.00244	0.36221	0.18217			
CHLORINE K(2)L(8)3S(2)3P(4) - 3P T.E.= -0.45904841D+03 P.E.= -0.91809217D+03 K.E.= 0.45904376D+03 V.T.= -0.20000101D+01						
S	1S	2S	3S	P	2P	3P
BASIS/ORB E	-105.36099	-11.07623	-1.47010	BASIS/ORB E	-8.53913	-0.93879
1S 16.41090	0.91179	-0.26596	-0.08505	2P 7.49526	0.67402	-0.19950
1S 23.56000	0.06669	-0.01276	-0.00263	2P 13.71160	0.04201	-0.01120
2S 7.13038	0.00610	0.82157	0.27571	3P 2.64828	0.00879	0.57258
2S 14.87010	0.02736	-0.12810	-0.04157	3P 1.65706	-0.00104	0.52126
3S 2.93541	0.00050	0.00866	-0.63782	3P 5.82970	0.34845	-0.11454
3S 1.97300	-0.00025	-0.00165	-0.49262			
3S 6.16710	-0.00208	0.32495	0.19392			
ARGON K(2)L(8)3S(2)3P(4) - 3P T.E.= -0.52530412D+03 P.E.= -0.10506054D+04 K.E.= 0.52530124D+03 V.T.= -0.20000055D+01						
S	1S	2S	3S	P	2P	3P
BASIS/ORB E	-119.73977	-13.42386	-2.18935	BASIS/ORB E	-10.66965	-1.56739
1S 17.20950	0.92327	-0.27689	-0.09394	2P 7.83036	0.69457	-0.22673
1S 25.05000	0.06809	-0.01112	-0.00250	2P 14.04190	0.05199	-0.01506
2S 7.52648	0.00829	0.85353	0.30483	3P 2.94667	0.01019	0.60346
2S 15.61240	0.01108	-0.12635	-0.04377	3P 1.97157	-0.00200	0.48912
3S 3.23552	0.00105	0.00840	-0.66127	3P 6.25519	0.31139	-0.11642
3S 2.27534	-0.00053	-0.00161	-0.47903			
3S 6.58755	-0.00354	0.29407	0.20488			
POTASSIUM K(2)L(8)3S(2)3P(4) - 3P T.E.= -0.59625862D+03 P.E.= -0.11925126D+04 K.E.= 0.59625396D+03 V.T.= -0.20300078D+01						
S	1S	2S	3S	P	2P	3P
BASIS/ORB E	-135.13272	-16.03627	-3.03003	BASIS/ORB E	-13.06611	-2.31694
1S 18.32650	0.92288	-0.28540	0.10093	2P 8.18139	0.71999	-0.25245
1S 26.39300	0.06207	-0.00630	0.00134	2P 14.50150	0.05824	-0.01823
2S 7.94689	0.00649	0.88130	-0.33218	3P 3.27370	0.00561	0.61494
2S 16.27770	0.01942	-0.13237	0.04909	3P 2.29934	-0.00004	0.48317
3S 3.57414	0.00086	0.00564	0.61932	3P 6.60497	0.27674	-0.11943
3S 2.64551	-0.00046	-0.00229	0.53017			
3S 7.02880	-0.00276	0.26899	-0.21411			
CALCIUM K(2)L(8)3S(2)3P(4) - 3P T.E.= -0.67190344D+03 P.E.= -0.13438038D+04 K.E.= 0.67190039D+03 V.T.= -0.20000045D+01						
S	1S	2S	3S	P	2P	3P
BASIS/ORB E	-151.53572	-18.91467	-3.98993	BASIS/ORB E	-15.72280	-3.18477
1S 19.38710	0.92515	-0.29038	0.10690	2P 8.54636	0.74240	-0.27623
1S 27.78140	0.05733	-0.00421	0.00065	2P 15.07740	0.06315	-0.02074
2S 8.33803	0.00510	0.92289	-0.36413	3P 3.60232	0.00387	0.61104
2S 16.96560	0.02294	-0.14080	0.05481	3P 2.64237	0.00056	0.493C4
3S 3.87629	0.00071	0.00477	0.60154	3P 6.57679	0.24555	-0.12006
3S 2.93464	-0.00038	-0.00014	0.50724			
3S 7.34729	-0.00214	0.23428	-0.22371			

See page 183 for Explanation of Tables and Notes for Tables 32, 42, and 43

## ROOTHAAN-HARTREE-FOCK ATOMIC WAVEFUNCTIONS

TABLE 27 (2). THE HARTREE-FOCK FUNCTIONS FOR S(3P) ISO-ELECTRICAL SERIES.

SCANDIUM K(2)L(8)3S(2)3P(4) - 3P  
 T.E.= -0.75223316D+03 P.E.= -0.15044631D+04 K.E.= 0.75222996D+03 V.T.= -0.20000042D+01

S	1S	2S	3S	P	2P	3P
BASIS/ORB E	-168.94610	-22.04827	-5.06406	BASIS/ORB E	-18.63709	-4.16880
1S 29.38180	0.92882	-0.29844	0.11343	2P 8.92300	0.78021	-0.29709
1S 29.20750	0.05462	-0.00100	-0.00041	2P 15.61860	0.06837	-0.02331
2S 8.78991	0.00494	0.93570	-0.38173	3P 3.91554	0.00354	0.61833
2S 17.68080	0.02179	-0.14282	0.05773	3P 2.97352	0.00061	0.49257
2S 4.19371	0.00078	0.00547	0.61816	3P 7.36544	0.21864	-0.12019
3S 3.30556	-0.00045	-0.00263	0.55763			
3S 7.86601	-0.00218	0.22191	-0.23261			

TITANIUM K(2)L(8)3S(2)3P(4) - 3P  
 T.E.= -0.837243870D+03 P.E.= -0.16744E52D+04 K.E.= 0.83724132D+03 V.T.= -0.20000030D+01

S	1S	2S	3S	P	2P	3P
BASIS/ORB E	-187.36234	-25.43606	-6.25423	BASIS/ORB E	-21.80733	-5.26802
1S 21.36580	-0.93225	-0.30321	0.11950	2P 9.31162	0.77639	-0.31616
1S 30.63950	-0.05251	0.00C24	-0.00144	2P 16.20060	0.07248	-0.02545
2S 9.25608	-0.00483	0.95299	-0.39835	3P 4.22742	0.00321	0.62495
2S 18.39220	-0.02017	-0.14E57	0.06080	3P 3.30493	0.00047	0.49257
3S 4.47515	-0.00086	0.00782	0.67815	3P 7.75568	0.19475	-0.12036
3S 3.58108	0.00051	-0.00158	0.51428			
3S 8.29105	0.00223	0.21075	-0.24919			

VANADIUM K(2)L(8)3S(2)3P(4) - 3P  
 T.E.= -0.92693284D+03 P.E.= -0.18538623D+04 K.E.= 0.92692949D+03 V.T.= -0.20000036D+01

S	1S	2S	3S	P	2P	3P
BASIS/ORB E	-206.78311	-29.06465	-7.55848	BASIS/CRB E	-25.23206	-6.48135
1S 22.33800	-0.93562	-0.30863	-0.12401	2P 9.71194	0.79152	-0.33321
1S 32.08680	-0.05087	0.00186	0.00173	2P 16.81720	0.07544	-0.02729
2S 9.73260	-0.00512	0.96266	0.41333	3P 4.52564	0.00266	0.66111
2S 19.11530	-0.01790	-0.15205	-0.06457	3P 3.60423	0.00054	0.46716
3S 4.78292	-0.00115	0.01061	-0.61913	3P 8.13532	0.17369	-0.12251
3S 3.97264	0.00072	-0.00282	-0.57983			
3S 8.79542	0.00253	0.20419	0.25672			

CHROMIUM K(2)L(8)3S(2)3P(4) - 3P  
 T.E.= -0.10212979D+04 P.E.= -0.20425923D+04 K.E.= 0.10212944D+04 V.T.= -0.20000035D+01

S	1S	2S	3S	P	2P	3P
BASIS/ORB E	-227.20757	-32.98467	-8.97612	BASIS/CRB E	-28.91037	-7.80824
1S 23.31070	-0.93851	-0.31221	0.12840	2P 10.12410	0.80483	-0.34917
1S 33.52370	-0.04949	0.00250	-0.00217	2P 17.46250	0.07756	-0.02857
2S 10.22330	-0.00534	0.974C1	-0.42659	3P 4.83287	0.00276	0.67532
2S 19.83780	-0.01589	-0.15786	0.06817	3P 3.92890	0.00030	0.46170
3S 5.09100	-0.00144	0.00867	0.61469	3P 8.52301	0.15534	-0.12384
3S 4.30774	0.00093	-0.00292	0.59822			
3S 9.23569	0.00277	0.19499	-0.27145			

MANGANESE K(2)L(8)3S(2)3P(4) - 3P  
 T.E.= -0.11203376D+04 P.E.= -0.22406726D+04 K.E.= 0.11203350D+04 V.T.= -0.20000023D+01

S	1S	2S	3S	P	2P	3P
BASIS/ORB E	-248.63488	-37.13778	-10.50680	BASIS/ORB E	-32.84159	-9.24825
1S 24.32280	-0.94099	-0.31565	-0.13239	2P 10.54660	0.81908	-0.36451
1S 34.97820	-0.04696	0.00361	0.00275	2P 18.12940	0.07823	-0.02929
2S 10.71210	-0.00488	0.98557	0.43932	3P 5.13805	-0.00175	0.72486
2S 20.55420	-0.01607	-0.16406	-0.07202	3P 4.21170	0.00251	0.42590
3S 5.39188	-0.00148	0.00728	-0.61306	3P 8.82277	0.13992	-0.12975
3S 4.64314	0.00099	-0.00232	-0.61311			
3S 9.67840	0.00257	0.19427	0.28479			

See page 183 for Explanation of Tables and Notes for Tables 32, 42, and 43

TABLE 27 (3). THE HARTREE-FOCK FUNCTIONS FOR S(<sup>3</sup>P) ISO-ELECTRICAL SERIES.

IRON K(2)L(8)3S(2)3P(4) - 3P T.E.= -0.12240505D+04 P.E.= -0.24480584D+04 K.E.= 0.12240478D+04 V.T.= -0.20300022D+01						
S	1S	2S	3S	P	2P	3P
BASIS/ORB E	-271.06501	-41.54347	-12.14996	BASIS/ORB E	-37.02510	-10.80088
1S 25.39940	0.94213	-0.31695	0.13546	2P 10.98110	0.83157	-0.38036
1S 36.33230	0.04337	0.00547	-0.00326	2P 18.92540	0.07751	-0.02873
2S 11.14360	0.00283	1.01316	-0.46282	3P 5.45618	0.00144	0.66811
2S 21.22840	0.01992	-0.17240	0.07827	3P 4.62716	0.00057	0.48647
3S 5.74011	0.00075	0.00182	0.61268	3P 9.23215	0.12444	-0.12597
3S 4.96653	-0.00051	0.00078	0.63541			
3S 9.98029	-0.00137	0.17459	-0.29579			
COBALT K(2)L(8)3S(2)3P(4) - 3P T.E.= -0.13324357D+04 P.E.= -0.26648684D+04 K.E.= 0.13324327D+04 V.T.= -0.20000023D+01						
S	1S	2S	3S	P	2P	3P
BASIS/ORB E	-294.49717	-46.20151	-13.90564	BASIS/GRB E	-41.46067	-12.46610
1S 26.38310	0.94426	-0.32203	0.13882	2P 11.42010	0.84062	-0.39241
1S 37.75770	0.04222	0.0616	-0.00363	2P 19.61280	0.07815	-0.02920
2S 11.63420	0.00284	1.02384	-0.47462	3P 5.76323	0.00232	0.67924
2S 21.94390	0.01866	-0.17800	0.08202	3P 4.55860	-0.00010	0.48442
3S 6.05260	0.00092	-0.00082	0.61045	3P 9.62536	0.11244	-0.12901
3S 5.29944	-0.00063	0.00230	0.65239			
3S 10.40120	-0.00146	0.17049	-0.30971			
NICKEL K(2)L(8)3S(2)3P(4) - 3P T.E.= -0.14454925D+04 P.E.= -0.28909814D+04 K.E.= 0.14454889D+04 V.T.= -0.20000025D+01						
S	1S	2S	3S	P	2P	3P
BASIS/ORB E	-318.93118	-51.11144	-15.77351	BASIS/ORB E	-46.14751	-14.24358
1S 27.36910	0.94629	-0.32482	-0.14197	2P 11.86360	0.84894	-0.40350
1S 39.19010	0.04105	0.0679	0.00401	2P 20.31230	0.07846	-0.02952
2S 12.14710	0.00282	1.03132	0.48405	3P 6.07049	0.00368	0.69123
2S 22.64780	0.01756	-0.18416	-0.08586	3P 5.28977	-0.00108	0.48150
3S 6.35390	0.00109	-0.00443	-0.60789	3P 10.02220	0.10152	-0.13240
3S 5.63306	-0.00076	0.00454	-0.66926			
3S 10.82980	-0.00152	0.17669	0.32511			
COPPER K(2)L(8)3S(2)3P(4) - 3P T.E.= -0.15632201D+04 P.E.= -0.31264361D+04 K.E.= 0.15632160D+04 V.T.= -0.20000026D+01						
S	1S	2S	3S	P	2P	3P
BASIS/ORB E	-344.36675	-56.27300	-17.75341	BASIS/ORB E	-51.08657	-15.13316
1S 28.35860	0.94805	-0.32156	-0.14488	2P 12.30990	0.85649	-0.41375
1S 40.60840	0.03996	0.06150	0.00439	2P 21.00760	0.07871	-0.02975
2S 12.64170	0.00274	1.04121	0.49453	3P 6.37845	0.00492	0.70389
2S 23.35900	0.01672	-0.18570	-0.08953	3P 5.62146	-0.00203	0.47806
3S 6.68023	0.00123	-0.00744	-0.60516	3P 10.41480	0.09167	-0.13622
3S 5.96515	-0.00088	0.00646	-0.68671			
3S 11.24690	-0.00154	0.16732	0.33690			
ZINC K(2)L(8)3S(2)3P(4) - 3P T.E.= -0.16856180D+04 P.E.= -0.33712318D+04 K.E.= 0.16856138D+04 V.T.= -0.20000024D+01						
S	1S	2S	3S	P	2P	3P
BASIS/ORB E	-370.80388	-61.6E591	-19.84526	BASIS/ORB E	-56.27643	-18.13476
1S 29.36780	0.94960	-0.32991	-0.14763	2P 12.75480	0.86037	-0.41906
1S 42.02040	0.03845	0.00824	0.00485	2P 21.67640	0.08019	-0.03138
2S 13.16340	0.00225	1.04789	0.50250	3P 6.68829	0.01593	0.70004
2S 24.05100	0.01684	-0.19632	-0.09342	3P 5.94987	-0.00919	0.48481
3S 7.00501	0.00108	-0.01192	-0.60068	3P 11.04380	0.08098	-0.13693
3S 6.29484	-0.00078	0.00538	-0.70623			
3S 11.66880	-0.00127	0.16872	0.35531			

See page 183 for Explanation of Tables and Notes for Tables 32, 42, and 43

## ROOTHAAN-HARTREE-FOCK ATOMIC WAVEFUNCTIONS

 TABLE 27 (4). THE HARTREE-FOCK FUNCTIONS FOR S(<sup>3</sup>P) ISO-ELECTRICAL SERIES.

GALLIUM K(2)L(8)3S(2)3P(4) - 3P  
 T.E.= -0.18126857D+04 P.E.= -0.36253665D+04 K.E.= 0.18126808D+04 V.T.= -0.20300027D+01

S	1S	2S	3S	P	2P	3P
BASIS/ORB E	-398.24205	-67.35009	-22.04884	BASIS/ORB E	-61.71739	-20.24817
1S 30.35700	0.95113	-0.33256	-0.15066	2P 13.19770	0.86716	-0.42788
1S 43.43670	0.03753	0.00900	0.00548	2P 22.34860	0.08069	-0.03176
2S 13.65000	0.00223	1.05819	0.51084	3P 6.99733	0.01792	0.71258
2S 24.77120	0.01605	-0.20123	-0.09600	3P 6.28031	-0.01060	0.48078
3S 7.39655	0.00117	-0.01333	-0.055426	3P 11.45360	0.07176	-0.14036
3S 6.62768	-0.00083	0.00994	-0.76986			
3S 12.08400	-0.00134	0.16406	0.37183			

GERMANIUM K(2)L(8)3S(2)3P(4) - 3P  
 T.E.= -0.19444229D+04 P.E.= -0.38888407D+04 K.E.= 0.19444177D+04 V.T.= -0.20000027D+01

S	1S	2S	3S	P	2P	3P
BASIS/ORB E	-426.68124	-73.26531	-24.36411	BASIS/ORB E	-67.40925	-22.47329
1S 31.35280	0.95252	-0.33503	-0.15304	2P 13.63440	0.87357	-0.43606
1S 44.84590	0.03653	0.00977	0.00585	2P 22.59730	0.08162	-0.03234
2S 14.15330	0.00204	1.06695	0.52000	3P 7.30823	0.02065	0.72459
2S 25.46720	0.01561	-0.20685	-0.09976	3P 6.60976	-0.01292	0.47695
3S 7.72052	0.00120	-0.01644	-0.54916	3P 11.87310	0.06232	-0.14348
3S 6.95845	-0.00086	0.01195	-0.78928			
3S 12.49620	-0.00127	0.16202	0.38525			

ARSENIC K(2)L(8)3S(2)3P(4) - 3P  
 T.E.= -0.20808294D+04 P.E.= -0.41616537D+04 K.E.= 0.20808244D+04 V.T.= -0.20000024D+01

S	1S	2S	3S	P	2P	3P
BASIS/ORB E	-456.12135	-79.43148	-26.79098	BASIS/ORB E	-73.35193	-24.81007
1S 32.34130	-0.95390	-0.33568	-0.15421	2P 14.06310	0.87964	-0.44400
1S 46.26620	-0.03573	0.00942	0.00550	2P 23.61030	0.08312	-0.03311
2S 14.77720	-0.00205	1.06258	0.52328	3P 7.61994	0.02341	0.73654
2S 26.17390	-0.01483	-0.21590	-0.10567	3P 6.94034	-0.01509	0.47322
3S 8.12734	-0.00141	-0.03091	-0.40236	3P 12.28410	0.05270	-0.14632
3S 7.36232	0.00101	0.02154	-0.94928			
3S 12.91790	0.00134	0.18115	0.40553			

SELENIUM K(2)L(8)3S(2)3P(4) - 3P  
 T.E.= -0.22219047D+04 P.E.= -0.44438040D+04 K.E.= 0.22218993D+04 V.T.= -0.20000024D+01

S	1S	2S	3S	P	2P	3P
BASIS/ORB E	-486.56230	-85.84445	-29.32943	BASIS/ORB E	-79.54532	-27.25846
1S 33.35870	-0.95501	-0.33833	-0.15602	2P 14.48040	0.88563	-0.45153
1S 47.65440	-0.03439	0.01058	0.00574	2P 24.19010	0.08526	-0.03419
2S 15.26350	-0.00142	1.07303	0.53478	3P 7.93652	0.02670	0.74818
2S 26.85790	-0.01528	-0.22088	-0.11012	3P 7.26654	-0.01758	0.46973
3S 8.62245	-0.00101	-0.03116	-0.23042	3P 12.70040	0.04230	-0.14883
3S 7.76177	0.00071	0.02052	-1.13294			
3S 13.32220	0.00099	0.17665	0.41359			

BROMINE K(2)L(8)3S(2)3P(4) - 3P  
 T.E.= -0.23676486D+04 P.E.= -0.47352916D+04 K.E.= 0.23676430D+04 V.T.= -0.20000023D+01

S	1S	2S	3S	P	2P	3P
BASIS/ORB E	-518.00363	-92.51620	-31.97944	BASIS/ORB E	-85.98935	-29.81846
1S 34.34630	0.95622	-0.34119	-0.15828	2P 14.78810	0.88771	-0.45559
1S 49.07000	0.03374	0.01162	0.00618	2P 24.26130	0.09739	-0.04046
2S 15.71890	0.00147	1.08576	0.54545	3P 8.41076	0.02291	0.64693
2S 27.56250	0.01464	-0.22430	-0.11295	3P 7.59541	-0.01322	0.58567
3S 8.95554	0.00120	-0.02903	-0.20249	3P 13.11280	0.02554	-0.15574
3S 8.09947	-0.00085	0.01919	-1.17226			
3S 13.73990	-0.00109	0.16639	0.42053			

See page 183 for Explanation of Tables and Notes for Tables 32, 42, and 43

TABLE 27 (5). THE HARTREE-FOCK FUNCTIONS FOR S(<sup>3</sup>P) ISO-ELECTRICAL SERIES.

KRYPTON K(2)L(8)3S(2)3P{4} - 3P						
T.E.= -0.25180610D+04 P.E.= -0.50361189D+04 K.E.= 0.2518C580D+04 V.T.= -C.20000012D+01						
S	1S	2S	3S	P	2P	3P
BASIS/ORB E	-550.44637	-99.43455	-34.74088	BASIS/ORB E	-92.66397	-32.48995
1S 35.42220	-0.95703	-0.34065	-0.16001	2P 15.23460	0.90079	-0.46710
1S 50.41030	-0.03126	0.01144	0.00672	2P 25.20520	0.09278	-0.03809
2S 16.45000	0.00057	1.07718	0.54061	3P 8.72058	0.03521	0.59836
2S 28.22980	-0.01769	-0.23911	-0.11906	3P 7.97967	-0.02265	0.63877
3S 9.27550	0.00039	-0.04969	-0.37111	3P 13.50910	0.01277	-0.15338
3S 8.33459	-0.00022	0.03125	-1.03174			
3S 14.12820	-0.00035	0.19877	0.46369			

See page 183 for Explanation of Tables and Notes for Tables 32, 42, and 43

## ROOTHAAN-HARTREE-FOCK ATOMIC WAVEFUNCTIONS

 TABLE 28 (1). THE HARTREE-FOCK FUNCTIONS FOR S(<sup>1</sup>D) ISO-ELECTRICAL SERIES.

SULFUR K(2)L(8)3S(2)3P(4) - 1D T.E.= -0.39745195D+03 P.E.= -0.79490785D+03 K.E.= 0.39745591D+03 V.T.= -0.19999500D+01						
S	1S	2S	3S	P	2P	3P
BASIS/ORB E	-92.01655	-9.01519	-0.88566	BASIS/ORB E	-6.69339	-0.41528
1S 15.81070	0.92256	-0.26909	-0.08121	2P 6.22009	0.74832	-0.19481
1S 23.03350	0.03806	-0.00246	0.00103	2P 11.37710	0.08730	-0.02153
2S 7.06367	-0.00190	0.76150	0.23362	3P 2.35939	0.00174	0.54906
2S 13.30130	0.05323	-0.15258	-0.04412	3P 1.30754	0.00150	0.56332
3S 2.62543	-0.00064	0.00549	-0.64569	3P 4.86352	0.22627	-0.07009
3S 1.64672	0.00028	-0.0023	-0.48067			
3S 5.80129	0.00190	0.41698	0.20332			

  

CHLORINE K(2)L(8)3S(2)3P(4) - 1D T.E.= -0.45898385D+03 P.E.= -0.91796342D+03 K.E.= 0.45897957D+03 V.T.= -0.20000093D+01						
S	1S	2S	3S	P	2P	3P
BASIS/ORB E	-105.37279	-11.06567	-1.47529	BASIS/CRB E	-8.54848	-0.91049
1S 16.45930	0.91946	-0.26385	-0.08523	2P 6.49508	0.81018	-0.24132
1S 24.06610	0.05802	-0.01294	-0.00248	2P 12.32240	0.08625	-0.02360
2S 7.27238	0.00668	0.78785	0.26211	3P 2.75959	-0.00851	0.53697
2S 14.92680	0.02806	-0.13149	-0.04155	3P 1.67378	0.00425	0.57679
3S 2.94124	0.00057	0.00981	-0.63298	3P 4.87993	0.16381	-0.07230
3S 1.97851	-0.00029	-0.00202	-0.49586			
3S 6.25809	-0.00228	0.36234	0.20731			

  

ARGON K(2)L(8)3S(2)3P(4) - 1D T.E.= -0.52522904D+03 P.E.= -0.10504512D+04 K.E.= 0.52522219D+03 V.T.= -0.20000130D+01						
S	1S	2S	3S	P	2P	3P
BASIS/ORB E	-119.75090	-13.43257	-2.19371	BASIS/ORB E	-10.67847	-1.53326
1S 17.33210	0.92695	-0.27790	-0.09480	2P 6.92892	0.82478	-0.27180
1S 25.45500	0.05891	-0.00862	-0.00141	2P 13.04240	0.08703	-0.02575
2S 7.65768	0.00782	0.81664	0.28914	3P 3.10281	-0.01117	0.54273
2S 15.62320	0.01765	-0.12759	-0.04325	3P 2.01193	0.00497	0.57437
3S 3.23731	0.00090	0.01306	-0.64052	3P 5.19003	0.14575	-0.07860
3S 2.29692	-0.00047	-0.00371	-0.49462			
3S 6.72686	-0.00317	0.33125	0.21665			

  

POTASSIUM K(2)L(8)3S(2)3P(4) - 1D T.E.= -0.59617349D+03 P.E.= -0.11923405D+04 K.E.= 0.59616697D+03 V.T.= -0.20000109D+01						
S	1S	2S	3S	P	2P	3P
BASIS/ORB E	-135.14324	-16.04629	-3.03394	BASIS/CRB E	-13.07410	-2.27756
1S 18.37380	0.92867	-0.28364	-0.10037	2P 7.41862	0.82845	-0.29441
1S 26.85260	0.05522	-0.00654	-0.00144	2P 13.76890	0.08606	-0.02690
2S 8.00371	0.00683	0.86783	0.32672	3P 3.44267	-0.01146	0.54370
2S 16.32900	0.02042	-0.13443	-0.04967	3P 2.34788	0.00526	0.57901
3S 3.52542	0.00092	0.00934	-0.67004	3P 5.62191	0.13998	-0.08766
3S 2.60340	-0.00050	-0.00221	-0.47787			
3S 7.06477	-0.00291	0.28428	0.21629			

  

CALCIUM K(2)L(8)3S(2)3P(4) - 1D T.E.= -0.67180865D+03 P.E.= -0.13436121D+04 K.E.= 0.67180342D+03 V.T.= -0.20000078D+01						
S	1S	2S	3S	P	2P	3P
BASIS/ORB E	-151.54565	-18.92171	-3.99264	BASIS/CRB E	-15.73042	-3.14035
1S 19.41460	0.93054	-0.29167	0.10812	2P 7.55337	0.81981	-0.30858
1S 28.22810	0.05180	-0.00288	-0.00019	2P 14.42860	0.08600	-0.02823
2S 8.45079	0.00584	0.88461	-0.34493	3P 3.75250	-0.00535	0.54766
2S 17.02790	0.02265	-0.13773	0.05222	3P 2.67327	0.00375	0.57546
3S 3.85213	0.00081	0.01288	0.64143	3P 6.25650	0.14237	-0.09457
3S 2.95663	-0.00046	-0.00415	0.51659			
3S 7.56228	-0.00251	0.26878	-0.23202			

See page 183 for Explanation of Tables and Notes for Tables 32, 42, and 43.

TABLE 28 (2). THE HARTREE-FOCK FUNCTIONS FOR S(1D) ISO-ELECTRICAL SERIES.

SCANDIUM K(2)L(8)3S(2)3P(4) - 1D T.E.= -0.75212881D+03 P.E.= -0.15042545D+04 K.E.= 0.75212569D+03 V.T.= -0.20000042D+01						
S	1S	2S	3S	P	2P	3P
BASIS/ORB E	-168.95562	-22.05566	-5.06752	BASIS/ORB E	-18.64447	-4.11949
1S 20.42530	0.93283	-0.25665	0.11393	2P 8.52449	0.81237	-0.32131
1S 29.59510	0.04957	-0.00148	-0.00090	2P 15.22120	0.08218	-0.02764
2S 8.91659	0.00506	0.90599	-0.36533	3P 3.98580	-0.00319	0.59736
2S 17.72120	0.02288	-0.14497	0.05671	3P 2.96598	0.00338	0.52474
3S 4.13930	0.00075	0.01030	0.67849	3P 6.85747	0.15071	-0.09513
3S 3.25520	-0.00044	-0.00307	0.49418			
3S 7.97797	-0.00217	0.25473	-0.24606			
TITANIUM K(2)L(8)3S(2)3P(4) - 1D T.E.= -0.83713018D+03 P.E.= -0.16742555D+04 K.E.= 0.83712530D+03 V.T.= -0.20000058D+01						
S	1S	2S	3S	P	2P	3P
BASIS/ORB E	-187.37160	-25.44608	-6.25744	BASIS/ORB E	-21.81437	-5.21377
1S 21.28950	-0.93722	-0.30410	-0.11896	2P 9.14480	0.79159	-0.32392
1S 30.98210	-0.05173	-0.00018	0.00072	2P 15.93590	0.08053	-0.02832
2S 9.30744	-0.00693	0.93647	0.39226	3P 4.29757	0.00450	0.5879
2S 18.41170	-0.01418	-0.14570	-0.06049	3P 3.30426	0.00041	0.53613
3S 4.46471	-0.00158	0.01160	-0.61880	3P 7.63233	0.16853	-0.11230
3S 3.64646	0.00097	-0.00412	-0.56405			
3S 8.39723	0.00352	0.22568	0.24684			
VANADIUM K(2)L(8)3S(2)3P(4) - 1D T.E.= -0.92680983D+03 P.E.= -0.18536183D+04 K.E.= 0.92680843D+03 V.T.= -0.20000015D+01						
S	1S	2S	3S	P	2P	3P
BASIS/ORB E	-206.79224	-29.09161	-7.56160	BASIS/ORB E	-25.23885	-6.42250
1S 22.35760	-0.93804	-0.30731	-0.12407	2P 9.81115	0.76471	-0.32130
1S 32.32850	-0.04821	0.00129	0.00183	2P 16.69790	0.07862	-0.02891
2S 9.81470	-0.00513	0.65010	0.40597	3P 4.56869	0.01417	0.60433
2S 19.09290	-0.01814	-0.15535	-0.06501	3P 3.62082	-0.00442	0.51845
3S 4.80477	-0.00116	0.00723	-0.61147	3P 8.44589	0.19336	-0.12745
3S 3.97174	0.00072	-0.00175	-0.58963			
3S 8.80822	0.00251	0.22191	0.26726			
CHROMIUM K(2)L(8)3S(2)3P(4) - 1D T.E.= -0.10211655D+04 P.E.= -0.20423414D+04 K.E.= 0.10211759D+04 V.T.= -0.19999899D+01						
S	1S	2S	3S	P	2P	3P
BASIS/ORB E	-227.21625	-32.99096	-8.97927	BASIS/ORB E	-28.91669	-7.74488
1S 23.37780	-0.93983	-0.31181	0.12904	2P 10.63000	0.70868	-0.30218
1S 33.70620	-0.04598	0.00302	-0.00285	2P 17.34080	0.08018	-0.03154
2S 10.32010	-0.00432	0.95768	-0.41610	3P 4.83816	0.02888	0.61520
2S 19.79200	-0.01896	-0.16123	0.06819	3P 3.94233	-0.01297	0.50551
3S 5.09202	-0.00101	0.00797	0.61745	3P 9.41069	0.24511	-0.15513
3S 4.30132	0.00066	-0.00242	0.59455			
3S 9.29734	0.00208	0.22011	-0.28191			
MANGANESE K(2)L(8)3S(2)3P(4) - 1D T.E.= -0.11201957D+04 P.E.= -0.22403970D+04 K.E.= 0.11202012D+04 V.T.= -0.19999951D+01						
S	1S	2S	3S	P	2P	3P
BASIS/ORB E	-248.64315	-37.14402	-10.50964	BASIS/ORB E	-32.84780	-9.18011
1S 24.35240	-0.94217	-0.31564	0.13318	2P 10.41310	0.67147	-0.29271
1S 35.12100	-0.04500	0.00392	-0.00334	2P 16.24930	0.15882	-0.06600
2S 10.79880	-0.00444	0.97178	-0.42986	3P 5.08483	0.04388	0.61242
2S 20.50070	-0.01719	-0.16660	0.07170	3P 4.30621	-0.02325	0.50553
3S 5.39566	-0.00125	0.00638	0.61760	3P 10.28570	0.19347	-0.13535
3S 4.63395	0.00083	-0.00169	0.60807			
3S 9.73290	0.00225	0.21202	-0.29447			

See page 183 for Explanation of Tables and Notes for Tables 32, 42, and 43

## ROOTHAAN-HARTREE-FOCK ATOMIC WAVEFUNCTIONS

TABLE 28 (3). THE HARTREE-FOCK FUNCTIONS FOR S(1D) ISO-ELECTRICAL SERIES.

IRON            K(2)L(8)3S(2)3P(4) - 1D  
 T.E.= -0.12238983D+04   P.E.= -0.24478761D+04   K.E.= 0.12239777D+04   V.T.= -0.19999351D+01

S	1S	2S	3S	P	ZP	3P
BASIS/ORB E	-271.07172	-41.54839	-12.15357	BASIS/ORB E	-37.02986	-10.72888
1S 25.48520	-0.94265	-0.31747	-0.13690	2P 10.27440	0.92642	-0.39122
1S 36.41680	-0.04010	0.00548	0.00451	2P 18.60090	0.09443	-0.04454
2S 11.36610	-0.00105	0.98031	0.43928	3P 5.40863	0.05583	0.63691
2S 21.15230	-0.02408	-0.17986	-0.07782	3P 4.57081	-0.03177	0.48612
3S 5.77475	0.00011	-0.00203	-0.60364	3P 11.26250	-0.02017	-0.06382
3S 4.95162	-0.00005	0.00388	-0.64454			
3S 10.10580	0.00018	0.21860	0.32117			

COBALT            K(2)L(8)3S(2)3P(4) - 1D  
 T.E.= -0.13322752D+04   P.E.= -0.26646260D+04   K.E.= 0.13323508D+04   V.T.= -0.19999433D+01

S	1S	2S	3S	P	ZP	3P
BASIS/ORB E	-294.50361	-46.20638	-13.90899	BASIS/ORB E	-41.46544	-12.38941
1S 26.44080	-0.94483	-0.32062	-0.14023	2P 10.73660	0.93687	-0.39535
1S 37.84110	-0.03993	0.00603	0.00472	2P 19.26300	0.09243	-0.04635
2S 11.84700	-0.00164	0.99271	0.45175	3P 5.64413	0.05957	0.64111
2S 21.87450	-0.02130	-0.18433	-0.08121	3P 4.95387	-0.03769	0.48278
3S 6.07475	-0.00025	-0.00501	-0.60308	3P 12.07060	-0.02836	-0.06637
3S 5.28626	0.00019	0.06508	-0.65793			
3S 10.53950	0.00063	0.21160	0.33226			

NICKEL            K(2)L(8)3S(2)3P(4) - 1D  
 T.E.= -0.14453236D+04   P.E.= -0.28907046D+04   K.E.= 0.14452810D+04   V.T.= -0.19999603D+01

S	1S	2S	3S	P	ZP	3P
BASIS/ORB E	-318.93787	-51.11647	-15.77650	BASIS/ORB E	-46.15290	-14.16213
1S 27.36660	-0.94705	-0.32353	-0.14282	2P 11.16130	0.96090	-0.40979
1S 39.27940	-0.04055	0.00597	0.00449	2P 19.93530	0.08884	-0.04613
2S 12.31200	-0.00290	1.00912	0.46756	3P 5.79148	0.06370	0.81123
2S 22.60110	-0.01718	-0.16884	-0.08531	3P 5.28827	-0.04556	0.31485
3S 6.40955	-0.00106	-0.01027	-0.58981	3P 12.73900	-0.04801	-0.06037
3S 5.62347	0.00073	0.00826	-0.68856			
3S 10.90950	0.00153	0.20171	0.34412			

COPPER            K(2)L(8)3S(2)3P(4) - 1D  
 T.E.= -0.15630424D+04   P.E.= -0.31261329D+04   K.E.= 0.1563C905D+04   V.T.= -0.19999692D+01

S	1S	2S	3S	P	ZP	3P
BASIS/ORB E	-344.37363	-56.27815	-17.75629	BASIS/ORB E	-51.09170	-16.04718
1S 28.33060	-0.94880	-0.32625	-0.14557	2P 11.63120	0.96690	-0.40960
1S 40.69050	-0.04024	0.00641	0.00465	2P 20.58640	0.08743	-0.04851
2S 12.80680	-0.00336	1.01956	0.47854	3P 5.99363	0.07355	1.02468
2S 23.31970	-0.01515	-0.19390	-0.08898	3P 5.62022	-0.05740	0.10513
3S 6.71897	-0.00152	-0.01403	-0.58814	3P 13.40100	-0.05200	-0.06798
3S 5.95705	0.00105	0.01072	-0.70422			
3S 11.32760	0.00191	0.15771	0.35671			

ZINC            K(2)L(8)3S(2)3P(4) - 1D  
 T.E.= -0.16854315D+04   P.E.= -0.33709012D+04   K.E.= 0.16854697D+04   V.T.= -0.19999773D+01

S	1S	2S	3S	P	ZP	3P
BASIS/ORB E	-370.81085	-61.69122	-19.84801	BASIS/CRB E	-56.28173	-18.04422
1S 29.30920	-0.95036	-0.32917	-0.14836	2P 12.10210	0.96903	-0.41130
1S 42.10050	-0.03957	0.00719	0.00501	2P 21.24250	0.08688	-0.05022
2S 13.28570	-0.00355	1.03146	0.48953	3P 6.19786	0.09725	1.46226
2S 24.03310	-0.01391	-0.19847	-0.09224	3P 5.95015	-0.08260	-0.32789
3S 7.03317	-0.00184	-0.01605	-0.58430	3P 13.55870	-0.05312	-0.07444
3S 6.28933	0.00130	0.01209	-0.72169			
3S 11.74880	0.00211	C.19C90	0.36794			

See page 183 for Explanation of Tables and Notes for Tables 32, 42, and 43

TABLE 28 (4). THE HARTREE-FOCK FUNCTIONS FOR S(1D) ISO-ELECTRICAL SERIES.

GALLIUM K(2)L(8)3S(2)3P(4) - 1D						
T.E.= -0.18124906D+04 P.E.= -0.36249746D+04 K.E.= 0.18124841D+04 V.T.= -0.20000036D+01						
S	1S	2S	3S	P	2P	3P
BASIS/ORB E	-398.25033	-67.35616	-22.05142	BASIS/ORB E	-61.72348	-20.15301
1S 30.19170	-0.95255	-0.33203	-0.15073	2P 12.47270	0.99681	-0.44740
1S 43.56950	-0.04111	0.0C705	0.00477	2P 21.93630	0.08438	-0.044E6
2S 13.73040	-0.00592	1.04436	0.50171	3P 6.34494	0.29800	6.14247
2S 24.78590	-0.00815	-0.19963	-0.09438	3P 6.28992	-0.28666	-5.00083
2S 7.30854	-0.00385	-0.01699	-0.58736	3P 14.13550	-0.07827	-0.05342
3S 6.63298	0.00283	0.01319	-0.72917			
3S 12.17710	0.00378	0.17967	0.37352			

  

GERMANIUM K(2)L(8)3S(2)3P(4) - 1D						
T.E.= -0.19442190D+04 P.E.= -0.38884262D+04 K.E.= 0.19442072D+04 V.T.= -0.20000061D+01						
S	1S	2S	3S	P	2P	3P
BASIS/ORB E	-426.68964	-73.27141	-24.36665	BASIS/CRB E	-67.41538	-22.37370
1S 31.17990	-0.95378	-0.33495	-0.15288	2P 12.90440	0.99725	-0.46041
1S 44.96620	-0.04030	0.0C808	0.00497	2P 22.58720	0.08606	-0.04413
2S 14.19150	-0.00598	1.05800	0.51501	3P 6.60870	-1.41093	*****
2S 25.48660	-0.00756	-0.203E2	-C.09833	3P 6.61957	1.42159	31.51196
3S 7.71040	-0.00443	-0.01846	-0.41795	3P 14.35830	-0.08070	-0.05254
3S 7.04026	0.00325	0.01415	-0.91083			
3S 12.58110	0.00398	0.17639	0.38050			

  

ARSENIC K(2)L(8)3S(2)3P(4) - 1D						
T.E.= -0.20806167D+04 P.E.= -0.41612315D+04 K.E.= 0.20806149D+04 V.T.= -0.20000009D+01						
S	1S	2S	3S	P	2P	3P
BASIS/ORB E	-456.12944	-79.43728	-26.79354	BASIS/ORB E	-73.35777	-24.70615
1S 32.22560	-0.95456	-0.33134	-0.15587	2P 13.33530	0.99738	-0.46787
1S 46.33580	-0.03829	0.00932	0.00598	2P 23.23530	C.08781	-0.04477
2S 14.68660	-0.00465	1.06876	0.52197	3P 7.01458	0.22654	4.83930
2S 26.17680	-0.00963	-0.21021	-0.10102	3P 6.94468	-0.21602	-3.67900
3S 8.04406	-0.00329	-0.01900	-0.53141	3P 14.56280	-0.08337	-0.05819
3S 7.29102	0.00235	0.013E2	-0.81726			
3S 12.98110	0.00312	0.16613	0.40023			

  

SELENIUM K(2)L(8)3S(2)3P(4) - 1D						
T.E.= -0.22216832D+04 P.E.= -0.44433812D+04 K.E.= 0.22216980D+04 V.T.= -0.19999933D+01						
S	1S	2S	3S	P	2P	3P
BASIS/ORB E	-486.57022	-85.85394	-29.33204	BASIS/ORB E	-79.55088	-27.15020
1S 33.37800	-0.95489	-0.33818	-0.15660	2P 13.71960	1.00817	-0.48446
1S 47.62420	-0.03400	0.01067	0.00617	2P 24.04770	0.08769	-0.04331
2S 15.33230	-0.00087	1.06749	0.52906	3P 7.57898	0.06734	1.18042
2S 26.82590	-0.01629	-0.22373	-0.11014	3P 7.25771	-0.05514	-0.00489
3S 8.61034	-0.00056	-0.03375	-0.29066	3P 14.53260	-0.09744	-0.06026
3S 7.72730	0.00041	0.02197	-1.07528			
3S 13.34680	0.00058	0.18665	0.42258			

  

BROMINE K(2)L(8)3S(2)3P(4) - 1D						
T.E.= -0.23674185D+04 P.E.= -0.47348318D+04 K.E.= 0.23674133D+04 V.T.= -0.2000022D+01						
S	1S	2S	3S	P	2P	3P
BASIS/ORB E	-518.01223	-92.52186	-31.98184	BASIS/ORB E	-85.99510	-29.70560
1S 34.19830	0.95717	-0.34C84	-0.15785	2P 15.23310	0.84024	-0.42142
1S 49.20590	0.03670	0.01008	0.00529	2P 24.61100	0.08934	-0.03983
2S 15.70550	0.00508	1.08214	0.54407	3P 7.84665	0.08140	1.53073
2S 27.62550	0.00806	-0.220C7	-0.11124	3P 7.61410	-0.07026	-0.34188
3S 8.97684	0.00431	-0.02841	-0.08238	3P 14.34100	0.08513	-0.15018
3S 8.15505	-0.00299	0.01932	-1.28329			
3S 13.79700	-0.00374	0.16647	0.41178			

  

KRYPTON K(2)L(8)3S(2)3P(4) - 1D						
T.E.= -0.25178221D+04 P.E.= -0.50356412D+04 K.E.= 0.25178191D+04 V.T.= -0.2000012D+01						
S	1S	2S	3S	P	2P	3P
BASIS/ORB E	-550.45474	-99.44030	-34.74330	BASIS/ORB E	-92.68980	-32.37274
1S 35.43590	-0.95699	-0.34076	-0.16006	2P 15.23750	0.90009	-0.46858
1S 50.40060	-0.03096	0.01162	0.00681	2P 25.20030	0.09281	-0.03769
2S 16.44690	0.00089	1.07784	0.54100	3P 8.71890	0.03260	0.64004
2S 28.22430	-0.01826	-0.23933	-0.11919	3P 7.91330	-0.01972	0.59572
3S 9.27371	0.00064	-0.04928	-0.37685	3P 13.50660	0.01342	-0.15076
3S 8.33140	-0.00039	0.03056	-1.02635			
3S 14.12550	-0.00058	0.198C6	0.46370			

See page 183 for Explanation of Tables and Notes for Tables 32, 42, and 43

## ROOTHAAN-HARTREE-FOCK ATOMIC WAVEFUNCTIONS

TABLE 29 (1). THE HARTREE-FOCK FUNCTIONS FOR S(1S) ISO-ELECTRICAL SERIES.

SULFUR            K(2)L(8)3S(2)3P(4) - 1S  
 T.E.= -0.39737433D+03 P.E.= -0.79475541D+03 K.E.= 0.39738108D+03 V.T.= -0.19999620D+01

S	1S	2S	3S	P	2P	3P
BASIS/ORB E	-92.03391	-9.03122	-0.89437	BASIS/ORB E	-6.70917	-0.38255
1S 16.04140	0.89728	-0.23842	-0.07272	2P 7.04366	0.64696	-0.16727
1S 23.23790	0.04084	-0.01683	-0.00300	2P 12.52260	0.04518	-0.01102
2S 6.87749	0.00432	0.74204	0.22790	3P 2.36721	0.01183	0.53847
2S 14.58340	0.07507	-0.14130	-0.04050	3P 1.28935	-0.00042	0.57414
3S 2.61892	0.00009	0.01172	-0.64965	3P 5.41525	0.37589	-0.10734
3S 1.64452	-0.00005	-0.00284	-0.47439			
3S 5.86635	-0.00081	0.40141	0.19807			

CHLORINE            K(2)L(8)3S(2)3P(4) - 1S  
 T.E.= -0.45888901D+03 P.E.= -0.91778018D+03 K.E.= 0.45889118D+03 V.T.= -0.19999953D+01

S	1S	2S	3S	P	2P	3P
BASIS/ORB E	-105.38806	-11.09568	-1.48250	BASIS/ORB E	-8.56238	-0.86632
1S 16.50270	0.91873	-0.26393	-0.08516	2P 7.28058	0.69682	-0.20362
1S 24.12620	0.05616	-0.01225	-0.00239	2P 13.27830	0.05162	-0.01496
2S 7.25424	0.00645	0.78843	0.26294	3P 2.82054	0.00752	0.49365
2S 14.96440	0.03121	-0.13075	-0.04155	3P 1.67738	0.00152	0.61604
3S 2.93413	0.00053	0.01083	-0.64073	3P 5.70891	0.31331	-0.11652
3S 1.97427	-0.00027	-0.00253	-0.48763			
3S 6.26635	-0.00218	0.35952	0.20601			

ARGON            K(2)L(8)3S(2)3P(4) - 1S  
 T.E.= -0.52511807D+03 P.E.= -0.10502333D+04 K.E.= 0.52511522D+03 V.T.= -0.20000054D+01

S	1S	2S	3S	P	2P	3P
BASIS/ORB E	-119.76558	-13.44564	-2.20006	BASIS/ORB E	-10.69147	-1.48259
1S 17.37300	0.92523	-0.27593	-0.09346	2P 7.57954	0.73072	-0.23689
1S 25.42370	0.05812	-0.00922	-0.00205	2P 13.74990	0.05961	-0.01827
2S 7.61577	0.00713	0.83305	0.29750	3P 3.15348	0.00338	0.50061
2S 15.60440	0.02096	-0.13057	-0.04549	3P 2.01097	0.00285	0.60899
3S 3.23614	0.0C081	0.00949	-0.64937	3P 6.01901	0.26716	-0.11533
3S 2.29380	-0.00043	-0.00267	-0.48796			
3S 6.65361	-0.00283	0.31724	0.21152			

POTASSIUM            K(2)L(8)3S(2)3P(4) - 1S  
 T.E.= -0.59604712D+03 P.E.= -0.11520910D+04 K.E.= 0.59604386D+03 V.T.= -0.20000055D+01

S	1S	2S	3S	P	2P	3P
BASIS/ORB E	-135.15748	-16.05E47	-3.03976	BASIS/ORB E	-13.08619	-2.21902
1S 18.39560	0.92779	-0.28525	-0.10196	2P 7.89755	0.75601	-0.26561
1S 26.81270	0.05489	-0.00534	-0.00046	2P 14.16180	0.06869	-0.02200
2S 8.02917	0.00647	0.85877	0.32072	3P 3.47478	0.00190	0.50792
2S 16.30540	0.02202	-0.13340	-0.04804	3P 2.33952	0.00318	0.60453
3S 3.56251	0.00082	0.01192	-0.63356	3P 6.35669	0.22789	-0.11253
3S 2.63166	-0.00044	-0.00334	-0.51450			
3S 7.11824	-0.00269	0.29205	0.22415			

CALCIUM            K(2)L(8)3S(2)3P(4) - 1S  
 T.E.= -0.67166738D+03 P.E.= -0.13433309D+04 K.E.= 0.67166355D+03 V.T.= -0.20000057D+01

S	1S	2S	3S	P	2P	3P
BASIS/ORB E	-151.55990	-18.93319	-3.99797	BASIS/ORB E	-15.74184	-3.07417
1S 19.37410	0.93152	-0.29026	0.10732	2P 8.23810	0.77913	-0.29150
1S 28.25440	0.05286	-0.00435	0.00050	2P 14.70990	0.07520	-0.02504
2S 8.41156	0.00644	0.89859	-0.35224	3P 3.81644	0.00263	0.50081
2S 17.04380	0.01997	-0.13850	0.05323	3P 2.67703	0.0260	0.61736
3S 3.84010	0.00100	0.00860	0.68056	3P 6.70743	0.19272	-0.11036
3S 2.92181	-0.00055	-0.00199	0.48211			
3S 7.47541	-0.0C0289	0.25674	-0.22940			

See page 183 for Explanation of Tables and Notes for Tables 32, 42, and 43

TABLE 29 (2). THE HARTREE-FOCK FUNCTIONS FOR S(<sup>1</sup>S) ISO-ELECTRICAL SERIES.

SCANDIUM K(2)L(8)3S(2)3P(4) - 1S T.E.= -0.75197313D+03 P.E.= -0.15039438D+04 K.E.= 0.751970650+03 V.T.= -0.20000033D+01						
S	1S	2S	3S	P	2P	3P
BASIS/ORB E	-168.96945	-22.06636	-5.07233	BASIS/CRB E	-18.65514	-4.04569
1S 20.44910	0.93251	-0.25672	0.11260	2P 8.59235	0.79875	-0.31615
1S 29.59990	0.04879	-0.00114	-0.00021	2P 15.23530	0.08135	-0.02748
2S 8.65990	0.00470	0.91905	-0.37469	3P 4.11827	0.00261	0.50204
2S 17.72420	0.02437	-0.14493	0.05862	3P 3.01143	0.00231	0.61998
3S 4.17388	0.00071	0.00996	0.61706	3P 7.04257	0.16254	-0.10418
3S 3.31479	-0.00042	-0.0290	0.55472			
3S 7.93115	-0.00201	0.24020	-0.23682			
TITANIUM K(2)L(8)3S(2)3P(4) - 1S T.E.= -0.83696032D+03 P.E.= -0.16739168D+04 K.E.= 0.83695647D+03 V.T.= -0.20000046D+01						
S	1S	2S	3S	P	2P	3P
BASIS/ORB E	-187.38531	-25.45673	-6.26225	BASIS/CRB E	-21.82497	-5.13307
1S 21.39650	0.93625	-0.30315	0.11913	2P 8.97011	0.81533	-0.33674
1S 31.04830	0.04807	0.00058	-0.00132	2P 15.77250	0.08615	-0.02990
2S 9.25607	0.00526	0.94713	-0.39593	3P 4.42618	-0.00033	0.52790
2S 18.45020	0.02048	-0.14698	0.06038	3P 3.31914	0.00326	0.60550
3S 4.43112	0.00099	0.01148	0.70291	3P 7.33040	0.13915	-0.10613
3S 3.57098	-0.00059	-0.00407	0.48378			
3S 8.36165	-0.00250	0.21326	-0.24554			
VANADIUM K(2)L(8)3S(2)3P(4) - 1S T.E.= -0.92662607D+03 P.E.= -0.18532484D+04 K.E.= 0.92662232D+03 V.T.= -0.20000041D+01						
S	1S	2S	3S	P	2P	3P
BASIS/ORB E	-206.80557	-29.10195	-7.56604	BASIS/CRB E	-25.24913	-6.33453
1S 22.41690	-0.93724	-0.30489	-0.12260	2P 9.34129	0.83082	-0.35699
1S 32.38830	-0.04638	0.00559	0.00124	2P 16.32300	0.09109	-0.03198
2S 9.72173	-0.00484	0.95761	0.41017	3P 4.73377	-0.00075	0.53950
2S 19.31180	-0.02138	-0.15164	-0.06399	3P 3.64298	0.00316	0.60328
3S 4.77347	-0.0103	0.01238	-0.61769	3P 7.61660	0.11546	-0.10469
3S 3.97702	0.00066	-0.00480	-0.57885			
3S 8.84293	0.00235	0.20525	0.25606			
CHROMIUM K(2)L(8)3S(2)3P(4) - 1S T.E.= -0.10209682D+04 P.E.= -0.20419299D+04 K.E.= 0.10209617D+04 V.T.= -0.20000053D+01						
S	1S	2S	3S	P	2P	3P
BASIS/ORB E	-227.22986	-33.00135	-8.98343	BASIS/CRB E	-28.92704	-7.64980
1S 23.24940	0.94157	-0.31252	0.12782	2P 9.72928	0.84185	-0.37327
1S 33.76730	0.04937	0.00193	-0.00149	2P 16.89140	0.09564	-0.03421
2S 10.17620	0.00686	0.98496	-0.43453	3P 5.08696	0.00295	0.52066
2S 19.82900	0.01167	-0.15675	0.06698	3P 3.98596	0.00144	0.63169
3S 5.09872	0.00216	0.00694	0.61813	3P 7.98900	0.09475	-0.10584
3S 4.30770	-0.00137	-0.00151	0.59758			
3S 9.16727	-0.00382	0.18809	-0.26662			
MANGANESE K(2)L(8)3S(2)3P(4) - 1S T.E.= -0.11199850D+04 P.E.= -0.22399618D+04 K.E.= 0.11199768D+04 V.T.= -0.20000073D+C1						
S	1S	2S	3S	P	2P	3P
BASIS/ORB E	-248.65740	-37.15399	-10.51381	BASIS/CRB E	-32.85783	-5.07827
1S 24.20200	-0.94425	-0.31642	-0.13284	2P 10.13950	0.85191	-0.38866
1S 35.20250	-0.04873	0.00265	0.00240	2P 17.58780	0.09741	-0.03511
2S 10.70650	-0.00761	0.98526	0.43871	3P 5.35340	0.01409	0.51325
2S 20.54730	-0.00875	-0.16141	-0.07068	3P 4.32564	-0.00403	0.63663
3S 5.39881	-0.00269	0.00756	-0.60952	3P 8.53765	0.07453	-0.09558
3S 4.64347	0.00177	-0.00244	-0.61676			
3S 9.68828	0.00435	0.19270	0.28513			

See page 183 for Explanation of Tables and Notes for Tables 32, 42, and 43

## ROOTHAAN-HARTREE-FOCK ATOMIC WAVEFUNCTIONS

TABLE 29 (3). THE HARTREE-FOCK FUNCTIONS FOR S(1S) ISO-ELECTRICAL SERIES.

IRON K(2)L(8)3S(2)3P(4) - 1S						
T.E.= -0.12236753D+04 P.E.= -0.24473414D+04 K.E.= 0.12236661D+04 V.T.= -0.20000075D+01						
S	1S	2S	3S	P	2P	3P
BASIS/ORB E	-271.08720	-41.55548	-12.15694	BASIS/ORB E	-37.04114	-10.61962
1S 25.18440	-0.94605	-0.32000	-0.13669	2P 10.55390	0.86021	-0.40197
1S 36.60680	-0.04763	0.00363	0.00293	2P 18.19590	0.09998	-0.03643
2S 11.16660	-0.00769	1.00121	0.45294	3P 5.66365	0.01727	0.51475
2S 21.26330	-0.00779	-0.16637	-0.07395	3P 4.65522	-0.00588	0.64286
3S 5.71145	-0.00307	0.0C664	-0.60445	3P 8.94136	0.05994	-0.09607
3S 4.97662	0.00207	-0.00209	-0.63619			
3S 10.11330	0.00453	0.18266	0.29643			
COBALT K(2)L(8)3S(2)3P(4) - 1S						
T.E.= -0.13320380D+04 P.E.= -0.26640666D+04 K.E.= 0.13320285D+04 V.T.= -0.20000072D+01						
S	1S	2S	3S	P	2P	3P
BASIS/ORB E	-294.51915	-46.21727	-13.91246	BASIS/ORB E	-41.47648	-12.27350
1S 26.20380	0.94724	-0.32219	0.13867	2P 10.97100	0.86793	-0.41419
1S 37.99600	0.04576	0.00427	-0.00267	2P 18.81130	0.10220	-0.03761
2S 11.63100	0.00682	1.02196	-0.47438	3P 5.96992	0.02073	0.52061
2S 21.96420	0.00892	-0.17438	0.08075	3P 4.98154	-0.00797	0.64481
3S 6.03668	0.00316	-0.00142	0.61098	3P 9.35076	0.04644	-0.09697
3S 5.30730	-0.00215	0.00279	0.65019			
3S 10.41250	-0.00412	0.17126	-0.30801			
NICKEL K(2)L(8)3S(2)3P(4) - 1S						
T.E.= -0.14450724D+04 P.E.= -0.28901346D+04 K.E.= 0.14450622D+04 V.T.= -0.20000070D+01						
S	1S	2S	3S	P	2P	3P
BASIS/ORB E	-318.95295	-51.12698	-15.78020	BASIS/ORB E	-46.16350	-14.03973
1S 27.20220	0.94865	-0.32552	-0.14205	2P 11.40170	0.87423	-0.42492
1S 39.38910	0.04446	0.00541	0.00326	2P 19.44320	0.10365	-0.03846
2S 12.10860	0.00654	1.03447	0.48634	3P 6.27847	0.02368	0.52342
2S 22.66300	0.00882	-0.17977	-0.08427	3P 5.31080	-0.00988	0.64970
3S 6.35153	0.00336	-0.00278	-0.60806	3P 9.77355	0.03578	-0.09690
3S 5.63889	-0.00233	0.00356	-0.66764			
3S 10.83360	-0.00404	0.16437	0.32052			
COPPER K(2)L(8)3S(2)3P(4) - 1S						
T.E.= -0.15627777D+04 P.E.= -0.31255452D+04 K.E.= 0.15627675D+04 V.T.= -0.20000066D+01						
S	1S	2S	3S	P	2P	3P
BASIS/ORB E	-344.38824	-56.28832	-17.75996	BASIS/ORB E	-51.10194	-15.91808
1S 28.16920	0.95033	-0.32851	-0.14499	2P 11.50110	0.87518	-0.43177
1S 40.80380	0.04394	0.00609	0.00356	2P 20.14970	0.10194	-0.03804
2S 12.57530	0.00698	1.04717	0.49855	3P 6.59055	0.02186	0.52609
2S 23.38490	0.00714	-0.18399	-0.08748	3P 5.64207	-0.00925	0.65584
3S 6.65830	0.00407	-0.00395	-0.60679	3P 10.21160	0.03679	-0.10690
3S 5.97364	-0.00289	0.00427	-0.68274			
3S 11.25060	-0.00445	0.15618	0.33113			
ZINC K(2)L(8)3S(2)3P(4) - 1S						
T.E.= -0.16851534D+04 P.E.= -0.33702973D+04 K.E.= 0.16851440D+04 V.T.= -0.20000056D+01						
S	1S	2S	3S	P	2P	3P
BASIS/ORB E	-370.82540	-61.70113	-19.85171	BASIS/ORB E	-56.29174	-17.90853
1S 29.26840	-0.95110	-0.32778	-0.14785	2P 12.36510	0.88544	-0.44210
1S 42.19030	-0.04018	0.0C595	0.00451	2P 21.02130	0.09793	-0.03675
2S 13.35820	-0.00469	1.01545	0.48254	3P 6.89631	0.02859	0.53146
2S 24.08440	-0.01167	-0.19874	-0.09192	3P 5.96790	-0.01370	0.65728
3S 7.14537	-0.00255	-0.01983	-0.41647	3P 10.65840	0.02668	-0.10934
3S 6.37072	0.00176	0.01455	-0.88660			
3S 11.80030	0.00287	0.20551	0.37240			

See page 183 for Explanation of Tables and Notes for Tables 32, 42, and 43

TABLE 29 (4). THE HARTREE-FOCK FUNCTIONS FOR S(<sup>1</sup>S) ISO-ELECTRICAL SERIES.

GALLIUM K(2)L(8)3S(2)3P(4) - 1S T.E.= -0.18121989D+04 P.E.= -0.36243889D+04 K.E.= 0.18121900D+04 V.T.= -0.20000050D+C1						
S	1S	2S	3S	P	2P	3P
BASIS/ORB E	-398.26324	-67.36516	-22.05518	BASIS/ORB E	-61.73253	-20.01078
1S 30.27900	-0.95219	-0.33021	-0.15023	2P 12.75110	0.68996	-0.45075
1S 43.56560	-0.03891	0.00682	0.00486	2P 21.47370	0.10349	-0.03927
2S 13.86420	-0.00412	1.02981	0.49296	3P 7.20198	0.03167	0.53848
2S 24.78360	-0.01211	-0.20508	-0.09618	3P 6.29363	-0.01570	0.65714
3S 7.47109	-0.00243	-0.02475	-0.40551	3P 11.10500	0.01367	-0.10901
3S 6.70284	0.00170	0.01774	-0.91255			
3S 12.20360	0.00257	0.20262	0.38590			
GERMANIUM K(2)L(8)3S(2)3P(4) - 1S T.E.= -0.19439141D+04 P.E.= -0.38878193D+04 K.E.= 0.19439052D+04 V.T.= -0.20000046D+01						
S	1S	2S	3S	P	2P	3P
BASIS/ORB E	-426.70234	-73.28223	-24.37037	BASIS/ORB E	-67.42426	-22.22481
1S 31.31030	-0.95312	-0.33305	-0.15225	2P 13.22110	0.89365	-0.45735
1S 44.92360	-0.03723	0.00816	0.00516	2P 22.17880	0.10242	-0.03910
2S 14.36110	-0.00311	1.04140	0.50551	3P 7.50468	0.03328	0.55037
2S 25.46250	-0.01347	-0.21138	-0.10132	3P 6.61770	-0.01721	0.65263
3S 7.96021	-0.00187	-0.02743	-0.25062	3P 11.55840	0.00989	-0.11393
3S 7.09573	0.00126	0.01842	-1.08101			
3S 12.59850	0.00202	0.19905	0.39602			
ARSENIC K(2)L(8)3S(2)3P(4) - 1S T.E.= -0.20802984D+04 P.E.= -0.41605898D+04 K.E.= 0.20802913D+04 V.T.= -0.20000034D+01						
S	1S	2S	3S	P	2P	3P
BASIS/ORB E	-456.14237	-79.44626	-26.79720	BASIS/ORB E	-73.36683	-24.55057
1S 32.36240	-0.95399	-0.33464	-0.15427	2P 13.7C730	0.89596	-0.46250
1S 46.28020	-0.03512	0.00898	0.00562	2P 22.89780	0.10081	-0.03876
2S 14.87110	-0.00156	1.05553	0.51794	3P 7.80539	0.03375	0.56648
2S 26.14530	-0.01572	-0.22014	-0.10673	3P 6.53890	-0.01806	0.64367
3S 8.28533	-0.00092	-0.03633	-0.38581	3P 12.02940	0.00873	-0.12001
3S 7.34759	0.00062	0.02287	-0.97564			
3S 12.88970	0.00101	0.19687	0.42219			
SELENIUM K(2)L(8)3S(2)3P(4) - 1S T.E.= -0.22213517D+04 P.E.= -0.44426969D+04 K.E.= 0.22213452D+04 V.T.= -0.20000029D+01						
S	1S	2S	3S	P	2P	3P
BASIS/ORB E	-486.58313	-85.86312	-29.33559	BASIS/ORB E	-79.56009	-26.98793
1S 33.37500	-0.95504	-0.33676	-0.15627	2P 14.13260	0.89873	-0.46817
1S 47.65790	-0.03396	0.00578	0.00595	2P 23.43760	0.10362	-0.04028
2S 15.38870	-0.00100	1.06345	0.52627	3P 8.11115	0.03497	0.57491
2S 26.84520	-0.01609	-0.22615	-0.11079	3P 7.26458	-0.01916	0.64145
3S 8.61585	-0.00064	-0.04053	-0.37963	3P 12.50980	0.00179	-0.12218
3S 7.67742	0.00044	0.02547	-0.99592			
3S 13.30000	0.00067	0.15642	0.43574			
BROMINE K(2)L(8)3S(2)3P(4) - 1S T.E.= -0.23670737D+04 P.E.= -0.47341424D+04 K.E.= 0.23670687D+04 V.T.= -0.20000022D+01						
S	1S	2S	3S	P	2P	3P
BASIS/ORB E	-518.02500	-92.53C70	-31.98552	BASIS/ORB E	-86.00402	-29.53691
1S 34.43660	-0.95595	-0.33911	-0.15840	2P 14.68040	0.90233	-0.47202
1S 49.01060	-0.03172	0.C1117	0.00662	2P 24.40060	0.09663	-0.03776
2S 15.91110	0.00069	1.07218	0.53441	3P 8.41118	0.03684	0.59224
2S 27.51790	-0.01854	-0.23334	-0.11522	3P 7.58508	-0.02120	0.63051
3S 8.94109	0.00053	-0.04372	-0.38840	3P 13.00090	0.00501	-0.13064
3S 7.99800	-0.00031	0.02740	-1.00156			
3S 13.71020	-0.00048	0.19563	0.44976			
KRYPTON K(2)L(8)3S(2)3P(4) - 1S T.E.= -0.25174643D+04 P.E.= -0.50249239D+04 K.E.= 0.25174596D+04 V.T.= -0.20000018D+01						
S	1S	2S	3S	P	2P	3P
BASIS/ORB E	-550.46730	-99.44894	-34.74690	BASIS/ORB E	-92.69849	-32.19736
1S 35.39070	-0.95712	-0.34043	-0.15987	2P 15.24210	0.89977	-0.47254
1S 50.43270	-0.03195	0.01103	0.00650	2P 25.21640	0.09246	-0.03643
2S 16.45720	-0.00016	1.07577	0.54002	3P 8.72443	0.03306	0.59191
2S 28.24230	-0.01634	-0.23862	-0.11889	3P 7.51837	-0.01927	0.63724
3S 9.27963	-0.00019	-0.05C83	-0.35928	3P 13.51490	0.01363	-0.14119
3S 8.34194	0.00016	0.03206	-1.04283			
3S 14.13450	0.00017	0.20035	0.46353			

See page 183 for Explanation of Tables and Notes for Tables 32, 42, and 43

## ROOTHAAAN-HARTREE-FOCK ATOMIC WAVEFUNCTIONS

 TABLE 30 (1). THE HARTREE-FOCK FUNCTIONS FOR C1(<sup>2</sup>P) ISO-ELECTRICAL SERIES.

CHLORINE K(2)L(8)3S(2)3P(5) - 2P						
T.E.= -0.45948181D+03 P.E.= -0.91896597D+03 K.E.= 0.45948417D+03 V.T.= -0.19999949D+01						
S	1S	2S	3S	P	2P	3P
BASIS/ORB E	-104.88405	-10.60719	-1.07267	BASIS/ORB E	-8.07194	-0.50617
1S 17.36120	0.91279	0.25342	0.07735	2P 7.67977	0.65334	-0.17929
1S 28.27580	0.01474	0.00538	0.00128	2P 14.06740	0.03507	-0.00875
2S 6.84172	0.00345	-0.88039	-0.28743	3P 2.61823	0.01075	0.57163
2S 15.47230	0.08794	0.14115	0.04481	3P 1.45933	-0.00103	0.54080
3S 2.97140	0.00009	-0.00751	0.62602	3P 5.93136	0.37721	-0.11467
3S 1.85605	-0.00005	0.00078	0.51750			
3S 5.99804	-0.00088	-0.25038	-0.16835			
ARGON K(2)L(8)3S(2)3P(5) - 2P						
T.E.= -0.52627435D+03 P.E.= -0.10525452D+04 K.E.= 0.52627086D+03 V.T.= -0.20000066D+01						
S	1S	2S	3S	P	2P	3P
BASIS/ORB E	-119.13381	-12.83628	-1.71135	BASIS/ORB E	-10.08383	-1.04543
1S 18.25010	0.92239	0.26244	0.08447	2P 7.95043	0.68234	-0.20940
1S 29.44590	0.01582	0.00433	0.00137	2P 14.19760	0.04695	-0.01291
2S 7.26099	0.00286	-0.90935	-0.31873	3P 2.95647	0.00922	0.57519
2S 16.15690	0.07578	0.14294	0.04957	3P 1.79986	-0.00048	0.52964
3S 3.29566	0.00003	-0.00758	0.61185	3P 6.30014	0.33055	-0.11664
3S 2.18528	-0.00003	0.00072	0.53681			
3S 6.40657	-0.00068	-0.22485	-0.17615			
POTASSIUM K(2)L(8)3S(2)3P(5) - 2P						
T.E.= -0.59789143D+03 P.E.= -0.11957780D+04 K.E.= 0.59788655D+03 V.T.= -0.20000081D+01						
S	1S	2S	3S	P	2P	3P
BASIS/ORB E	-134.40447	-15.34022	-2.47778	BASIS/ORB E	-12.36895	-1.71136
1S 19.16390	0.92749	0.26621	0.09076	2P 8.26153	0.70790	-0.23630
1S 30.53730	0.01783	0.00435	0.00152	2P 14.55970	0.05612	-0.01664
2S 7.68792	0.00342	-0.92772	-0.34296	3P 3.29602	0.00782	0.57288
2S 16.99110	0.06710	0.14398	0.05289	3P 2.13979	0.00000	0.53128
3S 3.61266	0.00020	-0.0C986	0.60154	3P 6.67201	0.29085	-0.11748
3S 2.51276	-0.00011	0.00160	0.55377			
3S 6.88001	-0.00115	-0.20655	-0.18596			
CALCIUM K(2)L(8)3S(2)3P(5) - 2P						
T.E.= -0.67431982D+03 P.E.= -0.13486336D+04 K.E.= 0.67431381D+03 V.T.= -0.20000089D+01						
S	1S	2S	3S	P	2P	3P
BASIS/ORB E	-150.68933	-18.11107	-3.36611	BASIS/ORB E	-14.91969	-2.49889
1S 20.09440	0.93177	0.27391	0.09750	2P 8.59741	0.72670	-0.25944
1S 31.75250	0.01922	0.00357	0.00108	2P 14.92440	0.06544	-0.02053
2S 8.14871	0.00392	-0.93318	-0.35705	3P 3.61506	0.00779	0.58101
2S 17.83130	0.06013	0.14443	0.05431	3P 2.46401	-0.00013	0.52548
3S 3.92914	0.00034	-0.01459	0.58786	3P 7.07101	0.25785	-0.11722
3S 2.84058	-0.00019	0.00365	0.57383			
3S 7.44289	-0.00158	-0.20030	-0.20075			
SCANDIUM K(2)L(8)3S(2)3P(5) - 2P						
T.E.= -0.75555079D+03 P.E.= -0.15110910D+04 K.E.= 0.75554022D+03 V.T.= -0.20000140D+01						
S	1S	2S	3S	P	2P	3P
BASIS/ORB E	-167.98388	-21.14300	-4.37184	BASIS/ORB E	-17.73044	-3.40385
1S 20.54920	0.95431	0.26526	0.10615	2P 8.92428	0.75449	-0.28982
1S 33.30740	0.02721	0.00535	0.00121	2P 15.62700	0.06956	-0.02100
2S 8.52122	0.01201	-0.95516	-0.37570	3P 3.81911	0.00991	0.62624
2S 18.70960	0.02074	0.13311	0.05084	3P 2.77621	-0.00185	0.47326
3S 4.16660	0.00242	-0.01911	0.65069	3P 7.44404	0.22030	-0.09963
3S 3.09813	-0.00126	0.00609	0.51849			
3S 7.98390	-0.00720	-0.17347	-0.20625			

See page 183 for Explanation of Tables and Notes for Tables 32, 42, and 43

TABLE 30 (2). THE HARTREE-FOCK FUNCTIONS FOR C1(<sup>2</sup>P) ISO-ELECTRICAL SERIES.

TITANIUM K(2)L(8)3S(2)3P(5) - 2P T.E.= -0.84157999D+03 P.E.= -0.16831555D+04 K.E.= 0.84157554D+03 V.T.= -0.20000053D+C1						
S	1S	2S	3S	P	2P	3P
BASIS/ORB E	-186.28611	-24.43500	-5.49557	BASIS/ORB E	-20.80054	-4.42678
1S 21.99730	0.93988	-0.28648	0.10905	2P 9.32265	0.74818	-0.29544
1S 34.04710	0.02013	-0.00159	0.00026	2P 15.71200	0.08433	-0.02879
2S 9.10678	0.00188	0.96070	-0.39417	3P 4.25461	0.01214	0.57739
2S 19.14620	0.05048	-0.15352	0.06222	3P 3.12917	-0.00231	0.53615
3S 4.53957	-0.00007	0.01346	0.58881	3P 7.98273	0.20735	-0.11595
3S 3.48730	0.00002	-0.00360	0.59487			
3S 8.32929	-0.00044	0.18589	-0.22617			
VANADIUM K(2)L(8)3S(2)3P(5) - 2P T.E.= -0.93240212D+03 P.E.= -0.16647978D+04 K.E.= 0.93239570D+03 V.T.= -0.20000069D+01						
S	1S	2S	3S	P	2P	3P
BASIS/ORB E	-205.59417	-27.98328	-6.73363	BASIS/ORB E	-24.12615	-5.56418
1S 22.88600	0.94441	-0.29343	0.11474	2P 9.73305	0.76520	-0.31425
1S 35.24770	0.02207	-0.00038	-0.00023	2P 16.38520	0.08552	-0.02983
2S 9.57132	0.02051	0.97163	-0.40870	3P 4.52993	0.01057	0.61333
2S 19.82750	0.04256	-0.15476	0.06442	3P 3.42606	-0.00194	0.50610
3S 4.85212	0.00019	0.01692	0.55189	3P 8.36583	0.18690	-0.11517
3S 3.84498	-0.00013	-0.00563	0.63807			
3S 8.84962	-0.00097	0.17746	-0.23418			
CHROMIUM K(2)L(8)3S(2)3P(5) - 2P T.E.= -0.10280147D+04 P.E.= -0.20560220D+04 K.E.= 0.10280074D+04 V.T.= -0.20000071D+01						
S	1S	2S	3S	P	2P	3P
BASIS/ORB E	-225.50691	-31.78700	-8.08591	BASIS/ORB E	-27.70662	-6.81601
1S 23.74720	0.94876	-0.29894	0.12008	2P 10.20790	0.77554	-0.32667
1S 36.40260	0.02474	-0.00067	-0.00061	2P 17.14650	0.08374	-0.02981
2S 10.05160	0.00356	0.98817	-0.42522	3P 4.83172	0.00921	0.62700
2S 20.46820	0.03376	-0.15916	0.06751	3P 3.74538	-0.00150	0.49906
3S 5.12983	0.00066	0.01250	0.62244	3P 8.78953	0.17691	-0.11904
3S 4.10729	-0.00039	-0.00368	0.58649			
3S 9.21163	-0.00178	0.16953	-0.25139			
MANGANESE K(2)L(8)3S(2)3P(5) - 2P T.E.= -0.11284154D+04 P.E.= -0.22568225D+04 K.E.= 0.11284071D+04 V.T.= -0.20000074D+01						
S	1S	2S	3S	P	2P	3P
BASIS/ORB E	-247.22334	-35.84454	-9.55182	BASIS/ORB E	-31.54083	-8.18150
1S 24.65060	0.95148	-0.30520	0.12461	2P 10.63340	0.78103	-0.33917
1S 37.55620	0.02667	0.00127	-0.00092	2P 17.69170	0.08819	-0.03254
2S 10.52930	0.00419	0.99838	-0.43958	3P 5.12934	0.01091	0.65435
2S 21.11060	0.02794	-0.16171	0.07084	3P 4.04165	-0.00249	0.47875
3S 5.544822	0.00104	0.01534	0.55304	3P 9.27637	0.16387	-0.12258
3S 4.49980	-0.00064	-0.00560	0.66080			
3S 9.71433	-0.00231	0.16275	-0.25620			
IRON K(2)L(8)3S(2)3P(5) - 2P T.E.= -0.12336027D+04 P.E.= -0.24671993D+04 K.E.= 0.12335966D+04 V.T.= -0.20000049D+01						
S	1S	2S	3S	P	2P	3P
BASIS/ORB E	-269.54283	-40.15635	-11.13070	BASIS/ORB E	-35.62811	-9.66015
1S 25.68240	0.95283	-0.31310	0.13039	2P 11.09670	0.78756	-0.35047
1S 38.75730	0.02518	0.00451	-0.00259	2P 18.39190	0.08843	-0.03310
2S 11.19270	0.00098	0.99249	-0.44432	3P 5.40983	0.01240	0.67771
2S 21.39890	0.02970	-0.17487	0.07781	3P 4.35485	-0.00357	0.46003
3S 5.75061	-0.00002	0.01163	0.54792	3P 9.76135	0.15472	-0.12411
3S 4.83256	-0.00002	-0.00405	0.67813			
3S 10.16470	-0.00027	0.18536	-0.28140			

See page 183 for Explanation of Tables and Notes for Tables 32, 42, and 43

## ROOTHAAN-HARTREE-FOCK ATOMIC WAVEFUNCTIONS

 TABLE 30 (3). THE HARTREE-FOCK FUNCTIONS FOR C1(<sup>2</sup>P) ISO-ELECTRICAL SERIES.

COBALT K(2)L(8)3S(2)3P(5) - 2P						
T.E.= -0.13435751D+04 P.E.= -0.26871450D+04 K.E.= 0.13435699D+04 V.T.= -0.20000039D+01						
S	1S	2S	3S	P	2P	3P
BASIS/ORB E	-292.86505	-44.72C72	-12.82232	BASIS/CRB E	-39.96798	-11.25164
1S 26.60950	0.95445	-0.31707	0.13358	2P 11.63890	0.79074	-0.35864
1S 39.95710	0.02668	0.00547	-0.00257	2P 19.27770	0.08369	-0.03175
2S 11.69850	0.00147	1.00769	-0.46217	3P 5.69028	0.01354	0.70245
2S 22.01830	0.02570	-0.18210	0.08386	3P 4.66833	-0.00456	0.44011
3S 6.05726	0.00031	0.00543	0.55182	3P 10.27440	0.15508	-0.13C15
3S 5.16429	-0.00023	-0.00C81	0.69038			
3S 10.50750	-0.00068	0.1E529	-0.29349			
NICKEL K(2)L(8)3S(2)3P(5) - 2P						
T.E.= -0.14583316D+04 P.E.= -0.29166567D+04 K.E.= 0.14583251D+04 V.T.= -0.20000044D+01						
S	1S	2S	3S	P	2P	3P
BASIS/ORB E	-317.18949	-49.53770	-14.62649	BASIS/ORB E	-44.56012	-12.95580
1S 27.55320	0.95461	-0.31596	0.13650	2P 12.14670	0.79425	-0.36670
1S 41.14190	0.02840	0.00349	-0.00260	2P 20.03440	0.08195	-0.03145
2S 12.19810	0.00308	1.00223	-0.45848	3P 5.97089	0.01360	0.73000
2S 23.07540	0.02251	-0.18203	0.08180	3P 4.98200	-0.00491	0.41793
3S 6.42851	0.00100	0.00410	0.51522	3P 10.76050	0.15235	-0.13475
3S 5.49538	-0.00065	0.00023	0.73946			
3S 11.04760	-0.00174	0.19015	-0.31533			
COPPER K(2)L(8)3S(2)3P(5) - 2P						
T.E.= -0.15778712D+04 P.E.= -0.31557355D+04 K.E.= 0.15778643D+04 V.T.= -0.20000044D+01						
S	1S	2S	3S	P	2P	3P
BASIS/ORB E	-342.51580	-54.6C668	-16.54292	BASIS/ORB E	-49.40402	-14.77230
1S 28.44480	0.95588	-0.32C80	-0.14036	2P 12.66360	0.79444	-0.37139
1S 42.25490	0.03095	0.00442	0.00306	2P 20.75920	0.08111	-0.03190
2S 12.69070	0.00422	1.01E35	0.47177	3P 6.27270	0.01480	0.74184
2S 23.67760	0.01735	-0.18696	-0.08545	3P 5.30447	-0.00584	0.41183
3S 6.75409	0.00170	0.00103	-0.51736	3P 11.29390	0.15177	-0.14167
3S 5.81772	-0.00110	0.00180	-0.75279			
3S 11.43700	-0.00258	0.18425	0.32822			
ZINC K(2)L(8)3S(2)3P(5) - 2P						
T.E.= -0.17021934D+04 P.E.= -0.34C43797D+04 K.E.= 0.17021863D+04 V.T.= -0.20000042D+01						
S	1S	2S	3S	P	2P	3P
BASIS/ORB E	-368.84373	-59.92747	-18.57143	BASIS/ORB E	-54.49948	-16.70095
1S 29.39400	0.95635	-0.32488	-0.14391	2P 13.17990	0.79536	-0.37625
1S 43.40780	0.03215	0.00556	0.00369	2P 21.48810	0.08006	-0.03210
2S 13.19280	0.00441	1.02702	0.48191	3P 6.56354	0.01542	0.76393
2S 24.31150	0.01520	-0.19225	-0.08880	3P 5.62155	-0.00649	0.39522
3S 7.07343	0.00196	-0.00056	-0.51362	3P 11.81140	0.15100	-0.14776
3S 6.14434	-0.00129	0.00257	-0.76962			
3S 11.86270	-0.00277	0.18C76	0.34085			
GALLIUM K(2)L(8)3S(2)3P(5) - 2P						
T.E.= -0.18312974D+04 P.E.= -0.36C25871D+04 K.E.= 0.18312897D+04 V.T.= -0.20000042D+01						
S	1S	2S	3S	P	2P	3P
BASIS/ORB E	-396.17323	-65.49577	-20.71182	BASIS/ORB E	-59.84627	-18.74156
1S 30.35750	0.95665	-0.32E31	-0.14691	2P 13.77170	0.79095	-0.37834
1S 44.57430	0.03299	0.00656	0.00417	2P 22.39380	0.07604	-0.03079
2S 13.71420	0.00442	1.03544	0.49131	3P 6.85202	0.02069	0.72652
2S 24.95500	0.01377	-0.19834	-0.09282	3P 6.03596	-0.01065	0.43363
3S 7.51198	0.00213	-0.00394	-0.40965	3P 12.42550	0.15823	-0.15366
3S 6.52501	-0.00137	0.00442	-0.88744			
3S 12.27830	-0.00288	C.18C83	0.35501			

See page 183 for Explanation of Tables and Notes for Tables 32, 42, and 43

TABLE 30 (4). THE HARTREE-FOCK FUNCTIONS FOR C1(<sup>2</sup>P) ISO-ELECTRICAL SERIES.

GERMANIUM K(2)L(8)3S(2)3P(5) - 2P						
T.E. = -0.19651828D+04 P.E. = -0.39303567D+04 K.E. = 0.19651759D+04 V.T. = -0.20300035D+01						
S	1S	2S	3S	P	2P	3P
BASIS/ORB E	-424.50376	-71.32350	-22.96409	BASIS/CRB E	-65.44428	-20.89410
1S 31.37200	0.95638	-0.33124	-0.14886	2P 14.25310	0.79650	-0.38505
1S 45.70930	0.03279	0.0C779	0.00433	2P 23.06940	0.07563	-0.03103
2S 14.22530	0.00316	1.04985	0.50790	3P 7.15358	0.01811	0.74940
2S 25.57620	0.01491	-0.20677	-0.09976	3P 6.35421	-0.00918	0.41825
3S 7.82905	0.00168	-0.01142	-0.42681	3P 12.85820	0.15293	-0.15856
3S 6.84682	-0.00109	0.0C852	-0.88934			
3S 12.58660	-0.00210	0.17794	0.36852			
ARSENIC K(2)L(8)3S(2)3P(5) - 2P						
T.E. = -0.21038492D+04 P.E. = -0.42076934D+04 K.E. = 0.21038442D+04 V.T. = -0.20000024D+01						
S	1S	2S	3S	P	2P	3P
BASIS/ORB E	-453.83555	-77.39833	-25.32811	BASIS/ORB E	-71.29324	-23.15846
1S 32.41130	-0.95639	-0.33370	-0.15124	2P 14.75380	0.79473	-0.38753
1S 46.91380	-0.03175	0.00902	0.00491	2P 23.75310	0.07668	-0.03204
2S 14.77220	-0.00166	1.05501	0.51499	3P 7.37708	0.02608	0.82197
2S 26.24430	-0.01686	-0.21430	-0.10441	3P 6.68206	-0.01574	0.34652
3S 8.15674	-0.00092	-0.01548	-0.40188	3P 13.47490	0.15152	-0.16028
3S 7.18852	0.00063	0.01C53	-0.92591			
3S 13.01710	0.00111	0.18200	0.38222			
SELENIUM K(2)L(8)3S(2)3P(5) - 2P						
T.E. = -0.22472962D+04 P.E. = -0.44945855D+04 K.E. = 0.22472893D+04 V.T. = -0.20000031D+01						
S	1S	2S	3S	P	2P	3P
BASIS/ORB E	-484.16818	-83.72434	-27.80379	BASIS/CRB E	-77.39322	-25.53454
1S 33.40900	-0.95645	-0.33650	-0.15371	2P 15.22350	0.80051	-0.39422
1S 48.07260	-0.03181	0.01012	0.00545	2P 24.36670	0.07694	-0.03238
2S 15.30860	-0.00101	1.06208	0.52295	3P 7.67843	0.02162	0.85054
2S 26.89750	-0.01701	-0.22111	-0.10877	3P 7.00675	-0.01278	0.32565
3S 8.47796	-0.00060	-0.01973	-0.39754	3P 13.87840	0.14574	-0.16448
3S 7.51740	0.00043	0.01347	-0.94346			
3S 13.42970	0.00071	0.18394	0.39617			
BROMINE K(2)L(8)3S(2)3P(5) - 2P						
T.E. = -0.23955235D+04 P.E. = -0.47910360D+04 K.E. = 0.23955126D+04 V.T. = -0.20000046D+01						
S	1S	2S	3S	P	2P	3P
BASIS/ORB E	-515.50182	-90.30123	-30.39112	BASIS/ORB E	-83.74393	-28.02233
1S 34.23890	-0.95700	-0.33976	-0.15731	2P 15.69650	0.80220	-0.39747
1S 49.26070	-0.03568	0.01008	0.00605	2P 24.55090	0.07853	-0.03376
2S 15.87260	-0.00420	1.06022	0.52026	3P 7.97133	0.02214	0.88698
2S 27.56600	-0.00994	-0.22383	-0.10864	3P 7.33651	-0.01352	0.30075
3S 8.80432	-0.00271	-0.01953	-0.36060	3P 14.38060	0.14171	-0.16879
3S 7.85539	0.00183	0.01362	-0.9854E			
3S 13.97890	0.00289	0.19120	0.40982			
KRYPTON K(2)L(8)3S(2)3P(5) - 2P						
T.E. = -0.25485308D+04 P.E. = -0.50570609D+04 K.E. = 0.25485301D+04 V.T. = -0.20000003D+01						
S	1S	2S	3S	P	2P	3P
BASIS/ORB E	-547.83629	-97.12872	-33.09001	BASIS/CRB E	-90.34518	-30.62171
1S 35.31400	-0.95704	-0.34116	-0.15902	2P 15.84450	0.81909	-0.40607
1S 50.48590	-0.03374	0.01111	0.00658	2P 25.24300	0.09096	-0.04103
2S 16.45080	-0.00207	1.06155	0.52429	3P 8.16957	0.05090	1.02943
2S 28.27210	-0.01329	-0.23192	-0.11328	3P 7.67386	-0.03795	0.14965
3S 9.13747	-0.00146	-0.02537	-0.31500	3P 15.14580	0.10456	-0.15232
3S 8.20744	0.00103	0.01745	-1.04051			
3S 14.42890	0.00148	C.19518	0.42332			

See page 183 for Explanation of Tables and Notes for Tables 32, 42, and 43

## ROOTHAAN-HARTREE-FOCK ATOMIC WAVEFUNCTIONS

 TABLE 31 (1). THE HARTREE-FOCK FUNCTIONS FOR Ar(<sup>1</sup>S) ISO-ELECTRICAL SERIES.

ARGON K(2)L(8)3S(2)3P(6) - 1S						
T.E.= -0.52681709D+03 P.E.= -0.10536331D+04 K.E.= 0.52681606D+03 V.T.= -0.20000020U+01						
S	1S	2S	3S	P	2P	3P
BASIS/ORB E	-118.60990	-12.32175	-1.27688	BASIS/ORB E	-9.57107	-0.59062
1S 18.15660	0.92887	-0.26950	0.08127	2P 8.12905	0.66383	-0.18977
1S 30.06590	0.01569	-0.00170	0.00198	2P 14.50200	0.04021	-0.01023
2S 6.77248	0.00326	1.05741	-0.37906	3P 2.90478	0.00924	0.58270
2S 16.04050	0.06832	-0.13361	0.05087	3P 1.60988	-0.00160	0.53591
3S 3.61984	0.00119	-0.01780	0.74213	3P 6.39570	0.35802	-0.11551
3S 2.08529	-0.00023	0.00321	0.59612			
3S 4.85534	-0.00196	0.08014	-0.28131			
POTASSIUM K(2)L(8)3S(2)3P(6) - 1S						
T.E.= -0.55901730D+03 P.E.= -0.11980285D+04 K.E.= 0.55901120D+03 V.T.= -0.20000102D+01						
S	1S	2S	3S	P	2P	3P
BASIS/ORB E	-133.75338	-14.70914	-1.96444	BASIS/CRB E	-11.73922	-1.17109
1S 18.98260	0.93931	-0.27701	0.08889	2P 8.61735	0.67152	-0.20999
1S 31.39050	0.01789	-0.00171	0.00173	2P 15.19580	0.04224	-0.01178
2S 7.30079	0.00420	1.04565	-0.39368	3P 3.24817	0.01009	0.58221
2S 16.70010	0.05305	-0.13733	0.05415	3P 1.94563	-0.00196	0.52576
3S 3.88331	0.00135	-0.00664	0.64114	3P 6.88378	0.34429	-0.12638
3S 2.40881	-0.00037	0.00268	0.61485			
3S 5.70995	-0.00255	0.08655	-0.21575			
CALCIUM K(2)L(8)3S(2)3P(6) - 1S						
T.E.= -0.67615405D+03 P.E.= -0.13522973D+04 K.E.= 0.67614326D+03 V.T.= -0.20000159D+01						
S	1S	2S	3S	P	2P	3P
BASIS/ORE E	-149.51653	-17.37023	-2.77870	BASIS/ORB E	-14.17950	-1.87741
1S 19.85610	0.94553	-0.28435	0.09576	2P 9.11433	C.67714	-0.22768
1S 32.43970	0.02016	-0.00105	0.00148	2P 15.86340	0.04420	-0.01304
2S 7.79921	0.00475	1.04968	-0.41086	3P 3.56861	0.01098	0.58722
2S 17.36070	0.04280	-0.14030	0.05767	3P 2.27163	-0.00245	0.52192
3S 4.18323	0.00150	-0.00078	0.60666	3P 7.37993	0.33327	-0.13455
3S 2.73133	-0.00048	0.00177	0.63178			
3S 6.35894	-0.00297	0.08860	-0.20777			
SCANDIUM K(2)L(8)3S(2)3P(6) - 1S						
T.E.= -0.75821457D+03 P.E.= -0.15164215D+04 K.E.= 0.75820691D+03 V.T.= -0.200001C1D+01						
S	1S	2S	3S	P	2P	3P
BASIS/ORB E	-167.09271	-20.29748	-3.71421	BASIS/CRB E	-16.88460	-2.70476
1S 20.71740	0.95026	-0.28616	0.10127	2P 9.61209	0.68169	-0.24276
1S 33.63060	0.02310	-0.00303	0.00170	2P 16.50940	0.04630	-0.01437
2S 8.32218	0.00707	1.03977	-0.41703	3P 3.91166	0.01208	0.57218
2S 18.28940	0.03256	-0.14371	0.05920	3P 2.61991	-0.00301	0.53707
3S 4.60777	0.00250	-0.00086	0.54911	3P 7.88243	0.32338	-0.14245
3S 3.09084	-0.00082	0.00245	0.69451			
3S 7.00851	-0.00492	0.10322	-0.22866			
TITANIUM K(2)L(8)3S(2)3P(6) - 1S						
T.E.= -0.84519051D+03 P.E.= -0.16903709D+04 K.E.= 0.84518042D+03 V.T.= -0.20000119D+01						
S	1S	2S	3S	P	2P	3P
BASIS/ORB E	-185.27932	-23.48730	-4.76862	BASIS/ORB E	-19.85124	-3.65052
1S 21.64990	0.95310	-0.29255	0.10731	2P 10.12070	0.67900	-0.25319
1S 34.75470	0.02435	-0.00181	0.00118	2P 16.90970	0.05120	-0.01679
2S 8.82635	0.00738	1.03769	-0.42797	3P 4.23842	0.01343	0.56819
2S 18.96180	0.02761	-0.14660	0.06193	3P 2.95011	-0.00368	0.54337
3S 4.90094	0.00238	0.00594	0.50138	3P 8.41308	0.31841	-0.15126
3S 3.43212	-0.00085	0.00071	0.72611			
3S 7.70277	-0.00502	0.10619	-0.22191			

See page 183 for Explanation of Tables and Notes for Tables 32, 42, and 43

TABLE 31 (2). THE HARTREE-FOCK FUNCTIONS FOR Ar(<sup>1</sup>S) ISO-ELECTRICAL SERIES.

VANADIUM		K(2)L(8)3S(2)3P(6) - 1S					
		T.E.= -0.93707615D+03 P.E.= -0.18741410D+04 K.E.= 0.93706487D+03 V.T.= -0.20000120D+01					
S	1S	2S	3S	P	2P	3P	
BASIS/ORB E	-204.47345	-26.93620	-5.93945	BASIS/ORB E	-23.07607	-4.71364	
1S 22.56550	0.95599	-0.25798	0.11263	2P 10.63190	0.68796	-0.26644	
1S 35.92840	0.02586	-0.00107	0.00086	2P 17.77070	0.04962	-0.01692	
2S 9.33647	0.00805	1.03711	-0.43894	3P 4.57247	0.01264	0.55900	
2S 19.64550	0.02204	-0.15012	0.06503	3P 3.28636	-0.00350	0.55688	
3S 5.20116	0.00261	0.00808	0.47716	3P 8.88729	0.30928	-0.15820	
3S 3.76303	-0.00105	0.00001	0.74939				
3S 8.27824	-0.00552	0.11161	-0.22807				
CHROMIUM		K(2)L(8)3S(2)3P(6) - 1S					
		T.E.= -0.10338673D+04 P.E.= -0.20677244D+04 K.E.= 0.10338571D+04 V.T.= -0.20000099D+C1					
S	1S	2S	3S	P	2P	3P	
BASIS/ORB E	-224.67356	-30.64231	-7.22560	BASIS/ORB E	-26.55737	-5.89179	
1S 23.61250	0.95455	-0.30233	0.11681	2P 11.13350	0.69445	-0.27920	
1S 36.95490	0.02543	0.00C57	0.00043	2P 1E.59860	0.04876	-0.01698	
2S 9.84692	0.00579	1.04251	-0.45429	3P 4.84528	0.01210	0.58683	
2S 20.26380	0.02520	-0.15773	0.07074	3P 3.58363	-0.00361	0.53279	
3S 5.47956	0.00186	0.0C715	0.48141	3P 9.36156	0.30009	-0.16233	
3S 4.07790	-0.00080	0.00C06	0.75320				
3S 8.72097	-0.00383	0.11506	-0.23825				
MANGANESE		K(2)L(8)3S(2)3P(6) - 1S					
		T.E.= -0.113556100D+04 P.E.= -0.22711124D+04 K.E.= 0.11355514D+04 V.T.= -0.20000085D+01					
S	1S	2S	3S	P	2P	3P	
BASIS/ORB E	-245.87807	-34.60376	-8.42586	BASIS/ORB E	-30.29342	-7.18419	
1S 24.59050	0.95651	-0.31353	0.12264	2P 11.63060	0.69854	-0.28830	
1S 38.09260	0.02530	0.00526	-0.00077	2P 19.17010	0.05128	-0.01836	
2S 10.37600	0.00331	1.06261	-0.48258	3P 5.15336	0.01296	0.58520	
2S 20.39820	0.02427	-0.16889	0.08098	3P 3.51419	-0.00424	0.53816	
3S 5.77218	0.00118	0.00460	0.48906	3P 9.87281	0.29343	-0.16727	
3S 4.40302	-0.00054	0.00C28	0.76202				
3S 8.97707	-0.00217	0.11276	-0.24786				
IRON		K(2)L(8)3S(2)3P(6) - 1S					
		T.E.= -0.124215500D+04 P.E.= -0.24E42995D+04 K.E.= 0.12421446D+04 V.T.= -0.20000084D+01					
S	1S	2S	3S	P	2P	3P	
BASIS/ORB E	-268.08665	-38.82017	-10.13997	BASIS/CRB E	-34.28383	-8.59064	
1S 25.57180	0.95557	-0.31C82	0.12452	2P 12.11950	0.70037	-0.29642	
1S 39.22050	0.02659	0.00274	-C.00009	2P 19.71650	0.05429	-0.01996	
2S 10.79600	0.00438	1.06763	-0.48970	3P 5.45962	0.01403	0.58280	
2S 21.59560	0.02313	-0.16E49	0.08041	3P 4.24593	-0.00502	0.54450	
3S 6.06523	0.00165	0.00405	0.53291	3P 10.38690	0.28657	-0.17161	
3S 4.67921	-0.00075	0.00C68	0.73572				
3S 9.43532	-0.00299	0.10393	-0.26571				
COBALT		K(2)L(8)3S(2)3P(6) - 1S					
		T.E.= -0.13536473D+04 P.E.= -0.27C72840D+04 K.E.= 0.13536368D+04 V.T.= -0.20000078D+01					
S	1S	2S	3S	P	2P	3P	
BASIS/ORB E	-291.29827	-43.29015	-11.76720	BASIS/CRB E	-38.52737	-10.11029	
1S 26.55100	0.95533	-0.31207	-0.12692	2P 12.60270	0.70262	-0.30364	
1S 40.35800	0.02753	0.00237	-0.00021	2P 20.26990	0.05725	-0.02169	
2S 11.18560	0.00470	1.08366	0.50580	3P 5.79404	0.01503	0.55896	
2S 22.54780	0.02206	-0.16878	-0.08211	3P 4.59792	-0.00572	0.57298	
3S 6.35969	0.00187	0.00817	-0.53594	3P 10.89950	0.27938	-0.17616	
3S 4.99612	-0.00088	-0.00102	-0.74141				
3S 9.88438	-0.00330	0.08366	0.26729				

See page 183 for Explanation of Tables and Notes for Tables 32, 42, and 43

## ROOTHAAN-HARTREE-FOCK ATOMIC WAVEFUNCTIONS

 TABLE 31 (3). THE HARTREE-FOCK FUNCTIONS FOR Ar(<sup>1</sup>S) ISO-ELECTRICAL SERIES.

NICKEL K(2)L(8)3S(2)3P(6) - 1S						
T.E.= -0.14700365D+04 P.E.= -0.29400619D+04 K.E.= 0.1470C254D+04 V.T.= -0.20000076D+01						
S	1S	2S	3S	P	2P	3P
BASIS/ORB E	-315.51260	-48.01327	-13.50728	BASIS/ORB E	-43.02367	-11.74288
1S 27.53210	0.95626	-0.31950	-0.13205	2P 13.07570	0.70520	-0.31056
1S 41.49660	0.02773	0.00546	0.00111	2P 20.81670	0.06049	-0.02349
2S 11.71880	0.00345	1.09083	0.51807	3P 6.11495	0.01622	0.54100
2S 22.95270	0.02130	-0.17635	-0.08750	3P 4.54438	-0.00660	0.59527
3S 6.65430	0.00142	0.00871	-0.53848	3P 11.41190	0.27164	-0.17951
3S 5.31668	-0.00071	-0.00171	-0.74859			
2S 10.32350	-0.00241	0.08726	0.27895			
COPPER K(2)L(8)3S(2)3P(6) - 1S						
T.E.= -0.15913216D+04 P.E.= -0.3182E346D+04 K.E.= 0.15913130D+04 V.T.= -0.20000054D+01						
S	1S	2S	3S	P	2P	3P
BASIS/ORB E	-340.72925	-52.98903	-15.35987	BASIS/ORB E	-47.77225	-13.48813
1S 28.46750	0.95657	-0.32318	-0.13601	2P 13.55370	0.70774	-0.31806
1S 42.51170	0.02963	0.00619	0.00175	2P 21.48510	0.06268	-0.02446
2S 12.30370	0.00354	1.08723	0.52176	3P 6.32692	0.02015	0.58994
2S 23.55150	0.01855	-0.18413	-0.09168	3P 5.24165	-0.00961	0.54774
3S 6.92864	0.00155	0.00220	-0.59849	3P 11.55320	0.26451	-0.17934
3S 5.58654	-0.00079	0.00086	-0.70710			
3S 10.73970	-0.00249	0.10515	0.30611			
ZINC K(2)L(8)3S(2)3P(6) - 1S						
T.E.= -0.17175014D+04 P.E.= -0.34349949D+04 K.E.= 0.17174535D+04 V.T.= -0.20000046D+01						
S	1S	2S	3S	P	2P	3P
BASIS/ORB E	-366.94769	-58.21701	-17.32465	BASIS/ORB E	-52.77276	-15.34560
1S 29.50650	0.95584	-0.32760	-0.13892	2P 13.94150	0.71499	-0.32780
1S 43.54040	0.02917	0.00841	0.00233	2P 21.92530	0.06843	-0.02677
2S 12.78870	0.00171	1.09811	0.53687	3P 6.60671	0.02239	0.57930
2S 24.16770	0.02083	-0.19022	-0.09730	3P 5.60047	-0.01162	0.56114
3S 7.20447	0.00071	0.00345	-0.59749	3P 12.44070	0.24914	-0.17593
3S 5.92065	-0.00040	0.00001	-0.71534			
3S 11.15430	-0.00116	0.10014	0.30578			
GALLIUM K(2)L(8)3S(2)3P(6) - 1S						
T.E.= -0.18485755D+04 P.E.= -0.36971420D+04 K.E.= 0.18485665D+04 V.T.= -0.20000049D+01						
S	1S	2S	3S	P	2P	3P
BASIS/ORB E	-394.16798	-63.69713	-19.40187	BASIS/ORB E	-58.02511	-17.31558
1S 30.44280	0.95647	-0.33103	-0.14150	2P 14.42300	0.71901	-0.33268
1S 44.73860	0.03059	0.00914	0.00240	2P 22.52450	0.06992	-0.02836
2S 13.26860	0.00250	1.10087	0.54477	3P 6.94084	0.02125	0.56627
2S 24.87800	0.01793	-0.19314	-0.10055	3P 5.93340	-0.01105	0.58097
3S 7.50769	0.00125	0.00694	-0.49248	3P 12.92550	0.24285	-0.18168
3S 6.33872	-0.00073	-0.00179	-0.81211			
3S 11.73450	-0.00179	0.10001	0.30328			
GERMANIUM K(2)L(8)3S(2)3P(6) - 1S						
T.E.= -0.19845429D+04 P.E.= -0.39690798D+04 K.E.= 0.19845369D+04 V.T.= -0.20000030D+01						
S	1S	2S	3S	P	2P	3P
BASIS/ORB E	-422.38965	-69.42886	-21.59089	BASIS/ORB E	-63.52885	-19.39748
1S 31.53010	0.95598	-0.33315	-0.14344	2P 14.75130	0.72703	-0.34211
1S 45.85340	0.02868	0.01059	0.00278	2P 22.87830	0.07822	-0.03190
2S 13.85740	-0.00013	1.10220	0.55353	3P 7.19166	0.02506	0.57775
2S 25.53340	0.02206	-0.20272	-0.10735	3P 6.27742	-0.01431	0.57203
3S 7.79773	-0.00021	0.00021	-0.50973	3P 13.42170	0.22363	-0.17573
3S 6.66120	0.00008	0.00140	-0.81036			
3S 12.09980	0.00013	0.11158	0.32165			

See page 183 for Explanation of Tables and Notes for Tables 32, 42, and 43

TABLE 31 (4). THE HARTREE-FOCK FUNCTIONS FOR Ar(<sup>1</sup>S) ISO-ELECTRICAL SERIES.

ARSENIC K(2)L(8)3S(2)3P(6) - 1S						
T.E.= -0.21254034D+04 P.E.= -0.42507984D+04 K.E.= 0.21253951D+04 V.T.= -0.20000039D+01						
S	1S	2S	3S	P	2P	3P
BASIS/ORB E	-451.61292	-75.41210	-23.89200	BASIS/CRB E	-69.28389	-21.59153
1S 32.38890	0.95726	-0.33632	-0.14684	2P 15.26290	0.73701	-0.34951
1S 47.19670	0.03150	0.01C56	0.00318	2P 23.81070	0.07368	-0.03066
2S 14.27000	0.00267	1.112E6	0.55997	3P 7.53304	0.02596	0.53357
2S 26.31900	0.01568	-0.20093	-0.10607	3P 6.64103	-0.01531	0.62185
3S 8.12524	0.00157	0.0C628	-0.45554	3P 13.89800	0.21705	-0.17969
3S 7.01594	-0.00097	-0.00293	-0.86581			
3S 12.65980	-0.00200	0.09644	0.32090			
SELENIUM K(2)L(8)3S(2)3P(6) - 1S						
T.E.= -0.22711562D+04 P.E.= -0.45423096D+04 K.E.= 0.22711533D+04 V.T.= -0.20000013D+01						
S	1S	2S	3S	P	2P	3P
BASIS/ORB E	-481.83713	-81.64663	-26.30480	BASIS/ORB E	-75.29003	-23.89737
1S 33.43490	0.55660	-0.33765	-0.15028	2P 15.68840	0.73658	-0.35251
1S 48.20810	0.03090	0.01128	0.00445	2P 24.27370	0.07956	-0.03384
2S 15.04980	0.00073	1.08778	0.54320	3P 7.82160	0.03310	0.48520
2S 26.92630	0.01811	-0.21419	-0.10996	3P 7.C2400	-0.02119	0.67211
3S 8.39784	0.00040	-0.00361	-0.47244	3P 14.47990	0.20912	-0.17954
3S 7.32437	-0.00029	0.00373	-0.85487			
3S 13.27720	-0.00056	0.14284	0.35458			
BROMINE K(2)L(8)3S(2)3P(6) - 1S						
T.E.= -0.24218011D+04 P.E.= -0.48435930D+04 K.E.= 0.24217919D+04 V.T.= -0.20000038D+01						
S	1S	2S	3S	P	2P	3P
BASIS/ORB E	-513.06254	-88.13252	-28.82933	BASIS/ORB E	-81.54734	-26.31496
1S 34.37080	-0.95625	-0.34081	-0.15297	2P 16.11570	0.74880	-0.36280
1S 49.23140	-0.03286	0.01215	0.00492	2P 24.92190	0.07937	-0.03370
2S 15.63140	-0.00116	1.08581	0.54860	3P 7.99115	0.03083	0.64850
2S 27.53060	-0.01591	-0.22165	-0.11468	3P 7.27401	-0.02073	0.51474
3S 8.67188	-0.00074	-0.00563	-0.50711	3P 14.87570	0.19713	-0.17863
3S 7.63264	0.00051	0.00718	-0.83300			
2S 13.69300	0.00089	0.15271	0.37169			
KRYPTON K(2)L(8)3S(2)3P(6) - 1S						
T.E.= -0.25773377D+04 P.E.= -0.51546655D+04 K.E.= 0.25773278D+04 V.T.= -0.20000039D+01						
S	1S	2S	3S	P	2P	3P
BASIS/ORB E	-545.28876	-94.86534	-31.46553	BASIS/ORB E	-88.05544	-28.84431
1S 35.38470	-0.95651	-0.34090	-0.15664	2P 16.32810	0.76668	-0.37536
1S 50.45350	-0.03233	0.01185	0.00634	2P 25.22680	0.08832	-0.03800
2S 16.44510	-0.00048	1.05976	0.52240	3P 8.27472	0.03419	0.65971
2S 28.25400	-0.01653	-0.23213	-0.11426	3P 7.61803	-0.02397	0.50852
3S 8.98073	-0.00033	-0.01573	-0.46178	3P 15.31540	0.16704	-0.16911
3S 7.97166	0.00027	0.01147	-0.87558			
3S 14.45090	0.00043	0.15793	0.40197			

See page 183 for Explanation of Tables and Notes for Tables 32, 42, and 43

## ROOTHAAN-HARTREE-FOCK ATOMIC WAVEFUNCTIONS

 TABLE 32 (1). THE HARTREE-FOCK FUNCTIONS FOR K(<sup>2</sup>S) ISO-ELECTRICAL SERIES.\*  

CALCIUM K(2)L(8)3S(2)3P(6)4S(1), 2S  
 T.E.= -0.67656989D+03 P.E.= -0.13531385D+04 K.E.= 0.67656863D+03 V.T.= -0.200000190+01

	1S	2S	3S	4S	P	2P	3P
BASIS/ORB E	-149.60959	-17.06681	-2.48511	-0.41632	BASIS/ORB E	-13.87423	-1.58162
1S 19.97610	-0.94180	-0.28206	0.09893	-0.02780	2P 9.12850	0.67668	-0.22488
1S 32.14530	-0.01800	-0.00095	-0.00055	0.00012	2P 15.91600	0.04326	-0.01326
2S 17.24190	-0.05095	-0.15C43	0.05325	-0.01522	3P 7.38744	0.33394	-0.13928
2S 8.40484	-0.00210	0.89576	-0.32893	0.09358	3P 3.67247	0.01296	0.52031
3S 7.46798	0.00046	0.257C3	-0.22503	0.06910	3P 2.38393	-0.00491	0.54690
3S 3.95877	0.00002	0.00926	0.71538	-0.20373	3P 1.72715	0.00156	0.04753
3S 3.01613	-0.00002	0.00151	0.09977	-0.10885			
4S 3.09060	0.00004	-0.00196	0.36973	-0.05597			
4S 1.42597	-0.00001	0.000C75	0.01979	0.60382			
4S 1.00258	0.00002	-0.00116	-0.02197	0.53477			
4S 0.86831	-0.00001	0.000C69	0.01261	-0.06991			

SCANDIUM K(2)L(8)3S(2)3P(6)4S(C)3D(1), 2D  
 T.E.= -0.75909219D+03 P.E.= -0.15181851D+04 K.E.= 0.75909290D+03 V.T.= -0.19999991D+01

	1S	2S	3S
BASIS/ORB E	-166.46696	-19.63899	-3.11665
1S 20.89830	-0.94614	0.28576	0.10216
1S 33.33600	-0.01921	-0.00C65	-0.00038
2S 17.87910	-0.04450	0.15215	0.05844
2S 8.53851	-0.00201	-0.99760	-0.38408
3S 7.43271	0.00073	-0.15526	-0.22367
3S 4.76901	-0.00028	-0.00182	0.39042
3S 3.33073	0.00025	-0.00434	0.62139
3S 2.60953	-0.00008	0.00113	0.20328

	2P	3P	D	3D
BASIS/ORB E	-16.22993	-2.12937	BASIS/ORB E	-0.90446
2P 9.59270	0.68789	-0.23455	3D 3.68416	0.34607
2P 16.59040	0.04505	-0.01472	3D 8.60768	0.02900
3P 7.84646	0.31764	-0.14678	3D 5.01174	0.04541
3P 4.11238	0.01246	0.46900	3D 1.85681	0.64945
3P 2.68927	-0.00393	0.57005	3D 1.00715	0.06832
3P 2.08292	0.00144	0.08356		

TITANIUM K(2)L(8)3S(2)3P(6)4S(C)3D(1), 2D  
 T.E.= -0.84674921D+03 P.E.= -0.16934992D+04 K.E.= 0.84675001D+03 V.T.= -0.19999991D+01

	1S	2S	3S
BASIS/ORB E	-184.51504	-22.68E41	-4.06863
1S 22.02320	-0.94366	0.28564	0.10674
1S 34.95600	-0.01663	-0.00053	-0.00108
2S 18.91320	-0.05095	0.15511	0.05810
2S 9.10692	-0.00041	-0.96647	-0.37400
3S 8.32663	-0.00063	-0.17E23	-0.22716
3S 4.88396	0.00075	-0.02114	0.43393
3S 3.41639	-0.00075	0.01C26	0.68717
3S 2.83054	0.00038	-0.00490	0.07039

	2P	3P	D	3D
BASIS/ORB E	-19.05461	-2.97535	BASIS/ORB E	-1.59312
2P 9.97373	0.70437	-0.24843	3D 2.22666	0.61402
2P 16.97770	0.05060	-0.01832	3D 9.19926	0.03463
3P 8.23656	0.29369	-0.16204	3D 4.45190	0.31729
3P 4.73340	0.00749	0.38494	3D 3.45709	0.11104
3P 3.05281	0.00100	0.71878	3D 1.37743	0.03178
3P 2.02182	-0.00050	0.03219		

\*Note: The Function for K is given in Table 1.

See page 183 for Explanation of Tables and Notes for Tables 32, 42, and 43

TABLE 32 (2). THE HARTREE-FOCK FUNCTIONS FOR K(<sup>2</sup>S) ISO-ELECTRICAL SERIES.

VANADIUM K{2}L{8}3S{2}3P{6}4S{1}3D{1}, 2D  
 T.E.= -0.93944540D+03 P.E.= -0.18788891D+04 K.E.= 0.93944369D+03 V.T.= -0.20000018D+01

S	1S	2S	3S
BASIS/ORB E	-203.58046	-26.00579	-5.14875
1S 22.98030	-0.94834	0.29873	0.11000
1S 36.37280	-0.01612	-0.00351	-0.00057
2S 19.36360	-0.04698	0.15933	0.08688
2S 9.29061	0.00141	-1.05908	-0.44277
3S 8.18536	-0.00218	-0.08622	-0.21151
3S 5.31087	0.00208	-0.02150	0.41803
3S 3.79841	-0.00166	0.01078	0.71787
3S 3.02661	0.00067	-0.00457	0.08970

P	2P	3P	D	3D
BASIS/ORB E	-22.14991	-3.54780	BASIS/ORB E	-2.40838
2P 10.45830	0.67382	-0.25019	3D 2.83724	0.52539
2P 16.75840	0.07011	-0.02514	3D 9.99502	0.03110
3P 8.98880	0.29443	-0.15557	3D 4.81778	0.33798
3P 4.882249	0.03170	0.41730	3D 2.18827	0.17308
3P 3.56805	-0.02674	0.29021	3D 6.30589	0.02473
3P 3.09750	0.01290	0.41276		

CHROMIUM K{2}L{8}3S{2}3P{6}4S{0}3D{1}, 2D  
 T.E.= -0.103717102D+04 P.E.= -0.20743418D+04 K.E.= 0.10371716D+04 V.T.= -0.19999986D+01

S	1S	2S	3S
BASIS/ORB E	-223.65680	-29.58525	-6.34594
1S 24.22170	-0.92662	-0.27591	0.10889
1S 35.48040	-0.02245	-0.00793	0.00108
2S 21.58370	-0.06292	-0.15924	0.06037
2S 10.05930	-0.00132	0.94235	-0.37682
3S 9.62411	-0.00040	0.19027	-0.24592
3S 5.88623	0.00122	0.02552	0.19304
3S 4.48391	-0.00126	-0.00534	0.64496
3S 3.68959	0.00054	0.00117	0.34935

P	2P	3P	D	3D
BASIS/ORB E	-25.50815	-5.04048	BASIS/ORB E	-3.34529
2P 10.12440	0.77473	-0.25500	3D 3.52004	0.36340
2P 17.04880	0.08952	-0.03423	3D 10.50170	0.03300
3P 9.22243	0.13680	-0.13114	3D 5.40218	0.30611
3P 6.73446	0.04766	0.09875	3D 2.73837	0.36498
3P 4.48391	-0.00826	0.59014	3D 6.92062	0.01382
3P 3.38030	0.00280	0.45054		

MANGANESE K{2}L{8}3S{2}3P{6}4S{0}3D{1}, 2D  
 T.E.= -0.11399165D+04 P.E.= -0.22798133D+04 K.E.= 0.11398969D+04 V.T.= -0.20000172D+01

S	1S	2S	3S
BASIS/ORB E	-244.74118	-33.43326	-7.66873
1S 24.92980	-0.94686	0.25658	0.11804
1S 38.09340	-0.02004	0.00035	-0.00100
2S 21.38670	-0.04283	0.1629	0.06763
2S 10.80940	-0.00044	-0.93606	-0.38834
3S 9.88210	-0.00047	-0.23044	-0.27692
3S 5.80650	0.00080	-0.01197	0.40828
3S 4.27806	-0.00134	-0.00124	0.61843
3S 3.90195	0.00088	0.00164	-0.02026

P	2P	3P	D	3D
BASIS/ORB E	-29.12594	-6.25032	BASIS/ORB E	-4.40114
2P 9.59025	-0.86981	-0.37796	3D 3.77129	0.09108
2P 16.49100	-0.14067	-0.04475	3D 11.31810	0.03224
3P 6.15812	0.01432	-0.26522	3D 5.68742	0.36541
3P 5.34788	-0.04549	0.87998	3D 3.30806	0.57051
3P 3.41677	0.03516	0.65656	3D 7.34649	0.01290
3P 3.01142	-0.02156	-0.21506		

See page 183 for Explanation of Tables and Notes for Tables 32, 42, and 43

## ROOTHAAN-HARTREE-FOCK ATOMIC WAVEFUNCTIONS

 TABLE 32 (3). THE HARTREE-FOCK FUNCTIONS FOR K(<sup>2</sup>S) ISO-ELECTRICAL SERIES.

IRON            K(2)L(8)3S(2)3P(6)4S(C)3D(1), 2D  
 T.E.= -0.12476808D+04 P.E.= -0.24953414D+04 K.E.= 0.12476606D+04 V.T.= -0.20300161D+01

	1S	2S	3S
BASIS/ORB E	-266.63086	-37.53424	-9.10330
1S	25.60170	0.95549	-0.30911
1S	39.12300	0.02584	0.00223
2S	11.12230	0.00485	1.00925
2S	21.54300	0.02399	-0.17501
3S	7.06020	0.00726	-0.05523
3S	9.59524	-0.00560	0.20017
3S	4.67247	0.00161	-0.011C7
3S	5.72700	-0.00572	0.04512
			0.08118

	2P	3P	D	3D
BASIS/ORB E	-32.99994	-7.57571	BASIS/ORB E	-5.57389
2P	10.00200	-0.87792	3D	3.75374
2P	17.19370	-0.14099	3D	11.50000
3P	6.14060	0.15153	3D	6.09290
3P	5.52310	-0.23953	3D	2.55156
3P	3.47900	-0.03058	3D	7.90000
3P	4.32900	0.11139		0.00674
		0.54623		

COBALT            K(2)L(8)3S(2)3P(6)4S(C)3D(1), 2D  
 T.E.= -0.13604610D+04 P.E.= -0.27209C32D+04 K.E.= 0.13604423D+04 V.T.= -0.20000137D+01

	1S	2S	3S
BASIS/ORB E	-289.92561	-41.89075	-10.65278
1S	26.50770	-0.96429	-0.32008
1S	41.84510	-0.02278	0.00611
2S	21.47940	-0.01644	-0.19257
2S	12.01850	-0.00623	0.97208
3S	10.67720	0.00493	0.23625
3S	6.35674	-0.00749	0.01555
3S	5.26993	0.00994	-0.01012
3S	4.60443	-0.00426	0.00419
			0.30580

	2P	3P	D	3D
BASIS/ORB E	-37.12906	-9.01597	BASIS/ORB E	-6.86250
2P	11.09900	0.88635	3D	4.60229
2P	19.76020	0.06038	3D	12.12350
3P	8.26871	0.06177	3D	6.84788
3P	6.62312	0.00905	3D	3.41431
3P	3.92525	0.01348	3D	2.29023
3P	4.45206	-0.02119		-0.01836
		0.84120		

NICKEL            K(2)L(8)3S(2)3P(6)4S(C)3D(1), 2D  
 T.E.= -0.15435124D+04 P.E.= -0.3C670238D+04  
 K.E.= 0.15435114D+04 V.T.= -0.20000007D+01

	1S
BASIS/ORB E	-358.22938
1S	28.13600
1S	41.39050
2S	22.89320
2S	12.77800
3S	10.82400
3S	6.83918
3S	5.57297
3S	4.84728
	0.00049
	0.00043
	-0.00045
	0.00018

	2P	C	3D
BASIS/ORB E	-50.88505	BASIS/ORB E	-14.32732
2P	11.45240	3D	4.54487
2P	19.42130	3D	10.55550
3P	11.46580	3D	6.87337
3P	6.36465	3D	3.16341
3P	3.97607	3D	3.53053
3P	4.84105		-0.10287
	-0.05020		

See page 183 for Explanation of Tables and Notes for Tables 32, 42, and 43

TABLE 32 (4). THE HARTREE-FOCK FUNCTIONS FOR K(<sup>2</sup>S) ISO-ELECTRICAL SERIES.

COPPER      K(2)L(8)3S(2)3P(6)4S(C)3D(1), 2D  
 T.E.= -0.16010545D+04 P.E.= -0.32021035D+04 K.E.= 0.16010491D+04 V.T.= -0.20000034D+01

	S	1S	2S	3S
BASIS/ORB E	-339.12294	-51.36850	-14.09278	
1S 28.40620	-0.55897	-0.32633	0.13615	
1S 42.60040	-0.02993	0.00750	-0.00291	
2S 23.05620	-0.01448	-0.19810	0.09316	
2S 12.99450	-0.00531	0.98800	-0.45534	
3S 11.54550	0.00404	0.22950	-0.29908	
3S 6.74091	-0.00851	0.00344	0.32787	
3S 5.90627	0.01055	0.00391	0.67073	
3S 5.09099	-0.00347	-0.00175	0.23244	

	P	2P	3P	D	3D
BASIS/ORB E	-46.15004	-12.23721	BASIS/ORB E	-9.78408	
2P 12.24950	0.82253	-0.36250	3D 4.62990	0.65660	
2P 20.33310	0.09649	-0.03636	3D 13.05800	0.04550	
3P 11.62330	0.08631	-0.10931	3D 9.49078	-0.03333	
3P 7.21903	0.04537	0.23639	3D 3.55127	-0.03028	
3P 4.26901	0.00836	0.03486	3D 7.35749	0.41375	
3P 5.40234	-0.02673	0.87140			

ZINC      K(2)L(8)3S(2)3P(6)4S(C)3D(1), 2D  
 T.E.= -0.17288647D+04 P.E.= -0.34577168D+04 K.E.= 0.17288521D+04 V.T.= -0.20000073D+01

	S	1S	2S	3S
BASIS/ORB E	-365.22616	-56.48803	-15.98241	
1S 29.48900	-0.95693	0.32571	0.13770	
1S 43.56550	-0.02903	-0.00562	-0.00288	
2S 23.81830	-0.01989	0.20225	0.10010	
2S 13.14890	-0.00148	-1.05235	-0.50371	
3S 11.56040	0.00112	-0.16344	-0.28948	
3S 6.91223	-0.00162	-0.00249	0.64930	
3S 5.67239	0.00244	-0.00169	0.63913	
3S 5.03785	-0.00118	0.00074	-0.02675	

	P	2P	3P	D	3D
BASIS/ORB E	-51.04044	-14.01739	BASIS/ORB E	-11.41573	
2P 11.92640	0.89860	-0.42572	3D 5.63712	0.55784	
2P 20.11720	0.12647	-0.04521	3D 13.54240	0.04217	
3P 10.73000	-0.02697	-0.05577	3D 7.89840	0.26922	
3P 6.89912	0.04129	0.51387	3D 3.21219	-0.05618	
3P 5.39422	-0.02009	0.64754	3D 4.03520	0.23577	
3P 3.01181	0.00202	-0.00353			

\*Note: The Function for K is given in Table 1.

See page 183 for Explanation of Tables and Notes for Tables 32, 42, and 43

## ROOTHAAN-HARTREE-FOCK ATOMIC WAVEFUNCTIONS

 TABLE 33 (1). THE HARTREE-FOCK FUNCTIONS FOR Sc<sup>+</sup>(<sup>3</sup>F) ISO-ELECTRONIC SERIES.

SCANDIUM K(2)L(8)3S(2)3P(6)4S(C)3D(2), 3F  
 T.E.= -0.75950974D+03 P.E.= -0.15190209D+04 K.E.= 0.75951114D+03 V.T.= -0.19999981D+C1

	S	1S	2S	3S
BASIS/ORB E	-165.98191	-19.13262	-2.63251	
1S	20.89120	-0.94637	0.28925	0.10129
1S	33.33330	-0.01935	-0.00030	-0.00049
2S	17.88050	-0.04400	0.15321	0.05754
2S	8.53919	-0.00212	-1.00086	-0.38003
3S	7.32747	0.00084	-0.15731	-0.23497
3S	4.70217	-0.00039	0.00571	0.47311
3S	3.23133	0.00037	-0.00591	0.49288
3S	2.63303	-0.00016	0.00378	0.26476

	P	2P	3P	D	3D
BASIS/ORB E	-15.72595	-1.66008	BASIS/ORB E	-0.45481	
2P	9.59010	0.68831	-0.23003	3D 3.47301	0.29546
2P	16.58910	0.04512	-0.01454	3D 8.60700	0.02387
3P	7.84754	0.31662	-0.14450	3D 4.90755	0.06672
3P	4.17069	0.01309	0.42309	3D 1.80631	0.50176
3P	2.82651	-0.00359	0.49102	3D 1.03675	0.29574
3P	2.08275	0.00114	0.21546		

TITANIUM K(2)L(8)3S(2)3P(6)4S(C)3D(2), 3F  
 T.E.= -0.84773045D+03 P.E.= -0.16954688D+04 K.E.= 0.84773836D+03 V.T.= -0.19999907D+01

	S	1S	2S	3S
BASIS/ORB E	-183.86082	-22.00125	-3.44530	
1S	22.21800	-0.93818	0.28538	0.10256
1S	35.26590	-0.01292	-0.00029	-0.00051
2S	19.08140	-0.06288	0.15774	0.05994
2S	8.94222	0.00237	-1.00643	-0.38900
3S	8.07512	-0.00316	-0.13435	-0.21436
3S	4.92646	0.00272	-0.01724	0.45022
3S	3.44649	-0.00272	0.00684	0.54504
3S	2.85534	0.00133	-0.00349	0.21166

	P	2P	3P	D	3D
BASIS/ORB E	-18.37304	-2.37321	BASIS/ORB E	-1.02382	
2P	10.02460	0.70314	-0.24112	3D 2.05875	0.57909
2P	17.12830	0.04749	-0.017C4	3D 9.27984	0.C2998
3P	8.23349	0.29913	-0.16052	3D 4.49086	0.28070
3P	4.63475	0.00713	0.43508	3D 3.24907	0.15546
3P	2.86619	0.00074	0.69230	3D 1.21368	0.09172
3P	1.36749	-0.00019	0.01506		

VANADIUM K(2)L(8)3S(2)3P(6)4S(0)3D(2), 3F  
 T.E.= -0.94113652D+03 P.E.= -0.18822790D+04 K.E.= 0.94114248D+03 V.T.= -0.19999937D+01

	S	1S	2S	3S
BASIS/ORB E	-202.78730	-25.17774	-4.42185	
1S	22.99560	-0.9462C	0.29397	0.10639
1S	36.39660	-0.01675	-0.00124	0.00017
2S	19.73170	-0.04758	0.15570	0.06541
2S	9.19475	-0.00080	-1.07054	-0.43891
3S	7.98035	-0.00020	-0.06853	-0.22105
3S	5.17853	0.00045	-0.01652	0.58537
3S	3.33366	-0.00064	0.01330	0.84313
3S	3.02860	0.00046	-0.00563	-0.18165

	P	2P	3P	D	3D
BASIS/ORB E	-21.32585	-3.24446	BASIS/ORB E	-1.73823	
2P	10.54650	0.66668	-0.23376	3D 2.81227	0.36443
2P	16.76970	0.06767	-0.02631	3D 9.81281	0.03298
3P	8.99295	0.30623	-0.17402	3D 4.82096	0.34944
3P	5.12169	0.01953	0.37704	3D 2.18658	0.34740
3P	3.21967	-0.00297	0.74974	3D 1.18344	0.01698
3P	1.48920	0.00046	0.01256		

See page 183 for Explanation of Tables and Notes for Tables 32, 42, and 43

TABLE 33 (2). THE HARTREE-FOCK FUNCTIONS FOR Sc<sup>+</sup>(<sup>3</sup>F) ISO-ELECTRONIC SERIES.

CHROMIUM K(2)L(8)3S(2)3P(6)4S(C)3D(2), 3F  
 T.E.= -0.10397014D+04 P.E.= -0.20793997D+04 K.E.= 0.10396983D+04 V.T.= -0.20000030D+01

S	1S	2S	3S
BASIS/ORB E	-222.73504	-28.63185	-5.53159
1S 23.75180	-0.93840	-0.28170	0.11000
1S 35.29560	-0.03149	-0.00525	0.00103
2S 21.47290	-0.03585	-0.15111	0.05488
2S 10.00700	-0.00811	0.55555	-0.37227
3S 9.57395	0.00565	0.17582	-0.24396
3S 5.85561	-0.00362	0.02662	0.25886
3S 4.46068	0.00354	-0.00639	0.44626
3S 3.67059	-0.00137	0.00175	0.48886

P	2P	3P	D	3D
BASIS/ORB E	-24.55465	-4.24631	BASIS/ORB E	-2.58159
2P 10.35760	0.72003	-0.27064	3D 3.50156	0.31772
2P 16.65110	0.09783	-0.03525	3D 10.44890	0.03301
3P 9.28790	0.20736	-0.13185	3D 5.37420	0.30800
3P 5.68777	0.03334	0.17897	3D 2.55367	0.43245
3P 4.46068	-0.01261	0.43082	3D 6.88472	0.00278
3P 3.27360	0.00225	C.52015		

MANGANESE K(2)L(8)3S(2)3P(6)4S(C)3D(2), 3F  
 T.E.= -0.11434111D+04 P.E.= -0.22868031D+04 K.E.= 0.11433920D+04 V.T.= -0.20000167D+01

S	1S	2S	3S
BASIS/ORB E	-243.69570	-32.35279	-6.76482
1S 24.94630	-0.94664	0.29625	0.11556
1S 38.11850	-0.01966	0.00030	-0.00095
2S 21.40050	-0.04368	0.16E37	0.06651
2S 10.81660	-0.00010	-0.93412	-0.38042
3S 9.88857	-0.00076	-0.23109	-0.26883
3S 5.81026	0.00104	-0.01488	0.41251
3S 4.28083	-0.00178	0.00249	0.55017
3S 3.90452	0.00117	-0.00087	0.24022

P	2P	3P	D	3D
BASIS/ORB E	-28.04903	-5.37029	BASIS/ORB E	-3.54748
2P 9.59452	-0.86850	-0.36717	3D 3.77373	0.20748
2P 16.48710	-0.14073	-0.04389	3D 11.32530	0.02711
3P 6.16215	0.01970	-0.33881	3D 5.31403	0.32827
3P 5.49413	-0.05186	0.87E13	3D 2.95470	0.46027
2P 3.41902	0.03346	0.73159	3D 7.35131	0.06031
3P 3.01340	-0.02087	-0.17237		

IRON K(2)L(8)3S(2)3P(6)4S(0)3D(2), 3F  
 T.E.= -0.12522587D+04 P.E.= -0.25045030D+04 K.E.= 0.12522442D+04 V.T.= -0.20000116D+01

S	1S	2S	3S
BASIS/ORB E	-265.66370	-36.33464	-8.11705
1S 25.57840	-0.95605	-0.30916	-0.12166
1S 39.12300	-0.02626	0.00213	0.00120
2S 21.54300	-0.02255	-0.17449	-0.07455
2S 11.12230	-0.00540	1.00899	0.43145
3S 9.59524	0.00620	0.156E3	0.33553
3S 7.06020	-0.00771	-0.04682	-0.31302
3S 4.48847	-0.00129	-0.00704	-0.83037
3S 5.72700	0.00554	0.03662	-0.15879

P	2P	3P	D	3D
BASIS/ORB E	-31.80326	-6.61243	BASIS/ORB E	-4.63257
2P 10.01270	-0.87755	-0.36E20	3D 3.75374	0.63525
2P 17.19370	-0.14019	-0.04324	3D 11.50000	0.03249
3P 6.14060	-0.66844	1.55086	3D 6.09290	0.30368
3P 6.29310	0.61375	-1.15789	3D 2.55156	0.07765
2P 3.47900	-0.02240	0.15472	3D 7.90000	0.02765
3P 4.32900	0.06798	0.59920		

See page 183 for Explanation of Tables and Notes for Tables 32, 42, and 43

## ROOTHAAN-HARTREE-FOCK ATOMIC WAVEFUNCTIONS

 TABLE 33 (3). THE HARTREE-FOCK FUNCTIONS FOR Sc<sup>+</sup>(<sup>3</sup>F) ISO-ELECTRONIC SERIES.

COBALT K(2)L(8)3S(2)3P(6)4S(0)3D(2), 3F  
 T.E.= -0.136624010+04 P.E.= -0.27224781D+04 K.E.= 0.13662380D+04 V.T.= -0.20000015D+01

S	1S	2S	3S
BASIS/ORB E	-288.63871	-40.57578	-9.58674
1S 26.95260	-0.95510	-0.3C152	0.12307
1S 42.39190	-0.01485	0.00367	-0.00172
2S 22.42860	-0.04106	-0.18332	0.07856
2S 11.86120	0.00324	0.95E53	-0.41247
3S 10.81570	-C.00310	0.22207	-0.27251
3S 6.63738	0.00346	0.02327	0.21135
3S 5.33873	-0.00354	-0.01C79	0.62360
3S 4.45537	0.00130	0.00354	0.37222

P	2P	3P	D	3D
BASIS/ORB E	-35.81609	-7.57157	BASIS/ORB E	-5.83546
2P 11.25700	0.86769	-0.36798	3D 4.32211	0.48390
2P 19.72540	0.07702	-0.02606	3D 12.25000	0.C3280
3P 8.35735	0.11992	-0.27592	3D 6.75937	C.30423
3P 6.84587	-0.03661	0.55712	3D 3.43753	C.24853
3P 4.40511	0.00553	0.77849	3D 2.13127	-0.00062
3P 3.04467	-0.00105	-0.00373		

NICKEL K(2)L(8)3S(2)3P(6)4S(0)3D(2), 3F  
 T.E.= -0.14853489D+04 P.E.= -0.29706956D+04 K.E.= 0.14853467D+04 V.T.= -0.20000015D+01

S	1S	2S	3S
BASIS/ORB E	-312.61840	-45.07407	-11.17168
1S 27.51000	-0.95824	-0.32546	0.13119
1S 41.38350	-0.02740	0.0C882	-0.00318
2S 21.99890	-0.02048	-0.20539	0.09510
2S 12.52420	-0.00151	0.95543	-0.45075
3S 10.82220	0.00125	0.23223	-0.29604
3S 6.83801	-0.00189	-0.01462	0.33123
3S 5.57203	0.00245	0.02184	0.46278
2S 4.84646	-0.00105	-0.00821	0.44657

P	2P	3P	D	3D
BASIS/ORB E	-40.08516	-9.44555	BASIS/ORB E	-7.15426
2P 11.45530	0.83975	-0.35665	3D 4.92433	0.23681
2P 19.22250	0.11205	-0.04288	3D 12.80490	0.03588
3P 11.46400	0.04924	-0.07432	3D 6.93858	0.33757
3P 6.48552	0.05693	0.34576	3D 3.15500	-0.03042
3P 3.97541	0.01729	0.05483	3D 3.93775	0.48323
3P 4.84023	-0.04429	0.72598		

COPPER K(2)L(8)3S(2)3P(6)4S(0)3D(2), 3F  
 T.E.= -0.16095838D+04 P.E.= -0.32191642D+04 K.E.= 0.16095804D+04 V.T.= -0.20000021D+01

S	1S	2S	3S
BASIS/ORB E	-337.60252	-49.82829	-12.87129
1S 28.41300	-0.95895	-0.32417	0.13339
1S 42.59070	-0.02978	0.00163	-0.00269
2S 23.07160	-0.01480	-0.15779	0.09245
2S 12.99750	-0.00505	0.98656	-0.44922
3S 11.54290	0.00381	0.22930	-0.28583
3S 6.73935	-0.00805	0.01221	0.36548
3S 5.90492	0.00998	-0.00551	0.45172
3S 5.08983	-0.00328	0.00126	0.40609

P	2P	3P	D	3D
BASIS/ORB E	-44.60948	-11.03401	BASIS/ORB E	-8.58840
2P 12.19980	0.82021	-0.34821	3D 4.55568	0.65523
2P 20.25800	0.10024	-0.04089	3D 13.14780	0.04167
3P 12.04360	0.07501	-0.10266	3D 9.44571	-0.02972
3P 7.56525	0.05517	0.17564	3D 3.50638	0.00225
3P 4.26804	0.00937	0.05796	3D 7.39986	0.38918
3P 5.39987	-0.02703	0.86093		

See page 183 for Explanation of Tables and Notes for Tables 32, 42, and 43

TABLE 33 (4). THE HARTREE-FOCK FUNCTIONS FOR SC<sup>+(3)F</sup> ISO-ELECTRONIC SERIES.

ZINC            K{2}L{8}3S{2}3P{6}4S{1}3D{2}, 3F  
 T.E.= -0.173894180+04 P.E.= -0.347786970+04 K.E.= 0.173892800+04 V.T.= -0.200000790+01

S	1S	2S	3S
BASIS/ORB E	-363.59028	-54.83775	-14.68504
1S 29.41610	-0.95819	-0.33106	0.13540
1S 43.67000	-0.03024	0.00582	-0.00257
2S 23.76000	-0.01592	-0.19780	0.09905
2S 13.11730	-0.00352	1.05512	-0.50051
3S 11.58710	0.00275	0.15527	-0.26527
3S 6.92900	-0.00399	0.01739	0.56166
3S 5.68600	0.00577	-0.01727	0.61446
3S 5.05000	-0.00276	0.00813	0.06839

P	2P	3P	D	3D
BASIS/ORB E	-49.38848	-12.73637	BASIS/ORB E	-10.13726
2P 11.95490	0.91173	-0.40622	3D 5.57808	0.49064
2P 20.36580	0.11773	-0.04510	3D 13.50000	0.04204
3P 11.63670	-0.03256	-0.05691	3D 7.80000	0.27726
3P 7.16210	0.03819	0.41217	3D 3.18191	-0.06423
3P 5.29935	-0.01544	0.74368	3D 4.01098	0.30862
3P 2.98910	0.00200	-0.00519		

See page 183 for Explanation of Tables and Notes for Tables 32, 42, and 43

## ROOTHAAN-HARTREE-FOCK ATOMIC WAVEFUNCTIONS

 TABLE 34 (1). THE HARTREE-FOCK FUNCTIONS FOR  $Ti^+(^4F)$  ISO-ELECTRONIC SERIES.

TITANIUM K(2)L(8)3S(2)3P(6)4S(C)3D(3), 4F  
 T.E.= -0.84818639D+03 P.E.= -0.16963743D+04 K.E.= 0.84818787D+03 V.T.= -0.19999983D+01

S	1S	2S	3S
BASIS/ORB E	-183.35059	-21.47095	-2.93668
1S	21.99140	-0.94468	0.10302
1S	34.90540	-0.01721	0.00018
2S	18.88570	-0.04887	0.15783
2S	9.13379	-0.00085	-0.96944
3S	8.15958	-0.00027	-0.18454
3S	4.87702	0.00047	-0.00863
3S	3.41148	-0.00035	0.45482
3S	2.62460	0.00015	0.57532
		0.00003	0.17406

P	2P	3P	D	3D
BASIS/ORB E	-17.84503	-1.87885	BASIS/ORB E	-0.52472
2P	10.06340	0.68764	3D	2.03289
2P	16.63140	0.05305	3D	9.18612
3P	8.29658	0.30949	3D	4.44554
3P	4.52656	0.00797	3D	3.36221
3P	2.75253	0.00057	3D	1.17302
3P	1.35410	-0.00016		0.28115
		0.02231		

VANADIUM K(2)L(8)3S(2)3P(6)4S(C)3D(3), 4F  
 T.E.= -0.94217916D+03 P.E.= -0.18843512D+04 K.E.= 0.94217209D+03 V.T.= -0.20000075D+01

S	1S	2S	3S
BASIS/ORB E	-202.11295	-24.47412	-3.77797
1S	22.68620	-0.95270	0.11022
1S	35.32790	-0.02422	-0.00152
2S	19.06680	-0.03037	0.15110
2S	9.16308	-0.00313	-1.09209
3S	8.08172	0.00232	-0.03887
3S	5.23907	-0.00212	-0.05049
3S	3.97752	0.00201	0.03883
3S	3.25320	-0.00076	0.01558
			0.51653

P	2P	3P	D	3D
BASIS/ORB E	-20.62563	-2.62C65	BASIS/ORB E	-1.11536
2P	10.61930	0.68354	3D	2.92393
2P	17.22680	0.05466	3D	9.46905
3P	8.83331	0.30923	3D	4.93457
3P	5.06617	0.00920	3D	1.82643
2P	3.10519	0.00115	3D	1.19855
3P	1.70725	-0.00036		0.01811
		0.02683		

CHROMIUM K(2)L(8)3S(2)3P(6)4S(C)3D(3), 4F  
 T.E.= -0.10414756D+04 P.E.= -0.20829510D+04 K.E.= 0.10414755D+04 V.T.= -0.20000001D+01

S	1S	2S	3S
BASIS/ORB E	-221.92108	-27.7E467	-4.78274
1S	24.20250	-0.92735	-0.27648
1S	35.46650	-0.02271	-0.00772
2S	21.57540	-0.06167	-0.15E56
2S	10.05530	-0.00153	0.94313
3S	9.62032	-0.00010	0.18E66
3S	5.65407	0.00071	0.02569
3S	4.08070	-0.00073	-0.01142
3S	3.32977	0.00034	0.00440
			0.25479

P	2P	3P	D	3D
BASIS/ORB E	-23.71129	-3.51998	BASIS/ORB E	-1.85257
2P	10.78810	0.67446	3D	3.31765
2P	16.80730	0.08743	3D	10.49770
3P	9.45924	0.27072	3D	5.29867
3P	5.87748	0.02244	3D	2.31223
3P	3.48935	-0.00137	3D	0.42213
3P	1.76997	0.00029	3D	0.01304
		0.02186		

See page 183 for Explanation of Tables and Notes for Tables 32, 42, and 43

TABLE 34 (2). THE HARTREE-FOCK FUNCTIONS FOR Ti<sup>+</sup>(<sup>4</sup>F) ISO-ELECTRONIC SERIES.

MANGANESE K(2)L(8)3S(2)3P(6)4S(C)3D(3), 4F  
 T.E.= -0.11460488D+04 P.E.= -0.22920775D+04 K.E.= 0.11460287D+04 V.T.= -0.20000176D+01

	S	1S	2S	3S
BASIS/ORB E	-242.75194	-31.37459	-5.92268	
1S	24.84230	-0.94878	0.29852	0.11463
1S	37.96040	-0.02183	0.00003	-0.00115
2S	21.31320	-0.03787	0.16659	0.06446
2S	10.77090	-0.00171	-0.54500	-0.37790
3S	9.84780	0.00054	-0.21891	-0.26139
3S	5.78655	-0.00011	-0.01785	0.45155
3S	4.26336	0.00024	0.0C769	0.25061
3S	3.88830	-0.00014	-0.0CC440	0.50268

	P	2P	3P	D	3D
BASIS/ORB E	-27.07456	-4.55163	BASIS/ORB E	-2.71939	
2P	9.59766	-0.86850	-0.35E63	3D 3.31066	0.46105
2P	16.50700	-0.14020	-0.04262	3D 11.07480	0.03299
3P	6.13677	0.02463	-0.35071	3D 5.61976	0.35250
3P	5.52664	-0.05807	0.85992	3D 2.50817	0.24770
3P	3.40487	0.03461	0.66682	3D 1.38483	0.00421
3P	3.0092	-0.02183	-0.07364		

IRON K(2)L(8)3S(2)3P(6)4S(C)3D(3), 4F  
 T.E.= -0.12558830D+04 P.E.= -0.25117437D+04 K.E.= 0.12558607D+04 V.T.= -0.20000178D+01

	S	1S	2S	3S
BASIS/ORB E	-264.59590	-35.23310	-7.18845	
1S	25.35820	-0.96066	-0.30562	-0.11922
1S	39.12300	-0.03045	0.00029	0.00021
2S	21.54300	-0.00948	-0.17256	-0.07396
2S	11.12230	-0.01092	1.01359	0.43024
3S	9.21524	0.01590	0.22549	0.40051
3S	7.06020	-0.02085	-0.1C787	-0.46248
3S	4.35047	-0.00262	-0.01C86	-0.82538
3S	5.72700	0.01316	0.06506	-0.08867

	P	2P	3P	D	3D
BASIS/ORB E	-30.70508	-5.7C715	BASIS/ORB E	-3.71015	
2P	10.02490	-0.87416	-0.37831	3D 3.55374	0.59613
2P	17.19370	-0.14040	-0.04151	3D 12.50000	0.02372
3P	6.14060	0.12197	-0.04301	3D 6.09290	0.32977
3P	5.52310	-0.2C768	0.47539	3D 2.55156	0.11538
3P	3.47900	-0.02835	0.29102	3D 7.90000	0.02246
3P	4.32900	0.10090	0.3E677		

COBALT K(2)L(8)3S(2)3P(6)4S(0)3D(3), 4F  
 T.E.= -0.13709715D+04 P.E.= -0.27419257D+04 K.E.= 0.13709542D+04 V.T.= -0.20300126D+01

	S	1S	2S	3S
BASIS/ORB E	-287.44959	-39.35428	-8.57486	
1S	26.48760	-0.96476	-0.31760	0.12532
1S	41.87560	-0.02312	0.00482	-0.00237
2S	21.72330	-0.01470	-0.18783	0.C7911
2S	12.00960	-0.00761	0.96228	-0.40700
3S	10.68530	0.00594	0.23506	-0.28282
3S	6.36143	-0.00891	0.01760	0.46366
3S	5.27380	0.01176	-0.00554	-0.03205
3S	4.60785	-0.00503	0.00410	0.78487

	P	2P	3P	D	3D
BASIS/ORB E	-34.59733	-6.98230	BASIS/ORB E	-4.82077	
2P	11.12970	0.88202	C.36819	3D 4.58C79	0.31204
2P	19.74940	0.07971	-0.02588	3D 12.22120	0.03229
3P	7.97617	0.09111	-0.38160	3D 6.72991	0.28450
3P	6.96926	-0.01783	0.65954	3D 3.42986	0.44563
3P	3.92815	0.00893	0.21E52	3D 2.12641	0.00434
3P	4.45534	-0.01232	0.57455		

See page 183 for Explanation of Tables and Notes for Tables 32, 42, and 43

## ROOTHAAN-HARTREE-FOCK ATOMIC WAVEFUNCTIONS

 TABLE 34 (3). THE HARTREE-FOCK FUNCTIONS FOR Ti<sup>+</sup>(<sup>4</sup>F), ISO-ELECTRONIC SERIES.

NICKEL K(2)L(8)3S(2)3P(6)4S(0)3D(3), 4F  
 T.E.= -0.14913059D+04 P.E.= -0.29826102D+04 K.E.= 0.14913043D+04 V.T.= -0.20000010D+01

S	1S	2S	3S
BASIS/ORB E	-311.30893	-43.73628	-10.07929
1S 27.49730	-0.95829	-0.32307	0.12842
1S 41.40210	-0.02774	0.00748	-0.00282
2S 22.20070	-0.01936	-0.20124	0.09034
2S 12.51830	-0.00261	0.99128	-0.43662
3S 10.82710	0.0020E	0.23599	-0.29706
3S 6.84109	-0.00301	-0.01746	0.40645
3S 5.57452	0.00377	0.02675	0.16201
3S 4.84863	-0.00160	-0.01031	0.67340

P	2P	3P	D	3D
BASIS/ORB E	-38.74925	-8.37465	BASIS/ORB E	-6.04950
2P 11.46020	0.84256	-0.34934	3D 4.93493	0.16554
2P 19.27960	0.11013	-0.04145	3D 12.81080	0.03394
3P 11.46890	0.04559	-0.07242	3D 6.94171	0.32941
3P 6.62174	0.05834	0.30999	3D 3.15641	0.03281
3P 3.97717	0.01715	0.14752	3D 3.93951	0.51015
3P 4.84240	-0.04224	0.66986		

COPPER K(2)L(8)3S(2)3P(6)4S(0)3D(3), 4F  
 T.E.= -0.16168829D+04 P.E.= -0.32337633D+04 K.E.= 0.16168803D+04 V.T.= -0.20000016D+01

S	1S	2S	3S
BASIS/ORB E	-336.17491	-48.37642	-11.70003
1S 28.42950	-0.95873	-0.32583	0.13110
1S 42.56680	-0.02948	0.0C772	-0.00271
2S 23.08470	-0.01568	-0.19786	0.05084
2S 13.00490	-0.00447	0.98489	-0.44085
3S 11.53670	0.00334	0.22578	-0.27975
3S 6.73554	-0.00708	0.01756	0.46459
3S 5.90162	0.00875	-0.01108	0.14576
3S 5.08699	-0.00289	0.00309	0.60957

P	2P	3P	D	3D
BASIS/ORB E	-43.15847	-9.88275	BASIS/ORB E	-7.39474
2P 12.19300	0.82084	-0.34101	3D 4.49003	0.61982
2P 20.25780	0.10022	-0.04015	3D 13.14040	0.03957
3P 12.05040	0.07263	-0.09571	3D 9.44042	-0.02511
3P 7.56098	0.05765	0.19086	3D 3.50439	0.06213
3P 4.26565	0.01065	0.16998	3D 7.39571	0.36998
3P 5.33662	-0.02843	0.77360		

ZINC K(2)L(8)3S(2)3P(6)4S(0)3D(3), 4F  
 T.E.= -0.17476989D+04 P.E.= -0.34953835D+04 K.E.= 0.17476846D+04 V.T.= -0.20000082D+01

S	1S	2S	3S
BASIS/ORB E	-362.04512	-53.27349	-13.43595
1S 29.40950	-0.95782	-0.32617	0.13035
1S 43.67940	-0.03063	0.00715	-0.00093
2S 24.24530	-0.01514	-0.18791	0.09373
2S 12.98160	-0.00488	1.05573	-0.49481
3S 11.58950	0.00378	0.13896	-0.24349
3S 6.93051	-0.00531	0.02303	0.53217
3S 5.68723	0.00760	-0.02165	0.49362
3S 5.05110	-0.00362	0.00986	0.20786

P	2P	3P	D	3D
BASIS/ORB E	-47.82379	-11.50564	BASIS/ORB E	-8.85550
2P 11.71230	0.92655	-0.40857	3D 5.52783	0.44672
2P 19.96690	0.13173	-0.04558	3D 13.63290	0.03684
3P 10.98390	-0.08012	-0.07599	3D 7.95942	0.26350
3P 8.02513	0.04936	0.30278	3D 3.21461	-0.04768
3P 5.33955	-0.00946	0.87885	3D 4.05186	0.36197
3P 3.01976	0.00145	0.00467		

See page 183 for Explanation of Tables and Notes for Tables 32, 42, and 43

TABLE 35 (1). THE HARTREE-FOCK FUNCTIONS FOR V<sup>+(5)D</sup> ISO-ELECTRONIC SERIES.

VANADIUM K(2)L(8)3S(2)3P(6)4S(C)3D(4), 5D  
 T.E.= -0.942669360+03 P.E.= -0.18E53290D+04 K.E.= 0.94265961D+03 V.T.= -0.20000103D+01

S	1S	2S	3S
BASIS/ORB E	-201.57752	-23.91907	-3.24461
1S 22.51160	-0.95577	0.30630	0.10866
1S 35.22130	-0.02853	-0.00277	-0.00053
2S 19.21270	-0.01955	0.148E3	0.06154
2S 9.23968	-0.00765	-1.07091	-0.42860
3S 8.02855	0.00674	-0.07128	-0.21199
3S 5.23391	-0.00649	-0.02673	0.50868
3S 3.93990	0.00554	0.01638	0.25824
3S 3.13236	-0.00194	-0.00656	0.47612

P	2P	3P	D	3D
BASIS/ORB E	-20.07280	-2.10106	BASIS/ORB E	-0.58442
2P 10.58920	0.67432	-0.21949	3D 2.93145	0.33876
2P 16.78480	0.06245	-0.02666	3D 9.75240	0.02740
3P 8.86537	0.30944	-0.19352	3D 4.89947	0.26091
3P 5.31114	0.01004	0.38646	3D 1.93482	0.31459
3P 3.11403	0.00193	0.73704	3D 1.26261	0.23526
3P 1.70944	-0.00048	0.04788		

CHROMIUM K(2)L(8)3S(2)3P(6)4S(C)3D(4), 5D  
 T.E.= -0.10425756D+04 P.E.= -0.20E51639D+04 K.E.= 0.10425883D+04 V.T.= -0.19999878D+01

S	1S	2S	3S
BASIS/ORB E	-221.22304	-27.05884	-4.11584
1S 23.89530	-0.93454	-0.28126	0.10551
1S 35.24250	-0.02900	-0.00810	0.00117
2S 21.44100	-0.04445	-0.15362	0.05581
2S 9.99196	-0.00520	0.96098	-0.36746
3S 9.55952	0.00298	0.17C24	-0.22357
3S 5.61823	-0.00148	0.03224	0.30261
3S 4.35735	0.00127	-0.01261	0.47754
3S 3.30865	-0.00035	0.00320	0.40922

P	2P	3P	D	3D
BASIS/ORB E	-22.98870	-2.87231	BASIS/ORB E	-1.19645
2P 10.56270	0.67579	-0.21199	3D 3.69953	0.25314
2P 16.48250	0.10345	-0.04730	3D 10.26870	0.03242
3P 9.56221	0.24160	-0.20450	3D 5.30439	0.25485
3P 6.23083	0.03302	0.30001	3D 2.32695	0.49184
3P 3.50921	-0.00177	0.83439	3D 1.47575	0.10781
3P 1.77028	0.00053	0.04E43		

MANGANESE K(2)L(8)3S(2)3P(6)4S(C)3D(4), 5D  
 T.E.= -0.11479047D+04 P.E.= -0.22957919D+04 K.E.= 0.11478871D+04 V.T.= -0.20000153D+01

S	1S	2S	3S
BASIS/ORB E	-241.91516	-30.506C8	-5.15033
1S 24.87930	-0.94814	0.29775	0.11383
1S 38.01670	-0.02101	0.000C7	-0.00176
2S 21.34430	-0.03987	0.16717	0.06154
2S 10.78720	-0.00105	-0.54130	-0.36575
3S 9.86232	-0.00000	-0.22219	-0.26765
3S 5.79499	0.00036	-0.01889	0.49578
3S 4.26958	-0.00059	0.0C896	-0.08577
3S 3.89408	0.00040	-0.00540	0.80025

P	2P	3P	D	3D
BASIS/ORB E	-26.20969	-3.80119	BASIS/ORB E	-1.95592
2P 9.60545	-0.86866	-0.35028	3D 3.60415	0.34299
2P 16.53070	-0.13928	-0.04167	3D 10.93990	0.C3216
3P 6.14581	0.02692	-0.38270	3D 5.67612	0.3C117
3P 5.56589	-0.06150	0.87627	3D 2.43C96	0.42553
3P 3.40991	0.03497	0.53558	3D 1.38690	0.01531
3P 3.00537	-0.02227	0.07692		

See page 183 for Explanation of Tables and Notes for Tables 32, 42, and 43

## ROOTHAAN-HARTREE-FOCK ATOMIC WAVEFUNCTIONS

 TABLE 35 (2). THE HARTREE-FOCK FUNCTIONS FOR V<sup>+</sup>(<sup>5</sup>D) ISO-ELECTRONIC SERIES.

IRON            K(2)L(8)3S(2)3P(6)4S(0)3D(4),    5D  
 T.E.= -0.12586249D+04   P.E.= -0.25172352D+04   K.E.= 0.12586103D+04   V.T.= -0.20900116D+01

S	1S	2S	3S
BASIS/ORB E	-263.62896	-34.23344	-6.32223
1S 25.35820	-0.96003	-0.3C289	-0.11298
1S 39.12300	-0.03080	-0.00328	-0.00210
2S 21.75300	-0.01022	-0.17802	-0.07891
2S 11.12230	-0.00943	1.02446	0.43910
3S 8.26524	0.02218	0.39047	0.73313
2S 6.71020	-0.03877	-0.45127	-1.39877
3S 4.30447	-0.00346	-0.03256	-0.96867
3S 5.72700	0.02449	0.25946	0.64120

P	2P	3P	D	3D
BASIS/ORB E	-29.70905	-4.86388	BASIS/ORB E	-2.84657
2P 10.04070	-0.87324	-0.36626	3D 3.65374	0.48287
2P 17.19370	-0.13957	-0.04145	3D 12.50000	0.02199
3P 6.14060	0.63125	-1.77106	3D 6.09290	0.30091
3P 6.01810	-0.69327	2.19398	3D 2.55156	0.27181
3P 3.47900	-0.02223	0.42052	3D 8.00000	0.02417
3P 4.32900	0.06871	0.26662		

COBALT            K(2)L(8)3S(2)3P(6)4S(0)3D(4),    5D  
 T.E.= -0.13747236D+04   P.E.= -0.27494347D+04   K.E.= 0.13747111D+04   V.T.= -0.20300091D+01

S	1S	2S	3S
BASIS/ORB E	-286.35758	-38.23005	-7.62088
1S 26.47790	-0.96456	-0.31260	0.12242
1S 41.89040	-0.02349	0.00222	-0.00188
2S 22.28460	-0.01356	-0.17635	0.07036
2S 11.85000	-0.00948	0.96383	-0.39480
3S 10.68930	0.00748	0.22064	-0.28327
3S 6.36371	-0.01081	0.01830	0.59608
3S 5.27568	0.01420	-0.00778	-0.43060
3S 4.60951	-0.00606	0.00281	1.05806

P	2P	3P	D	3D
BASIS/ORB E	-33.47630	-6.05123	BASIS/ORB E	-3.86099
2P 11.15010	0.87995	-0.36048	3D 4.58551	0.20655
2P 19.75940	0.07904	-0.02479	3D 12.38080	0.02948
3P 7.90641	0.10273	-0.31467	3D 6.64929	0.29690
3P 6.71133	-0.02963	0.64575	3D 3.43109	0.50971
3P 3.92956	0.00487	0.47544	3D 2.31215	0.04859
3P 4.45693	-0.00462	0.26562		

NICKEL            K(2)L(8)3S(2)3P(6)4S(0)3D(4),    5D  
 T.E.= -0.14961892D+04   P.E.= -0.29923771D+04   K.E.= 0.14961878D+04   V.T.= -0.20000010D+01

S	1S	2S	3S
BASIS/ORB E	-310.09529	-42.49221	-9.04170
1S 27.48610	-0.95861	-0.32341	0.12749
1S 41.41850	-0.02789	0.00763	-0.00340
2S 22.18220	-0.01864	-0.20087	0.08632
2S 12.51310	-0.00291	0.99195	-0.42456
3S 10.83150	0.00232	0.23320	-0.30269
3S 6.84382	-0.00335	-0.01155	0.51084
3S 5.57672	0.00418	0.02050	-0.18065
3S 4.85055	-0.00178	-0.00752	0.91758

P	2P	3P	D	3D
BASIS/ORB E	-37.50780	-7.35936	BASIS/ORB E	-4.99651
2P 11.46460	0.83347	-0.33752	3D 4.05443	0.44959
2P 19.14040	0.11416	-0.04245	3D 12.81600	0.03203
3P 11.47330	0.05104	-0.07423	3D 6.94447	0.32159
3P 6.63435	0.05772	0.31627	3D 3.15765	0.17368
3P 3.97873	0.01638	0.26550	3D 4.85873	0.10523
3P 4.84432	-0.04022	0.54377		

See page 183 for Explanation of Tables and Notes for Tables 32, 42, and 43

TABLE 35 (3). THE HARTREE-FOCK FUNCTIONS FOR V<sup>+</sup>(<sup>5</sup>D) ISO-ELECTRONIC SERIES.

COPPER      K{2}L{8}3S{2}3P{6}4S{C}3D{4},    50  
 T.E.= -0.16230161D+04   P.E.= -0.3246C309D+04   K.E.= 0.16230149D+04   V.T.= -0.20000007D+01

	S	1S	2S	3S
BASIS/ORB E	-334.84151	-47.01553	-10.58128	
1S	28.43140	-0.95807	0.32077	0.12885
1S	42.56490	-0.02982	-0.0C502	-0.00264
2S	23.57980	-0.01556	0.18765	0.08029
2S	12.86630	-0.00525	-0.98435	-0.42325
3S	11.53600	0.00356	-0.21473	-0.29239
3S	7.16620	-0.00224	-0.01224	0.42626
3S	5.08366	0.00194	0.00099	0.81728
3S	4.05293	-0.00078	-0.00038	-0.00914

	P	2P	3P	D	3D
BASIS/ORB E	-41.79936	-8.78527	BASIS/ORB E	-6.25028	
2P	12.19220	0.80501	-0.32439	3D 4.41690	0.54647
2P	20.05210	0.10715	-0.04215	3D 13.13950	0.03954
3P	12.30880	0.07965	-0.09897	3D 9.43981	-0.03385
3P	7.56049	0.06250	0.18150	3D 3.50416	0.14940
3P	4.26537	0.01070	0.29195	3D 7.39523	0.37338
3P	5.39315	-0.03003	0.65698		

ZINC      K{2}L{8}3S{2}3P{6}4S{C}3D{4},    50  
 T.E.= -0.17551987D+04   P.E.= -0.35103929D+04   K.E.= 0.17551942D+04   V.T.= -0.20000260D+01

	S	1S	2S	3S
BASIS/ORB E	-360.59265	-51.75753	-12.23751	
1S	29.44920	-0.95729	-0.32612	0.12795
1S	43.62250	-0.02992	0.0C761	-0.00090
2S	24.21350	-0.01720	-0.18553	0.09373
2S	13.01600	-0.00365	1.05190	-0.48705
3S	11.57490	0.00275	0.14440	-0.23611
3S	6.92138	-0.00386	0.02397	0.54366
3S	5.67981	0.00556	-0.02284	0.30867
3S	5.04448	-0.00265	0.01046	0.37543

	P	2P	3P	D	3D
BASIS/ORB E	-46.34861	-10.32718	BASIS/ORB E	-7.62061	
2P	11.62140	0.93132	-0.39695	3D 5.53407	0.32991
2P	19.78790	0.13779	-0.05277	3D 13.61560	0.03566
3P	10.74450	-0.12063	-0.14564	3D 7.86938	0.27553
3P	8.82008	0.07459	0.32494	3D 3.21037	-0.01020
3P	5.30267	-0.00496	0.91643	3D 4.14274	0.43841
3P	3.01579	0.00091	0.01685		

See page 183 for Explanation of Tables and Notes for Tables 32, 42, and 43

## ROOTHAAAN-HARTREE-FOCK ATOMIC WAVEFUNCTIONS

 TABLE 36 (1). THE HARTREE-FOCK FUNCTIONS FOR Cr<sup>+</sup>(<sup>6</sup>S) ISO-ELECTRONIC SERIES.

CHROMIUM K(2)L(8)3S(2)3P(6)4S(C)3D(5), 6S  
 T.E.= -0.10431388D+04 P.E.= -0.20862725D+04 K.E.= 0.10431337D+04 V.T.= -0.20000049D+01

	S	1S	2S	3S
BASIS/ORB E	-220.65383	-26.46591	-3.55058	
1S 23.91730	-0.93447	-0.278C7	0.10216	
1S 35.53690	-0.02799	-0.00558	0.00246	
2S 21.61760	-0.04518	-0.15343	0.05680	
2S 10.07520	-0.00622	0.93E24	-0.35805	
3S 9.63943	0.00371	0.19484	-0.21888	
3S 5.66534	-0.00185	0.03051	0.21875	
3S 4.39352	0.00141	-0.00935	0.62978	
3S 3.07388	-0.00030	0.00185	0.33407	

	P	2P	3P	D	3D
BASIS/ORB E	-22.40208	-2.32147	BASIS/ORB E	-0.64925	
2P 10.82120	0.68145	-0.23274	3D 3.22269	C.31097	
2P 16.87160	0.08244	-0.03141	3D 10.51780	0.02544	
3P 9.34648	0.27459	-0.16773	3D 5.35538	0.25990	
3P 5.57901	0.01576	0.34907	3D 2.38079	0.26295	
3P 3.48331	-0.00019	0.68539	3D 1.46678	0.31458	
3P 2.21454	0.00010	0.12689			

MANGANESE K(2)L(8)3S(2)3P(6)4S(C)3D(5), 6S  
 T.E.= -0.11491083D+04 P.E.= -0.22981974D+04 K.E.= 0.11490891D+04 V.T.= -0.20000167D+01

	S	1S	2S	3S
BASIS/ORB E	-241.18764	-29.75114	-4.45545	
1S 24.95320	-0.94657	-0.29616	0.10977	
1S 38.12890	-0.01952	-0.00022	-0.00055	
2S 21.40630	-0.04418	-0.16E46	0.06518	
2S 10.81970	0.00067	0.93413	-0.36791	
3S 9.89126	-0.00208	0.22835	-0.23561	
3S 7.02482	0.00241	0.0CE13	-0.07922	
3S 5.70696	-0.00139	0.01C79	0.61666	
3S 3.69431	0.00019	-0.00019	0.64997	

	P	2P	3P	D	3D
BASIS/ORB E	-25.45798	-3.12542	BASIS/ORB E	-1.28800	
2P 9.61830	-0.86962	-0.34328	3D 3.65559	0.27716	
2P 16.57800	-0.13746	-0.04C65	3D 10.72370	0.03372	
3P 6.16383	0.03006	-0.46266	3D 5.53874	0.29360	
3P 5.64417	-0.06466	0.93328	3D 2.37383	0.45627	
3P 3.47672	0.02339	0.46C89	3D 1.48214	0.08058	
3P 2.83848	-0.01188	0.178E2			

IRON K(2)L(8)3S(2)3P(6)4S(0)3D(5), 6S  
 T.E.= -0.12606141D+04 P.E.= -0.25211989D+04 K.E.= 0.12605848D+04 V.T.= -0.20000232D+01

	S	1S	2S	3S
BASIS/ORB E	-262.76302	-33.33624	-5.52184	
1S 25.56420	-0.95612	-0.30E21	0.11332	
1S 39.12300	-0.02669	0.00C53	0.00031	
2S 21.75300	-0.02145	-0.17232	0.07322	
2S 11.12230	-0.00E24	1.00260	-0.41624	
3S 9.59524	0.00687	0.19940	-0.27405	
3S 7.06020	-0.00800	-0.04601	0.10304	
3S 3.93600	-0.00059	-0.00275	0.63599	
3S 5.81447	0.00483	0.03302	0.51945	

	P	2P	3P	D	3D
BASIS/ORB E	-28.81539	-4.08514	BASIS/ORB E	-2.07326	
2P 10.07620	-0.86817	-0.35664	3D 3.65374	0.45214	
2P 17.19370	-0.13889	-0.04C49	3D 11.50000	0.03091	
3P 6.14060	0.02670	-0.66E27	3D 6.09290	0.29862	
3P 5.79810	-0.05797	1.19420	3D 2.35365	0.33661	
3P 3.51400	0.01824	0.56136	3D 1.40000	0.00050	
3P 2.82800	-0.00906	0.023E4			

See page 183 for Explanation of Tables and Notes for Tables 32, 42, and 43

TABLE 36 (2). THE HARTREE-FOCK FUNCTIONS FOR Cr<sup>+</sup>(<sup>6</sup>S) ISO-ELECTRONIC SERIES.

COBALT      K(2)L(8)3S(2)3P(6)4S(1)3D(5),    6S  
 T.E.= -0.13776283D+04    P.E.= -0.2755235CD+04    K.E.= 0.13776047D+04    V.T.= -0.20000171D+01

	S	1S	2S	3S
BASIS/ORB	E	-285.36147	-37.20202	-6.72644
1S	26.18190	-0.97429	-0.31456	0.12114
1S	42.33990	-0.02647	0.00057	-0.00109
2S	22.52580	0.00621	-0.16181	0.06352
2S	11.58690	-0.02076	0.99108	-0.39877
3S	10.80990	0.01819	0.16663	-0.25449
3S	7.16729	-0.01316	0.03143	0.20266
3S	5.33268	0.00944	-0.00760	0.54111
3S	4.09560	-0.00291	0.00268	0.47174

	P	2P	3P	D	3D
BASIS/ORB	E	-32.45171	-5.17939	BASIS/ORB	E
2P	11.14490	0.87564	-0.35515	3D	4.41665
2P	19.62130	0.08158	-0.02413	3D	12.35710
3P	8.19365	0.08457	-0.12383	3D	6.72163
3P	5.97651	-0.01102	0.61322	3D	2.91384
3P	3.73004	0.00243	0.61464	3D	1.66824
3P	2.97771	-0.00034	-0.02570		0.00739

NICKEL      K(2)L(8)3S(2)3P(6)4S(0)3D(5),    6S  
 T.E.= -0.15001345D+04    P.E.= -0.30002619D+04    K.E.= 0.15001274D+04    V.T.= -0.20000047D+01

	S	1S	2S	3S
BASIS/ORB	E	-308.97380	-41.33927	-8.05905
1S	27.43450	-0.95971	-0.32491	0.12730
1S	41.49410	-0.02871	0.00798	-0.00413
2S	22.09740	-0.01561	-0.20012	0.08170
2S	12.48910	-0.00432	0.99675	-0.41307
3S	10.85180	0.00343	0.22404	-0.31564
3S	7.33910	-0.00254	0.00265	0.37641
3S	5.00650	0.00246	0.00555	0.63106
3S	4.30321	-0.00131	-0.00218	0.25438

	P	2P	3P	D	3D
BASIS/ORB	E	-36.35796	-6.39544	BASIS/ORB	E
2P	11.48020	0.81810	-0.33263	3D	4.68693
2P	18.89400	0.12116	-0.04183	3D	12.84000
3P	11.08520	0.06880	-0.07147	3D	7.04258
3P	6.26531	0.04045	0.47486	3D	3.25301
3P	4.23478	-0.02985	0.60849	3D	1.61980
3P	3.54757	0.01514	0.04953		0.00272

COPPER      K(2)L(8)3S(2)3P(6)4S(0)3D(5),    6S  
 T.E.= -0.16281201D+04    P.E.= -0.32561916D+04    K.E.= 0.16280715D+04    V.T.= -0.20000298D+01

	S	1S	2S	3S
BASIS/ORB	E	-333.59556	-45.74237	-9.51428
1S	28.60900	-0.95537	-0.31913	0.12801
1S	42.35740	-0.02654	0.00587	-0.00395
2S	23.46670	-0.02531	-0.15E57	0.07977
2S	13.06970	-0.00004	0.96796	-0.40153
3S	11.48180	-0.00030	0.24789	-0.33035
3S	7.59359	0.00027	0.00029	0.39419
3S	5.06806	-0.00021	0.01326	0.81545
3S	4.53615	0.00014	-0.00783	0.04923

	P	2P	3P	D	3D
BASIS/ORB	E	-40.52792	-7.74C39	BASIS/ORB	E
2P	10.85490	0.83102	-0.37288	3D	4.42735
2P	17.49660	0.21963	-0.07255	3D	13.30220
3P	10.17440	-0.04187	-0.01709	3D	7.38623
3P	6.47093	0.01405	0.55266	3D	3.07577
3P	4.33879	-0.00045	0.60609	3D	1.89464
3P	3.05844	-0.00049	-0.01296		-0.00681

See page 183 for Explanation of Tables and Notes for Tables 32, 42, and 43

## ROOTHAAN-HARTREE-FOCK ATOMIC WAVEFUNCTIONS

 TABLE 36 (3). THE HARTREE-FOCK FUNCTIONS FOR Cr<sup>+</sup>(<sup>6</sup>S) ISO-ELECTRONIC SERIES.

ZINC            K(2)L(8)3S(2)3P(6)4S(0)3D(5),    6S  
 T.E.=-0.17615859D+04    P.E.=-0.35231641D+04    K.E.= 0.17615782D+04    V.T.=-0.20000043D+01

	1S	2S	3S
BASIS/ORB E	-359.22974	-50.40733	-11.08925
1S 29.52350	-0.95645	-0.32269	0.12921
1S 43.55170	-0.02843	0.00643	-0.00303
2S 24.17400	-0.02098	-0.20557	0.08736
2S 13.34150	-0.00150	1.01451	-0.44096
3S 11.55680	0.00098	0.20718	-0.32802
3S 7.85654	-0.00066	-0.00768	0.44060
3S 5.25233	0.00085	0.01716	0.89585
3S 4.68334	-0.00052	-0.01000	-0.05297

P	2P	3P	D	3D
BASIS/ORB E	-44.96011	-9.20011	BASIS/ORB E	-6.47390
2P 12.11190	0.86835	-0.38375	3D 4.73073	0.61169
2P 20.11080	0.12466	-0.03994	3D 13.78270	0.03078
3P 10.72640	0.01296	-0.05271	3D 7.85654	0.30506
3P 6.95494	0.02767	0.47448	3D 3.24375	0.13583
3P 4.79604	-0.00761	0.67226	3D 1.81305	-0.00588
3P 2.07831	0.00084	0.00083		

See page 183 for Explanation of Tables and Notes for Tables 32, 42, and 43

TABLE 37 (1). THE HARTREE-FOCK FUNCTIONS FOR  $Mn^+(5D)$  ISO-ELECTRONIC SERIES.

MANGANESE K(2)L(8)3S(2)3P(6)4S(C)3D(6), 5D  
 T.E.= -0.11495205D+04 P.E.= -0.22590304D+04 K.E.= 0.11495098D+04 V.T.= -0.20300093D+01

	S	1S	2S	3S
BASIS/ORB E	-240.63259	-25.18004	-3.89721	
1S 25.35960	-0.93786	-0.28772	0.10779	
1S 38.74670	-0.01159	-0.00096	-0.00123	
2S 21.74770	-0.06613	-0.17426	0.06297	
2S 10.99850	0.00586	0.85172	-0.35882	
3S 10.05060	-0.00526	0.27194	-0.27099	
3S 5.90450	0.03362	0.01743	0.37111	
3S 4.27100	-0.00287	-0.00180	0.57596	
3S 3.19300	0.00097	0.00062	0.25522	

	P	2P	3P	D	3D
BASIS/ORB E	-24.88890	-2.57906	BASIS/ORB E	-0.66729	
2P 9.67526	-0.86762	-0.33546	3D 3.61648	0.39420	
2P 16.63330	-0.13343	-0.03952	3D 10.18720	0.03436	
3P 6.26300	0.03434	-1.15102	3D 5.78370	0.21646	
3P 5.97500	-0.03850	1.56691	3D 2.10220	0.34577	
3P 3.53200	0.00945	0.53284	3D 1.41200	0.18803	
3P 2.58598	-0.00412	0.16135			

IRON K(2)L(8)3S(2)3P(6)4S(C)3D(6), 5D  
 T.E.= -0.12616558D+04 P.E.= -0.25232953D+04 K.E.= 0.12616394D+04 V.T.= -0.20300130D+01

	S	1S	2S	3S
BASIS/ORB E	-262.04677	-32.55685	-4.82954	
1S 25.71370	-0.95555	-0.31636	0.11613	
1S 39.05300	-0.02255	0.00748	-0.00233	
2S 20.81600	-0.03136	-0.18579	0.08114	
2S 11.13180	0.00214	1.04533	-0.43452	
3S 9.17491	-0.00258	0.17352	-0.30260	
3S 6.42077	0.00259	-0.02793	0.51965	
3S 4.70947	-0.00183	0.02014	0.27831	
3S 3.76114	0.00067	-0.00558	0.50592	

	P	2P	3P	D	3D
BASIS/ORB E	-28.07886	-3.40587	BASIS/ORB E	-1.31689	
2P 10.04700	-0.86260	-0.34696	3D 3.82038	0.39478	
2P 17.01000	-0.14532	-0.04298	3D 11.38040	0.03041	
3P 6.76323	0.01250	-0.22344	3D 6.12682	0.26069	
3P 5.86095	-0.04233	0.65419	3D 2.26586	0.42103	
3P 3.64334	0.01532	0.51538	3D 1.41149	0.04002	
3P 2.82298	-0.00682	0.12428			

COBALT K(2)L(8)3S(2)3P(6)4S(C)3D(6), 5D  
 T.E.= -0.13794459D+04 P.E.= -0.27588716D+04 K.E.= 0.13794256D+04 V.T.= -0.20000147D+01

	S	1S	2S	3S
BASIS/ORB E	-284.50437	-36.31654	-5.92399	
1S 26.24860	-0.97197	-0.31253	0.11864	
1S 42.23860	-0.02587	0.00015	-0.00076	
2S 22.47140	0.00177	-0.16942	0.06659	
2S 11.90340	-0.01732	0.94464	-0.37776	
3S 10.78270	0.01447	0.23487	-0.27445	
3S 7.15000	-0.01072	0.01199	0.19911	
3S 5.31983	0.00713	0.00410	0.58195	
3S 3.91429	-0.00192	-0.00052	0.43774	

	P	2P	3P	D	3D
BASIS/ORB E	-31.56989	-4.39691	BASIS/ORB E	-2.11373	
2P 11.14440	0.87655	-0.34847	3D 4.79634	0.34086	
2P 19.63950	0.08123	-0.02399	3D 12.32740	0.02683	
3P 8.08691	0.08768	-0.14664	3D 6.92523	0.19581	
3P 6.07049	-0.01509	0.61672	3D 2.85514	0.51593	
3P 3.70410	0.00344	0.55523	3D 1.66429	0.04686	
3P 2.97054	-0.00072	0.01708			

See page 183 for Explanation of Tables and Notes for Tables 32, 42, and 43

## ROOTHAAN-HARTREE-FOCK ATOMIC WAVEFUNCTIONS

 TABLE 37 (2). THE HARTREE-FOCK FUNCTIONS FOR  $Mn^+(^5D)$  ISO-ELECTRONIC SERIES.

NICKEL      K(2)L(8)3S(2)3P(6)4S(0)3D(6),    5D  
 T.E.= -0.15028610D+04   P.E.= -0.30057198D+04   K.E.= 0.15028589D+04   V.T.= -0.20300014D+01

	S	1S	2S	3S
BASIS/ORB E	-307.98488	-40.32070	-7.15924	
1S	27.40540	-0.96009	-0.32200	0.12549
1S	41.53670	-0.02931	0.00613	-0.00389
2S	22.35820	-0.01354	-0.19498	0.07627
2S	12.47560	-0.00595	0.98796	-0.39920
3S	10.86330	0.00471	0.22822	-0.32365
3S	7.34658	-0.00345	-0.00040	0.40395
3S	5.01159	0.00328	0.00962	0.47299
3S	4.30768	-0.00174	-0.00406	0.39219

	P	2P	3P	D	3D
BASIS/ORB E	-35.34265	-5.52C95	BASIS/ORB E	-3.04404	
2P	11.49170	0.82096	-0.32730	3D 5.17689	0.32876
2P	18.96880	0.11866	-0.04040	3D 12.85350	0.02918
3P	11.06240	0.06756	-0.07669	3D 7.22622	0.20683
3P	6.27175	0.04221	0.47007	3D 3.14751	0.52987
3P	4.24330	-0.03127	0.51C40	3D 1.62146	0.01592
3P	3.55121	0.01599	0.15572		

COPPER      K(2)L(8)3S(2)3P(6)4S(C)3D(6),    5D  
 T.E.= -0.16318811D+04   P.E.= -0.32637020D+04   K.E.= 0.16318209D+04   V.T.= -0.20000369D+01

	S	1S	2S	3S
BASIS/ORB E	-332.48020	-44.55760	-8.52408	
1S	28.60220	-0.95553	-0.31917	0.12676
1S	42.36210	-0.02665	0.00587	-0.00415
2S	23.46920	-0.02489	-0.19524	0.07761
2S	13.06830	-0.00020	0.96781	-0.39402
3S	11.48310	-0.00018	0.24699	-0.32907
3S	7.59442	0.00019	0.00162	0.40645
3S	5.06861	-0.00011	0.01228	0.63791
3S	4.53665	0.00008	-0.00707	0.21591

	P	2P	3P	D	3D
BASIS/ORB E	-39.38600	-6.77181	BASIS/ORB E	-4.10055	
2P	10.83100	0.82015	-0.38188	3D 4.53191	0.46360
2P	17.37700	0.22777	-0.06796	3D 13.23100	0.03022
3P	10.12420	-0.03703	0.03043	3D 7.37161	0.29669
3P	5.93494	0.01418	0.65777	3D 3.09457	0.31076
3P	3.86205	-0.00316	0.44756	3D 1.89485	-0.00282
3P	2.77258	0.00068	-0.03148		

ZINC      K(2)L(8)3S(2)3P(6)4S(0)3D(6),    5D  
 T.E.= -0.17665053D+04   P.E.= -0.35330145D+04   K.E.= 0.17665091D+04   V.T.= -0.19999978D+01

	S	1S	2S	3S
BASIS/ORB E	-357.99081	-49.14011	-10.01290	
1S	29.49000	-0.95701	-0.32234	0.12737
1S	43.59940	-0.02901	0.00557	-0.00284
2S	24.20060	-0.01912	-0.19577	0.08563
2S	13.35600	-0.00246	1.01103	-0.43288
3S	11.56900	0.00177	0.21003	-0.32347
3S	7.86520	-0.00125	-0.00729	0.43907
3S	5.25811	0.00150	0.01752	0.74602
3S	4.68845	-0.00093	-0.01C10	0.09572

	P	2P	3P	D	3D
BASIS/ORB E	-43.69539	-8.14530	BASIS/ORB E	-5.27830	
2P	11.99830	0.87648	-0.36533	3D 4.78618	0.49032
2P	19.95250	0.13039	-0.04621	3D 13.82600	0.02982
3P	11.75010	-0.00619	-0.05781	3D 7.80155	0.30065
3P	7.24466	0.03082	0.4C881	3D 3.38218	0.27083
3P	4.76395	-0.00636	0.73C57	3D 1.81505	-0.00206
3P	2.08064	0.00083	0.00520		

See page 183 for Explanation of Tables and Notes for Tables 32, 42, and 43

TABLE 38 (1). THE HARTREE-FOCK FUNCTIONS FOR  $\text{Fe}^+(\text{F})$  ISO-ELECTRONIC SERIES.

IRON            K(2)L(8)3S(2)3P(6)4S(0)3D(7), 4F  
 T.E.= -0.12622208D+04 P.E.= -0.25244161D+04 K.E.= 0.126219530D+04 V.T.= -0.20000202D+01

S	1S	2S	3S
BASIS/ORB E	-261.44787	-31.97969	-4.23202
1S 25.64570	-0.95477	-0.30896	0.11308
1S 39.05820	-0.02504	0.00279	-0.00082
2S 21.50810	-0.02669	-0.17658	0.07277
2S 11.10400	-0.00266	1.01666	-0.41261
3S 9.57945	0.00210	0.17708	-0.28501
3S 7.04857	-0.00152	-0.01278	0.26762
3S 3.48518	-0.00017	-0.00153	0.38558
3S 4.98635	0.00075	0.01094	0.62569

P	2P	3P	D	3D
BASIS/JRB E	-27.46385	-2.82515	BASIS/ORB E	-0.71284
2P 10.08990	-0.86577	-0.34654	3D 3.73410	0.36676
2P 17.16540	-0.13925	-0.03574	3D 11.40830	0.02845
3P 6.53068	-0.00764	-0.15962	3D 6.06825	0.25671
3P 5.60563	-0.02317	0.68776	3D 2.26526	0.35649
3P 3.48315	0.01092	0.49273	3D 1.41442	0.17372
3P 2.57346	-0.00474	0.09895		

COBALT            K(2)L(8)3S(2)3P(6)4S(0)3D(7), 4F  
 T.E.= -0.13806688D+04 P.E.= -0.27613523D+04 K.E.= 0.13806688D+04 V.T.= -0.20000106D+01

S	1S	2S	3S
BASIS/ORB E	-283.74624	-35.53517	-5.19555
1S 26.31870	-0.96949	-0.31369	0.11873
1S 42.13220	-0.02527	0.00137	-0.00161
2S 22.41430	-0.00320	-0.16824	0.06378
2S 11.70850	-0.01491	0.97792	-0.38327
3S 10.75420	0.01224	0.19024	-0.26754
3S 7.13183	-0.00773	0.02407	0.25673
3S 5.06381	0.00483	-0.00304	0.61568
3S 3.72268	-0.00146	0.00152	0.35528

P	2P	3P	D	3D
BASIS/ORB E	-30.79101	-3.68590	BASIS/ORB E	-1.38311
2P 11.14100	0.87045	-0.34593	3D 4.95296	0.36301
2P 19.42750	0.08485	-0.02343	3D 12.29630	0.02707
3P 8.32565	0.08327	-0.08083	3D 7.03565	0.14777
3P 5.75727	-0.00735	0.60577	3D 2.74850	0.49771
3P 3.57166	0.00256	0.54526	3D 1.69027	0.11388
3P 2.24143	-0.00029	0.02063		

NICKEL            K(2)L(8)3S(2)3P(6)4S(0)3D(7), 4F  
 T.E.= -0.15049162D+04 P.E.= -0.30098191D+04 K.E.= 0.15049029D+04 V.T.= -0.20000089D+01

S	1S	2S	3S
BASIS/ORB E	-307.08733	-39.39483	-6.32204
1S 27.24610	-0.96347	-0.32328	0.12275
1S 41.76990	-0.03180	0.00526	-0.00251
2S 22.22730	-0.00424	-0.15624	0.08099
2S 12.40170	-0.01033	1.01152	-0.41653
3S 10.50560	0.00899	0.21578	-0.32570
3S 7.38754	-0.00684	-0.01658	0.41617
3S 5.03946	0.00445	0.01575	0.55606
3S 4.00357	-0.00179	-0.00513	0.32155

P	2P	3P	D	3D
BASIS/ORB E	-34.42002	-4.70385	BASIS/ORB E	-2.20188
2P 11.55420	0.83944	-0.33646	3D 4.76011	0.37504
2P 19.37840	0.10481	-0.03241	3D 12.92740	0.02687
3P 10.51700	0.06609	-0.05558	3D 7.17214	0.22445
3P 6.07014	0.04029	0.53290	3D 2.83172	0.47501
3P 4.21162	-0.03546	0.29016	3D 1.63056	0.02722
3P 3.57112	0.01879	0.31455		

See page 183 for Explanation of Tables and Notes for Tables 32, 42, and 43

## ROOTHAAN-HARTREE-FOCK ATOMIC WAVEFUNCTIONS

 TABLE 38 (2). THE HARTREE-FOCK FUNCTIONS FOR  $\text{Fe}^+(\text{F})$  ISO-ELECTRONIC SERIES.

COPPER      K(2)L(8)3S(2)3P(6)4S(C)3D(7), 4F  
 T.E.= -0.16348882D+04   P.E.= -0.32697435D+04   K.E.= 0.16348553D+04   V.T.= -0.20000201D+01

S	1S	2S	3S
BASIS/ORB E	-331.45117	-43.53816	-7.58950
1S 28.55030	-0.95643	0.31691	0.12427
1S 42.43830	-0.02756	-0.00411	-0.00339
2S 23.51100	-0.02191	0.20183	0.07829
2S 13.24590	-0.00176	-0.94654	-0.38123
3S 11.50300	0.00096	-0.27931	-0.32913
3S 7.37587	-0.00065	0.00901	0.45222
3S 5.07770	0.00096	-0.02538	0.35514
3S 4.54483	-0.00059	0.01505	0.44697

P	2P	3P	D	3D
BASIS/ORB E	-38.33022	-5.85676	BASIS/ORB E	-3.15429
2P 10.43860	0.92546	-0.40950	3D 4.55911	0.43640
2P 17.72840	0.21128	-0.06480	3D 13.20120	0.02901
3P 10.15480	-0.14676	0.05698	3D 7.38487	0.27967
3P 6.17397	0.03506	0.60095	3D 2.94689	0.36295
3P 3.94292	-0.02707	0.58420	3D 1.82738	0.00512
3P 3.47631	0.01665	-0.05922		

ZINC      K(2)L(8)3S(2)3P(6)4S(C)3D(7), 4F  
 T.E.= -0.17705866D+04   P.E.= -0.35411630D+04   K.E.= 0.17705764D+04   V.T.= -0.20000058D+01

S	1S	2S	3S
BASIS/ORB E	-356.83564	-47.95526	-8.98828
1S 29.41180	-0.95833	-0.32156	0.12611
1S 43.70900	-0.03032	0.00483	-0.00275
2S 24.26180	-0.01481	-0.19817	0.08233
2S 13.38910	-0.00471	1.00361	-0.42071
3S 11.59710	0.00364	0.21762	-0.32750
3S 7.88508	-0.00262	-0.00873	0.44883
3S 5.27136	0.00302	0.01986	0.57018
3S 4.70017	-0.00187	-0.01144	0.26409

P	2P	3P	D	3D
BASIS/ORB E	-42.51346	-7.14244	BASIS/ORB E	-4.23343
2P 12.21530	0.85765	-0.36160	3D 4.79815	0.46845
2P 20.16540	0.12153	-0.03861	3D 13.78360	0.02875
3P 10.76670	0.03021	-0.06748	3D 7.82117	0.28437
3P 6.96467	0.02374	0.50244	3D 3.19763	0.32149
3P 4.49515	-0.00486	0.65384	3D 1.64789	-0.00147
3P 1.89572	0.00070	0.00253		

See page 183 for Explanation of Tables and Notes for Tables 32, 42, and 43

TABLE 39 (1). THE HARTREE-FOCK FUNCTIONS FOR  $\text{Co}^+(\text{F})$  ISO-ELECTRONIC SERIES.

COBALT      K(2)L(8)3S(2)3P(6)4S(0)3D(8), 3F  
 T.E.= -0.138112820D+04 P.E.= -0.276224750D+04 K.E.= 0.138111930D+04 V.T.= -0.200000640D+01

S	1S	2S	3S
BASIS/ORB E	-283.15239	-34.92573	-4.59802
1S 26.49780	-0.96415	-0.31241	0.11656
1S 41.86020	-0.02321	0.00234	-0.00139
2S 22.26840	-0.01479	-0.17772	0.06991
2S 11.86770	-0.00854	0.96368	-0.38280
3S 10.68120	0.00674	0.22015	-0.26588
3S 7.08540	-0.00457	0.01387	0.22682
3S 5.15265	0.00277	0.00153	0.64409
3S 3.60786	-0.00068	0.00036	0.35474

P	2P	3P	D	3D
BASIS/ORB E	-30.18352	-3.09574	BASIS/ORB E	-0.73473
2P 11.13470	0.87718	-0.34380	3D 4.99975	0.30194
2P 19.55780	0.08223	-0.02297	3D 11.56820	0.02985
3P 7.84410	0.09482	-0.13968	3D 7.01733	0.13832
3P 5.96817	-0.02589	0.63154	3D 2.97339	0.43113
3P 3.59600	0.00580	0.56483	3D 1.62864	0.28419
3P 2.22684	-0.00100	0.03548		

NICKEL      K(2)L(8)3S(2)3P(6)4S(0)3D(8), 3F  
 T.E.= -0.150602950D+04 P.E.= -0.301205340D+04 K.E.= 0.150602390D+04 V.T.= -0.200000370D+01

S	1S	2S	3S
BASIS/ORB E	-306.33325	-38.61855	-5.58998
1S 27.44620	-0.95915	-0.31765	0.11827
1S 41.47700	-0.02873	0.00412	-0.00129
2S 22.39170	-0.01623	-0.20486	0.08729
2S 12.49460	-0.00402	1.00594	-0.41967
3S 10.32110	0.00311	0.24400	-0.31399
3S 6.90563	-0.00283	-0.04791	0.53349
3S 5.00445	0.00237	0.03991	0.30346
3S 4.04433	-0.00094	-0.01434	0.45091

P	2P	3P	D	3D
BASIS/ORB E	-33.64689	-3.98788	BASIS/ORB E	-1.41822
2P 11.47560	0.82845	-0.325E2	3D 4.86729	0.35355
2P 19.07920	0.11591	-0.03683	3D 12.83450	0.02753
3P 11.22600	0.05842	-0.05319	3D 7.12212	0.20286
3P 6.26272	0.05802	0.37C67	3D 2.75130	0.48187
3P 4.83135	-0.03491	0.39265	3D 1.61913	0.08941
3P 3.40620	0.00823	0.37098		

COPPER      K(2)L(8)3S(2)3P(6)4S(0)3D(8), 3F  
 T.E.= -0.163681590D+04 P.E.= -0.327357890D+04 K.E.= 0.163676300D+04 V.T.= -0.200003240D+01

S	1S	2S	3S
BASIS/ORB E	-330.55359	-42.61550	-6.74521
1S 28.58670	-0.95582	0.31746	0.12340
1S 42.36400	-0.02695	-0.00478	-0.00368
2S 23.47030	-0.02399	0.20275	0.07789
2S 13.22290	-0.C.0056	-0.95177	-0.37999
3S 11.48360	0.00007	-0.27349	-0.32044
3S 7.19185	0.00000	0.00752	0.51000
3S 5.06885	0.00010	-0.02365	0.10261
3S 4.53686	-0.00006	0.01369	0.63909

P	2P	3P	D	3D
BASIS/ORB E	-37.41020	-5.03332	BASIS/ORB E	-2.25096
2P 10.82100	0.82056	-0.37C55	3D 4.69645	0.38122
2P 17.37540	0.22834	-0.06616	3D 13.07760	0.02913
3P 10.11900	-0.03875	0.02131	3D 7.37194	0.25907
3P 5.93912	0.01532	0.67304	3D 2.90714	0.41901
3P 3.66218	-0.00430	0.49145	3D 1.82419	0.04543
3P 2.96731	0.00186	-0.04439		

See page 183 for Explanation of Tables and Notes for Tables 32, 42, and 43

## ROOCHAAN-HARTREE-FOCK ATOMIC WAVEFUNCTIONS

TABLE 39 (2). THE HARTREE-FOCK FUNCTIONS FOR  $\text{Co}^+(^3\text{F})$  ISO-ELECTRONIC SERIES.

ZINC            K(2)L(8)3S(2)3P(6)4S(0)3D(8),    3F  
 T.E.= -0.17734664D+04    P.E.= -0.35469188D+04    K.E.= 0.17734524D+04    V.T.= -0.20000079D+01

S	1S	2S	3S	
BASIS/ORB E	-355.80688	-46.89867	-8.04492	
1S 29.34090	-0.95961	-0.32103	0.12566	
1S 43.79750	-0.03146	0.00389	-0.00299	
2S 24.31120	-0.01089	-0.19678	0.07848	
2S 13.41590	-0.03669	0.99770	-0.40849	
3S 11.61970	0.00528	0.22380	-0.33694	
3S 7.90114	-0.00383	-0.01013	0.47121	
3S 5.28206	0.00436	0.02186	0.39031	
3S 4.70964	-0.00270	-0.01253	0.42841	
P	2P	3P	D	3D
BASIS/ORB E	-41.46000	-6.21954	BASIS/ORB E	-3.21963
2P 12.35450	0.85765	-0.35553	3D 4.99306	0.39454
2P 20.48440	0.11031	-0.03420	3D 13.83710	0.02919
3P 10.50410	0.04582	-0.07899	3D 7.75046	0.26692
3P 6.94964	0.01958	0.52220	3D 3.12124	0.42017
3P 4.37277	-0.00384	0.64040	3D 1.71065	0.00695
3P 2.13152	0.00082	0.00645		

See page 183 for Explanation of Tables and Notes for Tables 32, 42, and 43

TABLE 40. THE HARTREE-FOCK FUNCTIONS FOR  $\text{Ni}^+(\text{D}_2)$  ISO-ELECTRONIC SERIES.

NICKEL      K(2)L(8)3S(2)3P(6)4S(C)3D(9), 2D  
 T.E.= -0.15065903D+04 P.E.= -0.30131781D+04 K.E.= 0.15065878D+04 V.T.= -0.20000316D+01

	S	1S	2S	3S
BASIS/ORB E	-305.70319	-37.97248	-4.96011	
1S	27.45160	-0.95953	0.32451	0.12109
1S	41.46910	-0.02838	0.00795	-0.00318
2S	22.12550	-0.01652	-0.20037	0.06235
2S	12.49710	-0.00366	0.95579	-0.40541
3S	10.84510	0.00280	0.22474	-0.28C80
3S	7.33471	-0.00207	0.00266	0.28960
3S	5.30118	0.00127	0.00461	0.61346
3S	3.75824	-0.00032	-0.00014	0.34474

	P	2P	3P	D	3D
BASIS/ORB E	-33.00252	-3.36587	BASIS/ORB E	-0.76920	
2P	11.47350	0.82345	3P	4.75253	0.33129
2P	19.06180	0.11781	3P	12.83200	0.02520
3P	11.48690	0.05987	3P	7.12077	0.20378
3P	6.33446	0.05874	3P	2.76709	0.41773
3P	4.83042	-0.03258	3P	1.57027	0.21053
3P	3.26358	0.00723		0.34528	

COPPER      K(2)L(8)3S(2)3P(6)4S(C)3D(9), 2D  
 T.E.= -0.16380834D+04 P.E.= -0.32761485D+04 K.E.= 0.16380651D+04 V.T.= -0.20000112D+01

	S	1S	2S	3S
BASIS/ORB E	-329.76836	-41.80541	-5.98293	
1S	28.44790	-0.95804	0.32104	0.12095
1S	42.54010	-0.02945	-0.00547	-0.00228
2S	23.56670	-0.01634	0.18777	0.07760
2S	12.88110	-0.00451	-0.98233	-0.40305
3S	11.52970	0.00285	-0.21631	-0.25376
3S	6.43914	-0.00306	-0.02331	0.80148
3S	5.08981	0.00496	0.02096	-0.67321
3S	4.55572	-0.00271	-0.01121	1.08895

	P	2P	3P	D	3D
BASIS/ORB E	-36.60370	-4.28735	BASIS/ORB E	-1.47153	
2P	12.07520	0.84736	3P	4.48665	0.41646
2P	20.14760	0.09934	3P	13.26420	0.02630
3P	10.15520	0.07609	3P	7.36110	0.25763
3P	5.96866	0.01339	3P	2.67500	0.35074
3P	3.67422	-0.00521	3P	1.84690	0.10582
3P	2.56840	0.00226		0.00279	

ZINC      K(2)L(8)3S(2)3P(6)4S(0)3D(9), 2D  
 T.E.= -0.17755800D+04 P.E.= -0.35511675D+04 K.E.= 0.17755874D+04 V.T.= -0.19999958D+01

	S	1S	2S	3S
BASIS/ORB E	-354.87396	-45.94032	-7.16917	
1S	29.71610	-0.95444	-0.32572	0.12624
1S	43.24000	-0.02456	0.01019	-0.00539
2S	24.00000	-0.03107	-0.20362	0.08126
2S	13.24730	0.00449	1.03472	-0.42230
3S	11.47710	-0.00410	0.18C84	-0.32212
3S	7.80000	0.00308	0.00437	0.51108
3S	5.21464	-0.00335	0.00438	0.28150
3S	4.65000	0.00210	-0.00146	0.50221

	P	2P	3P	D	3D
BASIS/ORB E	-40.50473	-5.36284	BASIS/ORB E	-2.32310	
2P	12.19890	0.85092	3P	5.39016	0.33216
2P	19.96580	0.12703	3P	13.50000	0.03178
3P	10.64670	0.03328	3P	7.73719	0.22709
3P	6.95210	0.02109	3P	3.16273	0.50083
3P	4.27494	-0.00356	3P	1.68861	0.04641
3P	2.10429	0.00082		0.01105	

See page 183 for Explanation of Tables and Notes for Tables 32, 42, and 43

## ROOTHAAN-HARTREE-FOCK ATOMIC WAVEFUNCTIONS

 TABLE 41. THE HARTREE-FOCK FUNCTIONS FOR Cu<sup>+</sup>(<sup>1</sup>S) ISO-ELECTRONIC SERIES.

COPPER      K(2)L(8)3S(2)3P(6)4S(C)3D(10), 1S  
 T.E.= -0.16387276D+04   P.E.= -0.32774473D+04   K.E.= 0.16387196D+04   V.T.= -0.20300049D+01

	S	1S	2S	3S
BASIS/ORB	E	-329.10745	-41.12805	-5.32511
1S	28.45300	-0.55851	-0.32587	0.12160
1S	42.53270	-0.02906	0.0C819	-0.00297
2S	23.10340	-0.01709	-0.19715	0.08245
2S	13.01550	-0.00297	0.98177	-0.40335
3S	11.52770	0.00168	0.23062	-0.25689
3S	6.72990	-0.00089	0.01499	0.55723
3S	4.61704	0.00078	-0.00405	0.54604
3S	3.53495	-0.00031	0.00151	0.11723

	P	2P	3P	D	3D
BASIS/ORB	E	-35.92860	-3.64181	BASIS/ORB	E
2P	12.36430	0.76853	-0.28521	3D	4.70557
2P	19.52640	0.11626	-0.04270	3D	13.47820
3P	11.52780	0.12971	-0.12476	3D	7.38627
3P	7.15679	0.02772	0.37278	3D	2.93665
3P	4.50992	-0.00468	0.66459	3D	0.36175
3P	2.86886	0.00165	0.13742		0.22921

ZINC      K(2)L(8)3S(2)3P(6)4S(C)3D(10), 1S  
 T.E.= -0.17769583D+04   P.E.= -0.35539053D+04   K.E.= 0.17769471D+04   V.T.= -0.20300063D+01

	S	1S	2S	3S
BASIS/ORB	E	-354.05714	-45.10123	-6.38021
1S	29.29720	-0.56049	0.32478	0.12210
1S	43.94410	-0.03203	-0.00559	-0.00194
2S	24.39300	-0.00890	0.18359	0.07832
2S	13.03440	-0.00735	-1.03866	-0.43354
3S	11.65720	0.00499	-0.15209	-0.24477
3S	7.07461	-0.00290	-0.01787	0.60751
3S	4.60368	0.00445	0.01169	0.55998
3S	4.15360	-0.00304	-0.0C836	0.07194

	P	2P	3P	D	3D
BASIS/ORB	E	-39.66834	-4.59014	BASIS/ORB	E
2P	12.35130	0.85325	-0.34501	3D	4.92159
2P	20.28450	0.11401	-0.03491	3D	13.92570
3P	10.10640	0.05264	-0.09628	3D	7.92771
3P	6.93875	0.01129	0.56458	3D	2.89899
3P	4.15538	-0.00084	0.61746	3D	0.37314
3P	1.88801	0.00035	0.01288		0.11920

See page 183 for Explanation of Tables and Notes for Tables 32, 42, and 43

TABLE 42(1). DOUBLE ZETA FUNCTIONS.

HELIUM	1S(2), 1S			
T.E.=	-0.28616726D+01			
P.E.=	-0.57233581D+01			
K.E.=	0.28616855D+01			
V.T.=	-0.19999955D+01			
S	1S			
EASIS/ORB E	-0.91794			
1S	2.91093	0.18069		
1S	1.45363	0.84378		
LITHIUM	1S(2)2S(1) 2S			
T.E.=	-0.74327214D+01	P.E.=	-0.14E65345D+02	BERYLLIUM 1S(2)2S(2), 1S
K.E.=	0.74326239D+01	V.T.=	-0.20000131D+01	T.E.= -0.14572369D+02 P.E.= -0.29145492D+02
S	1S	2S		K.E.= 0.14573123D+02 V.T.= -0.19999482D+C1
BASIS/ORB E	-2.47768	-0.19632		
1S	4.61679	0.15502	0.00303	BASIS/ORB E -4.73283 -0.30923
1S	2.46167	0.85766	-0.21999	1S 5.59108 0.15502 0.00303
2S	1.96299	-0.00309	0.94196	1S 3.35538 0.85766 -0.21999
2S	0.67198	0.00191	0.09904	2S 1.01122 -0.00309 0.94196
				2S 0.61000 0.00191 0.09904
BORON	1S(2)2S(2)2P(1), 2P			
T.E.=	-0.24527920D+02	P.E.=	-0.49056561D+02	
K.E.=	0.24528640D+02	V.T.=	-0.19559706D+01	
S	1S	2S	P	2P
BASIS/ORB E	-7.69443	-0.49408	BASIS/ORB E	-0.30989
1S	6.55557	0.19030	0.00754	2P 2.21734 0.21526
1S	4.24927	0.82091	-0.25C55	2P 1.00551 0.84052
2S	1.41314	-0.00364	0.87099	
2S	0.87564	0.00251	0.1E515	
CARBON	1S(2)2S(2)2P(2), 3P			
T.E.=	-0.37686749D+02	P.E.=	-0.75374545D+02	
K.E.=	0.37687796D+02	V.T.=	-0.19999722D+01	
S	1S	2S	P	2P
BASIS/ORB E	-11.32343	-0.70436	BASIS/ORB E	-0.43263
1S	7.52232	0.23126	0.01051	2P 2.73045 0.25946
1S	5.12306	0.77896	-0.26957	2P 1.25656 0.80264
2S	1.83068	-0.00349	0.79305	
2S	1.15282	0.00266	0.27351	
NITROGEN	1S(2)2S(2)2P(3), 4S			
T.E.=	-0.54397951D+02	P.E.=	-0.10879805D+03	
K.E.=	0.54400095D+02	V.T.=	-0.19599606D+01	
S	1S	2S	P	2P
BASIS/ORB E	-15.62541	-0.94316	BASIS/ORB E	-0.56587
1S	8.49597	0.27067	0.01358	2P 3.24933 0.28810
1S	5.98644	0.73875	-0.28352	2P 1.49924 0.77826
2S	2.26086	-0.00293	0.72569	
2S	1.42457	0.00253	0.34546	
XYLGEN	1S(2)2S(2)2P(4), 3P			
T.E.=	-0.74804323D+02	P.E.=	-0.14961146D+03	
K.E.=	0.74807160D+02	V.T.=	-0.19999621D+01	
S	1S	2S	P	2P
EASIS/ORB E	-20.66258	-1.24045	BASIS/ORB E	-0.62827
1S	9.46635	0.31054	0.01567	2P 3.69445 0.32221
1S	6.83768	0.69824	-0.29663	2P 1.65864 0.74483
2S	2.68801	-0.00245	0.7C761	
2S	1.67543	0.00237	0.37450	
FLUORINE	1S(2)2S(2)2P(5), 2P			
T.E.=	-0.99401309D+02	P.E.=	-0.19880692D+03	
K.E.=	0.99405613D+02	V.T.=	-0.19999567D+01	
S	1S	2S	P	2P
BASIS/ORB E	-26.37363	-1.56E51	BASIS/ORB E	-0.72391
1S	10.42450	0.35375	0.01669	2P 4.18389 0.35458
1S	7.65585	0.65460	-0.3C569	2P 1.85062 0.72794
2S	3.13578	-0.00216	0.67367	
2S	1.94456	0.00232	0.41439	

See page 183 for Explanation of Tables and Notes for Tables 32, 42, and 43

## ROOCHAAN-HARTREE-FOCK ATOMIC WAVEFUNCTIONS

TABLE 42 (2). DOUBLE ZETA FUNCTIONS.

NEON      1S(2)2S(2)2P(6), 1S  
 T.E.= -0.12853511D+03   P.E.= -0.257C7579D+03  
 K.E.= 0.12854068D+03   V.T.= -0.19999566D+01

S	1S	2S	P	2P
BASIS/ORB E	-32.75986	-1.92187	BASIS/ORB E	-0.84143
1S 11.42160	0.38645	0.01729	2P 4.6E773	0.36818
1S 8.50182	0.62142	-0.31229	2P 2.0E684	0.71748
2S 3.56883	-0.00158	0.65864		
2S 2.19285	0.00210	0.43410		

SODIUM      K(2)L(8)3S(1), 2S  
 T.E.= -0.16184999D+03   P.E.= -0.32370891D+03  
 K.E.= 0.16185893D+03   V.T.= -0.1999944ED+01

S	1S	2S	3S	P	2P
BASIS/ORB E	-40.46972	-2.79215	-0.18122	BASIS/ORB E	-1.51288
1S 12.58430	-0.37590	-0.02313	-0.00483	2P 5.47723	0.32517
1S 9.43884	-0.63135	0.32941	0.05111	2P 2.56267	0.73552
2S 3.85928	0.00127	-0.76696	-0.11828		
2S 2.39434	-0.00240	-0.32753	-0.06624		
3S 1.25277	0.00084	0.01346	0.27943		
3S 0.74608	-0.00040	-0.00506	0.78135		

MAGNESIUM      K(2)L(8)3S(2), 1S  
 T.E.= -0.19960701D+03   P.E.= -0.39922785D+03  
 K.E.= 0.19962084D+03   V.T.= -0.19999307D+01

S	1S	2S	3S	P	2P
BASIS/ORB E	-49.02390	-3.76418	-0.25232	BASIS/CRB E	-2.27832
1S 13.33360	0.47073	-0.01478	-0.00521	2P 6.23231	0.31239
1S 10.06420	0.53733	0.33E32	0.06842	2P 3.05066	0.74849
2S 4.40510	-0.00452	-0.69172	-0.13229		
2S 2.99542	0.00445	-0.40179	-0.11270		
3S 1.47233	-0.00113	0.00425	0.47238		
3S 0.89173	0.00056	-0.00147	0.61010		

ALUMINUM      K(2)L(8)3S(2)3P(1), 2P  
 T.E.= -0.24187307D+03   P.E.= -0.48373553D+03   K.E.= 0.24186247D+03   V.T.= -0.20000438D+01

S	1S	2S	3S	P	2P	3P
BASIS/ORB E	-58.49855	-4.90991	-0.39285	BASIS/CRB E	-3.21737	-0.20577
1S 14.22690	0.53116	-0.00862	-0.00452	2P 7.20781	0.25887	-0.04475
1S 10.72610	0.47771	0.34710	0.08395	2P 3.65413	0.78155	-0.14577
2S 5.00360	-0.00826	-0.57504	-0.11622	3P 1.68275	0.02695	0.26788
2S 3.63124	0.00702	-0.51913	-0.18811	3P 0.91381	-0.00726	0.80384
3S 1.77396	-0.00145	-0.00298	0.54265			
3S 1.10766	0.00072	0.00110	0.55020			

SILICON      K(2)L(8)3S(2)3P(2), 3P  
 T.E.= -0.28885116D+03   P.E.= -0.57769845D+03   K.E.= 0.28884729D+03   V.T.= -0.20000134D+01

S	1S	2S	3S	P	2P	3P
BASIS/ORB E	-68.80941	-6.15555	-0.53940	BASIS/CRB E	-4.25495	-0.29691
1S 15.14750	0.58207	-0.00134	-0.00278	2P 7.96908	0.24394	0.05078
1S 11.36710	0.42768	0.35322	0.09425	2P 4.13763	0.79331	0.17742
2S 5.61540	-0.01189	-0.46994	-0.08617	3P 1.81897	0.02398	-0.42160
2S 4.21229	0.00938	-0.62747	-0.25916	3P 1.06461	-0.00781	-0.65766
3S 2.05901	-0.00166	-0.00675	0.58430			
3S 1.29744	0.00060	0.00217	0.51874			

PHOSPHORUS      K(2)L(8)3S(2)3P(3), 4S  
 T.E.= -0.34071595D+03   P.E.= -0.68143182D+03   K.E.= 0.34071586D+03   V.T.= -0.20000003D+01

S	1S	2S	3S	P	2P	3P
BASIS/ORB E	-79.96651	-7.51000	-0.69596	BASIS/CRB E	-5.39978	-0.39142
1S 16.10360	0.61924	0.00449	-0.00085	2P 8.74488	0.22881	0.05255
1S 12.02450	0.39123	0.35903	0.10195	2P 4.63044	0.80448	0.20117
2S 5.19095	-0.01504	-0.40232	-0.05669	3P 2.06453	0.02246	-0.49076
2S 4.74121	0.01147	-0.69878	-0.32180	3P 1.22668	-0.00749	-0.59396
3S 2.35748	-0.00186	-0.00907	0.58464			
3S 1.49875	0.00087	0.00252	0.52875			

See page 183 for Explanation of Tables and Notes for Tables 32, 42, and 43

## CLEMENTI AND ROETTI

TABLE 42 (3). DOUBLE ZETA FUNCTIONS.

SULFUR K(2)L(6)3S(2)3P(4), 3P  
 T.E.= -0.397502290+03 P.E.= -0.795007370+03 K.E.= 0.397505090D+03 V.T.= -0.199995200+01

S	1S	2S	3S	P	2P	3P
BASIS/DRB E	-92.00112	-9.00305	-0.87897	BASIS/CRB E	-6.68121	-0.43694
1S 17.07720	0.64806	0.00897	0.00074	2P 9.51251	0.21613	-0.05241
1S 12.69440	0.36296	0.36485	0.10897	2P 5.12050	0.81370	-0.22012
2S 6.72875	-0.01770	-0.35985	-0.03080	3P 2.33793	0.02086	0.53768
2S 5.24284	0.01327	-0.74517	-0.37678	3P 1.33331	-0.00567	0.55152
3S 2.66221	-0.00199	-0.01053	0.59902			
3S 1.68771	0.00090	0.00255	0.52459			

CHLORINE K(2)L(8)3S(2)3P(5), 2P  
 T.E.= -0.45947960D+03 P.E.= -0.91896613D+03 K.E.= 0.45948653D+03 V.T.= -0.19999849D+C1

S	1S	2S	3S	P	2P	3P
BASIS/DRB E	-104.88066	-10.60582	-1.07203	BASIS/CRB E	-8.07052	-0.50569
1S 18.05050	0.67493	0.01381	0.00245	2P 10.28770	0.20413	-0.05139
1S 13.33580	0.33676	0.36959	0.11483	2P 5.61299	0.82243	-0.23772
2S 7.32724	-0.01993	-0.30580	-0.00455	3P 2.62421	0.02056	0.55540
2S 5.75219	0.01447	-0.80394	-0.42555	3P 1.47456	-0.00465	0.55168
3S 2.92737	-0.00202	-0.01184	0.62616			
3S 1.85365	0.00089	0.00260	0.50512			

ARGON K(2)L(6)3S(2)3P(6), 1S  
 T.E.= -0.52681511D+03 P.E.= -0.10536429D+04 K.E.= 0.52682776D+03 V.T.= -0.19999760D+C1

S	1S	2S	3S	P	2P	3P
BASIS/DRB E	-118.60610	-12.32009	-1.27622	BASIS/CRB E	-9.56937	-0.59006
1S 19.02850	0.69702	0.01736	0.00319	2P 11.07020	0.19302	-0.04943
1S 14.00310	0.31476	0.37488	0.12082	2P 6.10658	0.83132	-0.25138
2S 7.71149	-0.02226	-0.33163	0.00637	3P 2.90339	0.01947	0.56956
2S 6.18497	0.01649	-0.78247	-0.45891	3P 1.62255	-0.00525	0.54309
3S 3.21815	-0.00213	-0.01208	0.63577			
3S 2.02947	0.00090	0.00220	0.50569			

POTASSIUM K(2)L(8)3S(2)3P(6)4S(1), 2S  
 T.E.= -0.59916241D+03 P.E.= -0.11983487D+04 K.E.= 0.59918628D+03 V.T.= -0.19999602D+01

S	1S	2S	3S	4S	P	2P	3P
BASIS/DRB E	-133.52773	-14.48692	-1.74714	-0.14701	BASIS/DRB E	-11.51616	-0.95308
1S 20.01550	0.71805	-0.02321	0.00596	-0.00153	2P 11.89500	0.18002	-0.04829
1S 14.57250	0.29527	-0.37911	0.12781	-0.02396	2P 6.61653	0.84060	-0.28236
2S 8.50264	-0.02570	0.23483	0.03866	-0.01395	3P 3.29528	0.02192	0.53002
2S 6.74543	0.01813	0.88454	-0.51797	0.10973	3P 1.99426	-0.00612	0.57404
3S 3.47996	-0.00298	0.01616	0.64779	-0.15552			
3S 2.32676	0.00169	-0.00482	0.49058	-0.07884			
4S 1.20531	-0.00045	0.00111	0.00122	0.40578			
4S 0.72769	0.00021	-0.00050	0.00018	0.67568			

CALCIUM K(2)L(8)3S(2)3P(6)4S(2), 1S  
 T.E.= -0.67675594D+03 P.E.= -0.13535273D+04 K.E.= 0.67677129D+03 V.T.= -0.19999772D+C1

S	1S	2S	3S	4S	P	2P	3P
BASIS/DRB E	-149.35981	-16.82085	-2.24434	-0.19514	BASIS/DRB E	-13.62730	-1.33968
1S 21.01110	0.73425	-0.02705	0.00833	-0.00237	2P 12.63720	0.17359	-0.04871
1S 15.16510	0.28036	-0.38455	0.13447	-0.03144	2P 7.10158	0.84524	-0.30560
2S 9.30033	-0.02718	0.17672	0.05766	-0.02124	3P 3.57668	0.02196	0.55630
2S 7.26755	0.01792	0.94853	-0.56230	0.14647	3P 2.27430	-0.00651	0.54593
3S 3.69973	-0.00336	0.01651	0.70789	-0.20909			
3S 2.57011	0.00212	-0.00665	0.43258	-0.09647			
4S 1.43414	-0.00056	0.00144	-0.00150	0.51789			
4S 0.86666	0.00024	-0.00052	0.00054	0.58360			

See page 183 for Explanation of Tables and Notes for Tables 32, 42, and 43

## ROOTHAAN-HARTREE-FOCK ATOMIC WAVEFUNCTIONS

TABLE 42 (4). DOUBLE ZETA FUNCTIONS.

SCANDIUM K(2)L(8)3S(2)3P(6)4S(2)3D(1), 2D  
 T.E.= -0.75972637D+03 P.E.= -0.15194678D+04 K.E.= 0.75974144D+03 V.T.= -0.19999802D+01

S	1S	2S	3S	4S
BASIS/ORB E	-165.89347	-19.07477	-2.56216	-0.20824
1S 22.00770	0.74821	-0.02963	0.01021	-0.00294
1S 15.76440	0.26753	-0.39093	0.13830	-0.03176
2S 10.10970	-0.02767	0.14222	0.06604	-0.02337
2S 7.75457	0.01679	0.98849	-0.58442	0.15C7E
3S 3.92714	-0.00315	0.01879	0.75878	-0.22341
3S 2.73064	0.00199	-0.00679	0.38664	-0.07919
4S 1.53840	-0.00054	0.00151	-0.00290	0.51722
4S 0.91407	0.00022	-0.00058	0.00091	0.58703

P	2P	3P	D	3D
BASIS/ORB E	-15.66249	-1.5699C	BASIS/ORB E	-0.33810
2P 13.36440	0.16863	-0.04754	3D 4.22244	0.35922
2P 7.58430	0.64899	-0.31782	3D 1.74647	0.76601
3P 3.83578	0.02130	0.59075		
3P 2.43406	-0.00607	0.51579		

TITANIUM K(2)L(8)3S(2)3P(6)4S(2)3D(2), 3F  
 T.E.= -0.84838875D+03 P.E.= -0.16967931D+04 K.E.= 0.84840434D+03 V.T.= -0.19999816D+01

S	1S	2S	3S	4S
BASIS/ORB E	-183.26456	-21.41380	-2.86513	-0.21E07
1S 23.00460	0.76115	-0.03219	0.01231	-0.00354
1S 16.32720	0.25610	-0.35782	0.14109	-0.03133
2S 11.02380	-0.02810	0.11966	0.06627	-0.02283
2S 8.25215	0.01515	1.01969	-0.59431	0.14951
3S 4.14661	-0.00283	0.01867	0.80283	-0.23197
3S 2.79906	0.00178	-0.00660	0.34675	-0.06145
4S 1.61853	-0.00051	0.00156	-0.00519	0.51724
4S 0.94889	0.00021	-0.00059	0.00151	0.58740

P	2P	3P	D	3D
BASIS/ORB E	-17.78235	-1.78759	BASIS/ORB E	-0.43184
2P 14.08400	0.16437	-0.04698	3D 4.67000	0.36461
2P 8.06621	0.85197	-0.32699	3D 1.98614	0.75561
3P 4.09547	0.02098	0.61453		
3P 2.58122	-0.00570	0.49611		

VANADIUM K(2)L(8)3S(2)3P(6)4S(2)3D(3), 4F  
 T.E.= -0.94285728D+03 P.E.= -0.188573180+04 K.E.= 0.94287456D+03 V.T.= -0.19999817D+01

S	1S	2S	3S	4S
BASIS/ORB E	-201.49238	-23.86156	-3.17131	-0.22698
1S 24.00780	0.77112	-0.03347	0.01363	-0.00391
1S 16.92690	0.24724	-0.40471	0.14398	-0.03091
2S 11.81230	-0.02893	0.1C899	0.06862	-0.02311
2S 8.72824	0.01445	1.03E73	-0.60566	0.14E75
3S 4.39565	-0.00266	0.01879	0.81499	-0.23094
3S 2.94007	0.00164	-0.00E43	0.33836	-0.05400
4S 1.69734	-0.00047	0.00153	-0.00574	0.51328
4S 0.98281	0.00019	-0.00C57	0.00165	0.59195

P	2P	3P	D	3D
BASIS/ORB E	-20.00988	-2.0CE39	BASIS/ORB E	-0.49698
2P 14.80040	0.16050	-0.04557	3D 5.05186	0.37378
2P 8.54808	0.85462	-0.33456	3D 2.17279	0.74564
3P 4.35447	0.02092	0.63294		
3P 2.72423	-0.00545	0.48129		

See page 183 for Explanation of Tables and Notes for Tables 32, 42, and 43

TABLE 42 (5). DOUBLE ZETA FUNCTIONS.

CHROMIUM K(2)L(8)3S(2)3P(6)4S(1)3D(5), 7S  
 T.E.= -0.10432900D+04 P.E.= -0.20866414D+04 K.E.= 0.10433514D+04 V.T.= -0.19999912D+01

	S	1S	2S	3S	4S
BASIS/ORB E	-220.35549	-26.17140	-3.24860	-0.20772	
1S	24.98800	0.78557	-0.03871	0.01205	-0.00347
1S	17.51200	0.23217	-0.40506	0.14988	-0.02869
2S	11.63200	-0.03495	0.14836	0.08695	-0.02945
2S	9.15411	0.02129	0.99995	-0.63377	0.14584
3S	4.72727	-0.00315	0.02066	0.76690	-0.20226
3S	3.13745	0.00179	-0.00689	0.39279	-0.05242
4S	1.74438	-0.00046	0.00169	0.00001	0.45362
4S	0.96230	0.00018	-0.00047	-0.00021	0.65446

	P	2P	3P	D	3D
BASIS/ORB E	-22.10272	-2.01665	BASIS/ORB E	-0.33930	
2P	15.43840	0.16005	-0.04549	3D 5.13843	C.40714
2P	9.01929	0.85418	-0.33575	3D 2.07723	0.73242
3P	4.60146	0.02031	0.65095		
3P	2.78187	-0.00474	0.47024		

CHROMIJ4 K(2)L(8)3S(2)3P(6)4S(2)3D(4), 5D  
 T.E.= -0.10432709D+04 P.E.= -0.20865614D+04 K.E.= 0.10432905D+04 V.T.= -0.19999812D+01

	S	1S	2S	3S	4S
BASIS/JRB E	-220.57914	-26.42147	-3.48316	-0.23523	
1S	24.99790	0.78371	-0.03661	0.01587	-0.00449
1S	17.40750	0.23656	-0.41207	0.14630	-0.03020
2S	12.66540	-0.03076	0.10814	0.06564	-0.02208
2S	9.19252	0.01384	1.04709	-0.61122	0.14648
3S	4.54782	-0.00256	0.01863	0.81955	-0.22770
3S	3.09125	0.00155	-0.00613	0.33670	-0.04889
4S	1.77218	-0.00044	0.00144	-0.00569	0.50946
4S	1.01451	0.00017	-0.00054	0.00164	0.55636

	P	2P	3P	D	3D
BASIS/JRB E	-22.34831	-2.23420	BASIS/ORB E	-0.55218	
2P	15.50780	0.15725	-0.04503	3D 5.40992	0.38301
2P	9.02843	0.85675	-0.34059	3D 2.34014	0.73672
3P	4.61536	0.02094	0.64636		
3P	2.86678	-0.00523	0.47108		

MANGANESE K(2)L(8)3S(2)3P(6)4S(2)3D(5), 6S  
 T.E.= -0.11498140D+04 P.E.= -0.22996482D+04 K.E.= 0.11498342D+04 V.T.= -0.19999824D+01

	S	1S	2S	3S	4S
BASIS/JRB E	-240.51830	-29.08717	-3.79670	-0.24262	
1S	26.03260	0.78278	-0.03101	0.01282	-0.00382
1S	18.36130	0.23539	-0.41703	0.15105	-0.03038
2S	12.94970	-0.02930	0.05764	0.08390	-0.02686
2S	9.66930	0.01461	1.05386	-0.63643	0.14980
2S	4.94055	-0.00249	0.01561	0.79953	-0.21814
3S	3.29090	0.00145	-0.00624	0.36117	-0.05134
4S	1.84488	-0.00039	0.00140	-0.00464	0.50463
4S	1.04408	0.00015	-0.00052	0.00142	0.60238

	P	2P	3P	D	3D
BASIS/ORB E	-24.79128	-2.46116	BASIS/ORB E	-0.61762	
2P	16.20660	0.15453	-0.04415	3D 5.76739	0.38984
2P	9.50747	0.85843	-0.34631	3D 2.50969	0.72965
3P	4.87726	0.02106	0.65567		
3P	3.00841	-0.00506	0.46466		

See page 183 for Explanation of Tables and Notes for Tables 32, 42, and 43

## ROOCHAAN-HARTREE-FOCK ATOMIC WAVEFUNCTIONS

TABLE 42 (6). DOUBLE ZETA FUNCTIONS.

IRON K(2)L(8)3S(2)3P(6)4S(2)3D(6), 5D  
 T.E.=-0.12623715D+04 P.E.=-0.25247662D+04 K.E.= 0.12623947D+04 V.T.=-0.19999817D+01

S	1S	2S	3S	4S
BASIS/ORB E	-261.35264	-31.90532	-4.14242	-0.25129
1S 27.03350	0.79062	-0.03115	0.01291	-0.00392
1S 19.01040	0.22775	-0.42273	0.15437	-0.03027
2S 13.51700	-0.02991	0.09856	0.08859	-0.02829
2S 10.13050	0.01485	1.05733	-0.64916	0.15050
3S 5.21660	-0.00246	0.01978	0.79159	-0.21377
3S 3.47616	0.00141	-0.00608	0.37233	-0.05090
4S 1.92517	-0.00036	0.00132	-0.00372	0.50156
4S 1.07742	0.00014	-0.00049	0.00117	0.60709

P	2P	3P	D	3D
BASIS/ORB E	-27.39489	-2.71718	BASIS/ORB E	-0.61788
2P 16.90320	0.15201	-0.04331	3D 6.06828	0.40379
2P 9.98637	0.86001	-0.35165	3D 2.61836	0.71984
3P 5.13914	0.02116	0.66557		
3P 3.15454	-0.00492	0.45730		

COBALT K(2)L(8)3S(2)3P(6)4S(2)3D(7), 4F  
 T.E.=-0.13813205D+04 P.E.=-0.27626673D+04 K.E.= 0.13813469D+04 V.T.=-0.19999809D+01

S	1S	2S	3S	4S
BASIS/ORB E	-283.03962	-34.83013	-4.49019	-0.25907
1S 28.03440	0.79775	-0.03092	0.01268	-0.00394
1S 19.67470	0.22059	-0.42816	0.15765	-0.03008
2S 14.03660	-0.03042	0.10105	0.09411	-0.02990
2S 10.58910	0.01524	1.05867	-0.66201	0.15176
3S 5.50254	-0.00244	0.02000	0.77756	-0.20743
3S 3.67136	0.00137	-0.00591	0.38948	-0.05214
4S 2.00140	-0.00034	0.00123	-0.00262	0.49765
4S 1.10841	0.00013	-0.00046	0.00088	0.61250

P	2P	3P	D	3D
BASIS/ORB E	-30.08374	-2.97456	BASIS/ORB E	-0.63869
2P 17.58970	0.14999	-0.04255	3D 6.38612	0.41333
2P 10.46370	0.86117	-0.35652	3D 2.74495	0.71262
3P 5.40335	0.02130	0.67186		
3P 3.30123	-0.00480	0.45334		

NICKEL K(2)L(8)3S(2)3P(6)4S(2)3D(8), 3F  
 T.E.=-0.15067517D+04 P.E.=-0.30135342D+04 K.E.= 0.15067824D+04 V.T.=-0.19999796D+01

S	1S	2S	3S	4S
BASIS/ORB E	-305.58756	-37.87093	-4.84609	-0.26640
1S 29.03620	0.80410	-0.03033	0.01217	-0.00389
1S 20.35820	0.21401	-0.43324	0.16094	-0.02991
2S 14.50890	-0.03086	0.10437	0.10101	-0.03189
2S 11.04660	0.01581	1.05849	-0.67582	0.15289
3S 5.79629	-0.00244	0.02028	0.76084	-0.20048
3S 3.87206	0.00133	-0.00576	0.40933	-0.05423
4S 2.07712	-0.00031	0.00115	-0.00148	0.49292
4S 1.13888	0.00012	-0.00043	0.00057	0.61875

P	2P	3P	D	3D
BASIS/ORB E	-32.89703	-3.23877	BASIS/ORB E	-0.66185
2P 18.27370	0.14815	-0.04176	3D 6.70551	0.42120
2P 10.94080	0.86219	-0.36079	3D 2.87381	0.70658
3P 5.67113	0.02149	0.67532		
3P 3.45098	-0.00468	0.452C2		

See page 183 for Explanation of Tables and Notes for Tables 32, 42, and 43

TABLE 42 (7). DOUBLE ZETA FUNCTIONS.

COPPER      K(2)L(8)3S(2)3P(6)4S(1)3D(10), 2S  
 T.E.= -0.16387496D+04 P.E.= -0.32775576D+04 K.E.= 0.16388080D+04 V.T.= -0.19999644D+01

S	1S	2S	3S	4S
BASIS/ORB E	-328.72818	-40.72955	-4.92707	-0.21805
1S 30.00890	0.81459	-0.03032	0.01043	-0.00333
1S 21.03960	0.20211	-0.43728	0.16499	-0.02322
2S 14.46680	-0.05246	0.14332	0.11960	-0.03256
2S 11.44970	0.01900	1.02251	-0.70363	0.13085
3S 6.19332	-0.00247	0.01920	0.71019	-0.15333
3S 4.08469	0.00119	-0.00430	0.46887	-0.04224
4S 2.00757	-0.00023	0.00076	0.0024E	0.41432
4S 1.03682	0.00009	-0.0029	-0.00039	0.69833

P	2P	3P	D	3D
BASIS/ORB E	-35.53210	-3.24463	BASIS/ORB E	-0.40408
2P 18.92080	0.14782	-0.04046	3D 6.79466	0.44729
2P 11.41270	0.86178	-0.36302	3D 2.76527	0.69683
3P 5.99213	0.02120	0.65653		
3P 3.58401	-0.00401	0.47591		

COPPER      K(2)L(8)3S(2)3P(6)4S(2)3D(9), 2D  
 T.E.= -0.16388025D+04 P.E.= -0.32776418D+C4 K.E.= 0.16388393D+04 V.T.= -0.19999775D+01

S	1S	2S	3S	4S
BASIS/ORB E	-328.99678	-41.02E37	-5.21057	-0.27338
1S 30.03790	0.81001	-0.02557	0.01152	-0.00381
1S 21.04960	0.20779	-0.43812	0.16414	-0.02971
2S 14.95750	-0.03129	0.10877	0.10855	-0.03408
2S 11.50220	0.01647	1.05E51	-0.68990	0.15417
3S 6.09689	-0.00245	0.02056	0.74260	-0.19338
3S 4.07634	0.00130	-0.00560	0.43068	-0.05662
4S 2.15990	-0.00029	0.00108	-0.00031	0.48850
4S 1.16808	0.00012	-0.00040	0.00025	0.62466

P	2P	3P	D	3D
BASIS/ORB E	-35.82535	-3.51C16	BASIS/ORB E	-0.68608
2P 18.94890	0.14668	-0.04103	3D 7.02531	0.42787
2P 11.41670	0.86289	-0.36467	3D 3.00372	0.70140
3P 5.94246	0.02168	0.67E51		
3P 3.60403	-0.00458	0.45282		

ZIVC      K(2)L(8)3S(2)3P(6)4S(2)3D(10), 1S  
 T.E.= -0.17776699D+04 P.E.= -0.35553681D+C4 K.E.= 0.17777182D+04 V.T.= -0.19999728D+C1

S	1S	2S	3S	4S
BASIS/ORB E	-353.26006	-44.29530	-5.57917	-0.27973
1S 31.00410	0.82235	-0.03240	0.01167	-0.00387
1S 21.53360	0.19552	-0.44207	0.16822	-0.02963
2S 15.27860	-0.03303	0.14237	0.10794	-0.03517
2S 11.90690	0.01809	1.03103	-0.69930	0.15497
3S 6.42595	-0.00256	0.01960	0.71760	-0.18484
3S 4.29540	0.00131	-0.00488	0.46054	-0.06C80
4S 2.22120	-0.00028	0.00050	0.00099	0.48426
4S 1.19514	0.00011	-0.00C34	-0.00011	0.63C36

P	2P	3P	D	3D
BASIS/ORB E	-38.86147	-3.78452	BASIS/ORB E	-0.71910
2P 19.58350	0.14676	-0.04037	3D 7.34928	0.43305
2P 11.88520	0.86214	-0.36E77	3D 3.13941	0.69712
3P 6.25251	0.02167	0.66E42		
3P 3.79437	-0.00429	0.46896		

See page 183 for Explanation of Tables and Notes for Tables 32, 42, and 43

## ROOTHAAN-HARTREE-FOCK ATOMIC WAVEFUNCTIONS

TABLE 42 (8). DOUBLE ZETA FUNCTIONS.

GALLIUM K(2)L(8)M(18)4S(2)4P(1), 2P  
 T.E.= -0.19231110D+04 P.E.= -0.38462701D+04 K.E.= 0.19231591D+04 V.T.= -0.19999750D+C1

S	1S	2S	3S	4S
BASIS/ORB E	-378.78529	-48.11611	-6.35133	-0.41411
1S 32.01830	0.82518	-0.03C81	0.01074	-0.00383
1S 22.29170	0.19220	-0.44671	0.17209	-0.03695
2S 15.63200	-0.03427	0.14458	0.12555	-0.04462
2S 12.37300	0.01990	1.02852	-0.72713	0.18919
3S 6.77070	-0.00287	0.02144	0.68313	-0.20467
3S 4.61217	0.00152	-0.00564	0.49737	-0.09825
4S 2.45796	-0.00034	0.00105	0.00179	0.53552
4S 1.40096	0.00014	-0.00040	-0.00021	0.57761

P	2P	3P	4P	D	2D
BASIS/ORB E	-42.44418	-4.44178	-0.20388	BASIS/ORB E	-1.14385
2P 20.34850	0.14163	0.03887	0.00545	3D 7.89432	0.41899
2P 12.38730	0.86561	0.376C1	0.06156	3D 3.50951	0.69956
3P 6.52223	0.02461	-0.66314	-0.12614		
3P 4.03812	-0.00659	-0.46603	-0.05712		
4P 2.05958	0.00151	0.00008	0.40615		
4P 1.07094	-0.00059	-0.00117	0.70547		

GERMANIUM K(2)L(8)M(18)4S(2)4P(2), 3P  
 T.E.= -0.20752284D+04 P.E.= -0.41505077D+04 K.E.= 0.20752793D+04 V.T.= -0.19999755D+01

S	1S	2S	3S	4S
BASIS/ORB E	-405.21879	-52.1C755	-7.15781	-0.54499
1S 33.03290	0.82776	-0.02921	0.00975	-0.00363
1S 23.05870	0.18910	-0.45002	0.17604	-0.04269
2S 15.93780	-0.03608	0.14761	0.14947	-0.05591
2S 12.84330	0.02235	1.02553	-0.76207	0.21967
3S 7.14429	-0.00322	0.02324	0.63987	-0.21004
3S 4.95514	0.00174	-0.00637	0.54332	-0.13741
4S 2.69865	-0.00038	0.00113	0.00336	0.56895
4S 1.57530	0.00015	-0.00044	-0.00047	0.54799

P	2P	3P	4P	D	3D
BASIS/ORB E	-46.19540	-5.13046	-0.28286	BASIS/ORB E	-1.59494
2P 21.07540	0.13850	0.03796	0.00655	3D 8.41462	0.40755
2P 12.87440	0.86785	0.38339	0.07647	3D 3.86350	0.70200
3P 6.78204	0.02581	-0.67291	-0.15573		
3P 4.25056	-0.00757	-0.45638	-0.07358		
4P 2.28865	0.00185	0.00286	0.46689		
4P 1.25160	-0.00073	-0.00218	0.64373		

ARSEVIC K(2)L(8)M(18)4S(2)4P(3), 4S  
 T.E.= -0.22341207D+04 P.E.= -0.44682962D+04 K.E.= 0.22341756D+04 V.T.= -0.19999754D+C1

S	1S	2S	3S	4S
BASIS/ORB E	-432.56512	-56.27333	-8.00304	-0.67904
1S 34.02140	0.83493	-0.03C57	0.00968	-0.00358
1S 23.63560	0.16188	-0.45374	0.18058	-0.04779
2S 16.21470	-0.03911	0.18043	0.16277	-0.06470
2S 13.26110	0.02554	0.95684	-0.78977	0.24573
3S 7.55246	-0.00369	0.02286	0.59133	-0.20634
3S 5.31126	0.00198	-0.00642	0.59629	-0.17898
4S 2.92135	-0.00042	0.00106	0.00520	0.59342
4S 1.73605	0.00017	-0.00042	-0.00075	0.52513

P	2P	3P	4P	D	3D
BASIS/ORB E	-50.11890	-5.85571	-0.36543	BASIS/ORB E	-2.07915
2P 21.76420	0.13668	0.03730	0.00729	3D 8.91876	0.39775
2P 13.35530	0.86894	0.39C83	0.08855	3D 4.20700	0.70433
3P 7.05630	0.02669	-0.67775	-0.17846		
3P 4.50827	-0.00835	-0.45140	-0.08711		
4P 2.49741	0.00207	0.00410	0.51559		
4P 1.40781	-0.00082	-0.00235	0.59597		

See page 183 for Explanation of Tables and Notes for Tables 32, 42, and 43

TABLE 42 (9). DOUBLE ZETA FUNCTIONS.

SELENIUM K(2)L(8)M(18)4S(2)4P(4), 3P  
 $T.E. = -0.239975630 \times 10^4$     $P.E. = -0.479946256 \times 10^4$     $K.E. = 0.239970620 \times 10^4$     $V.T. = -0.200002090 \times 10^4$

S	1S	2S	3S	4S
BASIS/ORB E	-460.84203	-60.62154	-8.89672	-0.83038
1S 35.03650	0.83730	0.02947	0.00904	-0.00333
1S 24.36140	0.17934	0.45717	0.18425	-0.05237
2S 16.58670	-0.04169	-0.18352	0.18822	-0.07643
2S 13.73710	0.02839	-0.99413	-0.82574	0.27217
3S 7.95809	-0.00408	-0.02556	0.54177	-0.19665
3S 5.66700	0.00219	0.0C696	0.64805	-0.22229
4S 3.13670	-0.00045	-0.001C7	0.00737	0.61625
4S 1.88996	0.00018	0.00043	-0.00111	0.51289

P	2P	3P	4P	D	3D
BASIS/ORB E	-54.22432	-6.62806	-0.39878	BASIS/CRB E	-2.60822
2P 22.63360	0.13554	0.03716	0.00793	3D 9.29756	0.39689
2P 13.83180	0.86969	0.39689	0.09782	3D 4.53759	0.69736
3P 7.27814	0.02716	-0.7C559	-0.20151		
3P 4.68101	-0.00915	-0.42487	-0.09344		
4P 2.71504	0.00231	0.00713	0.55089		
4P 1.51140	-0.00085	-0.00348	0.57215		

BROMINE K(2)L(8)M(18)4S(2)4P(5), 2P  
 $T.E. = -0.257234150 \times 10^4$     $P.E. = -0.51447530 \times 10^4$     $K.E. = 0.257241150 \times 10^4$     $V.T. = -0.199997280 \times 10^4$

S	1S	2S	3S	4S
BASIS/ORB E	-490.04352	-65.17C42	-9.85231	-0.98689
1S 36.03660	0.84191	0.02572	0.00882	-0.00318
1S 25.00700	0.17460	0.46040	0.18819	-0.05662
2S 16.87210	-0.04542	-0.21C89	0.21485	-0.08983
2S 14.17400	0.03246	-0.96876	-0.86642	0.30019
3S 8.41984	-0.00455	-0.02652	0.48865	-0.18183
3S 6.03270	0.00239	0.00691	0.70642	-0.26809
4S 3.36095	-0.00047	-0.00100	0.00914	0.63100
4S 2.04437	0.00019	0.00040	-0.00126	0.50501

P	2P	3P	4P	D	3D
BASIS/ORB E	-58.52577	-7.45565	-0.45342	BASIS/ORB E	-3.19375
2P 23.14170	0.13321	-0.03585	0.00803	3D 9.89282	0.38160
2P 14.31790	0.87119	-0.40530	0.10760	3D 4.87426	0.70876
3P 7.60185	0.02823	0.68960	-0.21343		
3P 5.01779	-0.00982	0.43858	-0.10758		
4P 2.91993	0.00226	-0.00340	0.58215		
4P 1.62414	-0.00082	0.002E1	0.54721		

KRYPTON K(2)L(8)M(18)4S(2)4P(6), 1S  
 $T.E. = -0.275196130 \times 10^4$     $P.E. = -0.550399640 \times 10^4$     $K.E. = 0.2752C370D+04$     $V.T. = -0.19999725D+01$

S	1S	2S	3S	4S
BASIS/ORB E	-520.15004	-69.87604	-10.83231	-1.14770
1S 37.05330	0.84361	-0.02840	0.00821	-0.00289
1S 25.75570	0.17269	-0.46340	0.19148	-0.06033
2S 17.25280	-0.04864	0.20640	0.25359	-0.10658
2S 14.67150	0.03600	0.97277	-0.91500	0.32867
3S 8.84771	-0.00489	0.02845	0.44406	-0.16E31
3S 6.38152	0.00255	-0.00743	0.75348	-0.30973
4S 3.57716	-0.00049	0.00101	0.01088	0.64314
4S 2.19214	0.00020	-0.00041	-0.00141	0.49969

P	2P	3P	4P	D	3D
BASIS/ORB E	-62.98359	-8.31522	-0.52076	BASIS/ORB E	-3.80139
2P 23.77970	0.13296	-0.03521	0.00814	3D 10.36520	0.37459
2P 14.79240	0.87089	-0.41292	0.11560	3D 5.19958	0.71070
3P 7.93594	0.02875	0.66888	-0.21918		
3P 5.37145	-0.01018	0.45774	-0.12370		
4P 3.12737	0.00213	-0.00038	0.60391		
4P 1.74596	-0.00074	0.00115	0.53023		

See page 183 for Explanation of Tables and Notes for Tables 32, 42, and 43

## ROOCHAAN-HARTREE-FOCK ATOMIC WAVEFUNCTIONS

TABLE 42 (10). DOUBLE ZETA FUNCTIONS.

PU3IDIUM K(2)L(8)M(18)4S(2)4P(6)5S(1),2S  
 T.E.= -0.29382706D+04 P.E.= -0.58766569U+04 K.E.= 0.29383862D+04 V.T.= -0.19999607D+01

S	1S	2S	3S	4S	5S
BASIS/ORB E	-551.44108	-75.02269	-12.11679	-1.51855	-0.13748
1S 38.08620	0.84306	0.02679	0.00789	-0.00258	0.00018
1S 26.53380	0.17339	0.46596	0.19385	-0.06545	0.01441
2S 17.71900	-0.05375	-0.16593	0.31101	-0.13088	0.02387
2S 15.24460	0.04116	-1.01685	-0.97888	0.36825	-0.07354
3S 9.31323	-0.00563	-0.03252	0.38201	-0.14087	0.02451
3S 6.76640	0.00305	0.00905	0.81340	-0.37290	0.08837
4S 3.88610	-0.00072	-0.00150	0.01573	0.60120	-0.16671
4S 2.52497	0.00037	0.00078	-0.00322	0.53871	-0.07389
5S 1.38017	-0.00011	-0.00021	0.00082	0.00987	0.44807
5S 0.80400	0.00005	0.00009	-0.00033	-0.00177	0.65575

P	2P	3P	4P	D	3D
BASIS/ORB E	-67.88020	-9.47203	-0.80660	BASIS/ORB E	-4.70956
2P 24.49670	-0.13049	-0.03433	0.00881	3D 10.85480	0.36644
2P 15.27970	-0.87286	-0.41944	0.12882	3D 5.53471	0.71479
3P 8.15357	-0.02989	0.70117	-0.24895		
3P 5.54448	0.01168	0.42750	-0.13864		
4P 3.41258	-0.00280	-0.00364	0.61394		
4P 2.02457	0.00098	0.00200	0.51815		

STRONTIUM K(2)L(8)M(18)4S(2)4P(6)5S(2),1S  
 T.E.= -0.31314652D+04 P.E.= -0.626230696D+04 K.E.= 0.21316044D+04 V.T.= -0.19999556D+01

S	1S	2S	3S	4S	5S
BASIS/ORB E	-583.67150	-80.365C3	-13.45924	-1.89142	-0.17789
1S 39.13040	0.84283	0.02897	-0.00972	-0.00325	0.00051
1S 27.02730	0.17573	0.46544	-0.19558	-0.06576	0.01860
2S 18.76280	-0.05396	-0.11899	-0.26910	-0.11676	0.02762
2S 15.79910	0.02908	-1.06176	0.93656	0.36592	-0.09189
3S 9.60271	-0.00666	-0.03720	-0.31750	-0.11105	0.02284
3S 7.18092	0.00393	0.01235	-0.86413	-0.43220	0.12416
4S 4.16121	-0.00097	-0.00214	-0.02523	0.57550	-0.19858
4S 2.82050	0.00054	0.00118	0.60746	0.56587	-0.11545
5S 1.63036	-0.00015	-0.00031	-0.00182	0.01065	0.50870
5S 0.96129	0.00006	0.00012	0.00069	-0.00211	0.60912

P	2P	3P	4P	D	3D
BASIS/ORB E	-72.97067	-10.68480	-1.09404	BASIS/ORB E	-5.67255
2P 25.15590	-0.12964	-0.03360	0.00920	3D 11.33050	0.35953
2P 15.75860	-0.87325	-0.42620	0.14094	3D 5.86357	0.71783
3P 8.44083	-0.03065	0.70153	-0.26680		
3P 5.63430	0.01256	0.42682	-0.15845		
4P 3.65550	-0.00303	-0.00236	0.63968		
4P 2.25751	0.00108	0.00155	0.49438		

YTTRIUM K(2)L(8)M(18)4S(2)4P(6)5S(2)4D(1),2D  
 T.E.= -0.33316558D+04 P.E.= -0.66632573D+04 K.E.= 0.33316035D+04 V.T.= -0.20000151D+01

S	1S	2S	3S	4S	5S
BASIS/ORB E	-616.74073	-85.80013	-14.74862	-2.15568	-0.19240
1S 40.11580	0.84724	0.02616	0.00779	-0.00260	0.00024
1S 27.89200	0.16954	0.471E4	0.19968	-0.07386	0.02013
2S 18.61820	-0.06313	-0.13738	0.39867	-0.17842	0.04167
2S 16.28230	0.05052	-1.04024	-1.08346	0.44401	-0.11090
3S 10.27940	-0.00650	-0.03647	0.28585	-0.10215	0.01956
3S 7.48929	0.00339	0.00954	0.91142	-0.47128	0.13828
4S 4.28025	-0.00086	-0.00163	0.02095	0.66193	-0.23644
4S 2.91412	0.00050	0.00094	-0.00544	0.48944	-0.08058
5S 1.70525	-0.00014	-0.00024	0.00123	0.00503	0.55001
5S 0.99727	0.00005	0.00009	-0.00044	-0.00071	0.56862

See page 183 for Explanation of Tables and Notes for Tables 32, 42, and 43

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TABLE 42 (11). DOUBLE ZETA FUNCTIONS.

P	2P	3P	4P	D	3D	4D
BASIS/CRB E	-78.15338	-11.84405	-1.29296	BASIS/CRB E	-6.58759	-0.24636
2P 25.77750	-0.12980	-0.03314	0.00542	3D 12.56410	0.27450	-0.05914
2P 16.23110	-0.87277	-0.43270	0.15016	3D 6.69231	0.75566	-0.17771
3P 8.74733	-0.03112	0.69126	-0.27417	4D 3.83698	0.06489	0.29168
3P 6.17653	0.01311	0.43548	-0.17887	4D 1.73901	-0.00730	0.82942
4P 3.88511	-0.00292	0.00121	0.66392			
4P 2.42270	0.00102	0.00067	0.47714			

ZIRCONIUM K(2)L(8)M(18)4S(2)4P(6)5S(2)4D(2), 3F  
 T.E.= -0.35389632D+04 P.E.= -0.70778843D+04 K.E.= 0.35389210D+04 V.T.= -0.20002119D+01

S	1S	2S	3S	4S	5S
BASIS/CRB E	-650.69692	-91.36695	-16.04560	-2.41152	-0.20416
1S 41.14930	0.84551	0.02207	0.00549	-0.00166	-0.00006
1S 28.86350	0.17028	0.47330	0.20287	-0.07727	0.02115
2S 18.61520	-0.08796	-0.00318	0.73131	-0.32661	0.07698
2S 17.00340	0.07664	-1.16678	-1.42316	0.60222	-0.14888
3S 10.81480	-0.00668	-0.04120	0.25021	-0.08546	0.01439
3S 7.82175	0.00329	0.01C32	0.95072	-0.50987	0.15025
4S 4.45263	-0.00083	-0.00178	0.02106	0.70644	-0.25537
4S 3.03088	0.00048	0.00103	-0.00541	0.45298	-0.06341
5S 1.79574	-0.00014	-0.00027	0.00121	0.00293	0.55594
5S 1.04278	0.00005	0.00010	-C.00042	-0.00016	0.56329

P	2P	3P	4P	D	3D	4D
BASIS/CRB E	-83.46753	-13.01052	-1.48081	BASIS/CRB E	-7.50451	-0.33541
2P 26.46150	-0.12829	-0.03221	0.00935	3D 12.87330	0.28563	-0.07279
2P 16.71580	-0.87361	-0.43686	0.15773	3D 6.90015	0.75602	-0.17958
3P 9.02922	-0.03209	0.69050	-0.28207	4D 3.63923	0.04952	0.40742
3P 6.47917	0.01405	0.43514	-0.19325	4D 1.80383	-0.00936	0.72844
4P 4.10493	-0.00297	0.0C255	0.68300			
4P 2.57028	0.00102	0.00C24	0.46531			

NIOBIUM K(2)L(8)M(18)4S(2)4P(6)5S(1)4D(4), 6D  
 T.E.= -0.37535591D+04 P.E.= -0.75071036D+04 K.E.= 0.37535445D+04 V.T.= -0.20000039D+01

S	1S	2S	3S	4S	5S
BASIS/CRB E	-685.42717	-96.95468	-17.22915	-2.52251	-0.20875
1S 42.10000	0.85474	0.02631	0.01595	-0.00520	0.00067
1S 29.28610	0.16156	0.47521	0.19069	-0.07468	0.02014
2S 20.21050	-0.05355	-0.00110	0.50734	-0.21777	0.04870
2S 17.52380	0.04071	-1.17274	-1.20445	0.49826	-0.11954
3S 11.30650	-0.00475	-0.04369	0.28289	-0.09191	0.01480
3S 7.93250	0.00220	0.01052	0.93640	-0.53109	0.15309
4S 4.68352	-0.00059	-0.00214	-0.00348	0.74403	-0.26115
4S 3.10683	0.00032	0.00119	0.00775	0.43980	-0.05020
5S 1.84738	-0.00009	-0.00033	-0.00251	0.00030	0.55072
5S 1.06545	0.00004	0.00013	0.00098	-0.00245	0.56660

P	2P	3P	4P	D	3D	4D
BASIS/CRB E	-88.80264	-14.06438	-1.54330	BASIS/CRB E	-8.31010	-0.29120
2P 27.02880	-0.12958	-0.03210	0.00936	3D 13.24190	0.28957	-0.07597
2P 17.18380	-0.87226	-0.44424	0.16286	3D 7.16473	0.75583	-0.16949
3P 9.33211	-0.03257	0.68027	-0.28160	4D 3.59080	0.04018	0.48705
3P 6.81806	0.01457	0.44496	-0.20750	4D 1.71750	-0.00808	0.66705
4P 4.30633	-0.00276	0.00532	0.70164			
4P 2.65318	0.00092	-0.00017	0.45539			

NIOBIUM K(2)L(8)M(18)4S(2)4P(6)5S(1)4D(3), 4F  
 T.E.= -0.37535211D+04 P.E.= -0.75070227D+04 K.E.= 0.37535016D+04 V.T.= -0.20000052D+01

S	1S	2S	3S	4S	5S
BASIS/CRB E	-685.56273	-97.05768	-17.37180	-2.65766	-0.21350
1S 42.12940	0.85251	0.02468	0.00614	-0.00175	-0.00009
1S 29.31960	0.16371	C.47710	0.20685	-0.08084	0.02203
2S 19.00060	-0.09289	-0.12299	0.69949	-0.31829	0.07218
2S 17.34330	0.08151	-1.05312	-1.40638	0.60586	-0.14637
3S 11.39800	-0.00725	-0.04003	0.22534	-0.07144	0.00954
3S 8.14768	0.00333	0.00860	0.98334	-0.54526	0.15989
4S 4.64550	-0.00083	-0.00144	0.02125	0.73260	-0.26543
4S 3.16032	0.00048	0.00C85	-0.00527	0.43438	-0.05182
5S 1.87724	-0.00014	-0.00022	0.00116	0.00229	0.55664
5S 1.08160	0.00005	0.00C08	-0.00039	-0.00003	0.56308

See page 183 for Explanation of Tables and Notes for Tables 32, 42, and 43

## ROOTHAAN-HARTREE-FOCK ATOMIC WAVEFUNCTIONS

TABLE 42 (12). DOUBLE ZETA FUNCTIONS.

P	2P	3P	4P	D	3D	4D
BASIS/CRB E	-88.94441	-14.20526	-1.66546	BASIS/CRB E	-8.44978	-0.40171
2P 27.07440	-0.12863	-0.03172	0.00937	3D 13.34950	0.28092	-0.07824
ZP 17.18870	-0.87316	-0.44471	0.16447	3D 7.22241	0.76010	-0.19074
3P 9.35611	-0.03260	0.66820	-0.27773	4D 3.77410	0.04647	0.45834
3P 6.85943	0.01451	0.45617	-0.21698	4D 1.92510	-0.00916	0.67869
4P 4.33198	-0.00272	0.00669	0.69251			
4P 2.71923	0.00092	-0.00064	0.46252			

MOLYBDENUM K(2)L(8)M(18)4S(2)4P(6)5S(1)4D(5), 7S  
 T.E.= -0.39755121D+04 P.E.= -0.79510641D+04 K.E.= 0.39755520D+04 V.T.= -0.19999900D+01

S	1S	2S	3S	4S	5S
BASIS/CRB E	-721.18426	-102.83061	-18.56686	-2.74550	-0.21604
1S 43.11900	0.85604	0.02589	0.01572	-0.00463	0.00046
1S 29.95450	0.16059	0.47625	0.19354	-0.07817	0.02101
2S 20.72570	-0.05677	0.00983	0.53227	-0.22479	0.04897
2S 18.03350	0.04371	-1.18459	-1.23562	0.51185	-0.12085
3S 11.77890	-0.00509	-0.04497	0.25194	-0.06909	0.00770
3S 8.25940	0.00233	0.01043	0.96726	-0.57182	0.16437
4S 4.92494	-0.00062	-0.00206	-0.00176	0.74418	-0.26153
4S 3.26266	0.00033	0.00112	0.00721	0.44953	-0.05300
5S 1.94119	-0.00010	-0.00030	-0.00229	-0.00044	0.54776
5S 1.10333	0.00003	0.00012	0.00088	-0.00241	0.57494

P	2P	3P	4P	D	3D	4D
BASIS/CRB E	-94.42359	-15.26969	-1.71043	BASIS/CRB E	-9.26560	-0.34811
2P 27.66020	-0.12949	-0.03151	0.00930	3D 13.78860	0.27933	-0.07868
2P 17.65810	-0.87214	-0.44987	0.16888	3D 7.52281	0.76319	-0.18442
3P 9.62141	-0.03297	0.67763	-0.28403	4D 3.81446	0.04044	0.51194
3P 7.12790	0.01513	0.44755	-0.22320	4D 1.86369	-0.00856	0.64116
4P 4.53262	-0.00267	0.00673	0.70993			
4P 2.79279	0.00087	-0.00035	0.45480			

MOLYBDENUM K(2)L(8)M(18)4S(2)4P(6)5S(2)4D(4), 5D  
 T.E.= -0.39754131D+04 P.E.= -0.79558178D+04 K.E.= 0.39754048D+04 V.T.= -0.2000021D+01

S	1S	2S	3S	4S	5S
BASIS/CRB E	-721.34269	-102.99612	-18.73158	-2.90243	-0.22154
1S 43.13500	0.85525	0.02437	-0.00546	-0.00122	-0.00020
1S 30.00570	0.16080	0.47957	-0.21034	-0.08422	0.02275
2S 18.95150	-0.16753	-0.03273	-1.44499	-0.64747	0.14212
2S 17.99150	0.15707	-1.14085	2.16601	0.94537	-0.21758
3S 12.17620	-0.00797	-0.04328	-0.19306	-0.05363	0.00394
3S 8.48951	0.00317	0.00721	-1.02452	-0.58174	0.16828
4S 4.84153	-0.00081	-0.00123	-0.02196	0.75077	-0.27080
4S 3.29197	0.00047	0.00074	0.00530	0.42254	-0.04335
5S 1.95489	-0.00013	-0.00019	-0.00114	0.00211	0.55367
5S 1.11327	0.00005	0.00007	0.00036	-0.00003	0.56647

P	2P	3P	4P	D	3D	4D
BASIS/CRB E	-94.58792	-15.43267	-1.85044	BASIS/CRB E	-9.42712	-0.46515
2P 27.67580	-0.12924	-0.03131	0.00936	3D 13.83160	0.27564	-0.08183
2P 17.65980	-0.87229	-0.45025	0.17056	3D 7.55093	0.76391	-0.20165
3P 9.69072	-0.03300	0.64443	-0.26882	4D 3.95409	0.04441	0.49299
3P 7.25199	0.01487	0.48237	-0.24296	4D 2.04659	-0.00895	0.64576
4P 4.55830	-0.00245	0.01039	0.69862			
4P 2.86547	0.00081	-0.00144	0.46264			

TECHNETIUM K(2)L(8)M(18)4S(2)4P(6)5S(2)4D(5), 6S  
 T.E.= -0.42047590D+04 P.E.= -0.84055028D+04 K.E.= 0.42047438D+04 V.T.= -0.2000036D+01

S	1S	2S	3S	4S	5S
BASIS/CRB E	-758.03551	-109.06090	-20.12426	-3.14622	-0.22864
1S 44.14780	0.85717	0.02436	-0.00574	-0.00122	-0.00039
1S 30.64890	0.15919	0.48245	-0.21253	-0.08665	0.02317
2S 19.46600	-0.18953	0.07561	-1.66991	-0.74695	0.15732
2S 18.56990	0.17889	-1.24571	2.39544	1.05559	-0.23272
3S 12.71100	-0.00821	-0.04515	-0.16435	-0.03632	-0.00183
3S 8.82037	0.00312	0.00693	-1.05200	-0.61215	0.17501
4S 5.03917	-0.00079	-0.00115	-0.02299	0.76498	-0.27429
4S 3.42135	0.00045	0.00068	0.00548	0.41446	-0.03496
5S 2.01960	-0.00012	-0.00017	-0.00117	0.00195	0.55465
5S 1.14710	0.00005	0.00006	0.00039	-0.00003	0.56549

See page 183 for Explanation of Tables and Notes for Tables 32, 42, and 43

TABLE 42 (13). DOUBLE ZETA FUNCTIONS.

P	ZP	3P	4P	D	3D	4D
BASIS/ORB E	-100.39668	-16.69211	-2.03587	BASIS/ORB E	-10.43574	-0.53963
2P 28.27110	0.12997	-0.03094	0.00934	3D 14.30340	0.27130	-0.06486
2P 18.13010	0.87132	-0.45549	0.17609	3D 7.67405	0.76719	-0.21080
3P 10.03420	0.03332	0.60695	-0.25532	4D 4.12429	0.04216	0.52761
3F 7.65492	-0.01516	0.51437	-0.27141	4D 2.15492	-0.00878	0.61308
4P 4.73273	0.00215	0.01398	0.70225			
4P 3.00926	-0.00071	-0.00218	0.46457			

RUTHENIUMM K(2)L(8)M(18)4S(2)4P(6)5S(1)4D(7),5F  
T.E.= -0.44415000D+04 P.E.= -0.88831293D+04 K.E.= 0.44416294D+04 V.T.= -0.19999709D+01

S	1S	2S	3S	4S	5S
BASIS/ORB E	-795.48998	-115.13474	-21.39197	-3.23929	-0.21477
1S 45.15230	0.85792	0.02505	0.01478	-0.00440	0.00009
1S 31.28860	0.15944	0.48412	0.19976	-0.08303	0.02108
2S 21.75440	-0.06422	0.02199	0.57625	-0.24948	0.04658
2S 19.05640	0.05068	-1.20846	-1.28986	0.54903	-0.11541
3S 12.74980	-0.00585	-0.04728	0.18765	-0.03433	-0.00458
3S 8.95920	0.00255	0.00993	1.02792	-0.63077	0.17038
4S 5.32031	-0.00065	-0.00179	0.00449	0.76032	-0.25539
4S 3.55341	0.00034	0.00096	0.00454	0.43976	-0.03282
5S 2.04429	-0.00009	-0.00023	-0.00138	0.00387	0.52381
5S 1.13104	0.00003	0.00009	0.00054	-0.00163	0.59975

P	ZP	3P	4P	D	3D	4D
BASIS/ORB E	-106.21465	-17.82748	-2.08476	BASIS/ORB E	-11.32094	-0.39911
2P 28.90670	-0.12969	-0.03055	0.00920	3D 14.85860	0.26131	-0.08142
2P 18.60450	-0.87161	-0.46010	0.17977	3D 8.22517	0.77555	-0.20898
3P 10.19940	-0.03393	0.66516	-0.28126	4D 4.25911	0.04063	0.54954
3P 7.79423	0.01641	0.45860	-0.25852	4D 2.09384	-0.00776	0.6970
4P 4.99399	-0.00244	0.01134	0.71698			
4P 3.08530	0.00076	-0.00114	0.46151			

RUTHENIUMM K(2)L(8)M(18)4S(2)4P(6)5S(2)4D(6),5D  
T.E.= -0.44414569D+04 P.E.= -0.8882947D+04 K.E.= 0.44414878D+04 V.T.= -0.19999931D+01

S	1S	2S	3S	4S	5S
BASIS/ORB E	-795.65897	-115.31062	-21.56777	-3.40261	-0.23636
1S 45.14260	0.86083	0.02405	-0.00487	-0.00080	-0.00052
1S 31.32130	0.15515	0.48510	-0.21628	-0.08556	0.02371
2S 19.53240	-0.50389	0.73161	-5.04655	-2.27772	0.47572
2S 19.19750	0.49374	-1.90748	5.78266	2.59038	-0.55235
3S 12.99870	-0.00847	-0.04610	-0.16885	-0.03418	-0.00365
3S 9.09833	0.00328	0.007E3	-1.05406	-0.63224	0.18005
4S 5.24030	-0.00080	-0.00127	-0.02145	0.78130	-0.27878
4S 3.54529	0.00045	0.00074	0.00451	0.40631	-0.02845
5S 2.09134	-0.00012	-0.00C19	-0.00094	0.00135	0.55375
5S 1.18048	0.00004	0.00007	0.00031	0.00012	0.56681

P	ZP	3P	4P	D	3D	4D
BASIS/ORB E	-106.38925	-18.00148	-2.23353	BASIS/ORB E	-11.49327	-0.56249
2P 28.87910	-0.13054	-0.03C82	0.00934	3D 14.81660	0.26370	-0.08550
2P 18.59690	-0.87089	-0.460C2	0.18133	3D 8.21990	0.77208	-0.22148
3P 10.23210	-0.03349	0.64650	-0.27532	4D 4.35709	0.04208	0.53942
3P 7.85840	0.01598	0.47614	-0.26791	4D 2.26533	-0.00821	0.60615
4P 5.00093	-0.00227	0.01335	0.71350			
4P 3.14334	0.00072	-0.00186	0.46130			

RHODIUMM K(2)L(8)M(18)4S(2)4P(6)5S(1)4D(8), 4F  
T.E.= -0.46858548D+04 P.E.= -0.93718823D+04 K.E.= 0.46860275D+04 V.T.= -0.19999631D+01

S	1S	2S	3S	4S	5S
BASIS/ORB E	-834.01163	-121.53570	-22.85390	-3.48319	-0.21351
1S 46.18660	0.85853	0.02461	-0.01402	-0.00395	-0.00019
1S 31.95440	0.15926	0.48699	-0.20325	-0.08579	0.02106
2S 22.26790	-0.06863	0.04303	-0.59375	-0.25644	0.04301
2S 19.56960	0.05484	-1.2224	1.31118	0.56046	-0.10934
3S 13.24850	-0.00631	-0.04847	-0.15367	-0.01297	-0.01131
3S 9.31300	0.00270	0.0C65	-1.05822	-0.66159	0.17217
4S 5.53758	-0.00067	-0.00166	-0.00844	0.75619	-0.24682
4S 3.71126	0.00035	0.00088	-0.00295	0.44744	-0.02822
5S 2.08865	-0.00008	-0.00020	0.00091	0.00546	0.51187
5S 1.14158	0.00003	0.00007	-0.00037	-0.00145	0.61275

See page 183 for Explanation of Tables and Notes for Tables 32, 42, and 43

## ROOTHAAN-HARTREE-FOCK ATOMIC WAVEFUNCTIONS

TABLE 42 (14). DOUBLE ZETA FUNCTIONS.

P	2P	3P	4P	D	3D	4D
BASIS/ORB E	-112.35749	-19.15440	-2.27198	BASIS/ORB E	-12.39522	-0.43760
2P 29.52190	-0.12996	-0.03011	0.00916	3D 15.36120	C.25365	-0.08210
2P 19.07660	-0.87121	-0.46487	0.18449	3C E.57186	0.78066	-0.21591
3P 10.48970	-0.03445	0.65618	-0.27534	4D 4.48485	0.34084	0.56119
3P 8.13980	0.01709	0.46679	-0.27907	4D 2.21685	-0.00758	0.59964
4P 5.23245	-0.00230	0.01377	0.71563			
4P 3.23403	0.00070	-0.00148	0.46980			

RHODIUM K(2)L(8)M(18)4S(2)4P(6)5S(2)4D(7),4F  
 T.E.= -0.46857699D+04 P.E.= -0.93715969D+04 K.E.= 0.46858271D+04 V.T.= -0.19999678D+01

S	1S	2S	3S	4S	5S
BASIS/ORB E	-834.19640	-121.72759	-23.04545	-3.65925	-0.24324
1S 46.24830	0.85126	0.02025	0.00746	-0.00195	-0.00040
1S 32.26880	0.16653	0.48722	0.21130	-0.08849	0.02341
2S 22.15390	-0.07480	0.07498	0.56844	-0.25687	0.05116
2S 19.59290	0.06143	-1.24805	-1.27379	C.55E59	-0.12440
3S 13.30520	-0.00719	-0.04705	0.06855	0.02227	-0.01882
3S 9.53393	0.00313	0.00864	1.11709	-0.68222	0.19205
4S 5.44599	-0.00073	-0.00116	0.02918	0.77758	-0.27689
4S 3.70047	0.00041	0.00067	-0.00772	0.41166	-0.02671
5S 2.16003	-0.00011	-0.00016	0.00166	0.00239	0.55333
5S 1.21018	0.00004	0.00006	-0.00056	-0.00016	0.56869

P	2P	3P	4P	D	3D	4D
BASIS/ORB E	-112.54801	-19.34417	-2.43247	BASIS/ORB E	-12.56317	-0.60403
2P 29.52220	-0.13011	-0.03017	0.00919	3D 15.30820	0.25802	-0.08655
2P 19.07430	-0.87111	-0.46490	0.18622	3D 8.55394	0.77592	-0.23024
3P 10.52430	-0.03421	0.63496	-0.26903	4D 4.56078	0.04131	0.55764
3P 8.20983	0.01678	0.48678	-0.28802	4D 2.36478	-0.00775	0.59192
4P 5.22966	-0.00214	0.01579	0.71496			
4P 3.28803	0.00067	-0.00224	0.46599			

PALLADIUM K(2)L(8)M(18)4S(2)4P(6)5S(1)4D(9), 3D  
 T.E.= -0.49378503D+04 P.E.= -0.98759303D+04 K.E.= 0.4938C800D+04 V.T.= -0.19999535D+01

S	1S	2S	3S	4S	5S
BASIS/ORB E	-873.45256	-128.10981	-24.35575	-3.73192	-0.21279
1S 47.21250	0.85895	0.02417	-0.01307	-0.00322	-0.00069
1S 32.61940	0.15930	0.48980	-0.20699	-0.08892	0.02139
2S 22.78090	-0.07348	0.05404	-0.60773	-0.25836	0.03553
2S 20.08380	0.05944	-1.23193	1.32805	0.56561	-0.09871
3S 13.75600	-0.00682	-0.04965	-0.11852	0.01145	-0.02000
3S 9.67280	0.00285	0.00934	-1.08835	-0.69389	0.17561
4S 5.75241	-0.00069	-0.00151	-0.01299	0.75058	-0.24089
4S 3.86410	0.00034	0.00078	-0.00116	0.45772	-0.01961
5S 2.10039	-0.00008	-0.00016	0.00043	0.00563	0.51650
5S 1.13773	0.00003	0.00006	-0.00019	-0.00116	0.60800

P	2P	3P	4P	D	3D	4D
BASIS/ORB E	-118.67238	-20.52037	-2.46435	BASIS/ORB E	-13.50746	-0.47302
2P 30.13180	-0.13034	-0.02963	0.00918	3D 15.89960	C.24671	-0.08235
2P 19.54810	-0.87072	-0.46556	0.18877	3D 8.91475	0.78511	-0.23100
3P 10.78590	-0.03494	0.64440	-0.26417	4D 4.72335	0.04118	0.55761
3P 8.49060	0.01776	0.47795	-0.30538	4D 2.34159	-0.00697	0.59530
4P 5.48238	-0.00217	0.01595	0.70978			
4P 3.39145	0.00064	-0.00166	0.48390			

PALLADIUM K(2)L(8)M(18)4S(2)4P(6)5S(2)4D(8),3F  
 T.E.= -0.49377504D+04 P.E.= -0.98755766D+04 K.E.= 0.49378262D+04 V.T.= -0.19939846D+01

S	1S	2S	3S	4S	5S
BASIS/ORB E	-873.64893	-128.31353	-24.55915	-3.91741	-0.24957
1S 47.19700	0.86049	0.02212	-0.00629	-0.00098	-0.00071
1S 32.75030	0.15641	0.49C39	-0.21730	-0.09282	0.02424
2S 21.22740	-0.21137	0.46351	-2.02605	C.89009	0.16808
2S 20.32790	0.20021	-1.63717	2.75776	1.20482	-0.24234
3S 14.24460	-0.00830	-0.05C09	-0.09404	0.01160	-0.01686
3S 9.73253	0.00288	0.00619	-1.11496	-0.69147	0.19178
4S 5.65155	-0.00071	-C.00C89	-0.02448	0.78743	-0.27759
4S 3.83055	0.00040	0.00053	0.00513	0.4C929	-0.02257
5S 2.22301	-0.00010	-0.00012	-0.00102	0.00247	0.55209
5S 1.23780	0.00004	0.00004	0.00033	-0.00022	0.57052

See page 183 for Explanation of Tables and Notes for Tables 32, 42, and 43

## CLEMENTI AND ROETTI

TABLE 42 (15). DOUBLE ZETA FUNCTIONS.

P	2P	3P	4P	D	3D	4D
BASIS/DRB E	-118.87467	-20.72204	-2.63362	BASIS/ORB E	-13.70726	-0.64905
2P 30.11210	0.13084	-0.02985	0.00912	3D 15.79890	0.25252	-0.08721
2P 19.54470	0.87024	-0.46936	0.19072	3D 8.88823	0.77954	-0.23876
3P 13.82400	0.03487	0.61E53	-0.25893	4D 4.77173	0.04088	0.57074
3P 8.57409	-0.01756	0.50244	-0.31070	4D 2.47121	-0.00732	0.58201
4P 5.45747	0.06200	0.01E26	0.71537			
4P 3.43123	-0.00061	-0.00260	0.47121			

SILVER K(2)L(8)M(18)4S(2)4P(6)5S(2)4D(9),2D  
 T.E.= -0.51974836D+04 P.E.= -0.10395073D+05 K.E.= 0.51975893D+04 V.T.= -0.19999797D+C1

S	1S	2S	3S	4S	5S
BASIS/DRB E	-914.01686	-135.06830	-26.10897	-4.17748	-0.25514
1S 48.22300	0.86035	0.02142	-0.00657	-0.00088	-0.00085
1S 33.48410	0.15688	0.49212	-0.21823	-0.09450	0.02446
2S 21.92110	-0.21622	0.7C825	-2.15207	-0.93206	0.16791
2S 21.01540	0.20664	-1.87E44	2.87902	1.24616	-0.24044
3S 14.81370	-0.00821	-0.05406	-0.05856	0.03401	-0.02309
3S 10.12480	0.00275	0.00631	-1.14045	-0.71769	0.19611
4S 5.86134	-0.00068	-0.00C52	-0.02673	0.78481	-0.27424
4S 3.98061	0.00038	0.00054	0.00580	0.41555	-0.02195
5S 2.28782	-0.00009	-0.00C12	-0.00114	0.00332	0.548E7
5S 1.26528	0.00003	0.00004	0.00038	-0.00C47	0.57514

P	2P	3P	4P	D	3D	4D
BASIS/DRB E	-125.36910	-22.13517	-2.83722	BASIS/ORB E	-14.86547	-0.69643
2P 30.72360	0.13106	-0.02936	0.00901	3D 16.29020	0.24713	-0.08755
2P 20.01860	0.86984	-0.47374	0.19490	3D 9.22285	0.78298	-0.24721
3P 11.12790	0.03570	0.59684	-0.24408	4D 4.98896	0.04080	0.57980
3P 8.95172	-0.01846	0.52320	-0.23717	4D 2.58374	-0.00682	0.57560
4P 5.68857	0.00185	0.02C80	0.71367			
4P 3.57599	-0.00056	-0.00295	0.47829			

CADMIUM K(2)L(8)M(18)4S(2)4P(6)5S(2)4D(10),1S  
 T.E.= -0.54650971D+04 P.E.= -0.10530346D+05 K.E.= 0.54652485D+04 V.T.= -0.19999723D+01

S	1S	2S	3S	4S	5S
BASIS/DRB E	-955.29647	-141.98819	-27.69179	-4.43733	-0.25986
1S 49.23720	0.86367	0.02716	-0.00887	-0.00134	-0.00086
1S 33.62670	0.15596	0.49560	-0.22133	-0.09760	0.02502
2S 22.15630	-0.88095	3.43383	-7.99330	-3.29802	0.53511
2S 21.89490	0.86820	-4.60357	8.72078	3.61086	-0.60499
3S 15.83970	-0.01005	-0.064E2	-0.02258	0.05626	-0.02895
3S 10.47480	0.00260	0.00574	-1.16668	-0.73858	0.19743
4S 6.06675	-0.00074	-0.001C4	-0.02975	0.77922	-0.26918
4S 4.13401	0.00041	0.00063	0.00686	0.42287	-0.02225
5S 2.35199	-0.00010	-0.00015	-0.00134	0.00443	0.54361
5S 1.29201	0.00004	0.000C5	0.00045	-0.00C80	0.58195

P	2P	3P	4P	D	3D	4D
BASIS/DRB E	-132.02759	-23.58043	-3.04128	BASIS/CRB E	-16.05469	-0.75237
2P 31.32550	0.13145	-0.02892	0.00892	3D 16.78180	0.24205	-0.08712
2P 20.49210	0.86927	-0.47789	0.19873	3D 9.55761	0.78675	-0.25408
3P 11.44150	0.03667	0.56688	-0.22282	4D 5.21258	0.03981	0.58534
3P 9.34616	-0.01947	0.55215	-0.36902	4D 2.70557	-0.00747	0.57202
4P 5.92238	0.00170	0.02343	0.70999			
4P 3.72187	-0.00051	-0.00328	0.48697			

INDIUM K(2)L(8)M(18)4S(2)4P(6)5S(2)4D(10)5P(1),2P  
 T.E.= -0.57401392D+04 P.E.= -0.11480437D+05 K.E.= 0.57402983D+04 V.T.= -0.19999723D+01

S	1S	2S	3S	4S	5S
BASIS/DRB E	-997.78688	-149.38224	-29.61450	-4.97010	-0.36942
1S 50.32200	0.85541	0.02059	-0.00972	-0.00206	-0.00056
1S 34.79970	0.16487	0.45703	-0.21686	-0.09645	0.02784
2S 25.44340	-0.06597	0.06589	-0.40717	-0.17441	0.03490
2S 21.65860	0.05010	-1.24289	1.10895	0.48255	-0.11569
3S 15.79590	-0.00733	-0.05466	0.04755	0.05557	-0.04054
3S 10.88310	0.00257	0.00573	-1.20720	-0.77896	0.23558
4S 6.25917	-0.00067	-0.00072	-0.03832	0.77770	-0.30472
4S 4.34217	0.00039	0.00046	0.01135	0.42326	-0.04078
5S 2.57153	-0.00010	-0.00010	-0.00239	0.00469	0.58047
5S 1.47680	0.00004	0.00004	0.00082	-0.00081	0.54097

See page 183 for Explanation of Tables and Notes for Tables 32, 42, and 43

## ROOTHAAN-HARTREE-FOCK ATOMIC WAVEFUNCTIONS

TABLE 42 (16). DOUBLE ZETA FUNCTIONS.

P	2P	3P	4P	5P	D	3D	4D
BASIS/DRB E	-139.15792	-25.36403	-3.50109	-0.19500	BASIS/CRB E	-17.57882	-1.05700
2P 31.93030	0.13167	-0.02833	0.00882	-0.00207	3D 17.29770	0.23468	-0.08842
2P 20.96910	0.86872	-0.48209	0.20425	-0.03971	3D 9.91616	0.79077	-0.27105
3P 11.81160	0.03827	0.49885	-0.18111	0.02339	4D 5.48162	0.04233	0.59196
3P 9.82786	-0.02096	0.61717	-0.42463	0.10520	4D 2.94786	-0.00831	0.55977
4P 6.20856	0.00166	0.02971	0.67454	-0.18490			
4P 4.02633	-0.00059	-0.00571	0.51766	-0.05535			
5P 2.14213	0.00010	0.00118	0.01059	0.48741			
5P 1.14940	-0.00004	-0.00044	-0.00136	0.64146			

TIV K(2)L(8)M(18)4S(2)4P(6)5S(2)4D(10)5P(2),3P  
 T.E.= -0.60229057D+04 P.E.= -0.12045859D+05 K.E.= 0.60225537D+04 V.T.= -0.19999520D+01

S	1S	2S	3S	4S	5S
BASIS/DRB E	-1041.21500	-156.96985	-31.59201	-5.50737	-0.47376
1S 51.32820	0.85831	0.02336	-0.01106	-0.00219	-0.00046
1S 35.30960	0.16245	0.49810	-0.21791	-0.09909	0.03082
2S 25.66130	-0.07720	0.12073	-0.50876	-0.21542	0.04903
2S 22.29840	0.66101	-1.29381	1.21724	0.52995	-0.13881
3S 16.04490	-0.00800	-0.06098	0.04730	0.10715	-0.04782
3S 11.16180	0.00299	0.00892	-1.21081	-0.80792	0.26601
4S 6.52585	-0.00082	-0.00157	-0.03583	0.75852	-0.32433
4S 4.59222	0.00049	0.00057	0.00956	0.45049	-0.06647
5S 2.75261	-0.00013	-0.00024	-0.00182	0.00516	0.61109
5S 1.62500	0.00005	0.00009	0.00062	-0.00066	0.51290

P	2P	3P	4P	5P	D	3D	4D
BASIS/DRB E	-146.48070	-27.20207	-3.96430	-0.26292	BASIS/DRB E	-19.15623	-1.36420
2P 32.51230	0.13260	0.02844	0.00896	-0.00235	3D 17.76450	0.23210	-0.00043
2P 21.43490	0.86793	0.48520	0.20944	-0.04809	3D 10.23420	0.79204	-0.28709
3P 11.97260	0.04129	-0.51914	-0.17537	0.02558	4D 5.77494	0.04166	0.59080
3P 10.17870	-0.02451	-0.59418	-0.44676	0.12953	4D 3.20455	-0.00783	0.55777
4P 6.48388	0.00176	-0.03494	0.65806	-0.21213			
4P 4.27372	-0.00062	0.00752	0.53787	-0.08055			
5P 2.35868	0.00011	-0.00160	0.01085	0.53103			
5P 1.32009	-0.00004	0.00061	-0.00117	0.59385			

ANTIMONY K(2)L(8)M(18)4S(2)4P(6)5S(2)4D(10)5P(3),4S  
 T.E.= -0.63134618D+04 P.E.= -0.12626964D+05 K.E.= 0.63135026D+04 V.T.= -0.19999535D+01

S	1S	2S	3S	4S	5S
BASIS/DRB E	-1085.58162	-164.75132	-33.63009	-6.05880	-0.57938
1S 52.38770	0.85458	0.02123	-0.01068	-0.00159	-0.00061
1S 36.17790	0.16680	0.49927	-0.21850	-0.10143	0.03327
2S 26.56330	-0.07511	0.13274	-0.46966	-0.19385	0.04729
2S 22.84650	0.05843	-1.30142	1.17271	0.50816	-0.14271
3S 16.68810	-0.00828	-0.06297	0.07371	0.12643	-0.05616
3S 11.50190	0.00301	0.00790	-1.22759	-0.83271	0.29029
4S 6.75627	-0.00091	-0.00141	-0.03979	0.73908	-0.33696
4S 4.85126	0.00056	0.00090	0.01163	0.47071	-0.09158
5S 2.95931	-0.00014	-0.00021	-0.00211	0.00724	0.62750
5S 1.77118	0.00005	0.00008	0.06071	-0.00099	0.50176

P	2P	3P	4P	5P	D	3D	4D
BASIS/DRB E	-153.99632	-29.09998	-4.44064	-0.33270	BASIS/CRB E	-20.79168	-1.68367
2P 33.10660	0.13325	0.02619	-0.00895	-0.00252	3D 18.26140	0.22715	-0.05124
2P 21.90360	0.86732	0.48886	-0.21478	-0.05494	3D 10.57320	0.79485	-0.30209
3P 12.23390	0.04350	-0.49089	0.14325	0.01900	4D 6.05287	0.04250	0.59140
3P 10.59180	-0.02697	-0.62069	0.49349	0.15713	4D 3.44742	-0.00798	0.55503
4P 6.73800	0.00159	-0.03926	-0.64717	-0.23194			
4P 4.51085	-0.00056	0.00906	-0.55138	-0.10256			
5P 2.55958	0.00009	-0.00192	-0.01073	0.56097			
5P 1.47557	-0.00003	0.00073	0.00123	0.56328			

See page 183 for Explanation of Tables and Notes for Tables 32, 42, and 43

TABLE 42 (17). DOUBLE ZETA FUNCTIONS.

TELLURIUM K(2)L(8)M(18)4S(2)4P(6)5S(2)4D(10)5P(4),3P							
T.E.= -0.66117621D+04 P.E.= -0.13223550D+05 K.E.= 0.66117881D+04 V.T.= -0.19999961D+C1							
S	1S	2S	3S	4S	5S		
BASIS/ORB E	-1130.91017	-172.74970	-35.74911	-6.64274	-0.69812		
1S	53.41410	0.85494	0.02247	-0.01224	-0.00164	-0.00054	
1S	36.65220	0.16805	0.50255	-0.21916	-0.10386	0.03588	
2S	27.70620	-0.07028	0.09644	-0.38223	-0.15282	0.03862	
2S	23.28810	0.05185	-1.26196	1.08267	0.46827	-0.13952	
2S	17.29240	-0.00842	-0.04626	0.09620	0.14280	-0.06446	
3S	11.83340	0.00298	0.06724	-1.24158	-0.85599	0.31242	
4S	6.98359	-0.00098	-0.00137	-0.04292	0.72146	-0.34728	
4S	5.10844	0.00062	0.0091	0.01331	0.48561	-0.11618	
5S	3.14692	-0.00015	-0.00021	-0.00223	0.00922	0.64656	
5S	1.90779	0.00006	0.00007	0.00075	-0.00125	0.48917	
P		2P	3P	4P	5P	D	
BASIS/ORB E	-161.72780	-31.07822	-4.94856	-0.35773	BASIS/ORB E	-22.50667	-2.03417
2P	33.70530	0.13353	0.02776	-0.00690	3D	18.76030	0.22252
2P	22.38020	0.86677	0.45238	-0.21977	3D	10.90960	0.79768
3P	12.65670	0.04499	-0.35271	0.05366	4D	6.33002	0.04297
3P	11.13750	-0.02819	-0.75660	0.59295	4D	3.68881	-0.00799
4P	6.95455	0.00117	-0.04447	-0.64211	-0.24987		
4P	4.73195	-0.00040	0.01122	-0.55510	-0.11556		
5P	2.73570	0.00005	-0.00225	-0.01079	0.55341		
5P	1.55177	-0.00001	0.00082	0.00058	0.54018		
IODINE K(2)L(8)M(18)4S(2)4P(6)5S(2)4D(10)5P(5),2P							
T.E.= -0.69179602D+04 P.E.= -0.13835993D+05 K.E.= 0.69180324D+04 V.T.= -0.19999896D+01							
S	1S	2S	3S	4S	5S		
BASIS/ORB E	-1177.17759	-180.94172	-37.92740	-7.23930	-0.81832		
1S	54.56250	0.84102	0.01390	-0.00761	0.00074	-0.00140	
1S	38.32090	0.18099	0.49905	-0.22006	-0.10617	0.03801	
2S	28.25430	-0.07475	0.19663	-0.43892	-0.17218	0.04642	
2S	24.03020	0.05791	-1.34912	1.12547	0.48268	-0.14968	
3S	17.96370	-0.00911	-0.06814	0.12835	0.16604	-0.07442	
3S	12.19580	0.00317	0.06558	-1.25831	-0.87662	0.33411	
4S	7.21283	-0.00116	-0.00091	-0.05125	0.69025	-0.34761	
4S	5.39337	0.00077	0.0062	0.01831	0.51885	-0.14704	
5S	3.34077	-0.00018	-0.00012	-0.0300	0.01223	0.65683	
5S	2.04555	0.00006	0.00004	0.00102	-0.00167	0.48693	
P		2P	3P	4P	5P	D	
BASIS/ORB E	-169.65199	-33.11512	-5.46859	-0.40078	BASIS/ORB E	-24.27865	-2.39647
2P	34.29400	0.13437	0.02760	-0.00874	3D	19.24990	0.21810
2P	22.84260	0.86635	0.45588	-0.22517	3D	11.24950	0.79999
3P	12.58340	0.05458	-0.51541	0.08691	4D	6.62014	0.04294
3P	11.33970	-0.03883	-0.59356	0.57958	4D	3.93933	-0.00812
4P	7.24503	0.00162	-0.04652	-0.63142	-0.26392		
4P	4.97721	-0.00055	0.01163	-0.57484	-0.13607		
5P	2.92046	0.00007	-0.00223	-0.01155	0.61404		
5P	1.67111	-0.00002	0.00080	0.00004	0.52580		
XENON K(2)L(8)M(18)4S(2)4P(6)5S(2)4D(10)5P(6),1S							
T.E.= -0.72321189D+04 P.E.= -0.14464290D+05 K.E.= 0.72321716D+04 V.T.= -0.19999927D+C1							
S	1S	2S	3S	4S	5S		
BASIS/ORB E	-1224.38985	-189.33393	-40.16984	-7.85219	-0.94196		
1S	55.19780	0.88283	0.02662	-0.00975	-0.00305	0.00052	
1S	36.83430	0.13748	0.52247	-0.23772	-0.11091	0.03997	
2S	27.41490	-0.06292	-0.21509	-0.29885	-0.15595	0.05004	
2S	23.10230	0.04653	-1.01285	1.07239	0.52524	-0.17952	
3S	15.39770	-0.01093	-0.03640	0.02426	0.17335	-0.09006	
3S	12.34720	0.00679	0.01411	-1.23002	-0.96755	0.39334	
4S	7.42968	-0.00141	-0.00128	-0.03696	0.77528	-0.39661	
4S	5.41398	0.00085	0.00083	0.01020	0.46529	-0.13303	
5S	3.48079	-0.00021	-0.00019	-0.00164	0.00323	0.68685	
5S	2.14824	0.00007	0.00006	0.00053	0.00077	0.46092	
P		2P	3P	4P	5P	D	
BASIS/ORB E	-177.77535	-35.21575	-6.00442	-0.45508	BASIS/ORB E	-26.11320	-2.77391
2P	34.77350	-0.13825	-0.02841	-0.00874	3D	19.76100	0.21296
2P	23.27040	-0.86363	-0.49512	-0.23107	3D	11.59180	0.80346
3P	12.47320	-0.04804	0.92129	0.32077	4D	6.85814	0.04474
3P	10.97100	0.03457	0.18868	0.37935	4D	4.14854	-0.00852
4P	7.60110	-0.00263	0.04702	-0.62750	-0.27868		
4P	5.22922	0.00080	-0.01088	-0.60282	-0.15772		
5P	3.09473	-0.00011	0.00204	-0.01087	0.63444		
5P	1.78077	0.00003	-0.00070	0.00068	0.51034		

See page 183 for Explanation of Tables and Notes for Tables 32, 42, and 43

## ROOTHAAN-HARTREE-FOCK ATOMIC WAVEFUNCTIONS

TABLE 43 (1). SINGLE ZETA FUNCTIONS.

HELIUM	1S(2), 1S			
T.E.=	-0.28476562D+01			
P.E.=	-0.56953125D+01			
K.E.=	0.28476562D+01			
V.T.=	-0.20000000D+01			
S	1S			
BASIS/ORB E	-0.89648			
1S	1.68750	1.00000		
LITHIUM	1S(2)2S(1), 2S			
T.E.=	-0.74184820D+01	P.E.=	-0.14E36934D+02	
K.E.=	0.74184525D+01	V.T.=	-0.20000040D+01	
S	1S	2S		
BASIS/ORB E	-2.46019	-0.19489		
1S	2.69063	0.99759	0.20444	
2S	0.63961	0.01239	-1.01824	
BERYLLIUM	1S(2)2S(2), 1S			
T.E.=	-0.14556740D+02	P.E.=	-0.29113332D+02	
K.E.=	0.14556592D+02	V.T.=	-0.20000102D+01	
S	1S	2S		
BASIS/ORB E	-4.71712	-0.30864		
1S	3.66478	0.99759	0.20444	
2S	0.95603	0.01239	-1.01324	
BORON	1S(2)2S(2)2P(1), 2P			
T.E.=	-0.24498369D+02	P.E.=	-0.48956433D+02	
K.E.=	0.24498065D+02	V.T.=	-0.20000124D+01	
S	1S	2S	P	2P
BASIS/ORB E	-7.67787	-0.48391	BASIS/ORB E	-0.30038
1S	4.67939	0.99749	0.22442	2P 1.21066
2S	1.28808	0.01175	-1.02235	1.00000
CARBON	1S(2)2S(2)2P(2), 3P			
T.E.=	-0.37622389D+02	P.E.=	-0.75244409D+02	
K.E.=	0.37622021D+02	V.T.=	-0.20000098D+01	
S	1S	2S	P	2P
BASIS/ORB E	-11.30156	-0.67750	BASIS/ORB E	-0.40162
1S	5.67263	0.99744	0.23509	2P 1.56788
2S	1.60833	0.01143	-1.02470	1.00000
NITROGEN	1S(2)2S(2)2P(3), 4S			
T.E.=	-0.54268900D+02	P.E.=	-0.1C853713D+03	
K.E.=	0.54268235D+02	V.T.=	-0.20000122D+01	
S	1S	2S	P	2P
BASIS/ORB E	-15.59378	-0.89254	BASIS/ORB E	-0.50336
1S	6.66507	0.99740	0.24176	2P 1.91703
2S	1.9236E	0.01128	-1.02623	1.00000
OXYGEN	1S(2)2S(2)2P(4), 3P			
T.E.=	-0.74540365D+02	P.E.=	-0.149079E7D+03	
K.E.=	0.74539502D+02	V.T.=	-0.20000116D+01	
S	1S	2S	P	2P
BASIS/ORB E	-20.61394	-1.15C89	BASIS/ORB E	-0.50327
1S	7.65781	0.99739	0.24788	2P 2.22662
2S	2.24588	0.01108	-1.02767	1.00000
FLUORINE	1S(2)2S(2)2P(5), 2P			
T.E.=	-0.98942113D+02	P.E.=	-0.19788306D+03	
K.E.=	0.98940947D+02	V.T.=	-0.20000118D+01	
S	1S	2S	P	2P
BASIS/ORB E	-26.30293	-1.430E5	BASIS/ORB E	-0.52641
1S	8.65007	0.99737	0.252C2	2P 2.54997
2S	2.56387	0.01097	-1.02E66	1.00000
NEON	1S(2)2S(2)2P(6), 1S			
T.E.=	-0.12781218D+03	P.E.=	-0.25562286D+03	
K.E.=	0.12781068D+03	V.T.=	-0.20000117D+01	
S	1S	2S	P	2P
BASIS/ORB E	-32.66213	-1.73250	BASIS/ORB E	-0.56172
1S	9.64200	0.99735	0.25499	2P 2.87923
2S	2.87923	0.01091	-1.02937	1.00000

See page 183 for Explanation of Tables and Notes for Tables 32, 42, and 43

TABLE 43 (2). SINGLE ZETA FUNCTIONS.

SODIUM	K(2)L(8)3S(1), 2S					
T.E.=	-0.16112392D+03	P.E.=	-0.32224558D+03			
K.E.=	0.16112165D+03	V.T.=	-0.20000141D+01			
S	1S	2S	3S	P	2P	
BASIS/ORB E	-40.38100	-2.62086	-0.17525	BASIS/ORB E	-1.25414	
1S	10.62580	0.99721	0.26956	2P	3.40090	1.00000
2S	3.28573	0.01090	-1.03131		-0.14557	
3S	0.83570	-0.00098	-0.01188		1.00824	
MAGNESIUM	K(2)L(8)3S(2), 1S					
T.E.=	-0.19885779D+03	P.E.=	-0.39771257D+03			
K.E.=	0.19885479D+03	V.T.=	-0.20000151D+01			
S	1S	2S	3S	P	2P	
BASIS/ORB E	-48.93854	-2.59794	-0.24097	BASIS/ORB E	-2.03147	
1S	11.60880	0.99716	0.28151	2P	3.91288	1.00000
2S	3.69601	0.01065	-1.03479		-0.19985	
3S	1.10250	-0.00129	-0.00754		1.01703	
ALUMINUM	K(2)L(8)3S(2)3P(1), 2P					
T.E.=	-0.24115376D+03	P.E.=	-0.48230539D+03	K.E.=	0.24115163D+03	V.T.= -0.20000088D+01
S	1S	2S	3S	P	2P	3P
BASIS/ORB E	-58.37393	-4.70356	-0.34682	BASIS/ORB E	-2.95530	-0.17428
1S	12.59100	0.99715	0.29212	2P	4.48186	0.98155
2S	4.10672	0.01031	-1.03804		1.35545	0.08301
3S	1.37236	-0.00151	-0.00474		1.02775	-1.01361
SILICON	K(2)L(8)3S(2)3P(2), 3P					
T.E.=	-0.28808996D+03	P.E.=	-0.57617642D+03	K.E.=	0.28808646D+03	V.T.= -0.20000122D+01
S	1S	2S	3S	P	2P	3P
BASIS/ORB E	-68.69169	-5.94661	-0.49232	BASIS/ORB E	-4.00137	-0.26975
1S	13.57450	-0.99720	0.30060	2P	4.97254	0.98789
2S	4.51000	-0.00990	-1.04174		1.42841	0.06254
3S	1.63429	0.00166	0.00055		1.03878	-1.01165
PHOSPHORUS	K(2)L(8)3S(2)3P(3), 4S					
T.E.=	-0.33990988D+03	P.E.=	-0.67981500D+03	K.E.=	0.33990511D+03	V.T.= -0.20000140D+01
S	1S	2S	3S	P	2P	3P
BASIS/ORB E	-79.85319	-7.25658	-0.64337	BASIS/ORB E	-5.15547	-0.35848
1S	14.55770	-0.99727	0.30792	2P	5.48057	0.98835
2S	4.91251	-0.00944	-1.04525		1.62878	0.05732
3S	1.88058	0.00171	0.00457		1.04838	-1.01414
SULFUR	K(2)L(8)3S(2)3P(4), 3P					
T.E.=	-0.39662762D+03	P.E.=	-0.79324930D+03	K.E.=	0.39662169D+03	V.T.= -0.20000149D+01
S	1S	2S	3S	P	2P	3P
BASIS/ORB E	-91.68467	-8.77098	-0.81168	BASIS/ORB E	-6.43647	-0.38720
1S	15.54090	-0.99737	0.31428	2P	5.98848	0.98848
2S	5.31429	-0.00895	-1.04859		1.82733	0.05427
3S	2.12196	0.00171	0.00697		1.05715	-1.01621
CHLORINE	K(2)L(8)3S(2)3P(5), 2P					
T.E.=	-0.45852369D+03	P.E.=	-0.91704025D+03	K.E.=	0.45851656D+03	V.T.= -0.20000156D+01
S	1S	2S	3S	P	2P	3P
BASIS/ORB E	-104.75974	-10.35070	-0.98849	BASIS/ORB E	-7.82334	-0.43911
1S	16.52410	-0.99748	0.31982	2P	6.49658	0.98826
2S	5.71512	-0.00845	-1.05164		2.03679	0.05285
3S	2.35619	0.00168	0.01237		1.06477	-1.01855

See page 183 for Explanation of Tables and Notes for Tables 32, 42, and 43

## ROOTHAAN-HARTREE-FOCK ATOMIC WAVEFUNCTIONS

TABLE 43 (3). SINGLE ZETA FUNCTIONS.

ARGON K(2)L(8)3S(2)3P(3), 1S T.E.= -0.52576525D+03 P.E.= -0.10515209D+04 K.E.= 0.52575564D+03 V.T.= -0.20000183D+01							
S	1S	2S	3S	P	2P	3P	
BASIS/ORB E	-118.47941	-12.03770	-1.17470	BASIS/ORB E	-9.31763	-0.50634	
1S	17.50730	-0.99759	0.32468	2P	7.00409	0.98868	0.25959
2S	6.11518	-0.00796	-1.05441	3P	2.25467	0.04908	-1.02101
3S	2.58564	0.00163	0.01529		1.07143		
POTASSIUM K(2)L(8)3S(2)3P(6)4S(1), 2S T.E.= -0.59808987D+03 P.E.= -0.11961684D+04 K.E.= 0.59807849D+03 V.T.= -0.20000190D+01							
S	1S	2S	3S	4S	P	2P	3P
BASIS/ORB E	-133.42336	-14.20995	-1.66216	-0.13951	BASIS/ORB E	-11.29558	-0.89238
1S	18.49030	0.99771	-0.32843	0.11474	2P	7.51358	0.96687
2S	6.50283	0.00753	1.05820	-0.42507	3P	2.57520	0.05071
3S	2.89339	-0.00166	-0.02091	1.08271		-0.18055	-1.02755
4S	0.87356	0.00019	0.00255	0.02312		1.00596	
CALCIUM K(2)L(8)3S(2)3P(6)4S(2), 1S T.E.= -0.67563390D+03 P.E.= -0.13512566D+04 K.E.= 0.67562294D+03 V.T.= -0.20000152D+01							
S	1S	2S	3S	4S	P	2P	3P
BASIS/ORB E	-149.26717	-16.53599	-2.16325	-0.18210	BASIS/ORB E	-13.42627	-1.20205
1S	19.47290	-0.99784	-0.33175	0.12359	2P	8.02066	0.98552
2S	6.88753	-0.00707	1.06230	-0.45913	3P	2.68611	0.05128
3S	3.20054	0.00165	-0.02703	1.09665		-0.24678	-1.03384
4S	1.09947	-0.00025	0.00423	0.02177		1.02015	
SCANDIUM K(2)L(8)3S(2)3P(6)4S(2)3D(1), 2D T.E.= -0.75840414D+03 P.E.= -0.15167937D+04 K.E.= 0.75838958D+03 V.T.= -0.20000192D+01							
S	1S	2S	3S	4S			
BASIS/ORB E	-165.81242	-18.77249	-2.45393	-0.19013			
1S	20.45630	-0.99798	-0.33544	0.12811		-0.02482	
2S	7.28648	-0.00655	1.06519	-0.47418		0.09215	
3S	3.44734	0.00153	-0.0327	1.10386		-0.23728	
4S	1.15866	-0.00021	0.00439	0.02182		1.01819	
P	2P	3P	D	3D			
BASIS/ORB E	-15.47408	-1.50296	BASIS/ORB E	-0.18988			
2P	8.52719	0.98535	3D	2.37330	1.00000		
3P	3.13492	0.05014		-1.03706			
TITANIUM K(2)L(8)3S(2)3P(6)4S(2)3D(2), 3F T.E.= -0.84681561D+03 P.E.= -0.16536169D+04 K.E.= 0.8468C131D+03 V.T.= -0.20000169D+01							
S	1S	2S	3S	4S			
BASIS/ORB E	-183.18855	-21.08042	-2.71990	-0.19612			
1S	21.44020	-0.99812	-0.33887	0.13135		-0.02413	
2S	7.68816	-0.00604	1.06757	-0.48396		0.09014	
3S	3.67854	0.00138	-0.03257	1.10872		-0.22533	
4S	1.20441	-0.00018	0.00437	0.02215		1.01598	
P	2P	3P	D	3D			
BASIS/ORB E	-17.59528	-1.69262	BASIS/ORB E	-0.24338			
2P	9.03231	0.98537	3D	2.71329	1.00000		
3P	3.36777	0.04895		-1.03933			

See page 183 for Explanation of Tables and Notes for Tables 32, 42, and 43

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TABLE 43 (4). SINGLE ZETA FUNCTIONS.

VANADIUM K(2)L(8)3S(2)3P(6)4S(2)3D(3), 4F  
 T.E.= -0.940971970D+03 P.E.= -0.18819278D+04 K.E.= 0.94095587D+03 V.T.= -0.20300171D+C1

	S	1S	2S	3S	4S
BASIS/DRB E	-201.41977	-23.49023	-2.9629C	-0.20144	
1S	22.42430	-0.99826	-0.34202	0.13400	-0.02338
2S	8.69077	-0.00554	1.06563	-0.49142	0.06690
3S	3.90346	0.00123	-0.03441	1.11250	-0.21407
4S	1.24613	-0.00015	0.00430	0.02248	1.01405

	P	2P	3P	D	3D
BASIS/DRB E	-19.81969	-1.87978	BASIS/DRB E	-0.25642	
2P	9.53643	0.98546	0.33540	3D 2.99412	1.00000
3P	3.59475	0.04785	-1.04117		

CHROMIUM K(2)L(8)3S(2)3P(6)4S(2)3D(4), 5D  
 T.E.= -0.10410063D+04 P.E.= -0.20819887D+04 K.E.= 0.10405824D+04 V.T.= -0.20000230D+C1

	S	1S	2S	3S	4S
BASIS/DRB E	-220.50837	-26.00554	-3.24546	-0.20628	
1S	23.40850	-0.99840	-0.34452	0.13620	-0.02261
2S	8.49405	-0.00506	1.07144	-0.49724	0.08364
3S	4.12386	0.00109	-0.03589	1.11550	-0.20362
4S	1.28507	-0.00012	0.00419	0.02276	1.01239

	P	2P	3P	D	3D
BASIS/DRB E	-22.15077	-2.06636	BASIS/DRB E	-0.25083	
2P	10.03970	0.98557	0.34360	3D 3.25375	1.00000
3P	3.81763	0.04685	-1.04269		

MANGANESE K(2)L(8)3S(2)3P(6)4S(2)3D(5), 6S  
 T.E.= -0.11471067D+04 P.E.= -0.22542744D+04 K.E.= 0.11471678D+04 V.T.= -0.19999467D+01

	S	1S	2S	3S	4S
BASIS/DRB E	-240.44816	-28.61952	-3.50471	-0.21067	
1S	24.39600	-0.99851	-0.34748	0.13798	-0.02183
2S	8.89604	-0.00468	1.07304	-0.50169	0.08042
3S	4.33991	0.00098	-0.03722	1.11788	-0.19395
4S	1.32132	-0.00010	0.00408	0.02310	1.01096

	P	2P	3P	D	3D
BASIS/DRB E	-24.58224	-2.24939	BASIS/DRB E	-0.25159	
2P	10.54220	0.98570	0.34661	3D 3.50949	1.00000
3P	4.03606	0.04596	-1.04292		

IRON K(2)L(8)3S(2)3P(6)4S(2)3D(6), 5D  
 T.E.= -0.12590255D+04 P.E.= -0.25181498D+04 K.E.= 0.12590643D+04 V.T.= -0.20300158D+C1

	S	1S	2S	3S	4S
BASIS/DRB E	-261.28083	-31.38076	-3.78471	-0.21506	
1S	25.37760	-0.99867	-0.35002	0.13982	-0.02115
2S	9.30142	-0.00416	1.07455	-0.50627	0.07756
3S	4.55846	0.00082	-0.03625	1.12023	-0.18535
4S	1.35878	-0.00008	0.00396	0.02318	1.00978

	P	2P	3P	D	3D
BASIS/DRB E	-27.16080	-2.45145	BASIS/DRB E	-0.15690	
2P	11.04470	0.98580	0.35034	3D 3.72669	1.00000
3P	4.25861	0.04514	-1.04523		

See page 183 for Explanation of Tables and Notes for Tables 32, 42, and 43

## ROOTHAAN-HARTREE-FOCK ATOMIC WAVEFUNCTIONS

TABLE 43 (5). SINGLE ZETA FUNCTIONS.

COBALT K(2)L(8)3S(2)3P(6)4S(2)3D(7), 4F  
 T.E.= -0.1377374D+04 P.E.= -0.27547210D+04 K.E.= 0.13773466D+04 V.T.= -0.20000202D+01

	S	1S	2S	3S	4S
BASIS/ORB E	-282.96517	-34.24164	-4.06181	-0.21904	
1S	26.36220	-0.99879	-0.35225	0.14133	-0.02046
2S	9.70545	-0.00375	1.07569	-0.50981	0.07474
3S	4.77334	0.00069	-0.03919	1.12210	-0.17729
4S	1.39383	-0.00006	0.00033	0.02329	1.00874

	P	2P	3P	D	3D
BASIS/ORB E	-29.84064	-2.65C16	BASIS/ORB E	-0.08085	
2P	11.54650	0.98592	0.35309	3D 3.95211	1.00000
3P	4.47728	0.04440	-1.04629		

NICKEL K(2)L(8)3S(2)3P(6)4S(2)3D(8), 3F  
 T.E.= -0.15020487D+04 P.E.= -0.30040639D+04 K.E.= 0.15020152D+04 V.T.= -0.20000223D+01

	S	1S	2S	3S	4S
BASIS/ORB E	-305.50899	-37.21212	-4.34110	-0.22276	
1S	27.34700	-0.99891	-0.35435	0.14264	-0.01980
2S	10.10980	-0.00335	1.07710	-0.51267	0.07203
3S	4.98602	0.00056	-0.03998	1.12364	-0.16980
4S	1.42748	-0.00005	0.00370	0.02337	1.007E4

	P	2P	3P	D	3D
BASIS/ORB E	-32.63106	-2.85015	BASIS/ORB E	-0.00054	
2P	12.04780	0.98603	0.35540	3D 4.17688	1.00000
3P	4.69403	0.04373	-1.04721		

COPPER K(2)L(8)3S(2)3P(6)4S(1)3D(10), 2S  
 T.E.= -0.16323354D+04 P.E.= -0.32E45570D+04 K.E.= 0.16322215D+04 V.T.= -0.20000698D+01

	S	1S	2S	3S	4S
BASIS/ORB E	-328.62644	-39.96615	-4.22723	-0.17797	
1S	28.32880	-0.99905	-0.357C9	0.14225	-0.01203
2S	10.53380	-0.00288	1.07749	-0.50720	0.04331
3S	5.15648	0.00041	-0.03890	1.12240	-0.10137
4S	1.20818	-0.00002	0.00211	0.01855	1.00240

	P	2P	3P	D	3D
BASIS/ORB E	-35.21639	-2.67282	BASIS/ORB E	0.50637	
2P	12.55410	0.98653	0.35230	3D 4.20186	1.00000
3P	4.87625	0.04246	-1.04669		

ZINC K(2)L(8)3S(2)3P(6)4S(2)3D(10), 1S  
 T.E.= -0.17711509D+04 P.E.= -0.35422729D+04 K.E.= 0.17711220D+04 V.T.= -0.20000163D+01

	S	1S	2S	3S	4S
BASIS/ORB E	-353.16912	-43.47763	-4.90485	-0.22948	
1S	29.31700	-0.99914	-0.35816	0.14475	-0.01854
2S	10.91930	-0.00262	1.07915	-0.51676	0.06698
3S	5.40524	0.00034	-0.04116	1.12586	-0.15635
4S	1.49111	-0.00002	0.00345	0.02245	1.00E35

	P	2P	3P	D	3D
BASIS/ORB E	-38.53905	-3.25227	BASIS/ORB E	0.16625	
2P	13.04940	0.98626	0.35851	3D 4.62630	1.00000
3P	5.12205	0.04256	-1.04867		

See page 183 for Explanation of Tables and Notes for Tables 32, 42, and 43

TABLE 43 (6). SINGLE ZETA FUNCTIONS.

GALLIUM K(2)L(8)M(18)4S(2)4P(1), 2P T.E.= -0.19165167D+04 P.E.= -0.38329993D+04 K.E.= 0.19164826D+04 V.T.= -0.20300178D+01					
S	1S	2S	3S	4S	
BASIS/ORB E	-378.67149	-47.21719	-5.66106	-0.33249	
1S 30.30190	-0.99924	-0.35922	0.14750	-0.02540	
2S 11.30400	-0.00229	1.08102	-0.52744	0.09212	
3S 5.66469	0.00024	-0.04373	1.12961	-0.21404	
4S 1.75702	-0.00002	0.00493	0.02766	1.01259	
P	2P	3P	4P	D	3D
BASIS/ORB E	-42.08761	-3.91252	-0.16921	BASIS/ORB E	-0.24485
2P 13.54580	0.98563	0.36708	0.05679	3D 5.03101	1.00000
3P 5.40054	0.04336	-1.04537	-0.17336		
4P 1.55487	-0.00357	-0.04245	1.00662		
GERMANIUM K(2)L(8)M(18)4S(2)4P(2), 3P T.E.= -0.20685139D+04 P.E.= -0.41269846D+04 K.E.= 0.20684707D+04 V.T.= -0.20300209D+01					
S	1S	2S	3S	4S	
BASIS/ORB E	-405.11899	-51.16536	-6.48243	-0.45608	
1S 31.28660	-0.99934	-0.36017	0.15028	-0.03110	
2S 11.68650	-0.00198	1.08302	-0.53855	0.11331	
3S 5.92920	0.00014	-0.04660	1.13419	-0.26176	
4S 2.01132	-0.00001	0.00629	0.02886	1.01970	
P	2P	3P	4P	D	3D
BASIS/ORB E	-45.84340	-4.63313	-0.23985	BASIS/ORB E	-0.71582
2P 14.04140	0.98526	0.37549	0.06150	3D 5.41709	1.00000
3P 5.67085	0.04354	-1.04795	-0.18523		
4P 1.69547	-0.00390	-0.03978	1.00847		
ARSENIC K(2)L(8)M(18)4S(2)4P(3), 4S T.E.= -0.22272649D+04 P.E.= -0.44544855D+04 K.E.= 0.22272206D+04 V.T.= -0.20300199D+01					
S	1S	2S	3S	4S	
BASIS/ORB E	-432.47533	-55.2E449	-7.33536	-0.58189	
1S 32.27110	-0.99944	-0.36106	0.15303	-0.03585	
2S 12.06770	-0.00168	1.08507	-0.54971	0.13116	
3S 6.19669	0.00004	-0.04558	1.13931	-0.30098	
4S 2.23073	0.00001	0.00750	0.02887	1.02679	
P	2P	3P	4P	D	3D
BASIS/ORB E	-49.76961	-5.38364	-0.31383	BASIS/ORB E	-1.21395
2P 14.53720	0.98485	0.38419	0.07108	3D 5.79204	1.00000
3P 5.95096	0.04381	-1.0493	-0.21156		
4P 1.89323	-0.00451	-0.03946	1.01215		
SELENIUM K(2)L(8)M(18)4S(2)4P(4), 3P T.E.= -0.23927274D+04 P.E.= -0.47854054D+04 K.E.= 0.23926780D+04 V.T.= -0.20000206D+01					
S	1S	2S	3S	4S	
BASIS/ORB E	-460.76236	-59.59372	-8.23675	-0.71950	
1S 33.25540	-0.99954	-0.36190	0.15571	-0.04607	
2S 12.44770	-0.00139	1.08718	-0.56075	0.14725	
3S 6.46643	-0.00006	-0.05267	1.14477	-0.33559	
4S 2.43958	0.00003	0.0CE65	0.02824	1.03398	
P	2P	3P	4P	D	3D
BASIS/ORB E	-53.88556	-6.18308	-0.32934	BASIS/ORB E	-1.76002
2P 15.03270	0.98447	0.39279	0.07910	3D 6.15928	1.00000
3P 6.23478	0.04397	-1.05221	-0.23244		
4P 2.07162	-0.00497	-0.03903	1.01550		

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## ROOTHAAN-HARTREE-FOCK ATOMIC WAVEFUNCTIONS

TABLE 43 (7). SINGLE ZETA FUNCTIONS.

BROMINE K(2)L(8)M(18)4S(2)4P(5), 2P  
 T.E.= -0.25651131D+04 P.E.= -0.51301759D+04 K.E.= 0.25650628D+04 V.T.= -0.20000196D+01

S	1S	2S	3S	4S
BASIS/DRB E	-489.95869	-64.07188	-9.16893	-0.86082
1S	34.23960	-0.99963	-0.36268	0.15828
2S	12.82680	-0.00111	1.08931	-0.57151
3S	6.73739	-0.00016	-0.05580	1.15044
4S	2.63776	0.00006	0.00972	0.02728

P	2P	3P	4P	D	3D
BASIS/DRB E	-58.17027	-7.01358	-0.36795	BASIS/CRB E	-2.33577
2P	15.52810	0.98411	0.40120	3D	6.51988
3P	6.52213	0.04410	-1.05445		1.00000
4P	2.25690	-0.00541	-0.03889		

KRYPTON K(2)L(8)M(18)4S(2)4P(6), 1S  
 T.E.= -0.27445197D+04 P.E.= -0.54889823D+04 K.E.= 0.27444626D+04 V.T.= -0.20000208D+01

S	1S	2S	3S	4S
BASIS/DRB E	-520.06553	-68.71949	-10.13355	-1.00676
1S	35.22360	-0.59972	-0.36343	0.16074
2S	13.20530	-0.00063	1.09145	-0.58192
3S	7.00913	-0.00027	-0.05893	1.15617
4S	2.82874	0.00008	0.01C72	0.02616

P	2P	3P	4P	D	3D
BASIS/ORB E	-62.62432	-7.87688	-0.42092	BASIS/ORB E	-2.94305
2P	16.02320	0.98380	0.40551	3D	6.87521
3P	6.81157	0.04415	-1.05725		1.00000
4P	2.44237	-0.00577	-0.03677		

RUBIDIUM K(2)L(8)M(18)4S(2)4P(6)5S(1), 2S  
 T.E.= -0.29306931D+04 P.E.= -0.58613417D+04 K.E.= 0.29306485D+04 V.T.= -0.20000152D+01

S	1S	2S	3S	4S	5S
BASIS/DRB E	-551.37849	-73.83245	-11.42585	-1.38949	-0.12467
1S	36.20730	-0.99980	-0.36409	0.16293	0.05256
2S	13.57910	-0.00055	1.09397	-0.59170	-0.19589
3S	7.28177	-0.00038	-0.06299	1.16129	0.43977
4S	3.09637	0.00012	0.01265	0.02570	0.06848
5S	1.00690	-0.00001	-0.00138	-0.00195	-0.03762

P	2P	3P	4P	D	3D
BASIS/ORB E	-67.54255	-9.06645	-0.72316	BASIS/ORB E	-3.87551
2P	16.51920	0.98342	0.41681	3D	7.22639
3P	7.10122	0.04445	-1.05842		1.00000
4P	2.72005	-0.00662	-0.03774		

STRONTIUM K(2)L(8)M(18)4S(2)4P(6)5S(2), 1S  
 T.E.= -0.31237176D+04 P.E.= -0.62473646D+04 K.E.= 0.31236470D+04 V.T.= -0.20000226D+01

S	1S	2S	3S	4S	5S
BASIS/DRB E	583.62727	-79.13639	-12.77007	-1.76976	-0.15812
1S	37.19040	-0.99989	-0.36469	0.16500	-0.05783
2S	13.95050	-0.00027	1.09662	-0.60120	0.21677
3S	7.55440	-0.00050	-0.06733	1.16673	-0.48623
4S	3.36141	0.00017	0.01464	0.02455	1.06717
5S	1.21355	-0.00003	-0.00212	-0.00226	0.03769

See page 183 for Explanation of Tables and Notes for Tables 32, 42, and 43

TABLE 43 (8). SINGLE ZETA FUNCTIONS.

P	2P	3P	4P	D	3D
BASIS/ORB E	-72.65169	-10.30704	-1.02449	BASIS/ORB E	-4.85930
2P 17.01500	0.98310	0.42365	0.12448	3D 7.57534	1.00000
3P 7.38925	0.04466	-1.05990	-0.35478		
4P 2.98305	-0.00732	-0.03765	1.04200		

YTTRIUM K(2)L(8)M(18)4S(2)4P(6)5S(2)4D(1),2D  
T.E.=-0.332478060+04 P.E.=-0.664547510+04 K.E.= 0.33246945D+04 V.T.=-0.20000259D+C1

S	1S	2S	3S	4S	5S
BASIS/ORB E	-616.61797	-84.51913	-14.05638	-1.91702	-0.16204
1S 38.17470	-0.99997	-0.36492	0.16784	0.06102	0.01123
2S 14.31110	-0.00003	1.09938	-0.61470	-0.23032	-0.04251
3S 7.84999	-0.00061	-0.07167	1.17508	0.51191	0.09556
4S 3.56554	0.00020	0.01581	0.02286	-1.07541	-0.21785
5S 1.25113	-0.00003	-0.00210	-0.00181	-0.03796	1.01263

P	2P	3P	4P	D	3D	4D
BASIS/ORB E	-77.81721	-11.48694	-1.11744	BASIS/ORB E	-6.00404	0.74275
2P 17.50120	0.98273	0.43280	0.13340	3D 8.46554	0.89591	0.59603
3P 7.69747	0.04478	-1.06275	-0.37585	4D 3.98924	0.22306	-1.05268
4P 3.18638	-0.00755	-0.03763	1.04747			

ZIRCONIUM K(2)L(8)M(18)4S(2)4P(6)5S(2)4D(2),3F  
T.E.=-0.35313181D+04 P.E.=-0.70629930D+04 K.E.= 0.35316749D+04 V.T.=-0.19998990D+01

S	1S	2S	3S	4S	5S
BASIS/JRB E	-650.49962	-89.89860	-15.20012	-2.11807	-0.16581
1S 39.15970	-1.00005	-0.36571	0.16953	0.06336	0.01132
2S 14.69220	0.00021	1.10144	-0.62194	-0.23987	-0.04298
3S 8.11398	-0.00072	-0.07467	1.17991	0.53139	0.09635
4S 3.74497	0.00024	0.01673	0.02129	-1.08235	-0.21315
5S 1.30210	-0.00003	-0.00215	-0.00154	-0.03606	1.01212

P	2P	3P	4P	D	3D	4D
BASIS/ORB E	-83.01892	-12.53089	-1.26800	BASIS/ORB E	-6.69103	0.00747
2P 18.00280	0.98266	0.43735	0.13937	3D 8.50330	0.95637	0.38051
3P 7.96878	0.04458	-1.06479	-0.39141	4D 3.24828	0.14316	-1.01928
4P 3.35752	-0.00780	-0.03561	1.05244			

NIOBIUM K(2)L(8)M(18)4S(2)4P(6)5S(2)4D(3),4F  
T.E.=-0.37454826D+04 P.E.=-0.74915845D+04 K.E.= 0.37461019D+04 V.T.=-0.19998347D+C1

S	1S	2S	3S	4S	5S
BASIS/JRB E	-685.37177	-95.56253	-16.49387	-2.35703	-0.17144
1S 40.14380	-1.00013	-0.36642	0.17140	0.06612	0.01134
2S 15.07040	0.00046	1.10362	-0.63017	-0.25122	-0.04321
3S 8.39525	-0.00083	-0.07788	1.18540	0.55467	0.09658
4S 3.94192	0.00028	0.01775	0.01952	-1.09082	-0.20634
5S 1.35125	-0.00004	-0.00217	-0.00126	-0.03417	1.01128

P	2P	3P	4P	D	3D	4D
BASIS/JRB E	-88.49594	-13.72383	-1.45167	BASIS/ORB E	-7.59775	-0.17649
2P 18.50100	0.98252	0.44275	0.14652	3D 8.77373	0.97252	0.30456
3P 8.24985	0.04449	-1.06715	-0.40990	4D 3.07049	0.11149	-1.01297
4P 3.56611	-0.00808	-0.03380	1.05839			

MOLYBDENUM K(2)L(8)M(18)4S(2)4P(6)5S(2)4D(4),5D  
T.E.=-0.39670398D+04 P.E.=-0.79347231D+04 K.E.= 0.39676832D+04 V.T.=-0.19998378D+01

S	1S	2S	3S	4S	5S
BASIS/JRB E	-721.16290	-101.40659	-17.83249	-2.59061	-0.17565
1S 41.12710	-1.00021	0.36704	0.17315	0.06862	0.01158
2S 15.44590	0.00071	-1.10562	-0.63814	-0.26171	-0.04430
3S 8.65597	-0.00096	0.08116	1.19097	0.57602	0.09875
4S 4.13509	0.00032	-0.01878	0.01757	-1.09860	-0.20477
5S 1.40920	-0.00004	0.00224	-0.00101	-0.03343	1.01101

See page 183 for Explanation of Tables and Notes for Tables 32, 42, and 43

## ROOTHAAN-HARTREE-FOCK ATOMIC WAVEFUNCTIONS

TABLE 43 (9). SINGLE ZETA FUNCTIONS.

P	2P	3P	4P	D	3D	4D
BASIS/ORB E	-94.14929	-14.96117	-1.63137	BASIS/ORB E	-8.57232	-0.25233
2P 18.99590	0.98243	0.44811	0.15320	3D 9.10252	0.97748	0.27997
3P 8.53276	0.04428	-1.06941	-0.42682	4D 3.10504	0.09846	-1.01201
4P 3.75131	-0.00828	-0.03217	1.06403			
TECHNETIUM K(2)L(8)M(18)4S(2)4P(6)5S(2)4D(5),6S						
T.E.= -0.41960536D+04	P.E.= -0.83926142D+04	K.E.= 0.41965606D+04	V.T.= -0.19998792D+01			
S	1S	2S	3S	4S	5S	
BASIS/ORB E	-757.86609	-107.41401	-19.20122	-2.81865	-0.17934	
1S 42.11040	-1.00028	0.36761	0.17481	0.07083	0.01167	
2S 15.82060	0.00096	-1.1C198	-0.64574	-0.27113	-0.04480	
3S 8.92598	-0.00108	0.08438	1.19647	0.59495	0.09961	
4S 4.32446	0.00036	-0.01574	0.01559	-1.10574	-0.20126	
5S 1.45930	-0.00004	0.00228	-0.00076	-0.03274	1.01049	
P	2P	3P	4P	D	3D	4D
BASIS/ORB E	-99.96731	-16.228t1	-1.80794	BASIS/GRB E	-9.58427	-0.31914
2P 19.48910	0.98239	0.45329	0.15922	3D 9.44680	0.97939	0.27265
3P 8.81601	0.04397	-1.C7180	-0.44176	4D 3.21664	0.09175	-1.01248
4P 3.95074	-0.00842	-0.03064	1.06917			
RUTHENIUM K(2)L(8)M(18)4S(2)4P(6)5S(2)4D(6),5D						
T.E.= -0.44323604D+04	P.E.= -0.88651983D+04	K.E.= 0.44328379D+04	V.T.= -0.19998923D+01			
S	1S	2S	3S	4S	5S	
BASIS/GRB E	-795.49500	-113.60161	-20.61480	-3.05165	-0.18281	
1S 43.09340	-1.00036	0.36816	0.17641	0.07292	0.01168	
2S 16.19500	0.00121	-1.11012	-0.65321	-0.28013	-0.04502	
3S 9.19707	-0.00120	0.08755	1.20192	0.61279	0.09982	
4S 4.51136	0.00040	-0.02065	0.01373	-1.11257	-0.19695	
5S 1.50550	-0.00005	0.00230	-0.00054	-0.03208	1.00988	
P	2P	3P	4P	D	3D	4D
BASIS/GRB E	-105.96575	-17.54168	-1.99051	BASIS/ORB E	-10.64240	-0.31386
2P 19.98220	0.98236	0.45835	0.16488	3D 9.79467	0.98039	0.26984
3P 9.10071	0.04364	-1.07417	-0.45553	4D 3.34361	0.08764	-1.01307
4P 4.13787	-0.00851	-0.02927	1.07401			
RHODIUM K(2)L(8)M(18)4S(2)4P(6)5S(2)4D(7),4F						
T.E.= -0.46762637D+04	P.E.= -0.93529546D+04	K.E.= 0.46766909D+04	V.T.= -0.19999087D+01			
S	1S	2S	3S	4S	5S	
BASIS/GRB E	-834.03768	-119.95474	-22.05858	-3.28203	-0.18604	
1S 44.07690	-1.00043	0.36874	0.17802	0.07475	0.01154	
2S 16.57120	0.00144	-1.11215	-0.66055	-0.28808	-0.04463	
3S 9.45981	-0.00132	0.09047	1.20722	0.62789	0.09859	
4S 4.69063	0.00044	-0.02143	0.01214	-1.11844	-0.19069	
5S 1.54360	-0.00005	0.00228	-0.00036	-0.03112	1.00914	
P	2P	3P	4P	D	3D	4D
BASIS/GRB E	-112.13013	-18.88545	-2.17229	BASIS/ORB E	-11.73279	-0.32766
2P 20.47520	0.98237	0.46294	0.16995	3D 10.14570	0.98078	0.27099
3P 9.38224	0.04327	-1.07650	-0.46788	4D 3.49085	0.08504	-1.01397
4P 4.32100	-0.00858	-0.02774	1.07856			
PALLADIUM K(2)L(8)M(18)4S(2)4P(6)5S(2)4D(8),3F						
T.E.= -0.49278059D+04	P.E.= -0.98556706D+04	K.E.= 0.49278647D+04	V.T.= -0.19999881D+01			
S	1S	2S	3S	4S	5S	
BASIS/ORB E	-873.49315	-126.46999	-23.53215	-3.50938	-0.18848	
1S 45.05940	-1.00051	0.36921	0.17938	0.07642	0.01146	
2S 16.94370	0.00168	-1.11422	-0.66713	-0.29553	-0.04446	
3S 9.73775	-0.00144	0.09355	1.21240	0.64252	0.09799	
4S 4.87021	0.00049	-0.02228	0.01016	-1.12433	-0.18604	
5S 1.58350	-0.00005	0.00228	-0.00016	-0.03066	1.00854	

See page 183 for Explanation of Tables and Notes for Tables 32, 42, and 43

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TABLE 43 (10). SINGLE ZETA FUNCTIONS.

P	2P	3P	4P	D	3D	4D	
BASIS/ORB E -118.45862	-20.25887	-2.35221		BASIS/ORB E -12.85267	-0.34125		
2P 20.96780	0.98240	0.46746	0.17466	3D 10.49760	0.98090	0.27374	
3P 9.66553	0.04286	-1.07878	-0.47904	4D 3.64601	0.08329	-1.01497	
4P 4.50084	-0.00862	-0.02646	1.08269				
 SILVER K(2)L(8)M(18)4S(2)4P(6)5S(2)4D(9),2D T.E.=-0.51870705D+04 P.E.=-0.10374054D+05 K.E.= 0.51865838D+04 V.T.=-0.20300157D+01							
S	1S	2S	3S	4S	5S		
BASIS/ORB E -913.86457	-133.15531	-25.04264	-3.74096	-0.19194			
1S 46.04240	-1.00058	0.36971	0.18076	0.07800	0.01106		
2S 17.31790	0.00191	-1.11620	-0.67369	-0.30256	-0.04306		
3S 10.00800	-0.00156	0.09643	1.21741	0.65586	0.09461		
4S 5.04633	0.00053	-0.02301	0.00853	-1.12980	-0.17650		
5S 1.60641	-0.00005	0.00220	-0.00001	-0.02956	1.00752		
P	2P	3P	4P	D	3D	4D	
BASIS/ORB E -124.95731	-21.66990	-2.53773		BASIS/ORB E -14.00966	-0.36100		
2P 21.46070	0.98244	0.47174	0.17902	3D 10.84990	0.98080	0.27756	
3P 9.94825	0.04246	-1.08099	-0.48925	4D 3.80595	0.08227	-1.01559	
4P 4.67817	-0.00863	-0.02524	1.08654				
 CADMIUM K(2)L(8)M(18)4S(2)4P(6)5S(2)4D(10),1S T.E.=-0.54541908D+04 P.E.=-0.10908220D+05 K.E.= 0.54540294D+04 V.T.=-0.20300296D+01							
S	1S	2S	3S	4S	5S		
BASIS/ORB E -955.14246	-139.99588	-26.57984	-3.96758	-0.19413			
1S 47.02540	-1.00065	0.37020	0.18210	0.07943	0.01087		
2S 17.69250	0.00213	-1.11812	-0.68005	-0.30903	-0.04241		
3S 10.27870	-0.00167	0.09518	1.22227	0.66783	0.09290		
4S 5.21929	0.00057	-0.02370	0.00705	-1.13458	-0.17072		
5S 1.63800	-0.00005	0.00216	0.00011	-0.02897	1.00691		
P	2P	3P	4P	D	3D	4D	
BASIS/ORB E -131.61581	-23.10805	-2.71921		BASIS/ORB E -15.19317	-0.38621		
2P 21.95390	0.98248	0.47579	0.18303	3D 11.20240	0.98130	0.27942	
3P 10.23040	0.04205	-1.08313	-0.49848	4D 3.56929	0.07906	-1.01724	
4P 4.85267	-0.00863	-0.02409	1.09008				
 INDIUM K(2)L(8)M(18)4S(2)4P(6)5S(2)4D(10)5P(1),2D T.E.=-0.57290986D+04 P.E.=-0.11458125D+05 K.E.= 0.57290266D+04 V.T.=-0.20300126D+01							
S	1S	2S	3S	4S	5S		
BASIS/ORB E -997.63137	-147.32451	-28.47224	-4.49475	-0.27871			
1S 48.00850	-1.00072	0.37064	0.18318	0.08191	0.01501		
2S 18.06240	0.00235	-1.12038	-0.68560	-0.31984	-0.05884		
3S 10.54330	-0.00180	0.10284	1.22701	0.69170	0.12939		
4S 5.44279	0.00063	-0.02527	0.00504	-1.14200	-0.23443		
5S 1.90276	-0.00008	0.00311	0.00042	-0.03519	1.01367		
P	2P	3P	4P	5P	D	3D	4D
BASIS/ORB E -138.75153	-24.89956	-3.19006	-0.15335		BASIS/ORB E -16.73175	-0.69203	
2P 22.44850	0.98245	0.47909	0.19020	-0.03168	3D 11.55920	0.97926	0.29511
3P 10.50690	0.04195	-1.08465	-0.51854	0.08759	4D 4.23514	0.08159	-1.02068
4P 5.09263	-0.00903	-0.02319	1.09135	-0.19889			
5P 1.67700	0.00096	0.00146	0.04469	1.00834			
 TIV K(2)L(8)M(18)4S(2)4P(6)5S(2)4D(10)5P(2),3P T.E.=-0.60116720D+04 P.E.=-0.12023214D+05 K.E.= 0.60115422D+04 V.T.=-0.20000216D+01							
S	1S	2S	3S	4S	5S		
BASIS/ORB E -1041.07983	-154.86112	-30.43971	-5.04732	-0.37606			
1S 48.99140	-1.00078	0.37106	0.18420	0.08424	0.01838		
2S 18.43110	0.00256	-1.12266	-0.69095	-0.33014	-0.07240		
3S 10.80700	-0.00193	0.10655	1.23182	0.71462	0.15978		
4S 5.66432	0.00069	-0.02688	0.00280	-1.14990	-0.28564		
5S 2.12506	-0.00011	0.00395	0.00083	-0.03784	1.02107		

See page 183 for Explanation of Tables and Notes for Tables 32, 42, and 43

## ROOTHAAN-HARTREE-FOCK ATOMIC WAVEFUNCTIONS

TABLE 43 (11). SINGLE ZETA FUNCTIONS.

P	2P	3P	4P	5P	D	3D	4D
BASIS/ORB E	-146.10014	-26.76659	-3.68229	-0.21260	BASIS/ORB E	-1E.34426	-1.02294
2P 22.94230	0.98247	0.48243	0.19696	-0.03541	3D 11.91370	0.97752	0.31665
3P 10.78460	0.04172	-1.08644	-0.53708	0.09810	4D 4.49253	0.08344	-1.02413
4P 5.31542	-0.09022	-0.02200	1.09835	-0.21815			
5P 1.81924	0.00108	0.00145	0.04320	1.01097			

ANTIMONY K(2)L(8)M(18)4S(2)4P(6)5S(2)4D(10)5P(3),4S  
 T.E.= -0.63020043D+04 P.E.= -0.12603883D+05 K.E.= 0.63018784D+04 V.T.= -0.20000200D+01

S	1S	2S	3S	4S	5S
BASIS/ORB E	-1085.46447	-162.58834	-32.46261	-5.60660	-0.47541
1S 49.97410	-1.00085	0.37146	0.18518	0.08646	0.02123
2S 18.79940	0.00277	-1.12492	-0.69619	-0.34008	-0.08398
3S 11.07070	-0.00206	0.11C24	1.23666	0.73675	0.16596
4S 5.88451	0.00076	-0.02849	0.00048	-1.15809	-0.32812
5S 2.32277	-0.00013	0.00470	0.00126	-0.03916	1.02840

P	2P	3P	4P	5P	D	3D	4D
BASIS/ORB E	-153.64002	-28.68957	-4.18211	-0.27562	BASIS/ORB E	-20.01694	-1.36133
2P 23.43620	0.98249	-0.48560	0.20379	-0.04109	3D 12.26630	0.97596	0.33251
3P 11.06170	0.04150	1.08821	-0.55603	0.11418	4D 4.74362	0.08479	-1.02756
4P 5.54463	-0.00944	0.02674	1.10519	-0.24923			
5P 1.99857	0.00126	-0.00146	0.04332	1.01538			

TELLURIUM K(2)L(8)M(18)4S(2)4P(6)5S(2)4D(10)5P(4),3P  
 T.E.= -0.66000387D+04 P.E.= -0.13200106D+05 K.E.= 0.66000669D+04 V.T.= -0.19999957D+01

S	1S	2S	3S	4S	5S
BASIS/ORB E	-1130.80076	-170.52171	-34.55559	-6.18706	-0.58279
1S 50.95680	-1.00091	0.37187	0.18617	0.08860	0.02378
2S 19.15800	0.00298	-1.12716	-0.70140	-0.34971	-0.09444
3S 11.33540	-0.00220	0.11388	1.24151	0.75813	0.20975
4S 6.10363	0.00082	-0.03008	-0.00181	-1.16641	-0.36555
5S 2.50602	-0.00016	0.00540	0.00175	-0.03973	1.03572

P	2P	3P	4P	5P	D	3D	4D
BASIS/ORB E	-161.38636	-30.68324	-4.70324	-0.28526	BASIS/ORB E	-21.74691	-1.72164
2P 23.93030	0.98251	-0.48860	0.21045	-0.04604	3D 12.61730	0.97458	0.34709
3P 11.33770	0.04129	1.09002	-0.57482	0.12833	4D 4.99057	0.08578	-1.03098
4P 5.77571	-0.00965	0.01932	1.11240	-0.27480			
5P 2.15804	0.00141	-0.00137	0.04374	1.01930			

IODINE K(2)L(8)M(18)4S(2)4P(6)5S(2)4D(10)5P(5),2P  
 T.E.= -0.69059462D+04 P.E.= -0.13811744D+05 K.E.= 0.69057974D+04 V.T.= -0.20000215D+01

S	1S	2S	3S	4S	5S
BASIS/ORB E	-1177.07985	-178.64839	-36.70628	-6.77652	-0.59223
1S 51.93900	-1.00098	0.37223	0.18704	0.09061	0.02607
2S 19.53430	0.00319	-1.12942	-0.70626	-0.35E91	-0.10397
3S 11.59740	-0.00233	0.11763	1.24644	0.77896	0.23167
4S 6.32241	0.00089	-0.03172	-0.00445	-1.17503	-0.39903
5S 2.67900	-0.00018	0.00606	0.00229	-0.03992	1.04283

P	2P	3P	4P	5P	D	3D	4D
BASIS/ORB E	-169.32776	-32.73494	-5.23371	-0.31591	BASIS/ORB E	-23.53949	-2.09164
2P 24.42350	0.98256	-0.49155	0.21686	-0.05128	3D 12.96680	0.97355	0.36050
3P 11.61420	0.04104	1.09189	-0.59295	0.14337	4D 5.23364	0.08646	-1.03436
4P 6.00695	-0.00984	0.01786	1.11945	-0.30175			
5P 2.32200	0.00155	-0.00126	0.04444	1.02379			

See page 183 for Explanation of Tables and Notes for Tables 32, 42, and 43

TABLE 43 (12). SINGLE ZETA FUNCTIONS.

XENON       $K(2)L(8)M(18)4S(2)4P(\ell)5S(z)4D(10)5P(6),1S$   
 $T.E. = -0.721979230 \times 10^4$     $P.E. = -0.144393640 \times 10^5$     $K.F. = 0.721957160 \times 10^4$     $V.T. = -0.200003060 \times 10^1$

S	1S	2S	3S	4S	5S	E	3D	4D
BASIS/ORE E	-1224.29750	-186.96814	-38.91443	-7.37636	-0.80441			
1S	52.92110	-1.00104	0.37260	0.18792	0.09254	0.02816		
2S	19.90090	0.00340	-1.13164	-0.71111	-0.36779	-0.11274		
3S	11.86000	-0.00247	0.12131	1.25135	0.79905	0.25197		
4S	6.54017	0.00096	-0.03333	-0.00704	-1.18363	-0.42918		
5S	2.84389	-0.00021	0.00668	0.00263	-0.03987	1.04965		
P	2P	3P	4P	5P	E	3D	4D	
BASIS/ORE E	-177.46272	-34.84475	-5.77515	-0.35921	BASIS/ORE E	-25.38662	-2.47297	
2P	24.91690	0.98262	-0.45435	0.22319	-0.05555	3D	13.31490	0.97227
3P	11.88950	0.04079	1.09381	-0.61112	0.15703	4D	5.47336	0.08650
4P	6.23951	-0.01002	0.01625	1.12737	-0.32555			-1.03769
5P	2.48482	0.00168	-0.00105	0.04291	1.02858			

See page 183 for Explanation of Tables and Notes for Tables 32, 42, and 43

## ROOTHAAN-HARTREE-FOCK ATOMIC WAVEFUNCTIONS

TABLE 44 (1). THE HARTREE-FOCK FUNCTIONS FOR NEGATIVE IONS.

LITHIUM 1S(2)2S(2), 1S  
 T.E.= -0.74282299D+01 P.E.= -0.14856473D+02  
 K.E.= 0.74282431D+01 V.T.= -0.19999982D+01

S	1S	2S
BASIS/ORB E	-2.32274	-0.01453
1S 2.47472	0.69760	-0.10034
1S 4.69209	0.11212	-0.01100
2S 0.26763	-0.00003	0.35768
2S 0.53399	0.00016	0.56089
2S 1.01129	-0.00108	0.20478
2S 1.66285	0.00750	-0.07906

BORON 1S(2)2S(2)2P(2), 3P  
 T.E.= -0.24519192D+02 P.E.= -0.49038759D+02  
 K.E.= 0.24519567D+02 V.T.= -0.19999847D+01

S	1S	2S	P	2P
BASIS/ORB E	-7.42471	-0.24234	BASIS/ORB E	-0.02631
1S 4.56045	0.91238	-0.17174	2P 1.30678	0.16838
1S 8.11463	0.06652	-0.01398	2P 2.01088	0.15874
2S 1.61352	0.00164	0.61136	2P 0.86730	0.45444
2S 4.07580	0.03461	-0.07870	2P 0.42052	0.36294
2S 0.89624	-0.00016	0.49174	2P 5.32615	0.00839

BORON 1S(2)2S(2)2P(2), 1D  
 T.E.= -0.24490501D+02 P.E.= -0.48981375D+02  
 K.E.= 0.24490874D+02 V.T.= -0.19999847D+01

S	1S	2S	P	2P
BASIS/ORB E	-7.47048	-0.27477	BASIS/ORB E	-0.00746
1S 4.52878	0.92064	-0.18106	2P 1.21973	0.27221
1S 8.11937	0.06707	-0.01232	2P 2.21440	0.13293
2S 1.61332	0.00147	0.63594	2P 0.79969	0.37576
2S 3.94269	0.02445	-0.07870	2P 0.34316	0.41062
2S 0.91372	-0.00017	0.46783	2P 7.96796	0.00284

BORON 1S(2)2S(2)2P(2), 1S  
 T.E.= -0.24444257D+02 P.E.= -0.48924120D+02  
 K.E.= 0.24479863D+02 V.T.= -0.199995455D+01

S	1S	2S	P	2P
BASIS/ORB E	-7.48496	-0.28065	BASIS/ORB E	0.03501
1S 4.55781	0.90607	-0.16885	2P 0.58014	0.82758
1S 8.05650	0.06813	-0.01775	2P 2.03284	0.36695
2S 1.62299	0.00116	0.64870	2P 5.55241	0.02905
2S 4.11606	0.03786	-0.08987	2P 3.51561	-0.09048
2S 0.90583	-0.00001	0.45776		

CARBON 1S(2)2S(2)2P(3), 4S  
 T.E.= -0.37708790D+02 P.E.= -0.75418508D+02  
 K.E.= 0.37709718D+02 V.T.= -0.19999754D+01

S	1S	2S	P	2P
BASIS/ORB E	-10.95611	-0.37271	BASIS/ORB E	-0.07692
1S 5.46377	0.91913	-0.19336	2P 1.47046	0.38711
1S 9.26713	0.07441	-0.01195	2P 2.49958	0.20373
2S 2.14720	0.00216	0.55913	2P 0.88367	0.36913
2S 4.61245	0.01622	-0.08947	2P 0.53683	0.15834
2S 1.16992	0.00002	0.56499	2P 5.71052	0.01337

CARBON 1S(2)2S(2)2P(3), 2D  
 T.E.= -0.37642523D+02 P.E.= -0.75286423D+02  
 K.E.= 0.37643899D+02 V.T.= -0.19999634D+01

S	1S	2S	P	2P
BASIS/ORB E	-11.00452	-0.40236	BASIS/ORB E	-0.04752
1S 5.40466	0.91672	-0.18525	2P 1.48912	0.36478
1S 9.10160	0.08455	-0.01866	2P 2.56050	0.19570
2S 2.13245	0.00359	0.56181	2P 0.90514	0.35018
2S 4.89591	0.00623	-0.08757	2P 0.50131	0.23271
2S 1.18793	-0.00052	0.55374	2P 6.03766	0.01059

See page 183 for Explanation of Tables and Notes for Tables 32, 42, and 43

TABLE 44 (2). THE HARTREE-FOCK FUNCTIONS FOR NEGATIVE IONS.

CARBON      1S(2)2S(2)2P(3), 2P  
 T.E.= -0.37600849D+02    P.E.= -0.75201919D+02  
 K.E.= 0.37601070D+C2    V.T.= -0.19999941D+01

S	1S	2S	P	2P
BASIS/ORB E	-11.03915	-0.42446	BASIS/ORB E	-0.03152
1S 5.54095	C.89605	-0.17610	2P 1.42054	0.27325
1S 9.25408	0.07655	-0.02026	2P 2.50736	0.22851
2S 2.00064	0.00339	C.65079	2P 1.02701	0.34349
2S 5.27297	0.03958	-0.08394	2P 0.46783	0.31704
2S 1.13183	-0.00065	0.45051	2P 6.41149	0.00887

NITROGEN      1S(2)2S(2)2P(4), 3P  
 T.E.= -0.54321897D+02    P.E.= -0.10864458D+03  
 K.E.= 0.54322683D+C2    V.T.= -0.19999855D+01

S	1S	2S	P	2P
BASIS/ORB E	-15.24218	-C.5E050	BASIS/ORB E	-0.09356
1S 6.54283	0.92390	-0.20406	2P 1.62610	0.47311
1S 11.08920	0.05704	-0.00913	2P 3.01746	0.25346
2S 2.55856	0.00235	0.57977	2P 0.88922	0.31743
2S 5.61125	0.02992	-0.09224	2P 0.55566	0.08602
2S 1.41772	0.00008	0.54305	2P 7.14545	0.01135

NITROGEN      1S(2)2S(2)2P(4), 1D  
 T.E.= -0.54266877D+C2    P.E.= -0.10653399D+03  
 K.E.= 0.54267113D+02    V.T.= -0.19999956D+01

S	1S	2S	P	2P
BASIS/ORB E	-15.27194	-0.59809	BASIS/ORB E	-0.07734
1S 6.54760	0.92738	-0.20509	2P 1.61663	C.45987
1S 11.26030	0.05387	-0.00886	2P 3.00439	0.25808
2S 2.54587	0.00287	0.56925	2P 0.89447	0.30325
2S 5.64752	0.02920	-0.09157	2P 0.55010	0.11987
2S 1.41976	-0.00015	0.53188	2P 7.18013	C.01122

NITROGEN      1S(2)2S(2)2P(4), 1S  
 T.E.= -0.54186826D+02    P.E.= -0.10637425D+03  
 K.E.= 0.54187421D+02    V.T.= -0.19999890D+01

S	1S	2S	P	2P
BASIS/ORB E	-15.31766	-0.62592	BASIS/ORB E	-0.05564
1S 6.53685	0.92869	-0.20741	2P 1.61271	0.43105
1S 11.23540	0.05450	-0.00879	2P 3.01645	0.25988
2S 2.55303	0.00264	C.55E50	2P 0.98019	0.25278
2S 5.59056	0.02706	-0.05412	2P 0.56273	C.21269
2S 1.42845	-0.00008	0.52500	2P 7.29361	C.01028

OXYGEN      1S(2)2S(2)2P(5), 2P  
 T.E.= -0.74789510D+02    P.E.= -0.14558305D+03  
 K.E.= 0.74793543D+02    V.T.= -0.19999461D+01

S	1S	2S	P	2P
BASIS/ORB E	-20.19814	-0.81327	BASIS/ORB E	-0.12926
1S 7.61467	0.93779	-0.21102	2P 1.74399	C.52755
1S 13.42550	0.03825	-0.0061	2P 3.42975	0.30564
2S 3.21269	0.00206	0.51254	2P 0.86393	0.28894
2S 6.31491	0.03520	-0.11661	2P 0.40831	C.00890
2S 1.75076	0.00040	0.62579	2P 7.82044	0.01376

FLUORINE      1S(2)2S(2)2P(6), 1S  
 T.E.= -0.99459366D+02    P.E.= -0.19891818D+03  
 K.E.= 0.99458810D+02    V.T.= -0.200000C56D+01

S	1S	2S	P	2P
BASIS/ORB E	-25.82952	-1.07444	BASIS/ORB E	-0.18085
1S 8.93690	C.89308	-0.20022	2P 2.07537	0.47039
1S 14.84990	0.03498	-0.00852	2P 3.93342	0.30842
2S 3.27783	0.00446	0.62675	2P 1.46603	0.09885
2S 8.10301	0.08884	-0.05809	2P 0.95683	0.24705
2S 1.85159	-0.00055	0.48432	2P 8.32950	0.01686

See page 183 for Explanation of Tables and Notes for Tables 32, 42, and 43

## ROOTHAAN-HARTREE-FOCK ATOMIC WAVEFUNCTIONS

TABLE 44 (3). THE HARTREE-FOCK FUNCTIONS FOR NEGATIVE IONS.

SODIUM K(2)L(8)3S(2), 1S  
 T.E.= -0.16185466D+03 P.E.= -0.3237C748D+03  
 K.E.= 0.16185282D+03 V.T.= -0.2000C0114D+01

S	1S	2S	3S	P	2P
BASIS/ORB E	-40.33140	-2.64578	-0.01248	BASIS/CRB E	-1.37090
1S 11.15950	0.89439	-0.21712	0.02032	2P 2.38607	0.54750
1S 18.41410	0.02283	-0.00623	0.00184	2P 4.30498	0.43517
2S 4.13029	0.00357	0.79537	-0.09542	2P 7.85561	0.06623
2S 9.93556	0.10131	-0.11441	0.01576	2P 1.48218	0.03069
3S 0.95740	0.00005	0.00146	0.51172		
3S 0.41694	-0.00002	-0.00043	0.62617		
3S 3.13459	-0.00031	0.33351	-0.02914		

ALUMINUM K(2)L(8)3S(2)3P(2), 3P  
 T.E.= -0.241E7778D+03 P.E.= -0.48374708D+03 K.E.= 0.24186930D+03 V.T.= -0.20000351D+01

S	1S	2S	3S	P	2P	3P
BASIS/ORB E	-58.30804	-4.71618	-0.20881	BASIS/ORB E	-3.02515	-0.01987
1S 13.79900	0.84839	0.21618	0.04596	2P 5.46435	0.63482	-0.08627
1S 21.54950	0.01875	0.00554	0.00254	2P 10.70680	0.03672	-0.00539
2S 4.53176	0.00543	-0.99260	-0.24560	3P 1.73650	0.01651	0.15014
2S 12.46090	0.15756	0.12337	0.03159	3P 0.46976	0.00097	0.45612
3S 1.74144	0.00101	0.01560	0.63081	3P 3.91477	0.41163	-0.06269
3S 0.96820	-0.00035	-0.00434	0.49895	3P 1.00691	-0.00408	0.56028
3S 3.19359	-0.00214	-0.11562	-0.06895			

ALUMINUM K(2)L(8)3S(2)3P(2), 1D  
 T.E.= -0.241856450D+03 P.E.= -0.4837C484D+03 K.E.= 0.24184839D+03 V.T.= -0.20000333D+01

S	1S	2S	3S	P	2P	3P
BASIS/ORB E	-58.33647	-4.74443	-0.23104	BASIS/ORB E	-3.05298	-0.00542
1S 13.97120	0.84393	-0.21555	0.04656	2P 5.47383	0.63358	-0.08294
1S 23.04970	0.01169	-0.00477	0.00195	2P 10.69030	0.03643	-0.00541
2S 4.56195	0.00556	0.97501	-0.24502	3P 1.67224	0.01487	0.20512
2S 12.52550	0.17081	-0.12795	0.03269	3P 0.37241	0.00091	0.44089
3S 1.71930	0.00086	-0.00541	0.64886	3P 3.91347	0.41441	-0.06309
3S 0.97286	-0.00033	0.00283	0.47051	3P 0.89534	-0.00331	0.56960
3S 3.37099	-0.00210	0.12579	-0.06574			

ALUMINUM K(2)L(8)3S(2)3P(2), 1S  
 T.E.= -0.24183001D+03 P.E.= -0.48365392D+03 K.E.= 0.24182391D+03 V.T.= -0.20000253D+01

S	1S	2S	3S	P	2P	3P
BASIS/ORB E	-58.38652	-4.79423	-0.27301	BASIS/ORB E	-3.10224	0.00510
1S 13.82790	0.84612	0.21740	0.04659	2P 5.48652	0.62957	-0.07476
1S 21.50190	0.01860	0.00622	0.00307	2P 10.60660	0.03699	-0.00555
2S 4.53882	0.00546	-0.98882	-0.25465	3P 1.71100	0.01506	0.20539
2S 12.47890	0.16033	0.12408	0.03360	3P 0.26569	0.00070	0.51201
3S 1.69241	0.00094	0.01232	0.68776	3P 3.92701	0.41744	-0.06337
3S 0.98249	-0.00037	-0.00381	0.42473	3P 0.83403	-0.00242	0.58524
3S 3.26649	-0.00208	-0.11665	-0.05988			

SILICON K(2)L(8)3S(2)3P(3), 4S  
 T.E.= -0.28888946D+03 P.E.= -0.57778024D+03 K.E.= 0.28889078D+03 V.T.= -0.19999954D+01

S	1S	2S	3S	P	2P	3P
BASIS/ORB E	-68.55290	-5.89668	-0.30154	BASIS/CRB E	-3.99785	-0.06153
1S 14.56740	0.88233	-0.2285	0.05507	2P 6.14385	0.62570	-0.11472
1S 23.51120	0.01511	-0.00702	0.00226	2P 11.90820	0.03052	-0.00565
2S 5.29626	0.00405	0.89914	-0.24334	3P 2.65508	0.01892	0.18378
2S 13.04490	0.12306	-0.13346	0.03633	3P 0.68553	0.00117	0.39535
3S 1.99715	0.00019	-0.00159	0.65999	3P 4.49330	0.42008	-0.08562
3S 1.13024	-0.00008	0.00122	0.46340	3P 1.29404	-0.00563	0.55702
3S 4.34124	-0.00097	0.22216	-0.10102			

See page 183 for Explanation of Tables and Notes for Tables 32, 42, and 43

TABLE 44 (4). THE HARTREE-FOCK FUNCTIONS FOR NEGATIVE IONS.

SILICON K(2)L(8)3S(2)3P(3), 2C  
T.E.= -0.28884143D+03 P.E.= -0.57768052D+03 K.E.= 0.28883910D+03 V.T.= -0.20300081D+01

S	1S	2S	3S	P	2P	3P
BASIS/ORB E	-66.58104	-5.92369	-0.32005	BASIS/ORB E	-4.02446	-0.03850
1S 14.48850	0.68282	-0.23C68	0.05561	2P 6.13871	0.63142	-0.11494
1S 22.91870	0.C191C	-0.0C125	0.00256	2P 12.13250	C.02853	-0.00502
2S 5.29821	0.00474	0.89130	-0.24403	3P 1.76840	0.01403	0.39881
2S 13.05530	0.11749	-0.12923	0.C3598	3P C.52213	0.00166	0.24544
3S 1.97393	0.00029	0.00266	0.68531	3P 4.45895	0.42016	-0.07570
3S 1.12147	-0.00012	-0.0CC44	0.43377	3P C.98802	-0.00482	0.51768
3S 4.41726	-0.00136	0.225E4	-0.09929			

SILICON K(2)L(8)3S(2)3P(3), 2P  
T.E.= -0.28881109D+03 P.E.= -0.57762152D+03 K.E.= C.28881043D+03 V.T.= -0.20300023D+01

S	1S	2S	3S	P	2P	3P
BASIS/ORB E	-68.60075	-5.94276	-0.33370	BASIS/ORB E	-4.04328	-0.02529
1S 14.5797C	0.88313	-0.23059	-0.05687	2P 6.14676	0.63127	-0.11290
1S 24.03560	0.01374	-0.00561	-0.00173	2P 12.22840	0.02772	-0.00499
2S 5.29924	0.00435	0.89176	0.24401	3P 1.82361	0.01422	0.36040
2S 13.06070	0.12355	-0.13099	-0.03576	3P 0.49949	0.06143	0.29471
3S 2.00291	0.00024	0.00223	-0.66830	3P 4.46282	0.42072	-0.08107
3S 1.14914	-0.00010	-0.0CC27	-0.45252	3P 1.01971	-0.00398	0.52668
3S 4.41145	-0.00115	0.225E1	0.10482			

PHOSPHORUS K(2)L(8)3S(2)3P(4), 3P  
T.E.= -0.34069866D+03 P.E.= -0.68139573D+03 K.E.= 0.34069706D+03 V.T.= -0.20000047D+01

S	1S	2S	3S	P	2P	3P
BASIS/ORB E	-79.69252	-7.23214	-0.43643	BASIS/ORB E	-5.12342	-0.07694
1S 15.87100	C.65248	-0.21667	0.05553	2F 6.50443	0.64958	-0.13697
1S 22.95730	0.02274	-0.01476	0.00522	2P 12.07960	0.04098	-0.00878
2S 5.60345	0.00505	0.54590	-0.27924	3P 2.22280	0.01262	0.32280
2S 14.35170	0.14794	-0.14303	0.04254	3P 0.74701	0.00094	0.31012
3S 2.30974	0.00038	0.00257	0.67285	3P 4.90177	0.38147	-0.09181
3S 1.32517	-0.00015	-0.00024	0.46334	3P 1.36757	-0.00308	0.51737
3S 4.71910	-0.00172	0.1E375	-0.10443			

PHOSPHORUS K(2)L(8)3S(2)3P(4), 1D  
T.E.= -0.34065980D+03 P.E.= -0.68131913D+03 K.E.= 0.34065932D+03 V.T.= -0.20000014D+01

S	1S	2S	3S	P	2P	3P
BASIS/ORB E	-79.70889	-7.24769	-0.44659	BASIS/CRB E	-5.13880	-0.06381
1S 16.08400	0.847C6	-0.21516	-0.05530	2P 6.49275	0.65057	-0.13540
1S 23.88660	0.015C9	-0.01242	-0.04558	2P 12.05600	0.04160	-0.00930
2S 5.58736	0.00496	0.94978	0.28205	3P 2.35154	0.01261	0.26942
2S 14.44780	0.16307	-0.14651	-0.04379	3P C.72316	0.00085	0.33127
3S 2.29977	0.00036	0.00269	-0.68539	3P 4.50041	0.37886	-0.09590
3S 1.31996	-0.00014	-0.00017	-0.45039	3P 1.41307	-0.00161	0.56264
3S 4.69916	-0.00166	0.15E60	0.10223			

PHOSPHORUS K(2)L(8)3S(2)3P(4), 1S  
T.E.= -0.34060316D+03 P.E.= -0.68120940D+03 K.E.= 0.3406C624D+03 V.T.= -0.19999910D+01

S	1S	2S	3S	P	2P	3P
BASIS/ORB E	-79.73376	-7.27150	-0.46234	BASIS/ORB E	-5.16235	-0.04552
1S 16.01580	0.84572	-0.21106	0.05453	2P 6.48013	0.65101	-0.13468
1S 23.19830	0.01964	-0.01616	0.00563	2P 11.98780	0.04269	-0.00949
2S 5.60276	0.00511	0.54E55	-0.28276	3P 2.39798	0.01262	0.25080
2S 14.44130	0.15925	-0.14817	0.04432	3P 0.69954	0.00108	0.36387
3S 2.31239	0.00041	0.0009	0.68726	3P 4.89686	0.37663	-0.09583
3S 1.33091	-0.00016	0.00C77	0.45120	3P 1.43720	-0.00068	0.56214
3S 4.66520	-0.00175	0.1E3C4	-C.10732			

See page 183 for Explanation of Tables and Notes for Tables 32, 42, and 43

## ROOTHAAN-HARTREE-FOCK ATOMIC WAVEFUNCTIONS

TABLE 44 (5). THE HARTREE-FOCK FUNCTIONS FOR NEGATIVE IONS.

SULFUR K(2)L(8)3S(2)3P(5), 2P  
 T.E.= -0.39753820D+03 P.E.= -0.79507644D+03 K.E.= 0.39753824D+03 V.T.= -0.19999999D+01

	S	1S	2S	3S	P	2P	3P
BASIS/ORB	E	-91.67593	-8.67515	-0.57932	BASIS/ORB	E	-6.35496
1S	15.78440	0.92673	-0.25528	-0.07376	2P	7.07744	0.65156
1S	24.31730	0.03436	-0.00781	-0.00186	2P	12.99860	0.03916
2S	6.72829	0.00485	0.80034	0.24398	3P	2.62059	0.01316
2S	14.02420	0.04839	-0.13560	-0.04061	3P	0.89975	0.00095
3S	2.55720	0.00025	0.00504	-0.69742	3P	5.42495	0.37601
3S	1.48480	-0.00012	-0.00015	-0.43754	3P	1.65797	-0.00214
3S	5.68198	-0.00131	0.35078	0.17086			0.52358

CHLORINE K(2)L(8)3S(2)3P(6), 1S  
 T.E.= -0.45957670D+03 P.E.= -0.91915E21D+03 K.E.= 0.45957951D+03 V.T.= -0.19999939D+01

	S	1S	2S	3S	P	2P	3P
BASIS/ORB	E	-104.50515	-10.22891	-0.73295	BASIS/ORB	E	-7.69533
1S	17.24050	0.52389	-0.25955	-0.07613	2P	7.62972	0.65375
1S	28.92250	0.01357	-0.00339	-0.00122	2P	13.76380	0.03936
2S	6.81054	0.00274	0.90297	0.29244	3P	2.92646	0.01297
2S	15.17810	0.07693	-0.14667	-0.04564	3P	1.01565	0.00056
3S	2.87181	0.00002	0.00350	-0.69781	3P	5.93996	0.36998
3S	1.67233	-0.00002	0.00057	-0.45281	3P	1.83188	-0.00273
3S	5.86922	-0.00055	0.23387	0.15074			0.52436

POTASSIUM K(2)L(8)3S(2)3P(6)4S(2), 1S  
 T.E.= -0.59916174D+03 P.E.= -0.11983254D+04 K.E.= 0.59916364D+03 V.T.= -0.19999968D+01

	S	1S	2S	3S	4S	P	2P	3P
BASIS/ORB	E	-133.41306	-14.36554	-1.62885	-0.01018	BASIS/ORB	E	-11.39927
1S	19.10140	-0.93428	-0.27373	0.09160	-0.01250	2P	8.65250	0.66828
1S	31.03670	-0.01631	-0.00210	-0.00002	0.00005	2P	15.28720	0.04077
2S	16.70060	-0.06155	-0.14405	0.04941	-0.00655	3P	6.91281	0.34764
2S	7.58500	-0.00257	0.96848	-0.34368	0.04638	3P	3.44500	0.01326
3S	6.60786	0.00081	0.17448	-0.20565	0.03208	3P	2.26213	-0.00456
3S	3.99350	-0.00023	0.00040	0.46742	-0.07622	3P	1.66856	0.00142
3S	2.63830	0.00022	0.00707	0.63029	-0.06234			0.18819
4S	2.56824	-0.00009	-0.00332	0.09556	-0.00742			
4S	0.35204	0.00000	0.00004	0.00116	0.39228			
4S	1.26523	0.00000	0.00036	0.01226	0.24294			
4S	0.70452	-0.00000	-0.00015	-0.00414	0.56584			

SCANDIUM K(2)L(8)3S(2)3P(6)4S(1)3D(3), 5F  
 T.E.= -0.75959416D+03 P.E.= -0.15191967D+04 K.E.= 0.7596C258D+03 V.T.= -0.19995889D+01

	S	1S	2S	3S	4S	P	2P	3P	D	3D
BASIS/ORB	E	-165.63585	-18.79775	-2.28079	-0.05C69					
1S	33.23500	-0.02047	0.00113	0.00028	0.00026					
1S	20.88320	-0.94488	0.28661	0.10049	-0.01574					
2S	18.12350	-0.04354	0.14935	0.05705	-0.00993					
2S	8.48943	-0.00389	-1.00110	-0.38349	C.07117					
3S	7.42737	0.00242	-0.14633	-0.22026	0.05512					
3S	4.76561	-0.00155	-0.00176	0.40051	-0.10980					
3S	3.22922	0.00103	-0.00447	0.75353	-0.13528					
4S	2.45807	-0.00043	0.00152	0.07342	-0.03495					
4S	1.60010	0.00018	-0.00C72	-0.00556	C.36534					
4S	0.89199	-0.00006	0.00021	0.00075	0.6C876					
4S	0.51134	0.00002	-0.00008	-0.00084	C.15819					
P		2P	3P	D	3D	BASIS/ORB	E			
BASIS/ORB	E	-15.38901	-1.3C070	BASIS/ORB	E	0.01513				
2P	16.53770	0.04584	-0.01469	3D	9.91594	C.C0890				
2P	9.60190	0.68465	-0.23089	3D	5.28852	0.6800				
3P	7.87679	0.31870	-0.14473	3D	3.08552	C.27680				
3P	4.22985	0.01483	0.37319	3D	1.42520	0.46525				
3P	2.93731	-0.00424	0.55109	3D	0.51378	0.52167				
3P	2.00587	0.00108	0.20542							

See page 183 for Explanation of Tables and Notes for Tables 32, 42, and 43

TABLE 44 (6). THE HARTREE-FOCK FUNCTIONS FOR NEGATIVE IONS.

SCANDIUM K(2)L(8)3S(2)3P(6)4S(2)3D(2), 3F  
 T.E.= -0.75968834D+03 P.E.= -0.15193772D+04 K.E.= 0.75968885D+03 V.T.= -0.19999993D+01

	1S	2S	3S	4S
BASIS/ORB E	-165.61064	-18.76542	-2.26593	-0.01563
1S 20.88320	-0.94496	-0.28672	-0.10170	-0.01513
1S 33.23500	-0.02043	-0.00107	0.00050	-0.00025
2S 18.12350	-0.04344	-0.14916	-0.05427	-0.00557
2S 8.48943	-0.00407	1.00C72	0.37590	0.06140
3S 7.42737	0.00283	0.14722	0.24112	0.03285
3S 4.76561	-0.00273	-0.00137	-0.49712	-0.04716
3S 3.22292	0.00311	0.01066	-0.53957	-0.18774
4S 3.24712	-0.00162	-0.00509	-0.19821	0.04567
4S 1.53091	0.00010	0.00041	-0.01961	0.22489
4S 0.95061	-0.00005	-0.00020	0.00748	0.50042
4S 0.48055	0.00001	0.00005	-0.00174	0.46101

	2P	3P	D	3D
BASIS/ORB E	-15.36084	-1.28790	BASIS/ORB E	-0.06082
2P 9.60190	0.68539	-0.22100	3D 3.29727	0.31881
2P 16.53770	0.04561	-0.01430	3D 8.56811	0.02274
3P 7.86258	0.31916	-0.14123	3D 4.92754	0.06948
3P 4.08896	0.01419	0.443E1	3D 1.61541	0.54349
3P 2.85710	-0.00483	0.44710	3D 0.74381	0.28246
3P 2.08141	0.00137	0.23614		

TITANIUM K(2)L(8)3S(2)3P(6)4S(1)3D(4), 6D  
 T.E.= -0.84825608D+03 P.E.= -0.16565181D+04 K.E.= 0.84826199D+03 V.T.= -0.19999930D+01

	1S	2S	3S	4S
BASIS/ORB E	-182.91780	-21.04211	-2.49229	-0.02486
1S 34.98210	-0.01930	-0.00116	0.00018	-0.00003
1S 21.89210	-0.94689	-0.28854	-0.10351	-0.01641
2S 19.05820	-0.04212	-0.15133	-0.05616	-0.00919
2S 9.13738	-0.00439	0.95314	0.36183	0.05850
3S 8.38922	0.00246	0.18571	0.21785	0.03769
3S 4.92062	-0.00119	0.01997	-0.38044	-0.06485
3S 3.44234	0.00083	-0.00499	-0.74326	-0.15062
4S 2.54575	-0.00025	0.00152	-0.07414	0.04921
4S 1.37695	0.00008	-0.00035	0.00488	0.42702
4S 0.73246	-0.00003	0.00018	-0.00083	0.55985
4S 0.39059	0.00001	-0.00004	0.00097	0.17310

	2P	3P	D	3D
BASIS/ORB E	-17.41505	-1.43135	BASIS/ORB E	-0.00347
2P 16.97770	0.05017	-0.01655	3D 7.65000	0.03106
2P 10.06610	0.69039	-0.23550	3D 4.88000	0.12705
3P 8.34065	0.30696	-0.15041	3D 3.22000	0.23432
3P 4.45769	0.01270	0.47621	3D 1.80000	0.48218
3P 2.79633	-0.00220	0.61E13	3D 0.66000	0.43507
3P 1.57585	0.00057	0.04923		

TITANIUM K(2)L(8)3S(2)3P(6)4S(2)3D(3), 4F  
 T.E.= -0.84837194D+03 P.E.= -0.16567485D+04 K.E.= 0.84837658D+03 V.T.= -0.19999945D+01

	1S	2S	3S	4S
BASIS/ORB E	-182.95605	-21.08206	-2.54592	-0.01561
1S 21.89210	-0.94698	-0.28876	-0.10551	-0.01533
1S 34.98210	-0.01925	-0.00124	0.00125	0.00006
2S 19.05820	-0.04199	-0.15160	-0.05241	-0.00823
2S 9.13738	-0.00465	0.95370	0.35251	0.05345
3S 8.38922	0.00291	0.18838	0.23909	0.03603
3S 4.92062	-0.00242	0.02478	-0.48965	-0.06C85
3S 3.44234	0.00290	-0.01254	-0.51300	-0.14191
4S 3.42281	-0.00142	0.0C636	-0.20292	0.01552
4S 1.54746	0.00008	-0.00016	-0.01582	0.30442
4S 0.85387	-0.00003	0.00CC7	0.00564	0.541C5
4S 0.43290	0.00001	-0.00002	-0.00169	0.36232

See page 183 for Explanation of Tables and Notes for Tables 32, 42, and 43

## ROOTHAAN-HARTREE-FOCK ATOMIC WAVEFUNCTIONS

TABLE 44 (7) THE HARTREE-FOCK FUNCTIONS FOR NEGATIVE IONS.

P BASIS/ORB E	2P 2P 10.06610	3P 2P 16.97770	D 3P 8.28494	3D 3P 4.61861
-17.45540	0.6542E	-0.23286	3D 1.80010	-C.11795
10.06610	0.04885	-0.01765	3D 9.13523	C.47919
16.97770	0.30635	-0.16279	3D 4.74134	C.02666
8.28494	0.00847	0.4451C	3D 3.22933	C.16763
4.61861	0.00048	0.66503	3D 0.94420	C.29483
2.81843	-0.00014	0.03673		C.23942
1.46228				

VANADIUM K(2)L(8)3S(2)3P(6)4S(1)3D(5), 7S  
 T.E.= -0.94276611D+03 P.E.= -0.1EE55336D+04 K.E.= 0.94276745D+03 V.T.= -0.19999986D+01

S BASIS/ORB E	1S 1S 36.50460	2S 2S 22.92730	3S 3S 19.93340	4S 4S 9.18959
-201.07765	-0.01825	-0.00072	-0.00071	-0.00604
36.50460	-0.54740	-0.29149	-0.10335	0.00014
22.92730	-0.04309	-0.15360	-0.06225	-0.01256
19.93340	-0.00358	1.06653	0.42466	-0.00662
9.18959	0.00268	0.6889	0.21335	0.04838
5.22990	-0.00268	0.02164	-0.51736	0.03528
3.95410	0.00219	-0.00551	-0.45948	-0.04062
3.48325	-0.00064	0.00363	-0.28077	-0.03935
1.69704	0.00006	-0.00015	-0.00930	0.25C53
0.81953	-0.00002	0.00010	0.00233	0.55102
0.35497	0.00001	0.00002	0.00032	0.47545

P BASIS/ORB E	2P 2P 16.82340	3P 3P 10.66620	D 3P 9.04510	3D 3P 4.76700
-19.57082	0.06492	-0.02217	3D 10.13420	-C.04060
16.82340	0.65526	-0.22680	3D 4.82409	0.02229
10.66620	0.32256	-0.15572	3C 1.75219	0.24987
9.04510	0.02116	0.45525	3D 2.65557	C.38880
4.76700	-0.00631	0.55284	3D 0.60588	C.29177
3.06784				0.31437
1.91912	0.00183	0.05270		

VANADIUM K(2)L(8)3S(2)3P(6)4S(2)3D(4), 5D  
 T.E.= -0.94286192D+03 P.E.= -0.18857205D+04 K.E.= 0.94285857D+03 V.T.= -0.20300036D+01

S BASIS/ORB E	1S 1S 22.92730	2S 2S 36.50460	3S 3S 19.93340	4S 4S 9.18959
-201.16442	-0.94741	-0.29143	-0.10520	-0.01613
22.92730	-0.01824	-0.00074	0.00013	C.00009
36.50460	-0.04306	-0.15365	-0.05950	-C.00833
19.93340	-0.00368	1.06659	0.41793	0.C5962
9.18959	0.00291	0.06823	0.24529	0.04193
5.22990	-0.00364	0.02554	-0.74069	-0.11589
3.95410	0.00367	-0.01569	-0.05875	-C.02419
3.82455	-0.00137	0.00612	-0.49128	-C.05935
1.66643	0.00006	-0.00014	-0.01656	C.30528
0.86739	-0.00002	0.00006	0.00509	0.57602
0.42942	0.00001	-C.00002	-0.00158	0.34C88

P BASIS/ORB E	2P 2P 10.66620	3P 3P 16.82340	D 3P 8.91238	3D 3P 5.20502
-19.66480	0.66661	-0.21916	3D 1.66028	C.35205
10.66620	0.06064	-0.02556	3D 9.94251	C.02547
16.82340	0.31955	-0.18945	3D 4.89566	C.26495
8.91238	0.01073	0.39668	3D 2.79579	0.40513
5.20502	0.00146	0.71461	3D 0.96428	C.15368
3.10978	-0.00041	0.05431		
1.73974				

See page 183 for Explanation of Tables and Notes for Tables 32, 42, and 43

TABLE 44 (B). THE HARTREE-FOCK FUNCTIONS FOR NEGATIVE IONS.

CHROMIUM K(2)L(8)3S(2)3P(6)4S(1)3D(6), 6D  
 T.E.= -0.104309560+04 P.E.= -0.20862117E+04 K.E.= 0.10431161D+04 V.T.= -0.19999803D+01

S	1S	2S	3S	4S
BASIS/ORB E	-220.17880	-25.99244	-3.05587	0.00071
1S 35.32410	-0.02813	-0.0C545	-0.00154	-0.00032
1S 23.95240	-0.93258	-0.27788	-0.10365	-0.00754
2S 21.58460	-0.04764	-0.15454	-0.05518	-0.00485
2S 10.05970	-0.00526	0.94174	0.35525	0.02943
3S 9.62450	0.00297	0.18910	0.23186	0.01870
3S 5.88646	-0.00107	0.02624	-0.25457	-0.01892
3S 4.08245	0.00066	-0.00360	-0.83145	-0.08415
4S 2.98919	-0.00021	0.00094	-0.12147	0.00712
4S 1.87037	0.00007	-0.00011	0.00638	0.11716
4S 0.94379	-0.00002	0.00003	-0.00139	0.40242
4S 0.34232	0.00000	0.00003	0.00076	0.74973

P	2P	3P	D	3D
BASIS/ORB E	-21.92476	-1.82E39	BASIS/ORB E	-0.06955
2P 16.52020	0.10537	-0.03483	3D 9.99336	0.02519
2P 10.43800	0.69003	-0.24746	3D 5.43036	0.21917
3P 9.48080	0.23194	-0.12397	3D 3.05964	0.39929
3P 5.25013	0.03135	0.37123	3D 1.84377	0.27698
3P 3.42373	-0.00975	0.66555	3D 1.01811	0.32362
3P 1.95230	0.00242	0.1CE53		

CHROMIUM K(2)L(8)3S(2)3P(6)4S(2)3D(5), 6S  
 T.E.= -0.10433344D+04 P.E.= -0.20866543D+04 K.E.= 0.10432199D+04 V.T.= -0.20000138D+01

S	1S	2S	3S	4S
BASIS/ORB E	-220.22571	-26.04736	-3.12437	-0.01634
1S 23.95240	-0.93259	-0.27784	-0.10569	-0.01435
1S 35.32410	-0.02812	-0.0C546	-0.00046	-0.00016
2S 21.58460	-0.04762	-0.15455	-0.05277	-0.00751
2S 10.05970	-0.00531	0.94173	0.35002	0.04886
3S 9.62450	0.00303	0.18888	0.24425	0.03573
3S 5.88646	-0.00118	0.02691	-0.28934	-0.03924
3S 4.08245	0.00080	-0.0C426	-0.77767	-0.13E17
4S 3.33125	-0.00025	0.00115	-0.13905	0.00992
4S 1.69515	0.00005	-0.00003	-0.00510	0.28810
4S 0.92786	-0.00002	-0.00000	0.00158	0.53593
4S 0.46239	0.00001	0.00000	-0.00047	0.38825

P	2P	3P	D	3D
BASIS/ORB E	-21.97798	-1.89C65	BASIS/ORB E	-0.21291
2P 10.43800	0.71107	-0.21430	3D 1.84377	0.39864
2P 16.52020	0.09776	-0.04726	3D 10.38590	0.02718
3P 9.21546	0.21569	-0.23718	3D 5.32873	0.25019
3P 6.35620	0.01984	0.35E71	3D 3.19556	0.39150
3P 3.44954	0.00167	0.80242	3D 1.01811	0.12728
3P 1.86664	-0.00023	0.06E53		

MANGANESE K(2)L(8)3S(2)3P(6)4S(2)3D(6), 5D  
 T.E.= -0.11497279D+04 P.E.= -0.22994407D+04 K.E.= 0.11497128D+04 V.T.= -0.20000132D+01

S	1S	2S	3S	4S
BASIS/ORB E	-240.18544	-28.74030	-3.45207	-0.01755
1S 24.72480	-0.95114	-0.29885	-0.11151	-0.01553
1S 37.89080	-0.02428	-0.00099	0.00091	0.00023
2S 21.35640	-0.03091	-0.16413	-0.06107	-0.00809
2S 10.79350	-0.00440	0.93878	0.36271	0.04935
3S 9.86796	0.00264	0.22452	0.25491	0.04018
3S 5.79826	-0.00180	0.01708	-0.43796	-0.06999
3S 4.19459	0.00159	-0.00268	-0.61009	-0.10303
4S 3.69091	-0.00056	0.00070	-0.16615	-0.00507
4S 1.82224	0.00007	0.00008	-0.00772	0.29472
4S 0.96029	-0.00003	-0.00004	0.00214	0.55250
4S 0.47738	0.00001	0.00001	-0.00064	0.37456

See page 183 for Explanation of Tables and Notes for Tables 32, 42, and 43

## ROOTHAAN-HARTREE-FOCK ATOMIC WAVEFUNCTIONS

TABLE 44 (9). THE HARTREE-FOCK FUNCTIONS FOR NEGATIVE IONS.

	P	2P	3P	D	3D
BASIS/ORB E	-24.44732	-2.13042	BASIS/ORB E	-0.21346	
2P 9.62773	-0.85997	-0.33888	3D 3.59961	0.34691	
2P 16.38780	-0.14268	-0.04130	3D 11.21700	C.02646	
3P 6.14932	-0.02512	-0.23542	3D 5.69535	C.24781	
3P 5.40046	-0.00699	0.73859	3D 2.06789	0.43207	
3P 3.46864	0.00797	0.42153	3D 1.08101	C.14744	
3P 2.62955	-0.00374	0.19100			

IRON K(2)L(8)3S(2)3P(6)4S(2)3D(7), 4F  
 T.E.= -0.12623659D+04 P.E.= -0.25247211D+04 K.E.= 0.12623552D+04 V.T.= -0.20000084D+01

	S	1S	2S	3S	4S
BASIS/ORB E	-260.55759	-31.53823	-3.78243	-C.01855	
1S 25.51840	-0.95706	-0.30830	-0.11529	-0.01588	
1S 39.06320	-0.02764	0.00118	0.00143	0.00032	
2S 21.59970	-0.01909	-0.17353	-0.06745	-0.00878	
2S 11.15200	-0.00646	1.00375	0.39765	C.05336	
3S 9.62088	0.00637	0.19480	0.33002	C.05314	
3S 7.07909	-0.00498	-0.02076	-0.36320	-0.05928	
3S 4.73058	0.00245	0.01539	-0.73373	-0.11883	
4S 3.97297	-0.00079	-0.00398	-0.22107	-0.01768	
4S 1.93277	0.00012	0.00065	-0.00933	0.28948	
4S 0.99925	-0.00005	-0.00025	0.00253	0.56678	
4S 0.48555	0.00001	0.00008	-0.00076	0.37364	

	P	2P	3P	D	3D
BASIS/ORB E	-27.02044	-2.37025	BASIS/ORB E	-0.23027	
2P 10.12600	-0.86200	-0.34683	3D 2.63186	0.44959	
2P 17.12220	-0.13858	-0.03912	3D 11.53300	C.02714	
3P 6.15706	-0.05325	-0.25359	3D 6.12611	C.23512	
3P 5.53789	0.02352	0.81353	3D 4.21333	0.24210	
3P 3.45469	0.00204	0.45176	3D 1.34113	C.24584	
3P 2.58480	-0.00165	0.10754			

COBALT K(2)L(8)3S(2)3P(6)4S(2)3C(8), 3F  
 T.E.= -0.13813503D+04 P.E.= -0.27626858D+04 K.E.= 0.13813355D+04 V.T.= -0.20000107D+01

	S	1S	2S	3S	4S
BASIS/ORB E	-282.67305	-34.45260	-4.11993	-0.01927	
1S 26.67090	-0.95982	-0.31008	-0.11570	-0.01530	
1S 41.68130	-0.02071	0.00270	0.00144	C.00011	
2S 22.26180	-0.02541	-0.18466	-0.07339	-0.01025	
2S 12.01770	-0.00322	0.94510	0.37812	0.05171	
3S 10.67790	0.00220	0.25111	0.26645	0.03722	
3S 6.35720	-0.00289	0.00313	-0.37100	-0.03510	
3S 5.27022	0.00254	0.00715	-0.53213	-C.11560	
4S 4.33106	-0.00047	-0.00119	-C.32933	-0.02201	
4S 2.02193	0.00006	0.00027	-0.00925	0.27127	
4S 1.07773	-0.00002	-0.00011	0.00239	C.54070	
4S 0.52594	0.00001	0.00003	-0.00067	0.41333	

	P	2P	3P	D	3D
BASIS/ORB E	-29.70862	-2.61706	BASIS/ORB E	-0.24840	
2P 11.08370	-0.88613	-0.35020	3D 2.32037	0.45580	
2P 19.68480	-0.08159	-0.02208	3D 11.22190	0.03127	
3P 7.33256	-0.10124	-0.14816	3D 7.13505	0.14543	
3P 5.81458	0.04435	0.69310	3D 4.48356	0.43587	
3P 3.60408	-0.01094	0.45273	3D 1.16006	C.13555	
3P 2.74055	0.00321	0.10379			

See page 183 for Explanation of Tables and Notes for Tables 32, 42, and 43

TABLE 44 (10). THE HARTREE-FOCK FUNCTIONS FOR NEGATIVE IONS.

NICKEL K(2)L(8)3S(2)3P(6)4S(1)3D(10), 2S  
 T.E.= -0.15066533D+04 P.E.= -0.30133399D+04 K.E.= 0.15066866D+04 V.T.= -0.19999778D+01

S	1S	2S	3S	4S
BASIS/ORB E	-305.05390	-37.31716	-4.29536	0.01471
1S 27.78100	-0.95282	-0.31421	-0.11775	-0.00747
1S 40.98670	-0.02301	0.0C546	0.00263	-C.0CC70
2S 22.66670	-0.C3510	-0.205C3	-0.08236	-0.00965
2S 12.65000	0.00477	0.96E12	0.39029	0.037C8
3S 10.71570	-0.00483	0.27596	0.31321	0.00693
3S 6.77220	0.00799	-0.07110	-0.58461	0.06599
3S 5.51882	-0.00714	0.06756	-0.26652	-0.17864
4S 4.80234	0.00177	-0.01517	-0.42487	0.84570
4S 2.32600	-0.00040	0.00352	-0.04154	-0.11764
4S 1.89572	0.00025	-0.00218	0.01973	0.35248
4S 0.65772	-0.00001	0.00011	-0.00085	C.86860

P	2P	3P	D	3D
BASIS/ORB E	-32.34797	-2.7C572	BASIS/ORB E	-0.C8237
2P 11.00410	0.95073	-0.35581	3D 2.53064	0.41638
2P 19.19390	0.10627	-0.03E57	3D 12.70400	C.02470
3P 12.12620	-0.06298	-0.01468	3D 6.99305	C.21607
3P 6.69828	0.04289	0.19694	3D 4.47400	C.34094
3P 5.11685	-0.01670	0.51660	3D 1.16216	C.24791
3P 3.21297	0.00312	C.36E24		

NICKEL K(2)L(8)3S(2)3P(6)4S(2)3D(9), 2D  
 T.E.= -0.15068201D+04 P.E.= -0.30136389D+04 K.E.= 0.15068188D+04 V.T.= -0.20000008D+01

S	1S	2S	3S	4S
BASIS/ORB E	-305.20547	-37.48194	-4.46490	-0.01926
1S 27.81430	-0.96090	-0.3CE27	-0.11523	-0.01491
1S 44.58670	-0.C1555	0.00218	0.00102	0.000G1
2S 23.34670	-0.03076	-0.18432	-0.07448	-0.01C45
2S 12.27000	-0.00191	0.58E58	0.39682	0.05399
3S 11.03570	0.00143	0.20487	0.25488	C.03326
3S 6.97220	-0.00235	0.00520	-0.13376	0.01313
3S 6.02882	0.00199	0.003E1	-0.70785	-0.14908
4S 4.67204	-0.00023	-0.00010	-0.39984	-0.03678
4S 2.19800	0.00004	0.00C17	-0.01336	0.23111
4S 1.20128	-0.00001	-0.CCC7	0.00351	C.51544
4S 0.58498	0.00000	0.00002	-0.00094	0.47416

P	2P	3P	D	3D
BASIS/ORB E	-32.51013	-2.86569	BASIS/ORB E	-0.26612
2P 11.11020	0.89162	-0.33384	3D 2.51734	0.40873
2P 18.89350	0.12017	-0.04211	3D 12.36020	C.02903
3P 12.40020	-0.01335	-0.03104	3D 6.96520	0.22319
3P 6.28120	0.05161	0.33114	3D 4.44161	0.37582
3P 4.87510	-0.02800	0.45113	3D 1.33207	C.16568
3P 3.25707	0.00562	0.351E1		

COPPER K(2)L(8)3S(2)3P(6)4S(2)3D(10), 1S  
 T.E.= -0.16389633D+04 P.E.= -0.32779228D+04 K.E.= 0.16389595D+04 V.T.= -0.20000023D+01

S	1S	2S	3S	4S
BASIS/ORB E	-328.59757	-40.62473	-4.81669	-C.02053
1S 28.66390	-C.96554	-0.31472	-0.11864	-C.01472
1S 46.01330	-0.01721	0.00253	0.00177	-0.00004
2S 23.54910	-0.02152	-C.18355	-0.07236	-C.01C75
2S 13.14420	-0.00544	0.91229	0.36334	C.C5019
3S 12.16970	0.00390	C.26E28	0.25516	0.02945
3S 6.66320	-0.01643	0.20381	0.50756	0.27574
3S 6.37970	0.01575	-0.17E27	-1.35087	-0.41526
4S 4.73278	-0.00056	0.00522	-0.362C5	-0.01342
4S 2.06877	0.00007	-0.00048	-0.00826	0.30621
4S 1.07578	-0.00003	0.00022	0.00235	0.54152
4S 0.52675	0.00001	-0.000C7	-0.00071	0.38199

See page 183 for Explanation of Tables and Notes for Tables 32, 42, and 43

## ROOTHAAAN-HARTREE-FOCK ATOMIC WAVEFUNCTIONS

TABLE 44 (11): THE HARTREE-FOCK FUNCTIONS FOR NEGATIVE IONS.

P	2P	3P	D	3D
EASIS/ORB E	-35.42351	-3.12892	BASIS/ORB E	-0.26482
2P 12.00560	0.64289	-0.32699	3D 4.94422	0.28630
2P 19.85650	0.10744	-0.03511	3D 13.43500	0.02461
3P 10.59380	0.05969	-0.10122	3D 7.37639	0.22909
3P 7.21396	0.02605	0.37009	3D 3.06871	0.41919
2P 4.62416	-0.00495	0.64728	3D 1.58319	0.24055
3P 2.96292	0.00180	0.17149		

GALLIUM K(2)L(8)M(18)4S(2)4P(2), 1D  
 T.E.= -0.19232374D+04 P.E.= -0.38464737D+04 K.E.= 0.19232363D+04 V.T.= -0.20000006D+01

S	1S	2S	3S	4S
BASIS/ORB E	-378.64104	-47.99134	-6.21721	-0.25191
1S 28.82690	0.74466	-0.30181	-0.11810	-0.03087
1S 35.57530	0.25705	-0.02790	-0.00844	0.00114
2S 26.21740	0.00107	-0.15158	-0.06219	-0.01147
2S 13.25870	0.00146	1.03610	0.42686	0.09282
3S 12.53040	0.00001	0.12576	0.23523	0.06670
3S 7.46126	-0.00038	0.02280	-0.54242	-0.16148
3S 4.91690	0.00016	-0.00411	-0.67987	-0.16015
4S 2.62664	-0.00005	0.00109	-0.00816	0.43189
4S 1.57894	0.00004	-0.00067	0.00190	0.56766
4S 0.93381	-0.00001	0.00023	-0.00049	0.14553

P	2P	3P	4P	D	3D
BASIS/ORB E	-42.31718	-4.30548	0.00085	BASIS/ORB E	-1.01636
2P 12.93080	0.82781	0.32650	0.03770	3C 3.57013	0.43337
2P 20.85320	0.11779	0.04111	0.00575	3D 2.11748	0.15758
3P 12.14090	0.05933	0.09564	0.01714	3D 5.74013	0.32239
3P 7.76270	0.03197	-0.37395	-0.05916	3C 6.32827	0.21020
3P 4.93246	-0.00651	-0.72622	-0.08830	3D 14.27940	0.02746
4P 3.54767	0.00239	-0.07950	0.00777		
4P 1.97012	-0.00077	0.00230	0.33017		
4P 1.04769	0.00031	-0.00139	0.43275		
4P 0.57049	-0.00011	0.00034	0.44564		

GERMANIUM K(2)L(8)M(18)4S(2)4P(3), 4S  
 T.E.= -0.20753941D+04 P.E.= -0.41507846D+04 K.E.= 0.20753905D+04 V.T.= -0.20000017D+01

S	1S	2S	3S	4S
BASIS/ORB E	-404.99094	-51.89738	-6.93761	-0.31923
1S 30.16260	0.75054	-0.30393	-0.11301	-0.03007
1S 36.63480	0.24272	-0.02287	-0.01191	-0.00127
2S 26.91170	0.01196	-0.16400	-0.07275	-0.01663
2S 13.85020	-0.00082	1.03301	0.43857	0.10644
3S 12.83680	0.00151	0.13580	0.24254	0.07400
3S 7.87044	-0.00096	0.02040	-0.50645	-0.15942
3S 5.25304	0.00042	-0.00268	-0.71942	-0.19914
4S 2.86528	-0.00013	0.00073	-0.01282	0.44139
4S 1.77403	0.00009	-0.00047	0.00430	0.54422
4S 1.09401	-0.00003	0.00016	-0.00137	0.16124

P	2P	3P	4P	C	3D
EASIS/ORB E	-45.98359	-4.90916	-0.05893	BASIS/ORB E	-1.38217
2P 13.38070	0.83864	0.33375	0.05774	3C 3.80112	0.44948
2P 21.68540	0.11385	0.04085	0.00663	3D 2.27866	0.11888
3P 12.84680	0.04745	0.09104	0.01615	3D 6.05485	0.33375
3P 8.09620	0.03802	-0.36915	-0.06971	3D 8.77659	0.20665
3P 5.16251	-0.00960	-0.73712	-0.14282	3D 14.78120	0.02813
4P 3.73039	0.00372	-0.06652	0.03486		
4P 2.15725	-0.00152	0.00165	0.40749		
4P 1.25783	0.00071	-0.00089	0.48731		
4P 0.73871	-0.00024	0.00027	0.25156		

See page 183 for Explanation of Tables and Notes for Tables 32, 42, and 43

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TABLE 44 (12). THE HARTREE-FOCK FUNCTIONS FOR NEGATIVE IONS.

GERMANIUM K(2)L(8)M(18)4S(2)4P(3), 2D  
 T.E.= -0.207534700+04 P.E.= -0.415069300+04 K.E.= 0.207534330+04 V.T.= -0.200000180+01

S	1S	2S	3S	4S
BASIS/ORB E	-405.01686	-51.92291	-6.96306	-0.33770
1S 30.09100	0.75064	-0.30285	-0.11283	-0.03068
1S 36.66570	0.24434	-0.02445	-0.01232	-0.00109
2S 26.93850	0.00969	-0.16274	-0.07205	-0.01633
2S 13.83630	-0.00031	1.03386	0.43851	0.10691
3S 12.84970	0.00117	0.13779	0.24184	0.07505
3S 7.87820	-0.00083	0.02083	-0.50345	-0.16077
3S 5.25821	0.00036	-0.00280	-0.72193	-0.20074
4S 2.86806	-0.00011	0.00076	-0.01309	0.44090
4S 1.78429	0.00007	-0.00048	0.00439	0.55344
4S 1.07890	-0.00003	0.00016	-0.00134	0.15143

P	2P	3P	4P	D	3D
BASIS/ORB E	-46.00906	-4.93438	-0.03633	BASIS/CRB E	-1.40750
2P 13.40260	0.83619	0.33156	0.05612	3C 3.82844	0.44566
2P 21.69830	0.11340	0.04053	0.00659	3D 2.31740	0.12577
3P 12.85970	0.05067	0.05350	0.01660	3D 4.10082	0.32997
3P 8.10416	0.03784	-0.37016	-0.69115	3D 8.77888	0.20709
3P 5.15734	-0.00940	-0.73748	-0.13932	3D 14.78500	0.02803
4P 3.73407	0.00359	-0.06525	0.03249		
4P 2.16573	-0.00135	0.00062	0.40733		
4P 1.21020	0.00053	-0.00074	0.51156		
4P 0.64500	-0.00017	0.00004	0.25775		

ARSENIC K(2)L(8)M(18)4S(2)4P(4), 3P  
 T.E.= -0.22342224D+04 P.E.= -0.446E4354D+04 K.E.= 0.22342170D+04 V.T.= -0.20000024D+01

S	1S	2S	3S	4S
BASIS/ORB E	-432.32210	-56.04568	-7.76471	-0.43829
1S 30.56460	0.79002	0.34508	-0.13368	-0.03636
1S 38.62050	0.22158	-0.00031	-0.00029	0.00175
2S 26.33590	-0.01401	0.16E51	-0.07488	-0.01769
2S 14.90930	0.0721	-0.58E12	0.42118	0.10924
3S 13.48790	-0.00337	-0.21560	0.27439	0.09053
3S 8.16133	0.00099	-0.01765	-0.48388	-0.16750
3S 5.54645	-0.00044	0.00157	-0.73607	-0.22474
4S 3.04051	0.00012	-0.00054	-0.01411	0.47838
4S 1.95099	-0.00008	0.00036	0.00513	0.51392
4S 1.22355	0.00003	-0.00012	-0.00163	0.15211

P	2P	3P	4P	D	3D
BASIS/ORB E	-49.88998	-5.61658	-0.07327	BASIS/CRB E	-1.84839
2P 14.46800	0.78810	0.31513	0.6586	3D 4.23664	0.47322
2P 22.87540	0.09648	0.03405	0.00574	3D 2.57493	0.12084
3P 13.56260	0.12154	0.11E12	0.01998	3C 5.57131	0.28249
3P 8.39915	0.03994	-0.33518	-0.06541	3D 9.03544	0.21895
3P 5.59273	-0.01265	-0.72132	-0.17981	3C 15.30250	0.02971
4P 4.35379	0.00460	-0.05721	0.02892		
4P 2.43200	-0.00146	-0.00110	0.42199		
4P 1.47600	0.00069	-0.00061	0.46528		
4P 0.84940	-0.00021	0.00002	0.26633		

ARSENIC K(2)L(8)M(18)4S(2)4P(4), 1D  
 T.E.= -0.22341854D+04 P.E.= -0.446E3678D+04 K.E.= 0.22341824D+04 V.T.= -0.20000014D+01

S	1S	2S	3S	4S
BASIS/ORB E	-432.33671	-56.05586	-7.77876	-0.44813
1S 30.32060	0.79750	0.34354	-0.13432	-0.03658
1S 38.81960	0.22135	0.00364	-0.00105	0.00008
2S 26.50290	-0.02426	0.15543	-0.06956	-0.01827
2S 14.81290	0.01058	-0.98714	0.41832	0.11197
3S 13.57140	-0.00549	-0.20884	0.27128	0.08518
3S 8.21334	0.00178	-0.02154	-0.46427	-0.15214
3S 5.58177	-0.00081	0.00333	-0.75181	-0.24302
4S 3.17676	0.00023	-0.00052	-0.01616	0.40513
4S 2.05456	-0.00015	0.00058	0.00510	0.57194
4S 1.24069	0.00005	-0.00017	-0.00146	0.17263

See page 183 for Explanation of Tables and Notes for Tables 32, 42, and 43

## ROOTHAAAN-HARTREE-FOCK ATOMIC WAVEFUNCTIONS

TABLE 44 (13). THE HARTREE-FOCK FUNCTIONS FOR NEGATIVE IONS.

P	2P	3P	4P	C	3D
BASIS/ORB E	-49.90415	-5.63051	-0.06076	BASIS/ORB E	-1.86239
2P 14.60930	0.76141	0.31535	0.06345	3D 4.24821	0.47554
2P 23.14510	0.09000	0.03210	0.00575	3D 2.56696	0.12242
2P 13.64610	0.13452	0.11548	0.02337	3D 6.61305	0.28213
3P 8.45245	0.04202	-0.32294	-0.06747	3D 9.05214	0.21545
3P 5.62805	-0.01353	-0.73834	-0.17315	3D 15.32950	0.02953
4P 4.38140	0.00489	-0.10190	0.01628		
4P 2.45991	-0.00143	-0.00161	0.43415		
4P 1.40998	0.00059	-0.00075	0.50707		
4P 0.76740	-0.00018	-0.00013	0.23262		

ARSENIC K(2)L(8)M(18)4S(2)4P(4), 1S  
 T.E.= -0.22341313D+04 P.E.= -0.44682607D+04 K.E.= 0.22341295D+04 V.T.= -0.20000008D+01

S	1S	2S	3S	4S
BASIS/ORB E	-432.25830	-56.68118	-7.79986	-0.46306
1S 30.45500	0.79316	0.34427	-0.13418	-0.03514
1S 38.71000	0.22162	0.00156	-0.00054	-0.00091
2S 26.41100	-0.01854	0.16440	-0.07224	-0.02060
2S 14.86600	0.00874	-0.98647	0.41950	0.11532
3S 13.52540	-0.00433	-0.21479	0.27351	0.08296
3S 8.18470	0.00137	-0.61550	-0.47582	-0.15143
3S 5.56232	-0.00063	0.00266	-0.74241	-0.24700
4S 3.16580	0.00018	-0.00075	-0.01505	0.43041
4S 2.03129	-0.00012	0.00049	0.00491	0.54572
4S 1.29472	0.00004	-0.00016	-0.00157	0.17261

P	2P	3P	4P	C	3D
BASIS/ORB E	-49.92542	-5.65137	-0.04305	BASIS/ORB E	-1.88338
2P 14.53150	0.78518	0.31770	0.06415	3D 4.27314	0.47162
2P 22.99660	0.09350	0.03315	0.00573	3D 2.61574	0.12823
3P 13.60010	0.12733	0.11557	0.02144	3D 6.59007	0.27640
3P 8.42310	0.04094	-0.32559	-0.06622	3D 9.04295	0.21916
3P 5.60860	-0.01312	-0.73432	-0.17420	3D 15.31470	0.02948
4P 4.36620	0.00480	-0.09935	0.01954		
4P 2.49308	-0.00145	-0.00170	0.40406		
4P 1.45427	0.00056	-0.00120	0.50086		
4P 0.75790	-0.00016	-0.00036	0.28206		

SELENIUM K(2)L(8)M(18)4S(2)4P(5), 2P  
 T.E.= -0.23999042D+04 P.E.= -0.47558017D+04 K.E.= 0.23958974D+04 V.T.= -0.20000028D+01

S	1S	2S	3S	4S
BASIS/ORB E	-460.56477	-60.36656	-8.62935	-0.55568
1S 31.69100	0.83803	0.34668	-0.13299	-0.03758
1S 40.78910	0.17586	-0.00284	-0.00124	-0.00053
2S 27.22790	-0.01822	0.17042	-0.08016	-0.02327
2S 15.10370	0.01010	-1.03180	0.45350	0.13052
3S 13.64750	-0.00566	-0.16965	0.25982	0.08621
3S 8.43695	0.00222	-0.01757	-0.51134	-0.17437
3S 5.76402	-0.00104	0.00247	-0.72233	-0.25572
4S 3.33859	0.00033	-0.00074	-0.00899	0.45452
4S 2.21979	-0.00023	0.00052	0.00148	0.50413
4S 1.44724	0.00008	-0.00016	-0.00050	0.15284

P	2P	3P	4P	C	3D
BASIS/ORB E	-53.56693	-6.35971	-0.10123	BASIS/ORB E	-2.34762
2P 14.89160	0.79107	0.32625	0.07426	3D 4.61472	0.48271
2P 23.42820	0.05984	0.03555	0.00703	3D 2.86374	0.12133
3P 14.10790	0.11305	0.11021	0.02345	3D 7.14841	0.29718
3P 8.71082	0.04195	-0.33306	-0.07666	3D 9.71251	0.18569
3P 5.84405	-0.01398	-0.74110	-0.20000	3D 15.80930	0.02895
4P 4.58260	0.00506	-0.08657	0.02368		
4P 2.66211	-0.00156	-0.00193	0.46992		
4P 1.56157	0.00064	-0.00065	0.48894		
4P 0.89382	-0.00020	-0.00014	0.19639		

See page 183 for Explanation of Tables and Notes for Tables 32, 42, and 43

TABLE 44 (14). THE HARTREE-FOCK FUNCTIONS FOR NEGATIVE IONS.

BROMINE K(2)L(8)M(18)4S(2)4P(6), 1S  
 T.E.= -0.25725355D+04 P.E.= -0.51450662D+04 K.E.= 0.25725307D+04 V.T.= -0.20000019D+01

S	1S	2S	3S	4S
EASIS/ORB E	-489.72005	-64.66448	-9.53239	-0.68533
1S 32.83790	0.80855	0.37829	-0.14606	-0.04114
1S 41.13520	0.19674	-0.02717	0.00771	0.00051
2S 26.42870	-0.00607	0.20459	-0.10114	-0.03362
2S 15.94410	0.00564	-1.05731	0.48088	0.15017
3S 13.73830	-0.00262	-0.19545	0.28103	0.09054
3S 8.75244	0.00106	-0.00554	-0.54032	-0.17726
3S 5.99564	-0.00048	-0.00130	-0.71411	-0.29049
4S 3.63572	0.00014	0.00027	-0.00495	0.45299
4S 2.37420	-0.00009	-0.00013	-0.00132	0.55239
4S 1.51690	0.00003	0.00005	0.00023	0.15888

P	2P	3P	4P	D	3D
BASIS/ORB E	-58.21511	-7.13979	-0.13879	BASIS/CRB E	-2.88146
2P 15.80950	0.73379	0.30621	0.07770	3D 4.85590	0.46287
2P 23.96750	0.10307	0.03753	0.00719	3D 3.11959	0.11062
2P 14.97930	0.17236	0.12902	0.02682	3D 7.33254	0.31170
2P 8.60775	0.04791	-0.41356	-0.09153	3D 10.10240	0.19318
3P 5.87791	-0.02504	-0.6751	-0.22932	3D 16.28710	0.02960
4P 5.16140	0.01002	-0.06117	0.05351		
4P 2.81552	-0.00191	-0.01008	0.51702		
4P 1.68578	0.00091	0.00326	0.43505		
4P 1.04140	-0.00030	-0.00111	0.18693		

RUBIDIUM K(2)L(8)M(18)4S(2)4P(6)5S(2), 1S.  
 T.E.= 0.0 P.E.= 0.0 K.E.= 0.0 V.T.= 0.0

S	1S	2S	3S	4S	5S
EASIS/ORB E	-546.92571	-74.76596	-11.00602	-1.39851	-0.00771
1S 38.08620	0.84366	0.03542	0.01238	0.00441	0.00048
1S 26.53380	0.17692	0.45714	0.17482	0.06243	0.00970
2S 17.71900	-0.03858	-0.11601	0.31294	0.13559	0.01864
2S 15.24460	0.03126	-1.04461	-0.93386	-0.36833	-0.05353
3S 9.51323	-0.00486	-0.02487	0.29217	0.10442	0.01320
3S 6.76840	0.00206	0.01717	0.88030	0.41811	0.06880
4S 3.88610	-0.00057	-0.00271	0.02517	-0.59553	-0.11503
4S 2.52497	0.00033	0.00162	-0.00655	-0.54812	-0.06203
5S 1.51897	-0.00013	-0.00062	0.00214	-0.01012	0.19878
5S 0.93751	0.00007	0.00034	-0.00107	0.00099	0.45896
5S 0.50292	-0.00002	-0.00010	0.00031	-0.00009	0.54269

P	2P	3P	4P	D	3D
EASIS/ORB E	-65.11857	-8.91634	-0.68350	BASIS/CRB E	-4.29236
2P 24.49670	-0.12034	0.02893	0.00783	3D 11.83640	0.21430
2P 15.27970	-0.87341	0.41088	0.12959	3D 6.42176	0.67314
3P 8.15357	-0.05912	-0.60347	-0.21442	3D 3.73911	0.20900
3P 5.54448	0.03505	-0.52542	-0.19613		
4P 3.53562	-0.01393	0.02290	0.53783		
4P 2.18936	0.00837	-0.01704	0.55708		
4P 1.35316	-0.00289	0.00609	0.05966		

RUBIDIUM K(2)L(8)M(18)4S(2)4P(6)5S(2), 1S  
 T.E.= -0.29383372D+04 P.E.= -0.58764993D+04 K.E.= 0.29381621D+04 V.T.= -0.20000596D+01

S	1S	2S	3S	4S	5S
EASIS/ORB E	-551.33986	-74.92805	-12.01154	-1.40081	-0.00543
1S 38.08620	0.84303	0.02677	-0.00603	0.00257	0.00043
1S 26.53380	0.17342	0.46555	-0.19370	0.06567	0.00985
2S 17.71900	-0.05391	-0.16596	-0.31272	0.13120	0.02065
2S 15.24460	0.04134	-1.01033	0.98108	-0.36928	-0.05684
3S 9.51323	-0.00573	-0.03258	-0.38378	0.14119	0.02148
3S 6.76840	0.00315	0.00517	-0.81210	0.37444	0.05873
4S 3.88610	-0.00080	-0.00164	-0.01582	-0.60707	-0.11065
4S 2.52497	0.00047	0.00055	0.00343	-0.53301	-0.06971
5S 1.51897	-0.00019	-0.00036	-0.00118	-0.00970	0.23479
5S 0.93751	0.00012	0.00022	0.00065	0.00121	0.35863
5S 0.56292	-0.00004	-0.00008	-0.00022	-0.00016	0.58572

See page 183 for Explanation of Tables and Notes for Tables 32, 42, and 43

## ROOTHAAN-HARTREE-FOCK ATOMIC WAVEFUNCTIONS

TABLE 44 (15). THE HARTREE-FOCK FUNCTIONS FOR NEGATIVE IONS.

P	2P	3P	4P	D	3D
BASIS/ORB E	-67.78500	-9.366CS	-0.68732	BASIS/ORB E	-4.60915
2P 24.49670	-0.13056	0.03433	0.00898	3D 11.83640	0.25435
2P 15.27970	-0.87269	0.4162	0.12898	3D 6.42176	0.67672
3P 8.15357	-0.03066	-0.70163	-0.24651	3D 3.73911	0.16464
3P 5.54448	0.01291	-0.42161	-0.14744		
4P 3.53562	-0.00407	0.00531	0.54015		
4P 2.18936	0.00223	-0.00420	0.54591		
4P 1.35316	-0.00074	0.00129	0.5260		

YTTRIUM K(2)L(8)M(18)4S(2)4P(6)5S(1)4D(3), 5F  
 T.E.= -0.33315782D+04 P.E.= -0.66629769D+04 K.E.= 0.33313987D+04 V.T.= -0.20300539D+01

S	1S	2S	3S	4S	5S
BASIS/ORB E	-616.48461	-85.53824	-14.48117	-1.88526	-0.03139
1S 40.11580	0.84723	0.02617	0.00780	0.00283	0.00023
1S 27.89200	0.16556	0.47182	0.19966	C.01297	0.01535
2S 18.61820	-0.06325	-0.13705	0.39897	0.18077	0.03261
2S 16.28320	0.05064	-1.04054	-1.08369	-0.44509	-0.08576
3S 10.27940	-0.00654	-0.03656	0.26562	0.10460	0.01573
3S 7.48929	0.00342	0.00561	0.91162	0.46445	0.10486
4S 4.28025	-0.00089	-0.00170	0.02091	-0.64994	-0.17729
4S 2.91412	0.00053	0.00101	-0.00557	-0.49619	-0.06612
5S 1.74080	-0.00017	-0.00C29	0.00141	-0.01365	0.34929
5S 1.00726	0.00008	0.00014	-0.00065	C.00488	0.58922
5S 0.55072	-0.00003	-0.00005	0.00020	-0.00005	0.25891

P	2P	3P	4P	D	3D	4D
BASIS/ORB E	-77.89271	-11.57786	-1.03080	BASIS/CRB E	-6.32305	0.01673
2P 25.77780	-0.12988	0.03216	0.00937	3D 12.56410	0.27543	-0.04512
2P 16.23110	-0.87261	0.43272	0.14860	3D 6.69231	0.75297	-0.11107
3P 8.74733	-0.03178	-0.69120	-0.26971	4C 3.91742	0.06877	0.10812
3P 6.17653	0.01407	-0.435E2	-0.18144	4D 2.24038	-0.01007	0.46812
4P 3.97728	-0.00381	-0.00C27	0.55237	4D 0.89708	0.00171	0.66702
4P 2.54741	0.00189	-0.00151	0.52217			
4P 1.44003	-0.00049	0.00030	0.03786			

YTTRIUM K(2)L(8)M(18)4S(2)4P(6)5S(2)4D(2), 3F  
 T.E.= -0.3331637.0D+04 P.E.= -0.66620844D+04 K.E.= 0.33314475D+04 V.T.= -0.20000559D+01

S	1S	2S	3S	4S	5S
BASIS/ORB E	-616.52114	-85.57594	-14.52068	-1.92512	-0.01686
1S 40.11580	0.84723	0.02616	0.00779	0.00281	0.00018
1S 27.89200	0.16555	0.471E3	C.19968	0.07305	0.01429
2S 18.61820	-0.06318	-0.13739	0.39851	C.18045	0.02969
2S 16.28230	0.05056	-1.04022	-1.08324	-0.44490	-0.07889
3S 10.27940	-0.00651	-0.03650	0.28562	0.10443	0.01408
3S 7.48929	0.00340	0.00957	0.91162	0.46500	0.09779
4S 4.28025	-0.00087	-0.00166	0.02088	-0.65069	-0.16573
4S 2.91412	0.00051	0.00C57	-0.00545	-0.49616	-0.05781
5S 1.70006	-0.00015	-0.00027	0.00133	-0.01230	0.34450
5S 0.98030	0.00008	0.00013	-0.00062	0.00295	0.52536
5S 0.53057	-0.00003	-0.00004	0.00020	-0.00090	0.35250

P	2P	3P	4P	D	3D	4D
BASIS/ORB E	-77.93012	-11.61703	-1.07210	BASIS/ORB E	-6.36191	-0.04099
2P 25.77750	-0.12987	0.03216	0.00942	3D 12.56410	0.27520	-0.05287
2P 16.23110	-0.87262	0.43269	0.14874	3D 6.69231	0.75357	-0.14042
3P 8.74733	-0.03172	-0.69114	-0.26960	4D 3.88696	0.06845	0.17510
3P 6.17653	0.01397	-0.43580	-0.18251	4C 2.09713	-0.01088	0.5597C
4P 3.96593	-0.00376	-0.00C47	0.60478	4D 0.99427	0.00277	0.48248
4P 2.52060	0.00175	-0.00139	0.51828			
4P 1.39935	-0.00046	0.00C30	0.02803			

See page 183 for Explanation of Tables and Notes for Tables 32, 42, and 43

TABLE 44 (16). THE HARTREE-FOCK FUNCTIONS FOR NEGATIVE IONS.

ZIRCONIUM K(2)L(8)M(18)4S(2)4P(6)5S(1)4D(4), 6D  
 T.E.= -0.353892010D+04 P.E.= -0.70775712D+04 K.E.= 0.35386511D+04 V.T.= -0.20000760D+01

S	1S	2S	3S	4S	5S	
BASIS/ORB E	-650.38708	-91.05035	-15.72111	-2.08018	-0.02292	
1S 41.14930	0.84549	0.02206	-0.00552	0.00192	0.00031	
1S 28.88350	0.17031	0.47331	-0.20283	0.07625	0.01463	
2S 18.61520	-0.08824	-0.00339	-0.73171	0.32956	0.06303	
2S 17.00340	0.07693	-1.16654	1.42358	-0.60413	-0.11555	
3S 10.81480	-0.00676	-0.04134	-0.25031	0.08824	0.01508	
3S 7.82175	0.00337	0.01045	-0.95067	0.50213	0.10237	
4S 4.45263	-0.00090	-0.00192	-0.02122	-0.69227	-0.16903	
4S 3.03088	0.00057	0.00120	0.00582	-0.45947	-0.07040	
5S 1.94130	-0.00018	-0.00036	-0.00150	-0.01322	0.30059	
5S 1.08033	0.00007	0.00015	0.00055	0.00430	0.59144	
5S 0.56101	-0.00002	-0.00005	-0.00016	0.00056	0.34048	
P	2P	3P	4P	D	3D	4D
BASIS/ORB E	-83.15232	-12.68745	-1.16479	BASIS/ORB E	-7.18357	-0.01061
2P 26.46150	-0.12837	0.03222	0.00934	3D 12.87330	0.28711	-0.05741
2P 16.71580	-0.87366	0.43854	0.15566	3D 6.90015	0.75147	-0.14221
3P 9.02922	-0.03273	-0.69115	-0.27583	4D 3.94757	0.05065	0.21692
3P 6.47917	0.01498	-0.43506	-0.19725	4D 2.14927	-0.00711	0.54891
4P 4.19107	-0.00383	-0.00237	0.62269	4D 0.94903	0.00149	0.48665
4P 2.66573	0.00181	-0.00074	0.50531			
4P 1.51024	-0.00047	0.00008	0.03304			

ZIRCONIUM K(2)L(8)M(18)4S(2)4P(6)5S(2)4C(3), 4F  
 T.E.= -0.35389697D+04 P.E.= -0.70776921D+04 K.E.= 0.35387224D+04 V.T.= -0.20006990D+01

S	1S	2S	3S	4S	5S	
BASIS/ORB E	-650.45237	-91.11743	-15.79077	-2.15423	-0.01612	
1S 41.14930	0.84551	0.02207	-0.00550	0.00192	-0.00009	
1S 28.88350	0.17029	0.47329	-0.20286	0.07633	0.01474	
2S 18.61520	-0.08805	-0.00219	-0.73132	0.33027	0.05227	
2S 17.00340	0.07673	-1.16675	1.42315	-0.60473	-0.10200	
3S 10.81480	-0.00670	-0.04124	-0.25012	0.08831	0.00947	
3S 7.82175	0.00331	0.0136	-0.95083	0.50267	0.10441	
4S 4.45263	-0.00084	-0.00182	-0.02099	-0.69374	-0.17605	
4S 3.03088	0.00050	0.00107	0.00543	-0.46096	-0.04179	
5S 1.78084	-0.00016	-0.00032	-0.00138	-0.01051	0.33298	
5S 1.05281	0.00008	0.00017	0.00066	0.00260	0.48059	
5S 0.56285	-0.00003	-0.00006	-0.00021	-0.00080	0.40366	
P	2P	3P	4P	D	3D	4D
BASIS/ORB E	-83.21902	-12.75672	-1.23474	BASIS/ORB E	-7.25235	-0.09261
2P 26.46150	-0.12835	0.03222	0.00933	3D 12.87330	0.28661	-0.06593
2P 16.71580	-0.87369	0.43891	0.15621	3D 6.90015	0.75294	-0.15938
3P 9.02922	-0.03260	-0.69106	-0.27761	4D 3.79514	0.05269	0.28228
3P 6.47917	0.01478	-0.43508	-0.19589	4D 2.10680	-0.01152	0.57676
4P 4.17096	-0.00363	-0.00255	0.63513	4D 1.08515	0.00319	0.34339
4P 2.64187	0.00161	-0.00062	0.50183			
4P 1.38208	-0.00037	0.00009	0.02090			

NIOBIUM K(2)L(8)M(18)4S(2)4P(6)5S(1)4D(5), 7S  
 T.E.= -0.375353850D+04 P.E.= -0.75068002D+04 K.E.= 0.37532617D+04 V.T.= -0.20000737D+01

S	1S	2S	3S	4S	5S	
BASIS/ORB E	-685.19825	-96.72476	-16.99089	-2.27443	-0.01358	
1S 42.12940	0.85249	0.02467	0.00617	-0.00204	0.00039	
1S 29.31960	0.16375	0.47712	0.20680	-0.07964	0.01367	
2S 19.00060	-0.09327	-0.12327	0.69988	-0.32235	0.05770	
2S 17.34330	0.08191	-1.05279	-1.40677	0.60816	-0.10741	
3S 11.36880	-0.00737	-0.04017	0.22535	-0.07460	0.01229	
3S 8.14768	0.00342	0.00074	0.98334	-0.53619	0.09758	
4S 4.64550	-0.00092	-0.00158	0.02150	0.71701	-0.15538	
4S 3.16032	0.00059	0.00101	-0.00578	0.44188	-0.06627	
5S 2.08501	-0.00019	-0.00030	0.00148	0.01419	0.26354	
5S 1.12605	0.00007	0.00011	-0.00046	-0.00413	0.56638	
5S 0.54979	-0.00002	-0.00003	0.00012	-0.00164	0.43576	
P	2P	3P	4P	D	3D	4D

See page 183 for Explanation of Tables and Notes for Tables 32, 42, and 43

## ROOTHAAN-HARTREE-FOCK ATOMIC WAVEFUNCTIONS

TABLE 44 (17). THE HARTREE-FOCK FUNCTIONS FOR NEGATIVE IONS.

P	2P	3P	4P	D	3D	4D
EASIS/ORB E	-88.57315	-13.82597	-1.30093	BASIS/CRB E	-8.07311	-0.04557
2P 27.07440	-0.12872	0.03170	0.00937	3C 13.34950	0.28244	-0.06449
2P 17.18870	-0.87299	0.44483	0.16192	3D 7.22241	0.75550	-0.16479
3P 9.35611	-0.03337	-0.66883	-0.26966	4D 4.12888	0.04728	0.27055
3P 6.85943	0.01559	-0.45543	-0.22272	4C 2.25274	-0.00703	0.57804
4P 4.45292	-0.00365	-0.00670	0.61196	4D 1.05088	0.00151	0.39013
4P 2.86189	0.00175	0.00559	0.51374			
4P 1.68069	-0.00046	-0.00028	0.04381			

NIOBIUM K(2)L(8)M(18)4S(2)4P(6)5S(2)4D(4), 5D  
 T.E.= -0.37535547D+04 P.E.= -0.75C68510D+04 K.E.= 0.37532963D+04 V.T.= -0.20000688D+01

S	1S	2S	3S	4S	5S
EASIS/ORB E	-685.29678	-96.82626	-17.09467	-2.37550	-0.01556
1S 42.12940	0.85250	0.02468	-0.00616	0.00201	0.00001
1S 29.31960	0.16373	0.47710	-0.20662	0.07588	0.01491
2S 19.00060	-0.09309	-0.12305	-0.69972	0.32227	0.05085
2S 17.34330	0.08172	-1.05259	1.40661	-0.60863	-0.10162
3S 11.38800	-0.00721	-0.04010	-0.22536	0.07435	0.00758
3S 8.14768	0.00338	0.00668	-0.98333	0.53787	0.10749
4S 4.64550	-0.00088	-0.00151	-0.02133	-0.71561	-0.17580
4S 3.16032	0.00053	0.00553	0.00547	-0.44233	-0.04112
5S 1.92550	-0.00017	-0.00028	-0.00141	-0.00587	0.29717
5S 1.13310	0.00008	0.00014	0.00062	0.00201	0.49269
5S 0.60904	-0.00003	-0.00004	-0.00019	-0.00059	0.43436

P	2P	3P	4P	D	3D	4D
BASIS/ORB E	-88.67410	-13.92527	-1.40000	BASIS/ORB E	-8.17564	-0.13980
2P 27.07440	-0.12870	0.03170	0.00936	3D 13.34950	-0.28199	-0.07191
2P 17.18870	-0.87302	0.44481	0.16285	3D 7.22241	-0.75676	-0.17654
3P 9.35611	-0.03321	-0.66873	-0.27267	4C 3.97401	-0.04943	0.32644
3P 6.85943	0.01536	-0.45554	-0.22045	4C 2.23372	0.01125	0.57572
4P 4.41531	-0.00347	-0.00679	0.63460	4D 1.18633	-0.00315	0.28533
4P 2.82081	0.00160	0.00068	0.50386			
4P 1.57715	-0.00035	-0.00023	0.02626			

MOLYBDENUM K(2)L(8)M(18)4S(2)4P(6)5S(1)4D(6), 6D  
 T.E.= -0.39753877D+04 P.E.= -0.755C5571D+04 K.E.= 0.39751694D+04 V.T.= -0.20000549D+01

S	1S	2S	3S	4S	5S
EASIS/ORB E	-720.56814	-102.60939	-18.34042	-2.51479	-0.00318
1S 43.12250	0.25711	0.02665	-0.00670	-0.00168	-0.00010
1S 29.86310	0.15936	0.47513	-0.20969	-0.08321	0.01160
2S 19.16340	-0.14165	-0.02647	-1.17256	-0.51645	0.05809
2S 18.01280	0.13053	-1.14618	1.88870	0.81116	-0.09628
3S 12.17300	-0.00773	-0.04522	-0.17691	-0.04428	0.00078
3S 8.51353	0.00310	0.00811	-1.03364	-0.58218	0.08652
4S 4.87537	-0.00075	-0.00142	-0.02509	0.72010	-0.13242
4S 3.29379	0.00041	0.00061	0.00536	0.45C71	-0.02766
5S 0.44454	-0.00001	-0.00002	-0.00011	-0.00091	0.51652
5S 1.88877	-0.00010	-0.00018	-0.00109	C.00978	0.28737
5S 0.95273	0.00004	0.00007	0.00038	-0.002E4	0.50000

P	2P	3P	4P	D	3D	4D
BASIS/ORB E	-94.20348	-15.04342	-1.48344	BASIS/CRB E	-9.04059	-0.07298
2P 27.65600	-0.12974	0.03148	C.00544	3D 13.82640	0.27328	-0.06840
2P 17.65740	-0.87175	0.45C7	0.16788	3D 7.60981	0.75639	-0.18144
3P 9.66096	-0.03387	-0.65610	-0.26734	4C 4.46535	0.05462	0.26094
3P 7.20765	0.01619	-0.46655	-0.24234	4D 2.56091	-0.00938	0.56072
4P 4.68358	-0.00351	-0.01000	0.61733	4D 1.24765	0.00223	0.40053
4P 3.02488	0.00169	0.00165	0.51050			
4P 1.82653	-0.00045	-0.00028	0.04781			

See page 183 for Explanation of Tables and Notes for Tables 32, 42, and 43

TABLE 44 (18). THE HARTREE-FOCK FUNCTIONS FOR NEGATIVE IONS.

MOLYBDENUM K(2)L(8)M(18)4S(2)4P(6)5S(2)4D(5),6S T.E.= -0.397550650+04 P.E.= -0.75508301D+04 K.E.= 0.39753236D+04 V.T.= -0.20000460D+01						
S	1S	2S	3S	4S	5S	
BASIS/ORB E	-721.04863	-102.69304	-18.42783	-2.60610	-0.01688	
1S 43.12250	C.85710	0.02664	-0.00672	-0.00153	-0.00016	
1S 29.86310	0.15938	C.47514	-0.20966	-0.08370	0.01517	
2S 19.16340	-0.14179	-0.02670	-1.17328	-0.51401	0.07428	
2S 18.01280	0.13068	-1.14554	1.88947	C.80707	-0.12389	
3S 12.17300	-0.00776	-0.04526	-0.17714	-0.04252	0.00059	
3S 8.51353	0.03012	C.00E15	-1.03340	-C.58571	0.11307	
4S 4.87537	-0.00078	-0.00146	-0.02336	C.72569	-0.17327	
4S 3.29379	0.00044	0.000E5	G.00560	0.44722	-0.03512	
5S 1.92101	-0.00012	-0.00022	-0.00125	0.00621	0.34625	
5S 1.04014	0.00005	0.00010	0.00050	-0.00072	0.55634	
5S 0.52594	-0.00002	-0.00003	-0.00016	0.00018	0.34778	
P	2P	3P	4P	D	3D	4D
BASIS/ORB E	-94.28646	-15.13C15	-1.56782	BASIS/CRB E	-9.12638	-0.19918
2P 27.65600	-0.12573	0.02148	C.00945	3D 12.82640	0.27262	-0.07466
2P 17.65740	-C.87177	0.45003	0.16685	3D 7.60981	0.75841	-0.19257
3P 9.66096	-0.C3378	-0.65590	-0.26935	4D 4.27913	0.05647	0.32728
3P 7.20785	0.01606	-0.46714	-0.24163	4D 2.45975	-0.01454	0.58429
4P 4.65578	-0.00341	-0.01C11	0.63530	4D 1.33228	0.00414	0.27327
4P 2.99052	0.00163	0.00174	0.50442			
4P 1.77956	-0.00043	-0.00055	0.03199			
TECHNETIUM K(2)L(8)M(18)4S(2)4P(6)5S(1)4D(7),5F T.E.= -0.42046719D+04 P.E.= -0.84051325D+04 K.E.= 0.42044607D+04 V.T.= -0.20000502D+01						
S	1S	2S	3S	4S	5S	
BASIS/ORB E	-757.68144	-108.69368	-19.75260	-2.78003	0.00115	
1S 44.13570	C.85889	0.02642	-0.00697	-0.00157	0.00063	
1S 30.51100	0.15789	0.48219	-0.21182	-0.0E577	0.00652	
2S 19.65550	-0.16160	0.05040	-1.36464	-0.55696	0.07238	
2S 18.58460	0.15043	-1.22515	2.08632	C.89534	-0.09951	
3S 12.76560	-0.00812	-0.C4723	-0.14885	-0.02668	0.00725	
3S 8.84424	0.00050	0.00152	-1.06166	-0.61265	0.04994	
4S 5.06872	-0.00081	-0.00139	-0.02456	C.73776	-0.06639	
4S 3.42305	0.00049	0.00088	0.00627	0.43659	-0.05092	
5S 2.27855	-0.00013	-C.00C22	-0.00141	0.01160	0.16043	
5S 0.59685	0.00003	0.00005	0.00026	-0.00C66	0.43877	
5S 0.36075	-0.00001	-0.00001	-0.00005	-0.00C76	0.75084	
P	2P	3P	4P	D	3D	4D
BASIS/ORB E	-100.03198	-16.32258	-1.69183	BASIS/CRB E	-10.06904	-0.13520
2P 28.25180	-0.13046	0.02112	0.00945	3D 14.29850	0.26894	-0.07249
2P 18.12740	-0.87083	0.45531	0.17333	3D 7.92996	0.76069	-0.19439
3P 9.98674	-0.03426	-0.63121	-0.25699	4D 4.59671	0.05205	0.30672
3P 7.59462	0.01656	-0.49C14	-0.26821	4D 2.64324	-0.00996	0.55995
4P 4.91893	-0.00316	-0.01410	0.61955	4D 1.31803	0.00259	0.35248
4P 3.18222	0.00151	0.0C291	0.51247			
4P 1.94849	-0.00040	-0.00055	0.04939			
TECHNETIUM K(2)L(8)M(18)4S(2)4P(6)5S(2)4D(6),5L T.E.= -0.42029274D+04 P.E.= -0.83E64477D+04 K.E.= 0.41777203D+04 V.T.= -0.20060337D+01						
S	1S	2S	3S	4S	5S	
BASIS/ORB E	-758.60570	-109.35482	-20.00838	-2.85285	-0.01825	
1S 44.13570	C.85889	0.02626	-0.00679	-0.00176	-0.00011	
1S 30.51100	0.15799	0.48300	-0.21257	-0.0E576	0.01559	
2S 19.63550	-0.16697	0.05373	-1.40450	-0.63253	0.09370	
2S 18.58400	0.15575	-1.23083	2.12992	C.93453	-0.14516	
3S 12.76560	-0.00823	-0.04384	-0.15636	-C.03563	-0.00042	
3S 8.84424	0.00311	0.00E34	-1.06003	-C.60841	0.11769	
4S 5.06872	-0.00077	-0.00102	-0.01854	C.75C04	-0.18056	
4S 3.42305	0.00044	0.000E1	0.00335	C.42821	-0.02858	
5S 1.99366	-0.00012	-0.00116	-0.00075	0.00676	0.35441	
5S 1.07493	0.00005	0.00007	0.00031	-C.00070	0.55600	
5S 0.54271	-0.00002	-0.00002	-0.00010	0.00018	0.34056	

See page 183 for Explanation of Tables and Notes for Tables 32, 42, and 43

## ROOTHAAAN-HARTREE-FOCK ATOMIC WAVEFUNCTIONS

TABLE 44 (19). THE HARTREE-FOCK FUNCTIONS FOR NEGATIVE IONS.

P	2P	3P	4P	C	3D	4D
BASIS/ORB E	-100.72495	-16.26911	-1.71974	BASIS/ORB E	-10.37556	-0.21714
2P 28.25180	0.12455	0.10628	0.03537	3C 14.29850	0.27607	-0.07955
2P 18.12740	0.88209	0.28865	0.11397	3D 7.92996	0.75995	-0.19993
3P 99.86740	0.00060	-0.00606	-0.00199	4D 4.45180	0.04261	0.37675
3P 7.59482	0.01925	-1.15768	-0.57220	4D 2.54414	-0.00876	0.56894
4P 4.88685	-0.01350	0.34389	0.81695	4D 1.36971	0.00237	0.24660
4F 3.15037	0.00916	-0.24633	0.36274			
4P 1.88278	-0.00299	0.08433	0.09543			

RHODIUM K(2)L(8)M(18)4S(2)4P(6)5S(2)4D(8),3F  
 T.E.= -0.46858581D+04 P.E.= -0.93715643D+04 K.E.= 0.46E57061D+04 V.T.= -0.20000324D+01

S	1S	2S	3S	4S	5S
BASIS/ORB E	-833.86812	-121.39034	-22.70701	-3.33020	-0.01883
1S 46.18930	0.86002	0.02651	-0.01067	-0.00275	-0.00015
1S 31.53590	0.15971	0.49262	-0.21305	-0.08966	0.01593
2S 22.36960	-0.07088	-0.10496	-0.39418	-0.17044	0.02062
2S 19.25330	0.05606	-1.08386	1.11271	0.47411	-0.06980
3S 13.77310	-0.00783	-0.04105	-0.07489	0.01570	-0.01157
3S 9.52967	0.00290	0.00428	-1.11929	-0.67768	0.12656
4S 5.47461	-0.00072	-0.00048	-0.02805	0.75904	-0.17838
4S 3.69732	0.00040	0.00030	0.00680	0.43023	-0.02409
5S 2.13567	-0.00010	-0.00067	-0.00147	0.00567	0.34556
5S 1.13941	0.00005	0.00003	0.00058	-0.00065	0.55473
5S 0.56987	-0.00001	-0.00001	-0.00018	0.00017	0.35687

P	2P	3P	4P	D	3D	4D
BASIS/ORB E	-112.21239	-19.00704	-2.11719	BASIS/ORB E	-12.24774	-0.27515
2P 29.44890	-0.13182	0.03052	0.06940	3D 15.27760	0.25753	-0.08079
2P 19.06530	-0.86929	0.46445	0.18448	3C 8.59242	0.77019	-0.22498
3P 10.59930	-0.03473	-0.59451	-0.24240	4D 4.86839	0.05019	0.41315
3P 8.32836	0.01727	-0.52415	-0.31188	4D 2.77544	-0.01203	0.56535
4P 5.33965	-0.00251	-0.02075	0.64463	4D 1.49843	0.00378	0.21552
4P 3.45909	0.00115	0.00502	0.50601			
4P 2.12394	-0.00029	-0.00147	0.03730			

FALLADIUM K(2)L(8)M(18)4S(2)4P(6)5S(2)4D(9),2D  
 T.E.= -0.49378746D+04 P.E.= -0.98756008D+04 K.E.= 0.49377262D+04 V.T.= -0.20000301D+01

S	1S	2S	3S	4S	5S
BASIS/ORB E	-873.20553	-127.56669	-24.20519	-3.57448	-0.01911
1S 47.15980	0.86665	0.02566	-0.00825	-0.00147	-0.00036
1S 32.10000	0.15168	0.49212	-0.22047	-0.09425	0.01635
2S 21.04950	-0.22456	-0.00178	-1.67129	-0.71041	0.08311
2S 20.07510	0.21281	-1.17541	2.41399	1.02652	-0.13250
3S 14.43650	-0.01002	-0.05346	-0.09473	0.01424	-0.01158
3S 9.79756	0.00321	0.00667	-1.11897	-0.69100	0.12678
4S 5.67806	-0.00080	-0.00120	-0.02576	0.76919	-0.17780
4S 3.82464	0.00043	0.00071	0.00549	0.42718	-0.02098
5S 2.19708	-0.00011	-0.00017	-0.00116	0.00535	0.34327
5S 1.16559	0.00005	0.00007	0.00045	-0.00060	0.55463
5S 0.58051	-0.00002	-0.00002	-0.00014	0.00015	0.36170

P	2P	3P	4P	D	3D	4D
BASIS/ORB E	-118.52345	-20.36538	-2.30492	BASIS/ORB E	-13.35627	-0.31034
2P 30.03080	-0.13283	0.03277	0.00938	3D 15.75530	0.25304	-0.08205
2P 19.53300	-0.86817	0.46531	0.18896	3D 8.91908	0.77336	-0.23439
3P 10.94970	-0.03490	-0.55547	-0.21862	4D 5.07798	0.04891	0.43177
3P 8.75686	0.01743	-0.56679	-0.34641	4C 2.88952	-0.01117	0.56122
4P 5.56431	-0.00210	-0.02517	0.64324	4D 1.56195	0.00369	0.20241
4P 3.61882	0.00095	0.00654	0.50675			
4P 2.26669	-0.00024	-0.00193	0.04154			

See page 183 for Explanation of Tables and Notes for Tables 32, 42, and 43

TABLE 44 (20). THE HARTREE-FOCK FUNCTIONS FOR NEGATIVE IONS.

SILVER      K(2)L(8)M(18)4S(2)4P(6)5S(2)4D(10),1S  
 T.E.= -0.51976826D+04   P.E.= -0.1C395085D+05   K.E.= 0.51974022D+04   V.T.= -0.20000539D+01

	1S	2S	3S	4S	5S
BASIS/ORB E	-913.66154	-134.70583	-25.74092	-2.81681	-0.01917
1S 48.20370	0.86307	0.02356	-0.00749	-0.00151	-0.00043
1S 33.24800	0.15470	0.49268	-0.21894	-0.09389	0.01600
2S 22.09440	-0.15751	0.22646	-1.33441	-0.51973	0.06668
2S 20.76230	0.14577	-1.40058	2.06634	0.89432	-0.11448
3S 15.05540	-0.00862	-0.05302	-0.06009	0.02666	-0.01376
3S 10.12760	0.00265	0.03477	-1.14228	-0.70824	0.12649
4S 5.85959	-0.00067	-0.00067	-0.02676	0.77105	-0.17513
4S 3.98157	0.00037	0.00041	0.00576	0.42463	-0.01864
5S 2.27095	-0.00009	-0.00009	-0.00116	0.00883	0.33269
5S 1.20256	0.00004	0.00004	0.00044	-0.00196	0.55343
5S 0.59623	-0.00001	-0.00001	-0.00014	0.00060	0.37541

	2P	3P	4P	D	3D	4D
BASIS/ORB E	-125.00802	-21.76558	-2.49342	BASIS/ORB E	-14.50120	-0.35349
2P 30.63690	-0.13306	0.02940	0.00922	3D 16.24400	0.25145	-0.08300
2P 20.00970	-0.86753	0.47447	0.19317	3D 5.20435	0.77739	-0.24321
3P 11.43010	-0.03431	-0.45786	-0.16923	4L 5.31137	0.04136	0.44544
3P 9.24448	0.01642	-0.45634	-0.40591	4D 3.01632	-0.00799	0.56019
4P 5.81375	-0.00152	-0.02826	0.62993	4D 1.63286	0.00209	0.19229
4P 3.79881	0.00065	0.00680	0.52042			
4P 2.35358	-0.00014	-0.00189	0.04535			

INDIUM      K(2)L(8)M(18)4S(2)4P(6)5S(2)4D(10)5P(2),3P  
 T.E.= -0.57401599D+04   P.E.= -0.11480087D+05   K.E.= 0.57359270D+04   V.T.= -0.20000406D+01

	1S	2S	3S	4S	5S
BASIS/ORB E	-997.62056	-149.21676	-29.44170	-4.78536	-0.19599
1S 50.47740	0.84327	0.02770	-0.01142	-0.00011	-0.00092
1S 33.87640	0.18676	0.50516	-0.22263	0.10430	0.02849
2S 25.56180	-0.13060	0.05785	-0.39356	0.09184	0.00794
2S 22.18650	0.11154	-1.19508	1.05362	-0.36072	-0.07388
2S 18.73670	-0.01577	-0.10500	0.10166	-0.12695	-0.04308
3S 10.91680	0.00225	-0.00270	-1.20281	0.75256	0.21141
4S 6.24023	-0.00092	0.00058	-0.04707	-0.75546	-0.27424
4S 4.39832	0.00064	-0.00056	0.01811	-0.43010	-0.06662
5S 2.78806	-0.00023	0.00021	-0.00517	-0.00581	0.42473
5S 1.70359	0.00012	-0.00011	0.00255	0.00226	0.56275
5S 1.00391	-0.00004	0.00004	-0.00083	-0.00073	0.18293

	2P	3P	4P	5P	D	3D	4D
BASIS/ORB E	-138.99247	-25.19164	-3.32055	-0.02093	BASIS/ORB E	-17.40701	-0.87609
2P 31.88400	0.13281	0.02855	0.00920	-0.00157	3D 17.23440	0.24069	-0.08740
2P 20.96010	0.86767	0.48157	0.20374	-0.03216	3D 9.88166	0.78327	-0.27931
3P 11.84710	0.03814	-0.46657	-0.15823	0.01877	4D 5.92274	0.04233	0.44426
3P 9.91541	-0.02084	-0.64721	-0.44758	0.0814	4D 3.52746	-0.00718	0.58180
4P 6.23969	0.00152	-0.03319	0.66237	-0.13901	4D 2.06862	0.00161	0.14611
4P 4.05379	-0.00055	0.00721	0.52861	-0.05904			
5P 2.29457	0.00011	-0.00181	0.01139	0.31034			
5P 1.26579	-0.00005	0.00063	-0.00068	0.55850			
5P 0.64817	0.00002	-0.00027	0.00022	0.37132			

TIN      K(2)L(8)M(18)4S(2)4P(6)5S(2)4D(10)5P(3),4S  
 T.E.= -0.60229586D+04   P.E.= -0.12C45637D+05   K.E.= 0.60226783D+04   V.T.= -0.20000465D+01

	1S	2S	3S	4S	5S
BASIS/ORB E	-1041.00023	-156.75610	-31.37312	-5.28241	-0.26532
1S 51.31560	0.85768	-0.01622	-0.00608	-0.00041	-0.00067
1S 35.92780	0.15984	-0.45739	-0.22074	-0.09597	0.02919
2S 24.76870	-0.08793	-0.24919	-0.77561	-0.34271	0.08246
2S 22.33560	0.07497	1.41998	1.49219	0.66420	-0.17103
3S 15.46340	-0.00778	0.05487	0.02076	0.10033	-0.04342
3S 11.13190	0.00337	-0.01020	-1.19649	-0.81370	0.25670
4S 6.56056	-0.00090	0.00149	-0.03509	0.74835	-0.30202
4S 4.61749	0.00055	-0.00052	0.00948	0.46353	-0.07918
5S 2.85085	-0.00017	0.00026	-0.00220	0.00596	0.52218
5S 1.73190	0.00009	-0.00014	0.00109	-0.00082	0.52404
5S 1.04256	-0.00003	0.00005	-0.00036	0.00033	0.11354

See page 183 for Explanation of Tables and Notes for Tables 32, 42, and 43

## ROOTHAAN-HARTREE-FOCK ATOMIC WAVEFUNCTIONS

TABLE 44 (21). THE HARTREE-FOCK FUNCTIONS FOR NEGATIVE IONS.

P	2P	3P	4P	5P	D	3D	4D
EASIS/ORB E	-146.26712	-26.58365	-3.73974	-C.06651	BASIS/ORB E	-18.93823	-1.13936
2P 32.49040	0.13307	0.02849	-0.00914	-0.00199	3D 17.73890	0.23487	-0.08889
2P 21.43360	0.86731	0.46529	-0.20918	-0.04224	3D 10.22450	0.78701	-0.29396
3P 12.13300	0.03987	-0.43233	0.12861	0.01617	4D 6.15528	0.04333	0.46030
3P 10.32510	-0.02271	-0.68167	0.49136	0.11773	4D 3.70743	-0.00780	0.59010
4P 6.48721	0.00141	-0.03756	-0.65202	-C.17813	4D 2.18437	0.00174	0.11507
4P 4.28617	-0.00051	0.CCE66	-0.54080	-0.08093			
5P 2.46851	0.00010	-0.00230	-0.01115	C.38994			
5P 1.42807	-0.00005	0.00118	0.00081	0.55979			
5P 0.80171	0.00002	-0.00041	-0.00013	0.24714			

ANTIMONY K(2)L(8)M(18)4S(2)4P(6)5S(2)4D(10)5P(4),3P  
 T.E.= -0.63134692D+04 P.E.= -0.12626807D+05 K.E.= 0.63133382D+04 V.T.= -0.20000207D+01

S	1S	2S	3S	4S	5S
BASIS/ORB E	-1085.35277	-164.52118	-33.39963	-5.82541	-0.36119
1S 52.35240	0.85663	-0.01674	0.00698	-0.00112	-0.00046
1S 36.67060	0.16138	-0.49690	0.22039	-0.10021	0.03146
2S 25.75890	-0.07677	-C.25196	0.66887	-C.30830	0.08214
2S 22.88580	0.06271	1.42253	-1.38284	C.63370	-0.17890
3S 15.18140	-0.00815	0.06267	-0.07486	0.15012	-0.06503
3S 11.51870	0.00433	-0.01512	1.24254	-0.87614	0.29972
4S 6.80039	-0.00100	0.00299	0.04031	0.73514	-0.32249
4S 4.85397	0.00060	-0.00183	-0.01189	0.48104	-0.09756
5S 3.00470	-0.00021	0.00054	0.00272	0.00633	0.56884
5S 1.85062	0.00012	-0.00031	-0.00144	-0.00080	0.49208
5S 1.16611	-0.00004	0.00011	0.00050	0.00037	0.09446

P	2P	3P	4P	5P	D	3D	4D
BASIS/ORB E	-153.76652	-28.86584	-4.20757	-0.07224	BASIS/CRB E	-20.56165	-1.45039
2P 33.11500	0.13335	C.02811	-0.00892	-C.00220	3D 18.24510	-0.22596	-0.08902
2P 21.89930	0.86736	0.48522	-0.21498	-0.04934	3D 10.61820	-0.79020	-0.30646
3P 12.30790	0.04118	-0.45630	0.12997	C.01627	4D 6.36092	-0.05149	0.47729
3P 10.62610	-0.02462	-C.5337	0.50599	C.14551	4D 3.88266	0.01311	0.58873
4P 6.75090	0.00129	-C.03563	-0.63544	-0.20094	4D 2.31903	-0.00355	0.09173
4P 4.54506	-0.00043	0.CC956	-0.55957	-0.10C74			
5P 2.64586	0.00006	-0.00229	-0.01382	0.44335			
5P 1.53547	-0.00002	0.00114	0.00156	0.547C7			
5P 0.85446	0.00001	-0.00038	-0.00062	0.20892			

TELLURIUM K(2)L(8)M(18)4S(2)4P(6)5S(2)4D(10)5P(5),2P  
 T.E.= -0.66118159D+04 P.E.= -0.13223498D+05 K.E.= 0.66116818D+04 V.T.= -0.20000203D+01

S	1S	2S	3S	4S	5S
BASIS/ORB E	-1130.65163	-172.48558	-35.48963	-6.38060	-0.45742
1S 53.40020	0.85443	0.01624	-0.00764	-0.00061	-0.00077
1S 37.40130	0.16451	0.49E33	-0.22051	-0.10291	0.03424
2S 26.57900	-C.7957	0.26533	-0.64658	-0.28374	0.07685
2S 23.50060	0.06501	-1.43406	1.35514	C.60701	-0.17771
3S 16.36680	-0.00814	-0.06401	0.08885	0.15082	-0.06703
3S 11.83350	0.00364	0.01324	-1.24738	-C.87806	0.31474
4S 7.0C608	-0.00108	-0.00240	-0.04254	C.72480	-0.33809
4S 5.09670	0.00071	0.C0155	0.01327	0.49C83	-0.11385
5S 3.17024	-0.00022	-0.00C45	-0.00283	C.00E54	0.59784
5S 1.97669	0.00013	0.00C26	0.00155	-0.00155	0.47194
5S 1.28179	-0.00005	-0.00C10	-0.00054	0.00068	0.08588

P	2P	3P	4P	5P	D	3D	4D
BASIS/ORB E	-161.46840	-30.81511	-4.68687	-0.09643	BASIS/ORB E	-22.24735	-1.77233
2P 33.73260	0.13316	0.C2752	-0.C0868	-0.00234	3D 18.70500	0.22327	-0.09073
2P 22.37E40	0.86736	0.49292	-0.22032	-0.05582	3D 10.94040	0.79206	-0.31861
3P 12.56430	0.04479	-0.42434	0.09370	0.006C5	4D 6.59966	0.05047	0.48791
3P 11.03340	-0.02832	-0.66E21	0.55520	0.17069	4D 4.07175	-0.01218	0.59781
4P 6.97060	0.00128	-0.04324	-0.63661	-0.22378	4D 2.32945	0.00293	C.07018
4P 4.75722	-0.00043	0.011C8	-0.56065	-0.11562			
5P 2.82192	0.00006	-0.00259	-0.01319	0.48361			
5P 1.65235	-0.00002	0.C0128	0.00072	0.52216			
5P 0.93491	0.00001	-0.00043	-0.00059	0.175C5			

See page 183 for Explanation of Tables and Notes for Tables 32, 42, and 43

TABLE 44 (22). THE HARTREE-FOCK FUNCTIONS FOR NEGATIVE IONS.

IODINE      K{2}L{8}M{18}4S{2}4P{6}5S{2}4D{10}5P{6},1S  
 T.E.= -0.69180636D+04    P.E.= -0.13835907D+05    K.E.= C.69178439D+04    V.T.= -0.20000317D+01

S	1S	2S	3S	4S	5S			
BASIS/ORB E	-1176.89784	-180.66320	-37.64414	-6.95100	-0.55621			
1S 54.53840	0.84743	0.02470	0.01161	-0.00075	-0.00142			
1S 37.21140	0.17863	0.50255	0.22293	-0.10833	0.03872			
2S 27.72960	-0.10774	0.21764	0.53055	-0.19762	0.04171			
2S 24.21470	0.08782	-1.37712	-1.22252	0.50845	-0.14063			
3S 18.17370	-0.01170	-0.08087	-0.12428	0.16618	-0.07744			
3S 12.17740	0.00393	0.00888	1.25172	-0.87647	0.32897			
4S 7.34469	-0.00151	-0.00236	0.04869	0.61037	-0.31590			
4S 5.53794	0.00097	0.00158	-0.01540	0.59750	-0.16237			
5S 3.28271	-0.00022	-0.00033	0.00217	0.01730	0.66510			
5S 1.96900	0.00010	0.00015	-0.00094	-0.00381	0.46704			
5S 1.01114	-0.00003	-0.00004	0.00024	0.00109	0.02523			
<hr/>								
P	2P	3P	4P	5P	D	3D	4D	
BASIS/ORB E	-169.37354	-32.83241	-5.18084	-0.12914	BASIS/ORB E	-23.99646	-2.10841	
2P 34.37880	0.13186	0.02672	-0.00852	-0.00244	3D 19.30520	0.21647	-0.08997	
2P 22.87760	0.26773	0.45596	-0.22494	-0.06110	3D 11.26420	0.79953	-0.33355	
3P 13.26120	0.04333	-0.15551	-0.04434	-0.03086	4D 6.84713	0.04669	0.49964	
3P 11.69430	-0.02576	-0.94684	0.69696	0.22067	4D 4.27111	-0.00968	0.59566	
4P 7.11123	0.00071	-0.0512	-0.64980	-0.24495	4D 2.45411	0.00197	0.06008	
4P 4.93989	-0.00022	0.01554	-0.54177	-0.12261				
5P 3.00175	-0.00000	-0.00368	-0.01146	0.51217				
5P 1.77590	0.00001	0.00180	0.00081	0.52068				
5P 1.02667	-0.00000	-0.00061	-0.00026	0.15742				

See page 183 for Explanation of Tables and Notes for Tables 32, 42, and 43