

## GENERAL HARTREE–FOCK PROGRAM

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### PROGRAM SUMMARY

*Title of program:* HF86

*Catalogue number:* AATK

*Program obtainable from:* CPC Program Library, Queen's University of Belfast, N. Ireland (see application form in this issue)

*Computer:* Vax 11/780; *Installation:* Vanderbilt University, Nashville, TN 37235, USA

*Operation system:* VMS Version 4.4

*Programming language used:* FORTRAN 77

*Virtual memory:* 526 kbytes

*No. of bits in a word:* 32

*Peripherals used:* disk, printer, terminal

*No. of lines in combined program and test deck:* 4167

*Keywords:* atomic structure, numerical Hartree–Fock, bound state, Schrödinger equation, wavefunction, self-consistent field, energy level, spin–orbit parameter

#### *Nature of physical problem*

Numerical non-relativistic Hartree–Fock wavefunctions are determined for atoms in a bound state. These are used to predict a variety of atomic parameters.

#### *Method of solution*

The self-consistent field method of solution is employed. Two methods of solution of the differential equations are used, each improving only a single function at a time [1], and rotations are introduced explicitly to find an energy stationary with respect to a rotation of the orbital basis. Otherwise, the procedures are essentially the same as those in MCHF77 [2].

#### *Restrictions on the complexity of the problem*

The configuration may have up to five open shells.

#### *Unusual features of the program*

The program is designed for interactive use. Fractional occupation numbers may be used to indicate a linear combination of two configurations differing by one electron. There is no restriction on the  $l$ -quantum number. A help facility is available and once the SCF calculation is complete, the user may request the evaluation of a variety of parameters.

#### *Typical running time*

The CPU time on a VAX 11/780 for several cases is as follows:

- (i) He  $1s2s\ ^3S$ : 5.95s;
- (ii) Ra ( $Z = 88$ )  $7s^2$  ground state: 3 min and 59 s.

#### *References*

- [1] C. Froese Fischer, *Comput. Phys. Commun.* 15 (1977) 221.
- [2] C. Froese Fischer, *Comput. Phys. Commun.* 14 (1978) 145.

## LONG WRITE-UP

### 1. Introduction

Earlier versions of multiconfiguration Hartree–Fock programs [1–3] all have included the single configuration Hartree–Fock calculation as a special case. Many scientists use the program in this manner which is inefficient in that much of the complexity of the program is related to the multiconfiguration nature of the general case. A much shorter program, using less computer resources, can be developed for a Hartree–Fock calculation. At the same time, Hartree–Fock calculations are frequently quite short and are executed most conveniently in the interactive mode.

In this paper we describe a general Hartree–Fock program to be used in the interactive mode. Little or no data need be prepared in advance. The user is prompted for a minimum of information. A HELP facility is available during execution to clarify the meaning of requested data. Finally, once the Hartree–Fock calculation has been completed, the user may request the display of a variety of parameters or integrals.

The program uses the same numerical techniques as the earlier MCHF77 [3] program and the meaning of input parameters has not changed. In this description we will concentrate on the differences and refer the reader to the earlier publication for additional information.

Earlier versions of MCHF programs all stored the numerical values for a radial function as a row in a two-dimensional array. In a paging environment, it is more efficient to store by columns. In this version such a rearrangement has been implemented. For Ra, this change alone reduced execution time by 13%.

### 2. Allowed configurations

The dimensions are such that the number of radial functions (NWF) or electron shells must not exceed twenty (20). This could be reduced to ten (10) if memory is critical. Unlike the MCHF programs there is no restriction on the angular or  $l$ -quantum number, though the program only recognizes symbols up to 'n' or  $l = 10$ . The three

dimensional arrays  $a_{i,j,k}$  and  $b_{i,j,k}$ , the coefficients of  $F^k$  and  $G^k$  integrals in the energy expression, have been deleted and replaced by a single list. The third dimension of the former was dependent on the maximum allowed  $l$ -value and caused these arrays to grow unduly large.

The configuration is specified in the spectroscopic notation as, for example, in  $1s(2)2s(2)$ . The electron label contains up to three characters of which the first non-blank character is the symbolic character for  $n$ , the principal quantum number. Thus, the usual values 0 to 9 are represented by the characters '0' to '9' and the character for  $n = 10$ , in the ASCII code is the character ':'. Let 'n' be the character representing the  $n$  quantum number. Then, in FORTRAN77,

$$n = \text{ICHAR}('n') - \text{ICHAR}('0').$$

The program is not designed with high  $n$  in mind. In fact, the numerical accuracy degrades fairly rapidly as  $n$  increases [2]. The basic step-size parameter  $H$  (set in the INIT subroutine) should be decreased and the associated arrays (dimensioned 220 in the present program) should be increased by an equivalent factor. For high accuracy, the parameter RHO should be made more negative.

The character following 'n' in the label is the 'l' symbol, following spectroscopic conventions. A third character may be used as a subscript, if so desired. In MCHF calculations, non-orthogonal orbitals may be convenient and a subscript designates the set of orthogonal orbitals. For compatibility purposes this subscript has been retained.

For large atoms, there may be a long list of closed shells. These should be specified separately so that the "configuration" contains only shells outside the closed shells. The configurations may, of course, contain closed shells but the total number of shells is limited to at most five. A configuration consisting only of closed shells is best specified as a "blank" configuration.

After the electron label, the occupation of the shell is specified, enclosed in parentheses. Fractional occupation numbers are allowed and so it would be possible to perform transition state

calculations such as those proposed by Godefroid et al. [4] for transition probabilities. For example, for the transition  $1s(2)2s(2)-1s(2)2s(1)2p(1)$  the average occupation in the initial and final state is  $1s(2)2s(1.5)2p(0.5)$ . A calculation for this configuration may yield a simple, approximate transition probability but should not be considered reliable.

Initially, the program orders the orbitals in the following way: first the orbitals for the closed shells, then the orbitals for the other shells, each in the order given by the user. Not all the orbitals need be varied. In response to a query, the user may indicate which are to be varied in a number of ways: ALL or NONE have the obvious meanings, N = an integer, say  $i$ , will vary the last  $i$  in the list. (Actually, the program searches for the '=' sign and ignores all preceding characters.) Sometimes, however, a user may wish to keep the last orbital fixed, and vary only orbitals that appear earlier in the list. In this case, a comma delimited list of electron labels (no blanks) may be given. The orbitals for the latter are then moved to the end of the list.

The SCF procedure converges most rapidly if the orbitals are improved in the order of decreasing energy, that is, those for the more tightly bound electrons should be improved first. The orbitals that are to be varied are sorted into increasing quantum numbers and, within a given quantum number, into increasing angular quantum numbers.

It should be mentioned that in identifying the position of an orbital in a list as, for example, when a user specifies a comma delimited list of electron labels, the program matches electron labels derived from the input data of closed shells and other shells. This matching must match exactly. Though for much of the code, responses can be either in lower case or capital, the user may not specify an electron label at one time in one case and then switch to a different case. Also, it should be remembered that electron labels are three characters. Thus, when only two are used (as for the closed shells), it is advised that the blank be the character at the left; this is the strategy used by the program in converting the specification of the configuration to a list of electrons.

### 3. The energy expression

The program, strictly speaking, is more general than a Hartree-Fock program. In fact, it determines the stationary wavefunction for an energy expression where

$$E = E_{av} + \sum_{nl} \sum_{n'l'} \left\{ \sum_k a_{nl, n'l'}^{(k)} F^k(nl, n'l') + \sum_k b_{nl, n'l'}^{(k)} G^k(nl, n'l') \right\}$$

and  $E_{av}$  is determined by the configuration.

The average energy is defined in terms of interactions for all electron pairs, the contribution being proportional to the number of pairs. For, say  $q$ , equivalent electrons, the number is  $q(q-1)/2$ . As long as  $q > 1$ , this quantity will always be positive, but when  $q = 1/2$ , say, the number of self-interaction "pairs" is negative. In this program the self-interaction is computed on the assumption that the non-integral occupation is a weighted average of two configurations in which the occupation differs by one, as it would in a transition state calculation. Again, the interaction between two shells, both with non-integral occupation numbers, is computed on the assumption that the configuration is a linear combination of two configurations in which the second configuration is obtained from the first by the transfer of one electron to another shell. For example  $1s(2)2s(1.5)2p(.5)$  will have an energy expression the same as the average of  $1s(2)2s(2)$  and  $1s(2)2s(1)2p(1)$ ; on the other hand,  $1s(2)2s(1.75)2p(0.25)$  will have an energy expression equal to three-quarter of the energy of  $1s(2)2s(2)$  and one-quarter of the energy of  $1s(2)2s(1)2p(1)$ . A field-width of up to four characters is permitted for the occupation number.

The deviations to the average energy depend on the term value. The latter should be specified in spectroscopic notation, say 3P for  $S = 1$ ,  $L = 1$ . In some instances seniority [5] may also be required. For example, a configuration with three d-electrons has two 2D terms, designated 2D1 and 2D3, where the last character represents seniority. Table 1 contains a list of terms and their seniority numbers for commonly occurring shells. The seniority

Table 1  
Allowed terms and their seniority for shells of equivalent electrons

Shell	Terms and their seniority (in data entry format)
s(1)	2S1
p(1)	2P1
p(2)	3P2, 1D2, 1S0
p(3)	4S3, 2D3, 2P1
d(1)	2D1
d(2)	3F2, 3P2, 1G2, 1D2, 1S0
d(3)	4F3, 4P3, 2H3, 2G3, 2F3, 2D1, 2D3, 2P3
d(4)	5D4, 3H4, 3G4, 3F2, 3F4, 3D4, 3P2, 3P4, 1I4, 1G2, 1G4, 1F4, 1D2, 1D4, 1S0, 1S4
d(5)	6S5, 4G5, 4F3, 4D5, 4P3, 2I5, 2H3, 2G3, 2G5, 2F3, 2F5, 2D1, 2D3, 2D5, 2P3, 2S5
f(1)	2F1
f(2)	3H2, 3F2, 3P2, 1I2, 1G2, 1D2, 1S0
g(1)	2G1
g(2)	3L2, 3H2, 3F2, 3P2, 1K2, 1I2, 1G2, 1D2, 1S0

number is optional if the term is unique. Terms for electrons and “holes” are equivalent. Thus, the set of possible terms for d(7) is the same as for d(3), a filled d shell containing ten (10) electrons. Given the configuration and the term, the program can deduce the deviations from the average energy in the following cases:

- i) one open s-, p- or d-shell or a singly occupied l-shell;
- ii) a single s-electron and any other single l-electron;
- iii) a single s-electron and an open p- or d-shell;
- iv) a single l-electron and an open p-shell.

Any number of closed shells may also be present. The energy of a configuration with a single electron (or hole) outside closed shells has no deviations to the average energy. In other cases the program will attempt to deduce the deviations, but if it cannot do so it will request that the data be supplied (the format will be described by the program). In the case of a single l-electron outside an open p-shell, the program may request information about the parent term, if more than one coupling scheme is possible. Thus, many of the configurations normally encountered in spectroscopy can be determined in a term-dependent

manner without additional data other than the term value. Exceptions are f-shells with 2 to 13 electrons and open d-shells with a single outer electron with  $l > 0$ .

A term value of ‘Av’ may be used to indicate an average energy calculation. This term must be used whenever fractional occupations are present.

#### 4. Input/output of functions

The radial function determined by a calculation is saved on disk, in a file which the present program calls ‘WFN.OUT’. In order to save space as well as accuracy, the file is written unformatted. The file can be renamed (or copied to) ‘WFN.INP’. When such a file exists, any function in the file for the same electron as in the present calculation will be used as an initial estimate for the radial function of that electron. In other words, at the start of an SCF calculation the program “inquires” about the existence of a file called ‘WFN.INP’. If available, information in the file is used for determining initial estimates. If functions are for a different nuclear charge  $Z$ , they will be scaled.

A summary of the calculation is written to a file called ‘HF.LOG’ along with a number of parameters and calculations selected from the menu.

The file naming conventions are system dependent. The OPEN statements in the program should be modified so that the file names agree with system requirements.

#### 5. Some examples

Most computing environments allow users to prepare command files to contain commands and also responses to prompts. Table 2 contains an example for the VAX. In this table, the text to the right of the exclamation mark (!) is a summary of the prompt associated with the response in the form of a comment – it is not data and is not included in the data deck.

Table 3 depicts an interactive session for a simple case. For brevity the HELP response is not demonstrated since it produces a fair amount of

Table 2

An example of a command file with responses to queries. Additional comments have been added for clarity, and are not part of the data

---

```

! Case 1. A standard case using defaults and computing a
! spin-orbit parameter.
$ run hf
0,3P,8.          ! ATOM,TERM,Z
  1s 2s          ! closed shells
2p(4)            ! configuration
all              ! orbitals varied
y                ! default electron parameters
y                ! default remaining parameters
y                ! additional parameters
4                ! MENU selection
  2p             ! spin-orbit parameter
6                ! exit MENU
n                ! iso-electronic sequence
!
! Case 2. The He 1s2s 1S problem with input data over-
! riding defaults and continuing up the iso-
! electronic sequence to Li+.
$ RUN hf
He,1S,2.          ! ATOM,TERM,Z
                  ! closed shells
1s(1)2s(1)        ! configuration
=2                ! orbitals varied
n                 ! default electron parameters
0,,,,            ! S(1),IND(1),METH(1),ACC(1)
0,,,,            ! S(2),IND(2),METH(2),ACC(2)
n                 ! default remaining parameters
n                 ! default for NO, STRONG
200,t             ! values for NO, STRONG
y                 ! default for PRINT, SCFTOL
y                 ! default for NSCF, IC
y                 ! default for TRACE
n                 ! additional parameters
y                 ! iso-electronic sequence
Li+ 3.0           ! ATOM,Z, (ACC(I),I=1,NWF)
y                 ! default remaining parameters
n                 ! additional parameters
n                 ! iso-electronic sequence
!
! Case 3. Core with ambiguous parent term, showing the
! evaluation of an Rk (Slater) integral.
$ RUN hf
S,3P,16.          ! ATOM,TERM,Z
  1s 2s 2p 3s     ! closed shells
3p(3)3d(1)        ! configuration
3p,3d             ! orbitals varied
y                 ! default electron parameters
2D                ! ambiguous parent term
y                 ! default remaining parameters
y                 ! additional parameters
2                 ! MENU selection
R 1( 3s, 3p; 3p, 3d) ! Slater integral
6                 ! exit MENU
n                 ! iso-electronic sequence

```

---

output. Notice that the response to most questions may be one of 'Y', 'N', or 'H' for 'Yes', 'No', or 'HELP', respectively. The responses may be either uppercase or lowercase. Once the self-consistent

field iteration has converged some parameters are displayed, but the program also permits the user to request the evaluation of a variety of additional parameters. The 'MENU' is displayed in table 3.

Table 3

An example of an interactive session with UNIT = 6 assigned to the terminal

```

! Case 1. A standard case using defaults and computing a
!           spin-orbit parameter.
!
$ run hf

=====
HARTREE-FOCK . 36
=====

THE DIMENSIONS FOR THE CURRENT VERSION ARE:
      NWF= 20      NO=220

START OF CASE
=====

Enter ATOM, TERM, Z
Examples: O, 3P, 8. or Oxygen, AV, 8.
O, 3P, 8.

List the CLOSED shells in the fields indicated (blank line if none)
... etc.
1s 2s

Enter electrons outside CLOSED shells (blank line if none)
Example: 2s(1)2p(3)
2p(4)

There are 3 orbitals as follows:
1s 2s 2p

Orbitals to be varied: ALL/NONE/=i (last i)/comma delimited list/H
all

Default electron parameters ? (Y/N/H)
y

Default values for remaining parameters? (Y/N/H)
y

WEAK ORTHOGONALIZATION DURING THE SCF CYCLE= T
SCF CONVERGENCE TOLERANCE (FUNCTIONS) = 1.00D-08
NUMBER OF POINTS IN THE MAXIMUM RANGE = 220

ITERATION NUMBER 1
-----

SCF CONVERGENCE CRITERIA (SCFTOL*SQRT(Z*NWF)) = 4.9D-08

      EL      ED      AZ      NORM      DPM
1s      46.0435196      43.5733556      0.9379554      1.63D-01
2s      4.0525312      11.3236894      1.0590813      3.57D-01
2p      2.2781257      17.0286774      0.7908316      5.83D-01
2p      0.5379463      11.3024487      9.5349310      3.81D-01
2p      1.5000736      13.5459804      1.5216043      1.76D-01

< 1s| 2s>= 1.4D-02

LEAST SELF-CONSISTENT FUNCTION IS 2s :WEIGHTED MAXIMUM CHANGE = 5.05D-01

```

Table 3 (continued)

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ITERATION NUMBER 2				
-----				
SCF CONVERGENCE CRITERIA (SCFTOL*SQRT(Z*NWF)) = 9.8D-08				
EL	ED	AZ	NORM	DPM
1s	41.2725155	43.1398593	1.0201570	1.62D-02
2s	2.5318731	9.9077768	1.1201016	1.07D-01
2p	1.3928113	14.5691471	1.0128710	6.42D-02
2s	2.4849893	9.7685569	1.0043315	6.38D-03
2p	1.2649134	14.6117438	1.0013086	8.72D-03
< 1s  2s>=-2.4D-04				
LEAST SELF-CONSISTENT FUNCTION IS 1s :WEIGHTED MAXIMUM CHANGE = 2.29D-02				
ITERATION NUMBER 3				
-----				
SCF CONVERGENCE CRITERIA (SCFTOL*SQRT(Z*NWF)) = 2.0D-07				
EL	ED	AZ	NORM	DPM
1s	41.3415035	43.1558699	0.9998800	4.91D-04
2s	2.4906623	9.7931425	0.9995464	7.03D-04
2p	1.2649904	14.6353888	0.9997630	2.26D-03
2p	1.2637762	14.6379892	1.0000058	3.51D-04
2s	2.4888866	9.7899989	1.0000882	1.58D-04
< 1s  2s>=-9.9D-06				
LEAST SELF-CONSISTENT FUNCTION IS 2p :WEIGHTED MAXIMUM CHANGE = 7.01D-04				
ITERATION NUMBER 4				
-----				
SCF CONVERGENCE CRITERIA (SCFTOL*SQRT(Z*NWF)) = 3.9D-07				
EL	ED	AZ	NORM	DPM
1s	41.3373611	43.1551573	0.9999982	2.37D-05
2s	2.4887265	9.7905851	0.9999954	1.52D-05
2p	1.2638884	14.6399062	0.9999793	1.47D-04
2p	1.2638181	14.6402784	0.9999979	3.90D-05
2p	1.2638144	14.6405072	0.9999987	1.82D-05
< 1s  2s>= 1.3D-06				
LEAST SELF-CONSISTENT FUNCTION IS 2p :WEIGHTED MAXIMUM CHANGE = 3.65D-05				

---

It would be a relatively simple matter to extend the menu to other properties. The more frequently used parameters are included – arbitrary moments, Slater and magnetic integrals, spin-orbit parameters, electron density at the nucleus, etc. and transition integrals.

Unfortunately, the default values do not always guarantee convergence. The most troublesome simple case is  $1s2s\ ^1S$  for helium. At least one of several non-default options is needed to get this case to converge – the same effective nuclear charge for generating initial estimates, a strong

Table 3 (continued)

---

 ITERATION NUMBER 5
 

---

SCF CONVERGENCE CRITERIA (SCFTOL\*SQRT(Z\*NWF)) = 7.8D-07

EL	ED	AZ	NORM	DPM
1s	41.3373116	43.1551785	1.0000000	6.99D-07
2s	2.4886315	9.7904928	1.0000014	4.35D-06
2p	1.2638161	14.6406220	0.9999989	6.71D-06
2p	1.2638124	14.6406411	1.0000000	1.57D-06
2s	2.4886294	9.7904942	1.0000000	1.91D-07

&lt; 1s| 2s&gt;= 3.4D-08

LEAST SELF-CONSISTENT FUNCTION IS 2p :WEIGHTED MAXIMUM CHANGE = 3.13D-06

---

 ITERATION NUMBER 5
 

---

SCF CONVERGENCE CRITERIA (SCFTOL\*SQRT(Z\*NWF)) = 1.6D-06

EL	ED	AZ	NORM	DPM
1s	41.3373143	43.1551771	1.0000000	4.89D-08
2s	2.4886295	9.7904939	1.0000000	5.32D-08
2p	1.2638126	14.6406530	0.9999999	7.21D-07

&lt; 1s| 2s&gt;= 8.3D-09

LEAST SELF-CONSISTENT FUNCTION IS 2p :WEIGHTED MAXIMUM CHANGE = 1.44D-06

---

 ITERATION NUMBER 7
 

---

SCF CONVERGENCE CRITERIA (SCFTOL\*SQRT(Z\*NWF)) = 3.1D-06

EL	ED	AZ	NORM	DPM
1s	41.3373140	43.1551771	1.0000000	6.56D-10
2s	2.4886293	9.7904937	1.0000000	1.20D-08
2p	1.2638124	14.6406577	1.0000000	2.37D-07

&lt; 1s| 2s&gt;= 4.8D-09

TOTAL ENERGY (a.u.)

Non-Relativistic	-74.80939845	Potential	74.80939821
Relativistic Shift	-0.04890388	Kinetic	-149.61879666
Relativistic	-74.85830233	Ratio	-2.000000003

Additional parameters ? (Y/N/H)

y

orthogonality requirement so that functions are orthogonal at every stage, and setting IC = 0 so that, after both 1s and 2s are improved, radial

functions are rotated to satisfy a stationary energy requirement. Though convergence can be obtained, it should be mentioned that the Hartree-



Table 3 (continued)

---

```

      These various functions are available:

        1 - EXPECTATION VALUES OF R**K
        2 - SLATER OR MAGNETIC INTEGRALS
        3 - ELECTRON DENSITY AT THE NUCLEUS
        4 - SPIN-ORBIT PARAMETER
        5 - TRANSITION INTEGRALS
        6 - EXIT TO MAIN PROGRAM

      Input number corresponding to your selection:
4
      INPUT IDENTIFYING LABEL FOR ELECTRON: Example
2p          FORMAT(1X,A3)
2p

      SPIN-ORBIT PARAMETER FOR 2p =  6.7673298D-04 a.u.
                                   148.525 cm-1

      These various functions are available:

        1 - EXPECTATION VALUES OF R**K
        2 - SLATER OR MAGNETIC INTEGRALS
        3 - ELECTRON DENSITY AT THE NUCLEUS
        4 - SPIN-ORBIT PARAMETER
        5 - TRANSITION INTEGRALS
        6 - EXIT TO MAIN PROGRAM

      Input number corresponding to your selection:
6

      Do you wish to continue along the sequence ?
n

      END OF CASE
      =====

      FORTRAN STOP
      CFF          job terminated at  3-AUG-1986 15:13:07.14

      Accounting information:
      Buffered I/O count:      40      Peak working set size:  757
      Direct I/O count:       59      Peak page file size:   1052
      Page faults:           547      Mounted volumes:       0
      Charged CPU time:      0 00:00:12.83  Elapsed time:      0 00:00:28.64

```

---

Fock energy is not an upperbound (Brillouin's theorem is not satisfied) in this case. Similar convergence problems can be anticipated for any  $(nl)^q(n'l)^q$  configuration, when two open shells of the same symmetry have the same occupation number, and similar techniques may be needed to achieve convergence.

Node counting can be another problem. In the He 1s2s <sup>1</sup>S problem, the 1s orbital acquires on extra node [5] which should be ignored for node

counting purposes. The routine, NODEC, searches for  $DPM = \max |\bar{P}(r_i)|$  where  $\bar{P}(r) = P(r)/\sqrt{r}$ . Any local maximum of  $|\bar{P}(r_i)| \leq 0.05DPM$  is ignored. The coefficient of 0.05 is appropriate for the helium problem, but cases involving d orbitals have been found where this coefficient had to be reduced to 0.02. The TRACE option, if turned on, provides information about the diagonal energy parameter and the associated node count. If insurmountable difficulties are encountered, this coef-

ficient could be changed. Use of `Meth(I) = 3` avoids all node counting but may result in convergence to an undesired solution.

A recent review of SCF theory and algorithms has been published [7].

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**TEST RUN OUTPUT****A listing of the output file, HF.LOG**

HARTREE-FOCK WAVE FUNCTIONS FOR O 3P Z = 8.0

Core = 1s( 2) 2s( 2)  
 Configuration = 2p( 4)

## INPUT DATA

	WAVE FUNCTION	PROCEDURE
	NL SIGMA METH ACC OPT	
1	1s 1 0 1.0 1 0.0 0	
2	2s 2 0 3.0 1 0.0 0	
3	2p 2 1 5.5 1 0.0 0	

## INITIAL ESTIMATES

NL	SIGMA	E(NL)	AZ(NL)	FUNCTIONS
1s	1.00	0.000	39.686	SCREENED HYDROGENIC
2s	3.00	0.000	10.277	SCREENED HYDROGENIC
2p	5.50	0.000	8.896	SCREENED HYDROGENIC

NUMBER OF FUNCTIONS ITERATED = 3  
 MAXIMUM WEIGHTED CHANGE IN FUNCTIONS = 0.47D-06

	ATOM O		TERM 3P			
nl	E(nl)	I(nl)	KE(nl)	Rel(nl)	S(nl)	Az(nl)
1s	41.3373140	-31.924159	29.213212	-0.022340	0.447	43.155177
2s	2.4886293	-7.013941	3.108231	-0.002552	2.746	9.790493
2p	1.2638124	-6.347258	2.541628	-0.000629	3.942	14.640658

  

nl	Delta(R)	1/R**3	1/R	R	R**2
1s	148.203	0.0000	7.64217	0.19859	0.05315
2s	7.628	0.0000	1.26527	1.14196	1.58122
2p	0.000	4.9741	1.11111	1.23220	1.97498

## TOTAL ENERGY (a.u.)

Non-Relativistic	-74.80939845	Potential	74.80939821
Relativistic Shift	-0.04890388	Kinetic	-149.61879666
Relativistic	-74.85830233	Ratio	-2.000000003

SPIN-ORBIT PARAMETER FOR 2p = 6.7673298D-04 a.u.  
 148.525 cm<sup>-1</sup>