
A practical guide to ATSP2K

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Contents

Chapter 1

The ATSP2K package

1.1 Application programs and tools

The new version of the ATSP2K package [1] consists of a number of application programs and tools. The application programs and tools, along with the underlying theory, are described in the original write-ups [2-13]. See also the book Computational Atomic Structure by Froese Fischer, Brage, and Jönsson [14].

Below is a partial list of programs in the package:

1. Routines that generate a configuration state list (CSL):
 - (a) **genc1** – generate a configuration state list (CSL) from lists of reference configurations
 - (b) **lsgen** – generate a CSL using rules
 - (c) **lsreduce** – include only CSFs that have at least one non-zero matrix element with a CSF of a reference list
2. **nonh** – compute angular coefficients
3. **nonhz** – compute angular coefficients assuming a partition of the configuration state list into zero- and first order spaces (optional)
4. **mchf** – determine orbitals and mixing coefficients
5. **mchf_C** – determine orbitals and mixing coefficients, assuming **c.lst** on disc (medium size calculations, to be used ONLY if ordinary **mchf** fails on current operating system)
6. **mchf_HC** – determine orbitals and mixing coefficients, assuming **c.lst** and **hmx.lst** (large size calculations, to be used ONLY if ordinary **mchf** fails on current operating system)
7. **bpic** – perform Breit-Pauli CI calculation, where matrix elements computed on the fly
8. **bp_ang** + **bp_mat** + **bp_eiv** – perform Breit-Pauli CI calculation, by separating angular integration and save on disc, the construct matrix and diagonalize (fine eigenvalues). Suitable in smaller cases for an iso-electronic sequence.
9. Routines for computing transition probabilities:
 - (a) **trans** – perform transition calculations in a single orthonormal basis
 - (b) **biotr** – perform biorthogonal transformation and subsequent transition calculation between states.
10. **hfs** – compute hyperfine interactions

A number of generally short programs have been developed as tools to facilitate a computational procedure.

1. **comp**: Given the **name** of a set of files, and a tolerance, this program displays the composition of each state in the file by listing the CSFs and their expansion coefficients in order of decreasing magnitude provided the magnitude is greater than the tolerance. The **name.c** option usually may not apply (seen **condens** below). This composition information may be of importance in determining the multi-reference set or the extent of correlation. It is also essential for resolving naming conflicts.
2. **condens**: Given the **name** of a case, the source for the expansion coefficients (usually .l or .j) and whether results are to be sorted, the program produces a file **cfg.out** that includes only those CSFs for which $\sqrt{\sum_i c_i^2} \geq T$, where T is the cut-off tolerance. Since **mchf** no longer produces a **cfg.out** with the expansion coefficients included, the **name.c** option cannot usually be applied. The coefficients are included in the condensed output file, **cfg.out**. To restore this file to the present .c format (without expansion coefficients), move the file to **clist.inp** and run **lsgen** selecting the “r” mode (for restore). Note that condensing may destroy the “closed under de-excitation” requirement of **biotr** but when the tolerance is sufficiently small, no problems have been encountered. In a systematic method, where maximum principal quantum number is increased by unity from one iteration to the next, it is unlikely that a CSF with a high n will remain and the equivalent CSF with a lower n be deleted.
3. **tables**: This is a program written in C++ that takes a **name.lsj** file, usually a concatenated file of all the .lsj transition files for a given atom or ion, and finds the energy level structure of the levels and the multiplet transition arrays. The tables posted at the web-site <http://atoms.vuse.vanderbilt.edu> are examples of tables produced by the **tables** program. When an energy level is present in the .lsj file with **two** different energies, the higher level is considered to be unphysical. It and all data associated with this level are removed from the table. The user may also specify certain levels as “unphysical” in which case they will be removed. Finally, the program computes the lifetimes of the levels from the transition data provided in the file.
4. **T_dependence**: Given a .c and a corresponding .j file, this program displays the term dependence of each state included in the file [?]. This gives an indication of LS term mixing in the wave function of a state. The Breit-Pauli programs all assign labels to states according to the largest expansion coefficient. When this process produces the same label for two different states a careful analysis is needed. The LS value should be that term with the largest composition and within that LS , the largest expansion coefficient identifies the label. For more on labeling, see [?].
5. **relabel** This utility reads radial functions in turn from **wfn.inp**. For each function, the user may enter either a blank, “d”, or a new 3-character label for which the respective action is to write the radial function unchanged into **wfn.out**, skip (or delete) the radial function, write the radial function changing the displayed label to the entered label.
6. **select** This routine selects those CSFs from a designated list that contain orbitals specified by the user. This may be useful when expansions that have been condensed are extended with new CSFs to be included to first-order. The selected CSFs may be appended to the condensed list.
7. **w_format** and **w_unformat**: Binary file formats are not always compatible in going from one system environment to another. **w_format** takes a **wfn.inp** file (in .w format) and produces a formatted **wfn.fmt** file. The program **w_unformat** reads **wfn.fmt** and produces the binary file (in .w format) **wfn.out**. Some loss of accuracy can be expected in the process but the radial functions are tabulated to 11-digits of accuracy.

References

1. ATSP2K: C. Froese Fischer, G. Tachiev, G. Gaigalas, M.R. Godefroid *Comput. Phys. Commun.* 176 559 (2007)
2. MCHF_LIBRARIES: C.Froese Fischer, *Comput. Phys. Commun.* 64 399 (1991)
3. MCHF_GENCL: C. Froese Fischer, B. Liu, *Comput. Phys. Commun.* 64 406 (1991)
4. MCHF_NONH: A. Hibbert, C. Froese Fischer, *Comput. Phys. Commun.* 64 417 (1991)
5. MCHF_88: C. Froese Fischer, *Comput. Phys. Commun.* 64 431 (1991)
6. MCHF_BREIT: A. Hibbert, R. Glass, C. Froese Fischer *Comput. Phys. Commun.* 64 455 (1991)
7. MCHF_CI: C. Froese Fischer, *Comput. Phys. Commun.* 64 473 (1991)
8. MCHF_MLTPOL: C. Froese Fischer, M.R. Godefroid, A. Hibbert, *Comput. Phys. Commun.* 64 486 (1991)
9. MCHF_LSTR AND MCHF_LSJTR: C.Froese Fischer, M.R. Godefroid, *Comput. Phys. Commun.* 64 501 (1991)
10. MCHF_AUTO: C.Froese Fischer, T. Brage, *Comput. Phys. Commun.* 74 381 (1993)
11. MCHF_HFS: P. Jönsson, C.-G. Wahlstrom, C.Froese Fischer, *Comput. Phys. Commun.* 74 399 (1993)
12. MCHF_ISOTOPE: C. Froese Fischer, L. Smentek-Mielczarek, N. Vaeck, G. Miecnik, *Comput. Phys. Commun.* 74 415 (1993)
13. MCHF_LSGEN: L. Sturesson and C. Froese Fischer, *Comput. Phys. Commun.* 74 432 (1993)
14. C. Froese Fischer, T. Brage, P. Jönsson, *Computational Atomic Structure - an MCHF approach*, IoP, (1997)

1.2 File naming conventions, program and data flow

Passing of information between different programs is done through files. This process is greatly facilitated through file naming conventions. A name is associated with the results and an extension that defines the contents and format of the file. Thus the file name becomes **name.extension**. Common extensions are listed in Table 1.1.

To run ATSP2K a number of programs need to be run in a pre-determined sequence. Figure 1.1 displays a typical sequence of block version program calls to evaluate different expectation values. The resulting flow of files is displayed in Figure 1.2.

Table 1.1: Table of common extensions.

<i>extension</i>	<i>data in the file</i>
.c	configuration state function (CSF) expansion
.w	radial wave functions (numerical values in binary form)
.l	expansion coefficients from a non-relativistic (LS) calculation
.j	expansion coefficients from a Breit-Pauli (LSJ) calculation
.h	hyperfine data
.t	term dependence of a .j file
.ls	transition probability data a non-relativistic (LS) calculation
.lsj	transition probability data a Breit-Pauli (LSJ) calculation

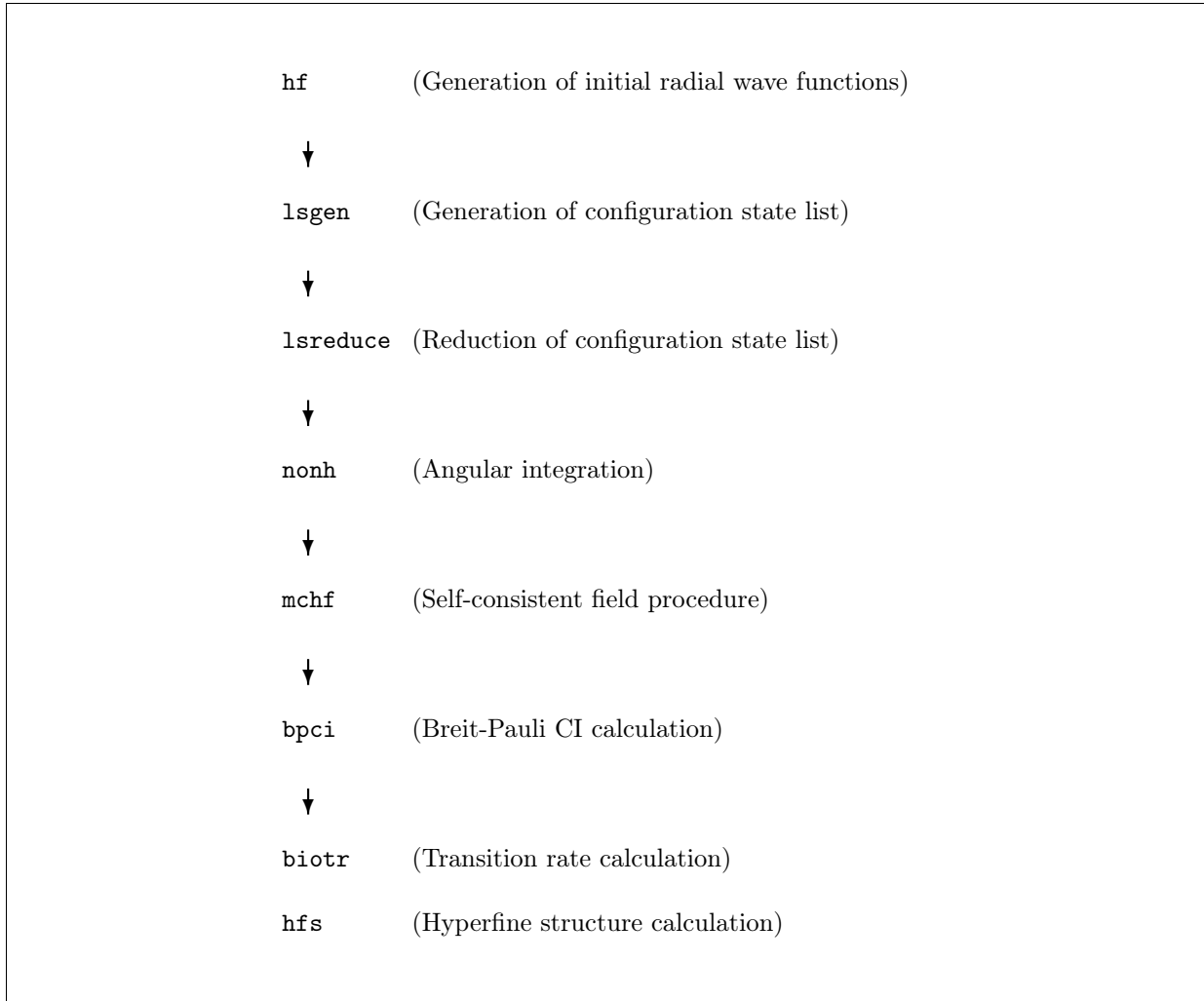


Figure 1.1: Typical sequence of block version program calls to evaluate different expectation values such as transition rates and hyperfine structure constants.

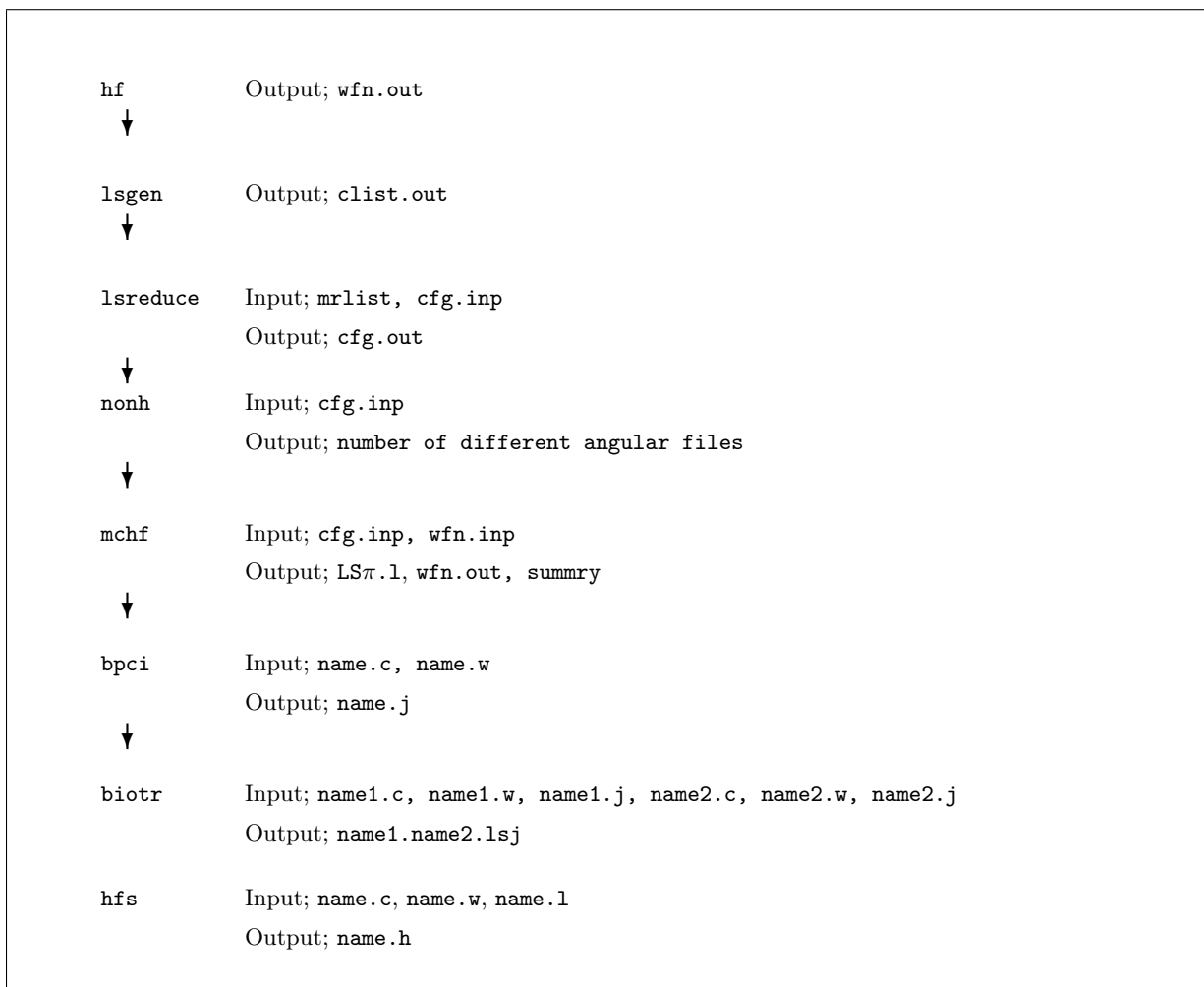


Figure 1.2: Flow of files for a normal sequence of program runs.

1.3 Generating lists of configuration state functions

Exploring different correlation models and generating lists of configuration state functions (CSFs) is a major task of the computation. The ATSP2K provides several programs for performing this task. For generating small lists of CSFs it is often best to use the **genc1** program. To generate expansion based on the notion of excitations from subshells to an active set of orbitals it is often advantageous to use the **lsgen** program. Different restrictions can be put on the excitations and it is possible to describe core-valence correlation where at most one excitation is allowed from subshells of the core. To make sure that the generated CSFs interacts with the CSFs in multireference the program **lsreduce** should be used. Before continuing the reader is advised to study the write-up of the **lsreduce** program [L. Sturesson and C. Froese Fischer, Comput. Phys. Commun. 74, 432 (1993)].

1.4 Spectroscopic orbitals

The “spectroscopic orbitals” are those where node counting is required to ensure that the self-consistent field procedure converges to the desired solution [C. Froese Fischer, T. Brage, P. Jönsson, Computational Atomic Structure - an MCHF approach, IoP, 1997]. Spectroscopic orbitals build the reference CSFs and often have occupation numbers near unity or more. All other orbitals are “correlation orbitals”. If the self-consistent field procedure fails for spectroscopic orbitals, i.e. the wrong number of nodes are obtained with a subsequent program halt.

Chapter 2

Running the application programs

In this chapter we demonstrate the use of the application programs of ATSP2K in three cases described below. The use of the tools of the ATSP2K package is described in the next chapter. The data written to the output files are explained and discussed in chapter 4.

2.1 First example: $1s^22s\ ^2S$ and $1s^22p\ ^2P$ in Li I

The first example is for $1s^22s\ ^2S_{1/2}$ and $1s^22p\ ^2P_{1/2,3/2}$ in Li.

Overview

1. Perform HF calculation for $1s^22s\ ^2S$.
2. Generate $n = 3$ CAS configuration list for $1s^22s\ ^2S$.
3. Perform angular integration.
4. Perform self-consistent field calculation.
5. Save output to 2S_CAS_3.
6. Calculate hfs.
7. Generate $n = 3$ CAS Breit configuration list for $1s^22s\ ^2S_{1/2}$.
8. Perform CI Breit-Pauli calculation
9. Perform HF calculation for $1s^22p\ ^2P$.
10. Generate $n = 3$ CAS configuration list for $1s^22p\ ^2P$.
11. Perform angular integration.
12. Perform self-consistent field calculation.
13. Save output to 2P_CAS_3.
14. Calculate hfs.
15. Generate $n = 3$ CAS Breit configuration list for $1s^22p\ ^2P_{1/2,3/2}$.
16. Perform CI Breit-Pauli calculation
17. Compute the transition rates from the CI wave functions.

Program input

In the test-runs input is marked by >> and >>3, for example, indicate that the user should input 3 and then strike the return key. When >> is followed by blanks just strike the return key.

```
*****
*          RUN HF FOR 1s(2)2s 2S          *
*          OUTPUT FILE: wfn.out, hf.log    *
*****
```

>>HF

```
=====
H A R T R E E - F O C K . 96
=====
```

```
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.
>>Li,2S,3.
```

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

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

```
There are 2 orbitals as follows:
1s 2s
```

```
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
```

```
.....
```

ITERATION NUMBER 7

```

-----

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

C( 1s 2s) = 0.00000 V( 1s 2s) = -2.19991 EPS = 0.000000
E( 2s 1s) = 0.00573 E( 1s 2s) = 0.00286

          EL          ED          AZ          NORM          DPM
        1s      4.9554830      9.2603703      1.0000000      1.43D-08
        2s      0.3926457      1.4468006      0.9999999      1.28D-08

< 1s| 2s>= 8.7D-09

TOTAL ENERGY (a.u.)
-----
Non-Relativistic      -7.43272693      Kinetic      7.43272693
Relativistic Shift    -0.00054376      Potential    -14.86545385
Relativistic          -7.43327069      Ratio        -2.000000000

Additional parameters ? (Y/N/H)
>>n

Do you wish to continue along the sequence ?
>>n

END OF CASE
=====

*****
*          COPY FILES                                     *
*          Keep a copy of the wfn.out in 2SeDF.w file for reference      *
*          Keep a copy of hf.log in 2SDF.log                             *
*****

cp wfn.out wfn.inp
cp wfn.out 2SeDF.w
cp hf.log 2SDF.log

*****
*          RUN LSGEN TO GENERATE N = 3 CAS CONFIGURATION LIST FOR 2S      *
*          OUTPUT FILES: clist.out, clist.log                             *
*****

New list, add to existing list, expand existing list, optimized sorting, restored order or quit? (*)
>>
Breit or MCHF? (B/*)
>>
Default, symmetry or user specified ordering? (*s/u)
>>
Highest principal quantum number, n? (1..15)
>>3

```

```

Highest orbital angular momentum, l? (s..d)
>>d
Are all these nl-subshells active? (n/*)
>>
Limitations on population of n-subshells? (y/*)
>>
Highest n-number in reference configuration? (1..3)
>>2
Number of electrons in 1s? (0..2)
>>2
Number of electrons in 2s? (0..2)
>>1
Number of electrons in 2p? (0..6)
>>0
Resulting term? (1S, 3P, etc.)
>>2S
Number of excitations = ? (0..3)
>>3
27 configuration states have been generated.
Generate a second list? (y/*)
>>
27 configuration states in the final list.
The generated file is called clist.out.
FORTRAN STOP

```

```

*****
*          COPY FILES          *
*      IT IS ADVISABLE TO SAVE THE LSGEN LOG-FILE TO HAVE A RECORD ON      *
*      HOW THE CONFIGURATION LISTS GENERATION WAS DONE                     *
*****

```

```

>>cp clist.log 2SeCAS3.log
>>cp clist.out cfg.inp

```

```

*****
*      RUN NONH TO GENERATE ENERGY EXPRESSION                            *
*      INPUT FILES: cfg.inp                                                *
*      OUTPUT FILES: cfg.h, yint.lst, c.lst, ih.=n.lst                    *
*****

```

```

>>nonh

```

```

input file is cfg.inp ...

```

```

=====
N O N H      2000
=====

```

THERE ARE 6 ORBITALS AS FOLLOWS:

1s 2s 2p 3s 3p 3d

THERE ARE 0 CLOSED SUBSHELLS COMMON TO ALL CONFIGURATIONS AS FOLLOWS:

Allocating space for 214 integrals
 processing 2Se with 27 configurations
 277 non-zero matrix elements
 92 NF 76 NG 446 NR 109 NL
 723 Total number of integrals

end-of-file clist!!!

```
*****
*      RUN MCHF TO OBTAIN SELF CONSISTENT SOLUTIONS      *
*      INPUT FILES: wfn.inp (optional), cfg.inp, angular files *
*      OUTPUT FILES: wfn.out, 2Se.l, summry              *
*                                                         *
*      NOTE1: Mixing coefficients written to a file named by LS-symmetry *
*      and parity, in this case 2Se.l                    *
*                                                         *
*      NOTE2: We force the program to iterate to higher precision than *
*      default which is a good thing for small calculations *
*****
```

>>mchf

```
=====
          M C H F   ... 2000
=====
```

THE DIMENSIONS FOR THE CURRENT VERSION ARE:
 NWD= 60 NO=220 Lagrange Multipliers=800

START OF CASE
 =====

ATOM, Z in FORMAT(A, F) :
 >>Li,3.
 cfg.inp has configurations for 1 terms

Enter eigenvalues and weights: one line per term, eigenvalues with weights
 in parenthesis and separated by commas, default is 1.0
 2Se
 >>1

There are 6 orbitals as follows:
 1s 2s 2p 3s 3p 3d

Enter orbitals to be varied: (ALL,NONE,SOME,NIT=,comma delimited list)

>>all

Enter those that are spectroscopic

>>1s,2s

Default electron parameters ? (Y/N)

>>y

Default values for other parameters? (Y/N)

>>n

Default values (NO,REL,STRONG) ? (Y/N)

>>y

Li 3. 220 6 6 0 F

Default values for PRINT, CFGTOL, SCFTOL ? (Y/N)

>>n

Input free FORMAT(L, F, F)

>>.f.,1.e-50,1.e-50

Default values for NSCF, IC ? (Y/N)

>>n

Input free FORMAT(I, I)

>>300,0

Default values for ACFG,LD,TRACE? (Y/N)

>>y

.....

ITERATION NUMBER 111

CONVERGENCE CRITERIA:ENERGY (CFGTOL) = 1.0D-50
 :FUNCTION(SCFTOL*SQRT(Z*NWF))= 4.2D-50

E(2s 1s) =	0.02212	E(1s 2s) =	0.01109
E(3s 1s) =	28.98616	E(1s 3s) =	0.03558
E(3s 2s) =	4.20140	E(2s 3s) =	0.01028
E(3p 2p) =	51.03003	E(2p 3p) =	5.25729

	EL	ED	AZ	NORM	DPM
< 1s 2s>=	4.2D-11				
< 1s 3s>=	-4.5D-10				
1s		5.0342669	9.2695740	1.0000000	5.17D-10
< 2s 3s>=	-7.3D-09				
< 1s 2s>=	1.0D-08				
2s		0.3956318	1.4529828	1.0000000	1.41D-08
< 2p 3p>=	6.0D-09				
2p		15.9592124	4.7810460	1.0000000**	9.70D-09
< 1s 3s>=	-4.4D-07				
< 2s 3s>=	-5.6D-08				
3s		16.2077493	14.8282834	1.0000000**	5.32D-07

```

< 2p| 3p>=-6.7D-09
          3p      30.8279905      66.8115267      1.0000000** 2.45D-08
          3d      35.1829408      88.8117857      1.0000000** 2.94D-10

      ETOTAL=      -7.47318427      Loops,DeltaE,Res.: 2 3.955D-16 7.343D-09
1 0.9984151      2 0.0004030      3 0.0002912      4 -0.0024959
5 0.0016210      6 -0.0009009      7 0.0029624      8 -0.0015623

      Sum of ETOTAL :      -7.47318427
DeltaE = 1.77635683940025046E-015 Sum_Energy = -7.4731842652568732

ENERGY (a.u.)
-----
      Total      -7.473184265
      Potential  -14.946368479
      Kinetic     7.473184213
      Ratio       2.000000007

*****
*      SAVE OUTPUT FILES      *
*****

>>cp wfn.out 2SeCAS3.w
>>cp cfg.inp 2SeCAS3.c
>>cp 2Se.l 2SeCAS3.l
>>cp summry 2SeCAS3.s

*****
*      RUN HFS TO COMPUTE HYPERFINE INTERACTION CONSTANTS      *
*      INPUT FILES: 2SeCAS3.c, 2SeCAS3.w, 2SeCAS3.l      *
*      OUTPUT FILES: 2SeCAS3.h      *
*      *      *      *      *      *      *      *      *      *      *
*      NOTE1: THE OPTION MCHF IS OBSOLETE AND ADERES TO THE OLD OUTPUT      *
*      FORMAT OF MCHF. NOW YOU NEED ALWAYS ASK FOR INPUT FROM A CI      *
*      CALCULATION.      *
*      *      *      *      *      *      *      *      *      *      *
*      NOTE2: THE HFS PROGRAM ONLY COMPUTES THE HYPERFINE INTERACTION      *
*      FROM ONE STATE AND YOU HAVE TO SPECIFY THE POSITION OF THE LEADING      *
*      CSF OF THIS STATE. AT SOME POINT SOMEONE SHOULD RECODE THE MODULE      *
*****

Name of state ...
>>2SeCAS3

Hyperfine structure calculation

Electron density at the nucleus ? (Y/N)
>>y
Indicate the type of calculation
0 => diagonal A and B factors only;
1 => diagonal and off-diagonal A and B factors;
>>0
Input from an MCHF (M) or CI (C) calculation ?

```

```
>>C
  Is the CI calculation J dependant ? (Y/N)
>>n
  Give the index of the dominant cfg in the CI
  expansion for which the hfs is to be calculated ?
>>1
  Give 2*I and nuclear dipole and quadrupole moments (in n.m. and barns)
>>2,1,1
```

The configuration set

STATE (WITH 27 CONFIGURATIONS):

THERE ARE 6 ORBITALS AS FOLLOWS:

1s 2s 2p 3s 3p 3d

THERE ARE 0 CLOSED SUBSHELLS COMMON TO ALL CONFIGURATIONS AS FOLLOWS:

.....

```
ja =      10
ja =      20
PER TEST
```

END OF CASE

=====

Total CPU time was 0.000 minutes

```
*****
*      RUN LSGEN TO GENERATE N = 3 CAS BREIT CONFIGURATION LIST FOR 2S      *
*      OUTPUT FILES: clist.out, clist.log                                   *
*****
```

```
New list, add to existing list, expand existing list, optimized sorting, restored order or quit? (*)
>>
Breit or MCHF? (B/*)
>>B
Default, symmetry or user specified ordering? (*s/u)
>>
Highest principal quantum number, n? (1..15)
>>3
Highest orbital angular momentum, l? (s..d)
>>d
Are all these nl-subshells active? (n/*)
>>
```

```

Limitations on population of n-subshells? (y/*)
>>
Highest n-number in reference configuration? (1..3)
>>2
Number of electrons in 1s? (0..2)
>>2
Number of electrons in 2s? (0..2)
>>1
Number of electrons in 2p? (0..6)
>>0
Maximum 2*J-value? (0..)
>>1
Minimum 2*J-value? (0..1)
>>1
Maximum (2*S+1)-value? (1..9)
>>9
Minimum (2*S+1)-value? (1..9)
>>1
Maximum resulting angular momentum? (S..N/N=*)
>>
Minimum resulting angular momentum? (S..N/S=*)
>>
Number of excitations = ? (0..3)
>>3
79 configuration states have been generated.
Generate a second list? (y/*)
>>
79 configuration states in the final list.
The generated file is called clist.out.
FORTRAN STOP

```

```

*****
*          COPY FILES          *
*      IT IS ADVISABLE TO SAVE THE LSGEN LOG-FILE TO HAVE A RECORD ON      *
*      HOW THE CONFIGURATION LISTS GENERATION WAS DONE                     *
*****

```

```

>>cp clist.log 2SeCAS3BREIT.log
>>cp clist.out 2SeCAS3BREIT.c

```

```

*****
*          COPY WAVE FUNCTION FILES TO PREPARE FOR THE BREIT-PAULI RUN      *
*****

```

```

>>cp 2SeCAS3.w 2SeCAS3BREIT.w

```

```

*****
*          RUN CI BREIT-PAULI          *
*      INPUT FILES: 2SeCAS3BREIT.c, 2SeCAS3BREIT.w          *
*      OUTPUT FILES: 2SeCASBREIT.j          *
*****

```

```

>>bpci
Enter ATOM, relativistic (Y/N) with mass correction (Y/N)

```

```
>>2SeCAS3BREIT,y,n
  Restarting (Y/y) ?
>>n
  Use existing Matrix and <atom>.l/j initial guess (Y/y)?
>>n

  Enter Maximum and minimum values of 2*J
>>1,1

  Enter eigenvalues: one line per term, eigenvalues separated by commas
2*J = 1
>>1
```

```
=====
  B R E I T - P A U L I
=====
```

```
Indicate the type of calculation
0 => non-relativistic Hamiltonian only;
1 => one or more relativistic operators only;
2 => non-relativistic operators and selected relativistic:
>>2
  All relativistic operators ? (Y/N)
>>y
```

```
THE TYPE OF CALCULATION IS DEFINED BY THE FOLLOWING PARAMETERS -
BREIT-PAULI OPERATORS          IREL   = 2
PHASE CONVENTION PARAMETER     ICSTAS = 1
```

```
-----
THE CONFIGURATION SET
-----
```

```
STATE (WITH 79 CONFIGURATIONS):
-----
```

```
THERE ARE 6 ORBITALS AS FOLLOWS:
```

```
1s 2s 2p 3s 3p 3d
```

```
THERE ARE 0 CLOSED SUBSHELLS COMMON TO ALL CONFIGURATIONS AS FOLLOWS:
```

```
All Interactions? (Y/N):
>>y
```

```
Default Rydberg constant (y/n)
>>y
```

.....

```

Allocating space for          783  integrals
Alcmat allocations for idisk=          0 nze =          659
J =          1          1
Entering LSJMAT with 2J =          1  NUME =          1
LSJMAT with idisk=          0 Nze =          2636

```

Summary of Davidson Performance

```

=====
Number of Iterations:          10
Shifted Eigval's:  -0.2830587230149465
Delta Lambda:      3.3306690738754696E-016
Residuals:         7.8543171982727995E-009

```

```

      1 Eigenvalues found
Finished with Davidson
Leaving LSJMAT
onlydvd  F
ILS =          0
Finished with the file

```

\begin{verbatim}

```

*****
*          RUN HF FOR 1s(2)2p 2P          *
*          OUTPUT FILE: wfn.out, hf.log    *
*****

```

>>HF

```

=====
H A R T R E E - F O C K . 96
=====

```

THE DIMENSIONS FOR THE CURRENT VERSION ARE:

NWF= 20 NO=220

START OF CASE

=====

```

Enter ATOM,TERM,Z
Examples: 0,3P,8. or Oxygen,AV,8.
>>Li,2P,3.

```

List the CLOSED shells in the fields indicated (blank line if none)

```

... .. etc.
>>1s

```

Enter electrons outside CLOSED shells (blank line if none)

Example: 2s(1)2p(3)

>>2p(1)

There are 2 orbitals as follows:

1s 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

.....

ITERATION NUMBER 5

SCF CONVERGENCE CRITERIA (SCFTOL*SQRT(Z*NWF)) = 3.9D-07

EL	ED	AZ	NORM	DPM
1s	5.0614517	9.2618326	0.9999999	2.29D-08
2p	0.2573450	0.4261374	1.0000000	9.86D-09

TOTAL ENERGY (a.u.)

Non-Relativistic	-7.36506966	Kinetic	7.36506968
Relativistic Shift	-0.00053279	Potential	-14.73013934
Relativistic	-7.36560245	Ratio	-1.999999997

Additional parameters ? (Y/N/H)

>>n

Do you wish to continue along the sequence ?

>>n

END OF CASE

=====

```

*****
*          COPY FILES          *
*    Keep a copy of the wfn.out in 2PoDF.w file for reference    *
*    Keep a copy of hf.log in 2PoDF.log                          *
*****

```



```
cp wfn.out wfn.inp
cp wfn.out 2PoDF.w
cp hf.log 2PoDF.log
```

```
*****
*          RUN LSGEN TO GENERATE N = 3 CAS CONFIGURATION LIST FOR 2P          *
*          OUTPUT FILES: clist.out, clist.log                                *
*****
```

```
New list, add to existing list, expand existing list, optimized sorting, restored order or quit? (*)
>>
Breit or MCHF? (B/*)
>>
Default, symmetry or user specified ordering? (*s/u)
>>
Highest principal quantum number, n? (1..15)
>>3
Highest orbital angular momentum, l? (s..d)
>>d
Are all these nl-subshells active? (n/*)
>>
Limitations on population of n-subshells? (y/*)
>>
Highest n-number in reference configuration? (1..3)
>>2
Number of electrons in 1s? (0..2)
>>2
Number of electrons in 2s? (0..2)
>>0
Number of electrons in 2p? (0..6)
>>1
Resulting term? (1S, 3P, etc.)
>>2P
Number of excitations = ? (0..3)
>>3
44 configuration states have been generated.
Generate a second list? (y/*)
>>
44 configuration states in the final list.
The generated file is called clist.out.
FORTRAN STOP
```

```
*****
*          COPY FILES                                                         *
*          IT IS ADVISABLE TO SAVE THE LSGEN LOG-FILE TO HAVE A RECORD ON    *
*          HOW THE CONFIGURATION LISTS GENERATION WAS DONE                   *
*****
```

```
>>cp clist.log 2PoCAS3.log
>>cp clist.out cfg.inp
```

```
*****
*          RUN NONH TO GENERATE ENERGY EXPRESSION                          *
*****
```

```

*          INPUT FILES: cfg.inp                      *
*          OUTPUT FILES: cfg.h, yint.lst, c.lst, ih.=n.lst      *
*****

```

```
>>nonh
```

```
input file is cfg.inp ...
```

```

=====
      N O N H      2000
=====

```

```
THERE ARE 6 ORBITALS AS FOLLOWS:
```

```
1s 2s 2p 3s 3p 3d
```

```
THERE ARE 0 CLOSED SUBSHELLS COMMON TO ALL CONFIGURATIONS AS FOLLOWS:
```

```

Allocating space for      214 integrals
processing 2Po with      44 configurations
      649 non-zero matrix elements
      152 NF      166 NG      1083 NR      191 NL
      1592 Total number of integrals

```

```
end-of-file clist!!!
```

```

*****
*          RUN MCHF TO OBTAIN SELF CONSISTENT SOLUTIONS          *
*          INPUT FILES: wfn.inp (optional), cfg.inp, angular files *
*          OUTPUT FILES: wfn.out, 2Po.l, summry                  *
*                                                                *
*          NOTE1: Mixing coefficients written to a file named by LS-symmetry *
*          and parity, in this case 2Po.l                        *
*                                                                *
*          NOTE2: We force the program to iterate to higher precision than *
*          default which is a good thing for small calculations    *
*****

```

```
>>mchf
```

```

=====
      M C H F      ... 2000
=====

```

```
THE DIMENSIONS FOR THE CURRENT VERSION ARE:
```

```
NO=60      NO=220      Lagrange Multipliers=800
```

```

START OF CASE
=====

ATOM, Z in FORMAT(A, F) :
>>Li,3.
  cfg.inp has configurations for          1  terms

Enter eigenvalues and weights: one line per term, eigenvalues with weights
in parenthesis and separated by commas, default is 1.0
2Po
>>1

There are  6 orbitals as follows:
  1s  2s  2p  3s  3p  3d
Enter orbitals to be varied: (ALL,NONE,SOME,NIT=,comma delimited list)
>>all
Enter those that are spectroscopic
>>1s,2p

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

Default values for other parameters? (Y/N)
>>n

Default values (NO,REL,STRONG) ? (Y/N)
>>y

Li          3.   220  6  6  0  F

Default values for PRINT, CFGTOL, SCFTOL ? (Y/N)
>>n
Input free FORMAT(L, F, F)
>>.f.,1.e-50,1.e-50

Default values for NSCF, IC ? (Y/N)
>>n
Input free FORMAT(I, I)
>>300,0

Default values for ACFG,LD,TRACE? (Y/N)
>>y

.....

      ITERATION NUMBER  62
      -----

CONVERGENCE CRITERIA:ENERGY  (CFGTOL)          =  1.0D-50
                      :FUNCTION(SCFTOL*SQRT(Z*NWF))=  4.2D-50

```

```

E( 2s 1s) =    25.62110   E( 1s 2s) =    0.03566
E( 3s 1s) =   125.27085   E( 1s 3s) =    0.00805
E( 3s 2s) =    72.76330   E( 2s 3s) =    3.36051
E( 3p 2p) =     2.18254   E( 2p 3p) =    0.00707

```

	EL	ED	AZ	NORM	DPM
< 1s 2s>=	9.9D-10				
< 1s 3s>=	-5.8D-11				
1s		5.1380025	9.2694030	1.0000000	1.23D-09
< 2s 3s>=	-2.8D-07				
< 1s 2s>=	-3.6D-07				
2s		15.1297623	9.8051412	1.0000000**	8.16D-07
< 2p 3p>=	-7.7D-11				
2p		0.2587501	0.4284629	1.0000000	1.50D-10
< 1s 3s>=	4.6D-08				
< 2s 3s>=	-3.2D-07				
3s		32.0103498	25.1021580	1.0000000**	3.78D-07
< 2p 3p>=	-2.0D-10				
3p		17.5853816	23.8010905	1.0000000**	2.18D-09
3d		32.5391413	81.3500754	1.0000000**	1.10D-09

```

ETOTAL=    -7.40458774   Loops,DeltaE,Res.:  2  3.608D-15  5.517D-08
1  0.9984119      2  0.0003758      3 -0.0006572      4 -0.0014719
5 -0.0042385      6 -0.0027196      7 -0.0003308      8 -0.0001325

```

```

Sum of ETOTAL :          -7.40458774
DeltaE =  6.21724893790087663E-015 Sum_Energy =  -7.4045877355330409

```

ENERGY (a.u.)

Total	-7.404587736
Potential	-14.809175438
Kinetic	7.404587702
Ratio	2.000000005

```

*****
*          SAVE OUTPUT FILES          *
*****

```

```

>>cp wfn.out 2PoCAS3.w
>>cp cfg.inp 2PoCAS3.c
>>cp 2Po.l 2PoCAS3.l
>>cp summry 2PoCAS3.s

```

```

*****
*          RUN HFS TO COMPUTE HYPERFINE INTERACTION CONSTANTS          *
*          INPUT FILES: 2PoCAS3.c, 2PoCAS3.w, 2PoCAS3.l                *
*          OUTPUT FILES: 2PoCAS3.h                                     *
*                                                                      *
*          NOTE1: THE OPTION MCHF IS OBSOLETE AND ADHERES TO THE OLD OUTPUT *
*          FORMAT OF MCHF. NOW YOU NEED ALWAYS ASK FOR INPUT FROM A CI  *
*          CALCULATION.                                                *

```

```

*
*          NOTE2: THE HFS PROGRAM ONLY COMPUTES THE HYPERFINE INTERACTION
*          FROM ONE STATE AND YOU HAVE TO SPECIFY THE POSITION OF THE LEADING
*          CSF OF THIS STATE. AT SOME POINT SOMEONE SHOULD RECODE THE MODULE
*
*****

```

```

Name of state ...
>>2PoCAS3

```

Hyperfine structure calculation

```

Electron density at the nucleus ? (Y/N)
>>y
Indicate the type of calculation
0 => diagonal A and B factors only;
1 => diagonal and off-diagonal A and B factors;
>>0
Input from an MCHF (M) or CI (C) calculation ?
>>C
Is the CI calculation J dependant ? (Y/N)
>>n
Give the index of the dominant cfg in the CI
expansion for which the hfs is to be calculated ?
>>1
Give 2*I and nuclear dipole and quadrupole moments (in n.m. and barns)
>>2,1,1

```

The configuration set

STATE (WITH 44 CONFIGURATIONS):

THERE ARE 6 ORBITALS AS FOLLOWS:

1s 2s 2p 3s 3p 3d

THERE ARE 0 CLOSED SUBSHELLS COMMON TO ALL CONFIGURATIONS AS FOLLOWS:

.....

```

ja =      10
ja =      20
ja =      30
ja =      40

```

PER TEST

END OF CASE

=====

Total CPU time was 0.000 minutes

```
*****
*          RUN LSGEN TO GENERATE N = 3 CAS BREIT CONFIGURATION LIST FOR 2P          *
*          OUTPUT FILES: clist.out, clist.log                                     *
*****
```

```
New list, add to existing list, expand existing list, optimized sorting, restored order or quit? (*)
>>
  Breit or MCHF? (B/*)
>>B
  Default, symmetry or user specified ordering? (*s/u)
>>
  Highest principal quantum number, n? (1..15)
>>3
  Highest orbital angular momentum, l? (s..d)
>>d
  Are all these nl-subshells active? (n/*)
>>
  Limitations on population of n-subshells? (y/*)
>>
  Highest n-number in reference configuration? (1..3)
>>2
  Number of electrons in 1s? (0..2)
>>2
  Number of electrons in 2s? (0..2)
>>0
  Number of electrons in 2p? (0..6)
>>1
  Maximum 2J-value? (0..)
>>3
  Minimum 2J-value? (0..1)
>>1
  Maximum (2S+1)-value? (1..9)
>>9
  Minimum (2S+1)-value? (1..9)
>>1
  Maximum resulting angular momentum? (S..N/N=*)
>>
  Minimum resulting angular momentum? (S..N/S=*)
>>
  Number of excitations = ? (0..3)
>>3
  114 configuration states have been generated.
  Generate a second list? (y/*)
>>
  114 configuration states in the final list.
  The generated file is called clist.out.
  FORTRAN STOP
```

```
*****
*          COPY FILES                                                              *
*          IT IS ADVISABLE TO SAVE THE LSGEN LOG-FILE TO HAVE A RECORD ON        *
```

```

*          HOW THE CONFIGURATION LISTS GENERATION WAS DONE          *
*****

>>cp clist.log 2PoCAS3BREIT.log
>>cp clist.out 2PoCAS3BREIT.c

*****
*          COPY WAVE FUNCTION FILES TO PREPARE FOR THE BREIT-PAULI RUN      *
*****

>>cp 2PoCAS3.w 2PoCAS3BREIT.w

*****
*          RUN CI BREIT-PAULI                                          *
*          INPUT FILES: 2PoCAS3BREIT.c, 2PoCAS3BREIT.w                *
*          OUTPUT FILES: 2PoCASBREIT.j                                *
*****

>>bpci
  Enter ATOM, relativistic (Y/N) with mass correction (Y/N)
>>2PoCAS3BREIT,y,n
  Restarting (Y/y) ?
>>n
  Use existing Matrix and <atom>.l/j initial guess (Y/y)?
>>n

  Enter Maximum and minimum values of 2*J
>>3,1

  Enter eigenvalues: one line per term, eigenvalues separated by commas
2*J =   3
>>1
  Enter eigenvalues: one line per term, eigenvalues separated by commas
2*J =   1
>>1

=====
  B R E I T - P A U L I
=====

Indicate the type of calculation
0 => non-relativistic Hamiltonian only;
1 => one or more relativistic operators only;
2 => non-relativistic operators and selected relativistic:
>>2
All relativistic operators ? (Y/N)
>>y

THE TYPE OF CALCULATION IS DEFINED BY THE FOLLOWING PARAMETERS -
BREIT-PAULI OPERATORS          IREL   = 2
PHASE CONVENTION PARAMETER     ICSTAS = 1
-----

```

THE CONFIGURATION SET

STATE (WITH 114 CONFIGURATIONS):

THERE ARE 6 ORBITALS AS FOLLOWS:

1s 2s 2p 3s 3p 3d

THERE ARE 0 CLOSED SUBSHELLS COMMON TO ALL CONFIGURATIONS AS FOLLOWS:

All Interactions? (Y/N):

>>y

Default Rydberg constant (y/n)

>>y

.....

Allocating space for 783 integrals

jb = 100

Alcmat allocations for idisk= 0 nze = 1124

J = 3 1

Entering LSJMAT with 2J = 3 NUME = 1

LSJMAT with idisk= 0 Nze = 8992

Summary of Davidson Performance

=====

Number of Iterations: 9

Shifted Eigval's: -3.95974915438215003E-002

Delta Lambda: 6.10622663543836097E-016

Residuals: 1.09932870175402541E-008

1 Eigenvalues found

Finished with Davidson

Leaving LSJMAT

J = 1 1

Entering LSJMAT with 2J = 1 NUME = 1

LSJMAT with idisk= 0 Nze = 8992

Summary of Davidson Performance

=====

Number of Iterations: 9

Shifted Eigval's: -3.95976088106196750E-002

Delta Lambda: 3.33066907387546962E-016

Residuals: 1.10031822657079236E-008


```

1 Eigenvalues found
Finished with Davidson
Leaving LSJMAT
onlydvd F
ILS = 0
Finished with the file

*****
* RUN BIOTR TO COMPUTE TRANSITION RATES *
* INPUT FILES: 2SoCAS3BREIT.c, 2SoCAS3BREIT.w, 2SoCAS3BREIT.j *
* 2PoCAS3BREIT.c, 2PoCAS3BREIT.w, 2PoCAS3BREIT.j *
* OUTPUT FILES: 2SoCAS3BREIT.2PoCASBREIT.lsj *
*****

>>biotr

=====
T R A N S B I O 99
=====

Name of Initial State
>>2SeCAS3BREIT
Name of Final State
>>2PoCAS3BREIT
intermediate printing (y or n) ?
>>n
Relativistic calculation ? (y/n)
>>y
Type of transition ? (E1, E2, M1, M2, .. or *)
>>E1
.....

-----
Pair number 1

Initial CSF : 1s(2).2s_2S J = 0.5
Final CSF : 1s(2).2p_2P J = 1.5

2*j = 1 lbl = 1 total energy = -7.4738052
2*j = 3 lbl = 1 total energy = -7.4051932

LENGTH FORMALISM:
-----

SL = 2.2537890D+01

```

```

FINAL OSCILLATOR STRENGTH (GF)          = 1.0308323D+00
TRANSITION PROBABILITY IN EMISSION (Aki) = 3.8973684D+07

```

```

VELOCITY FORMALISM:
-----

```

```

SV                                     = 2.1851565D+01
FINAL OSCILLATOR STRENGTH (GF)        = 9.9944136D-01
TRANSITION PROBABILITY IN EMISSION (Aki) = 3.7786856D+07

```

```

npair = 2

```

```

-----
Pair number 2

```

```

Initial CSF : 1s(2).2s_2S                J = 0.5
Final   CSF : 1s(2).2p_2P                J = 0.5

```

```

2*j = 1 lbl = 1 total energy = -7.4738052
2*j = 1 lbl = 1 total energy = -7.4051945

```

```

LENGTH FORMALISM:
-----

```

```

SL                                     = 1.1268927D+01
FINAL OSCILLATOR STRENGTH (GF)        = 5.1540601D-01
TRANSITION PROBABILITY IN EMISSION (Aki) = 3.8971507D+07

```

```

VELOCITY FORMALISM:
-----

```

```

SV                                     = 1.0925995D+01
FINAL OSCILLATOR STRENGTH (GF)        = 4.9972136D-01
TRANSITION PROBABILITY IN EMISSION (Aki) = 3.7785540D+07

```

```

Type of transition ? (E1, E2, M1, M2, .. or *)
*
STOP END OF CASE

```