
A practical guide to GRASP2K

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Preface

This is a practical guide to GRASP2K, version version 1_1 [P. Jönsson, G. Gaigalas, J. Bieroń, C. Froese Fischer, and I.P. Grant, Comput. Phys. Commun xxxxx]. The guide assumes that the GRASP2K package has been correctly installed according to the instructions in the `README` file in the main directory of the package and that the *executables are on the path*. All calculations are done with non-interacting blocks of given parity and J value. The programs used (Version 2 and Version 3) all adhere to this format. Only the operation of scalar programs is discussed. For a description on how to run the Message Passing Interface (MPI) codes see previous write-up [P. Jönsson, X. He, C. Froese Fischer, and I. P. Grant Comput. Phys. Commun. 177, 597-692 (2007)].

To run the scripts the `GRASP` environment variable must be set. If you are using the gfortran compiler this is done by issuing the command

```
source ./make_environment_gfort
```

in the GRASP2K installation directory (issue similar command if you use the ifort or Portland compiler).

Sample Disclaimer: Certain commercial equipment, instruments, software, or materials are identified in this paper in order to specify the computational procedure adequately. Such identification is not intended to imply recommendation or endorsement by the National Institute of Standards and Technology, nor is it intended to imply that the materials or equipment identified are necessarily the best available for the purpose.

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Chapter 1

The GRASP2K package

1.1 Application programs and tools

The new version of the GRASP2K package 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 [1 – 6]. The new GRASP2K contains three program versions for backward compatibility. Version 1 (V1) programs retain all the previous GRASP92 formats. In order to deal more efficiently with large scale calculations Version 2 (V2) codes were developed where the interaction matrix is considered to be a series of non-interacting blocks of given parity and J value, with selected eigenvalues determined from each. In the new version of GRASP2K programs are referred to as Version 3 (V3) programs [3]. They have the same block format as in V2, but angular integrations are based on second quantization in the coupled tensorial form, angular momentum theory in three spaces (orbital, spin and quasispin), and a generalized graphical technique. The theoretical background can be found in [7 – 9]. Also the new version implements a fast program `jj2lsj` that transforms a portion of the wave function in jj -coupling to a basis of LSJ -coupled configuration state functions. In the default mode, at least 99 % is transformed but the user can readily request that 99.9 % is transformed, see [10 – 11]. Labels in LSJ -coupling are used by several programs in the package. This will be discussed in detail later on.

When available, calculations using Version 3 programs are recommended. In order to distinguish V1, V2, and V3 executables, the Makefiles produce binary files with 'version number' at the end of filename, i.e., `mcp1`, `mcp2`, `mcp3`, `mcp2_mpi`, etc. The programs which exist in only one version do not have a 'version number'. MPI codes are available mainly for Version 2 parts of the package. These have names such as `mcp2_mpi`. Below is a partial list of programs in the package:

1. `iso` – define nuclear properties
2. Routines that generate a configuration state list (CSL):
 - (a) `cs1` – generate a configuration state list (CSL) from lists of reference configurations
 - (b) `jjgen` – generate a CSL using rules
 - (c) `jjreduce3` – include only CSFs that have at least one non-zero matrix element with a CSF of a reference list
 - (d) `xcs1` – discard the CSFs defined in the second configuration symmetry list file from the first one and output the rest
 - (e) `mrgcs1` – merge two configuration lists to one list weeding out all duplicates
3. `mcp3` – compute angular coefficients
4. `erwf` – estimate relativistic wave functions

5. `rscf2` – determine orbitals and mixing coefficients
6. `rci3` – perform CI calculation with Breit and other corrections
7. `jj2lsj` – a program for converting a portion of the wave function expansion in *jj*-coupled configuration states to *LSJ*-coupled CSFs.
8. Routines for computing transition probabilities:
 - (a) `oscl` – perform transition calculations in a single orthonormal basis
 - (b) `biotra3`, `biotra2_mpi` – perform biorthogonal transformations between states.
 - (c) `bioscl3`, `bioscl2_mpi` – compute oscillator strengths between biorthogonal states. If the program `jj2lsj` has been run the labels of the states in the output files are in *LSJ*-coupling.
9. `rhfs3` – compute hyperfine interactions and Landé g_J factors
10. `sms2` – compute isotope shifts (this program is obsolete and should be replaced by the `ris3` program [C. Nazé et al. Comput. Phys. Commun. (2012) submitted])

A number of generally short programs have been developed as tools to facilitate a computational procedure. Some are routines for converting files from V2 to V1 form (for backward compatibility) or from parallel to serial versions.

1. `cndens2` – condense a mixing file and associated `.c` file by deleting configuration states with a mixing coefficient below a cut-off, for block-format.
2. `extmix` – prints the numerical values of the expansion coefficients (in block format), above a cut-off value) along with the corresponding configuration states, in descending order of magnitude, if requested.
3. `jsplit` – split a configuration state list into blocks by J and parity.
4. `mchfmcdf` – convert an multiconfiguration Hartree-Fock (MCHF) radial orbital file `wfn.inp` file to GRASP2K orbital file `rwfn.out` that can be used with `erwf`.
5. `plotmcd` – extracts a single radial orbital from a radial orbital file(.w) and prints out in format for plot.
6. `readrwf` – convert a file of binary radial wave functions to ASCII form (for porting to other environments), or vice versa.
7. `rlevels` – list the levels in a series of mixing files, in the order of increasing energy and report levels (in cm^{-1}) relative to the lowest. If the program `jj2lsj` has been run the levels are given in *LSJ*-coupling notation.
8. `rsave` – a script file such that the command `rsave name` moves `rwfn.out` to `name.w`, `rmix.out` to `name.m`, `rcsl.inp` to `name.c` and `rscf.sum` to `name.s` .
9. `rotate_pair` – a routine that rotates orbitals, useful for testing purposes.

A number of small scripts with self-explanatory names are included in directory `$(GRASP)/src`:

1. `Cleanup.oa` — remove object and auxiliary files in all subdirectories
2. `Cleanup.oaexe` — remove object, auxiliary, and executable files
3. `Grep` — issue a `grep` command through all fortran files in all subdirectories
4. `Grepall` — issue a `grep` command through all files in all subdirectories

5. `qcompile` — quick recompile (equivalent to `make`)
6. `recompile` — remove object, executable, and auxiliary files, and recompile from scratch
7. `Search` — search for a file in all `GRASP` subdirectories (equivalent to `find .. -name`)

The script `recompile` includes a feature to generate soft-links (via `ln -s` linux command) which link the latest version of each program (i.e. executable file with 'version number') to the generic name (executable file without 'version number'), as explained in the second paragraph of this section.

References

1. GRASP92: F. A. Parpia, C. Froese Fischer, I. P. Grant, *Comput. Phys. Commun.* 94, 249-271 (1996)
2. GRASP2K: P. Jönsson, X. He, C. Froese Fischer, and I. P. Grant. *Comput. Phys. Commun.* 176, 597-692 (2007)
3. GRASP2K new version: P. Jönsson, G. Gaigalas, J. Bieroń, C. Froese Fischer, I.P. Grant, *Comput. Phys. Commun* xxxxx
4. HFS92: P. Jönsson F.A. Parpia and C. Froese Fischer, *Comput. Phys. Commun.* 96, 301 (1996)
5. SMS92: P. Jönsson and C. Froese Fischer, *Comput. Phys. Commun.* 94, 249 (1997)
6. JJGEN: L. Sturesson, P. Jönsson and C. Froese Fischer, *Comput. Phys. Commun.* 177, 539 (2007)
7. G. Gaigalas, Z.B. Rudzikas and C. Froese Fischer, *Journal of Physics B At. Mol. Phys.* 30, 3747 (1997)
8. G. Gaigalas, S. Fritzsche and I.P. Grant, *Comput. Phys. Commun.* 139, 263 (2001)
9. G. Gaigalas, S. Fritzsche, Z. Rudzikas, *Atomic Data and Nuclear Data Tables.* 76, 235 (2000)
10. G. Gaigalas, T. Žalandauskas, and Z. Rudzikas, *At. Data and Nucl. Data Tables* 84, 99 (2003)
11. G. Gaigalas, T. Žalandauskas, and S. Fritzsche, *Comput. Phys. Commun.* 157, 239 (2004)

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. Consider transition probability calculations between two groups of results, say one odd group and one even group. Three files are needed for each group in such a calculation - the configuration state list, the radial wave functions, and the expansion (or mixing) coefficients - or a total of six files. The GRASP2K package uses a convention similar to the one for the MCHF package [C. Froese Fischer, G. Tachiev, G. Gaigalas, and M.R. Godefroid, *Comput. Phys. Commun.* 176, 559 (2007)]. A name is associated with the results for each group 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. The tool `rsave` makes use of these default extensions.

To run GRASP2K a number of programs need to be run in a pre-determined sequence. Figure 2 displays a typical sequence of block version program calls to evaluate different expectation values. The resulting flow of files is displayed in Figure 3.

Table 1.1: Table of common extensions.

| Extension | Type of file |
|----------------------|---|
| <code>c</code> | Configuration state list. |
| <code>w</code> | Binary file of radial functions. |
| <code>m</code> | Binary file of expansion or mixing coefficients produced by <code>rscf</code> or its variants. |
| <code>cm</code> | Binary file of mixing coefficients produced by <code>rci</code> or its variants. |
| <code>bw</code> | A <code>.w</code> file after biorthogonal transformation using <code>biotra</code> or its variants. |
| <code>bm</code> | A <code>.m</code> file after biorthogonal transformation using <code>biotra</code> or its variants. |
| <code>cbm</code> | A <code>.cm</code> file after biorthogonal transformation using <code>biotra</code> or its variants. |
| <code>lsj.lbl</code> | File containing composition of wave functions in <i>LSJ</i> -coupling. |
| <code>t</code> | Transition probability data from <code>rscf</code> mixing coefficients or its variants. |
| <code>t.lsj</code> | Transition probability data from <code>rscf</code> mixing coefficients or its variants. Labels in <i>LSJ</i> -coupling. |
| <code>ct</code> | Transition probability data from <code>rci</code> mixing coefficients or its variants. |
| <code>ct.lsj</code> | Transition probability data from <code>rci</code> mixing coefficients or its variants. Labels in <i>LSJ</i> -coupling. |
| <code>h</code> | Hyperfine structure data and Landé factors from <code>rscf</code> mixing coefficients or its variants. |
| <code>ch</code> | Hyperfine structure data and Landé factors from <code>rci</code> mixing coefficients or its variants. |
| <code>hoffd</code> | Off-diagonal hyperfine structure data from <code>rscf</code> mixing coefficients or its variants. |
| <code>choffd</code> | Off-diagonal hyperfine structure data from <code>rci</code> mixing coefficients or its variants. |
| <code>i</code> | Isotope shift data from <code>rscf</code> mixing coefficients or its variants. |
| <code>ci</code> | Isotope shift data from <code>rci</code> mixing coefficients or its variants. |

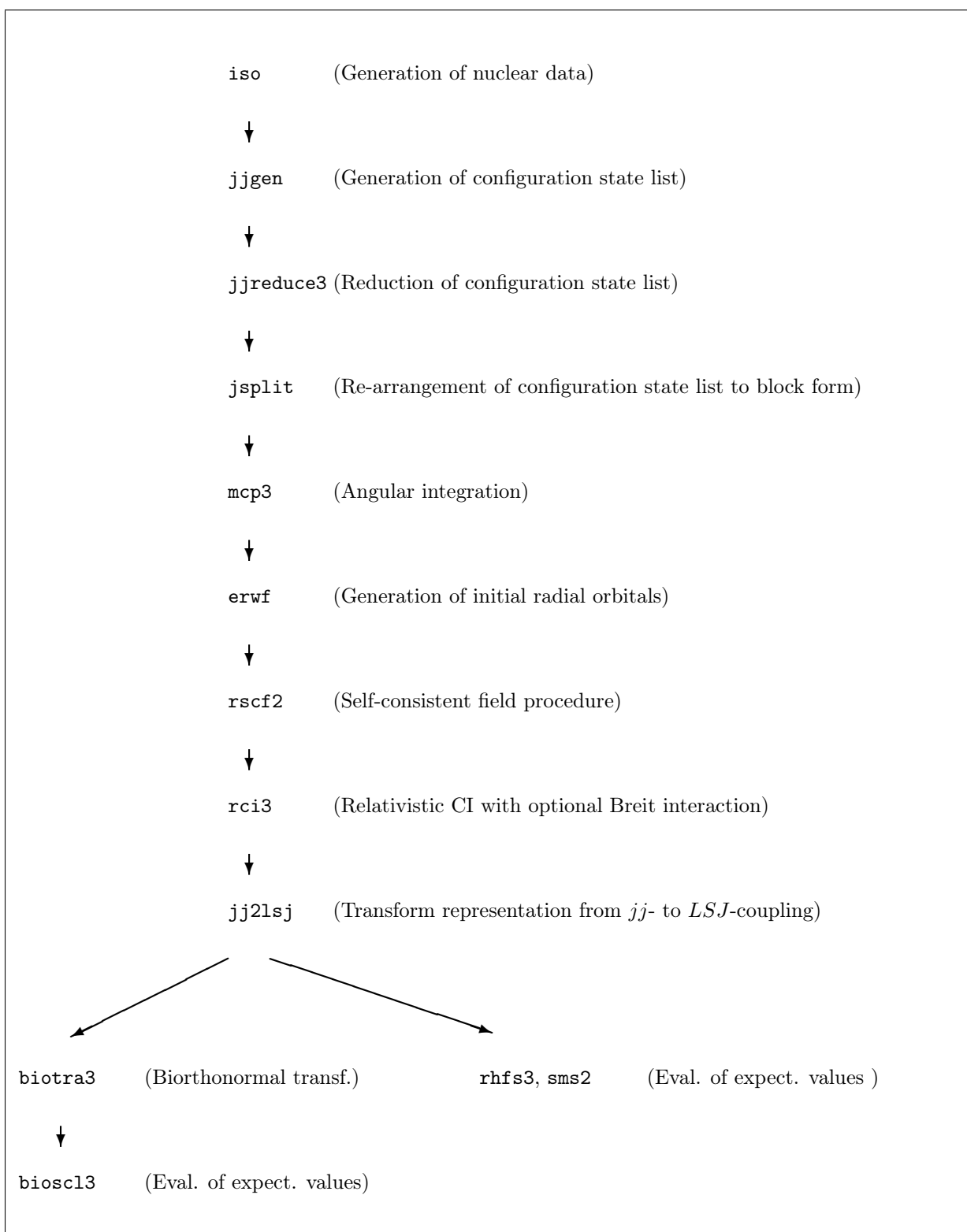


Figure 1.1: Typical sequence of block version program calls to evaluate different expectation values.

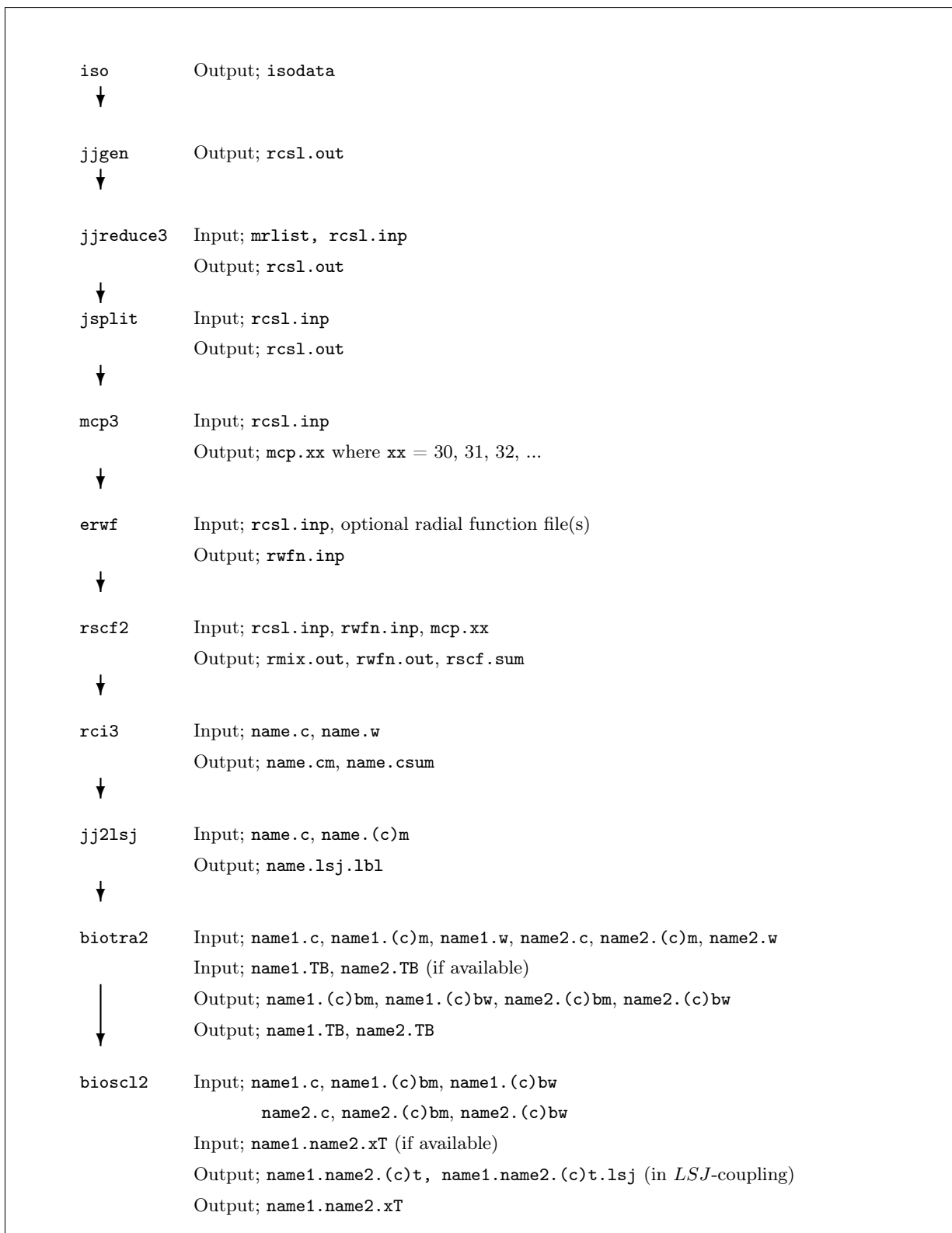


Figure 1.2: Flow of files for a normal sequence of program runs in the block version. Extensions (c) indicate data files from rci3 mixing coefficients.

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 GRASP2K provides several programs for performing this task. For generating small lists of CSFs it is often best to use the CSL 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 `jjgen` 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 `jjreduce3` should be used. Before continuing the reader is advised to study the write-up of the `jjgen` program [L. Stuesson, P. Jönsson and C. Froese Fischer, *Comput. Phys. Commun.* 177, 539 (2007)]. The write-up provides a number of examples on how to generate expansions capturing different correlation effects.

1.4 Providing initial estimates of the radial functions

The program application `erwf` generates initial estimates for radial orbitals. These estimates may be generated using a Thomas-Fermi potential. Alternatively, the initial radial functions can be taken as screened hydrogenic functions. Converted Hartree-Fock (HF) or multiconfiguration Hartree-Fock (MCHF) or radial functions from previous runs may also be used. It is the experience of the authors that the use of converted HF or MCHF functions generally give very good starting values and that this may cut down on the number of needed iterations in the self-consistent-field procedure. The conversion of HF or MCHF radial functions is done by `mchfmcdf`. In the present implementation, prior to normalization,

$$\begin{aligned} P(n\kappa; r) &= P^{MCHF}(nl; r) \\ Q(n\kappa; r) &= \frac{\alpha}{2} \left(\frac{d}{dr} + \frac{\kappa}{r} \right) P(n\kappa; r), \end{aligned}$$

which means that the relativistic orbital pair is strictly kinetically matched [I.P. Grant, *Relativistic Quantum Theory of Atoms and Molecules*, Springer 2007, p. 291].

1.5 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, it is often helpful to start from converted HF or MCHF radial orbitals rather than orbitals generated in a Thomas-Fermi potential or the simple screened hydrogenic orbitals.

1.6 Transverse photon interaction and self-energy correction

Relativistic corrections beyond the Dirac-Coulomb approximation for a many-electron system are implemented using assumptions based on one-electron concepts. For example, the transverse photon frequency is assumed to be the difference between the diagonal energy parameters. This may be an appropriate assumption for singly occupied orbitals but is not correct for multiply occupied ones and certainly is not true for correlation orbitals. For these reasons transverse photon interaction is often computed in the low-frequency limit by multiplying the frequency with a scale factor. The scale factor is often set to 10^{-6} . Similarly, the self-energy correction is computed from a screened-hydrogenic approximation, a model that does not apply well to correlation orbitals that

are far from hydrogenic. The `rci3` code allows the user to specify the largest principal quantum number for which CSFs are to be considered in the self-energy corrections. For small calculations with a few correlation orbitals this cut-off is set to the largest principal quantum number of the included orbitals. In large calculations with many correlation orbitals the cut-off is typically set to a number somewhat larger than the highest principal quantum number of the spectroscopic orbitals.

1.7 Trouble shooting: convergence

Convergence in the self-consistent field procedure is a major issue. It is advisable to first do a calculation with the most important configuration state functions defining the multireference. If there are problems converging spectroscopic orbitals then start from converted HF or MCHF radial functions. If convergence problems remain the user may increase the nuclear charge Z and perform the calculation for some more highly charged ion. The, hopefully, converged radial functions from this run can then be used for another calculation, where the nuclear charge has been slightly decrease. The radial functions from this run are, provided they are converged, used in a new calculation where the nuclear charge has been decreased further etc. If this still does not led to convergence the user may override the default options in the self-consistent field procedure. There a number of options to aid convergence such as increasing the orbital damping. After the calculation for the multireference has been successfully finished the user may introduce correlation orbitals layer by layer. Each time only the outermost layer is optimized and the remaining orbitals are kept frozen.

1.8 Trouble shooting: angular data from the `biotra`, `bioscl` and `rhfs3` programs

The `biotra` and `bioscl` programs and their variants as well as the `hfs3` program save angular data on file. If angular files are available the programs read these files and the execution time is reduced considerably. If, for some reason, there are incomplete files with angular coefficients these programs will end with some error message when trying to process the angular data files. In these cases the user should remove the angular files (they all have a capital **T** in the extension) and rerun the case again.

Chapter 2

Running the application programs

In this chapter we demonstrate the use of the application programs of GRASP2K in three cases described below. The use of the tools of the GRASP2K package is described in the next chapter. The data written to the output files are explained and discussed in chapter 4. Output files from the runs are available in the directories `manual/example1`, `manual/example2`, `manual/example3`. Scripts for running the examples can be found there, too. Please note that the executable all must be on the path! Also, to run the scripts the environment variable `GRASP` needs to be set. If you have set up the package with the `gfortran` compiler this is done by issuing the command

```
source ./make_environment_gfort
```

in the GRASP2K installation directory. A similar command should be issued if you have used the `ifort` or `portland` compilers.

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. Define nuclear data.
2. Generate configuration list containing three CSFs: $1s^22s^2S_{1/2}$, $1s^22p^2P_{1/2,3/2}$.
3. Perform angular integration.
4. Generate initial estimates of radial orbitals.
5. Perform self-consistent field calculation on the weighted average (EOL) of $1s^22s^2S_{1/2}$, $1s^22p^2P_{1/2,3/2}$.
6. Save output to `2s_2p_DF`.
7. Generate $n = 3$ complete active space configuration expansion for $1s^22s^2S_{1/2}$.
8. Perform angular integration.
9. Generate initial estimates of radial orbitals.
10. Perform self-consistent field calculation on $1s^22s^2S_{1/2}$.
11. Save output to `2s_3`.
12. Perform CI calculations in which Breit and QED effects are added.
13. Generate $n = 3$ complete active space configuration expansion for $1s^22p^2P_{1/2,3/2}$.

14. Perform angular integration.
15. Generate initial estimates of radial orbitals.
16. Perform self-consistent field calculation on the weighted average (EOL) of $1s^2 2p^2 P_{1/2,3/2}$.
17. Save output to 2p_3.
18. Perform CI calculations in which Breit and QED effects are added.
19. Run rlevels to view energy separations.
20. Calculate isotope and hyperfine calculations using the CI wave functions.
21. Compute the transition rates from the CI wave functions. Calculation in two steps: biorthogonal transformation and evaluation of transition matrix elements using standard Racah algebra methods.

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 ISO TO GENERATE NUCLEAR DATA          *
*          OUTPUT FILE: isodata                       *
*****

>>iso
  Enter the atomic number:
>>3
  Enter the mass number (0 if the nucleus is to be modelled as a point source):
>>7
  The default root mean squared radius is      2.16921046879772      fm;
  the default nuclear skin thickness is      2.300000000000000      fm;
  Revise these values?
>>n
  Enter the mass of the neutral atom (in amu) (0 if the nucleus is to be static):
>>6.941
  Enter the nuclear spin quantum number (I) (in units of h / 2 pi):
>>1.5
  Enter the nuclear dipole moment (in nuclear magnetons):
>>3.2564268
  Enter the nuclear quadrupole moment (in barns):
>>-0.040

*****
*          RUN JJGEN TO GENERATE CONFIGURATION LIST FOR 2S AND 2P WITH          *
*          THREE CSFs: 1s(2)2s J=1/2, 1s(2)2p- J=1/2, 1s(2)2p J=3/2          *
*          OUTPUT FILES: clist.out, clist.log                                   *
*                                                                              *
*          DETAILED INFORMATION ON HOW TO RUN THE JJGEN PROGRAM IS AVAILABLE  *
*          FROM THE ORIGINAL ARTICLE                                          *
*          L. Stuesson, P. Jönsson and C. Froese Fischer                      *
*          JJGEN: A flexible program for generating lists of jj-coupled       *
*          configuration state functions.                                       *
*****
```


* Computer Physics Communications, 177, 539 (2007). *

```
>>jjgen
  Version 2
    * : new list
    e : expand existing list
    q : quit
>>
  Default, reverse, symmetry or user specified ordering? (*r/s/u)
>>
  Highest principal quantum number, n? (1..15)
>>2
  Highest orbital angular momentum, l? (s..p)
>>p
  Are all these nl-subshells active? (n/*)
>>
  Limitations on population of n-subshells? (y/*)
>>
  Highest n-number in reference configuration? (1..2)
>>2
  Predefine open, closed or no core? (o/c/*)
>>
  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 2*J-number? lower, higher (J=1 -> 2*J=2 etc.)
>>1,1
  Number of excitations = ? (0..3)
>>0
  One configuration state has been generated.
  One configuration state in the final list.

  You have the possibility to generate another list
  This list must have the same 2*J values as
  previous lists of the same parity
  Generate another list? (y/*)
>>y
  Highest n-number? (1..15)
>>2
  Highest l-number? (s..p)
>>p
  Are all these nl-subshells active? (n/*)
>>
  Limitations on population of n-subshells? (y/*)
>>
  Highest n-number in reference configuration? (1..2)
>>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 2*J-number? lower, higher (J=1 -> 2*J=2 etc.)
>>1,3
  Number of excitations = ? (0..3)
>>0
  2 configuration states have been generated.
  3 configuration states in the final list.
```

```
You have the possibility to generate another list
This list must have the same 2*J values as
previous lists of the same parity
Generate another list? (y/*)
```

```
>>
  The merged file is called clist.out.
```

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

```
>>cp clist.log 2s_2p_DF.log
>>cp clist.out rcs1.inp
```

```
*****
*          RUN JSPLIT          *
*          OUTPUT FILE: rcs1.out          *
*          *          *          *
*          NOTE: IF JJGEN IS USED FOR GENERATION CHECKS ON DUPLICATES *
*          GENERALLY NOT NEEDED          *
*****
```

```
>>jsplit
  Perform duplicate check and remove them ?
>>n
```

```
          3 blocks were found
nb  J/P  ncf
    1  1/2+      1
    2  1/2-      1
    3  3/2-      1
```

```
*****
*          COPY FILES          *
*****
```

```
>>cp rcs1.out rcs1.inp
```

```
*****
*          RUN MCP3 TO GENERATE ENERGY EXPRESSION          *
*          OUTPUT FILES: mcp.xxx          *
*****
```

```
>>mcp3
```

```
=====
MCP3: Execution Begins ...
=====
```

```
Default settings? (y/n)
>>y
Block          1 , ncf =          1
Block          2 , ncf =          1
Block          3 , ncf =          1
Loading CSL file ... Header only
There are/is          4 relativistic subshells;
```

```
.....
```

```
=====
MCP3: Execution Finished ...
=====
```

```
Wall time:
    30 seconds
```

```
Finish Date and Time:
  Date (Yr/Mon/Day): 2011/09/20
  Time (Hr/Min/Sec): 23/55/47.390
  Zone: +0200
```

```
MCP3: Execution complete.
```

```
*****
*          RUN ERWF TO GENERATE INITIAL ESTIMATES FOR RADIAL FUNCTIONS          *
*          OUTPUT FILE: rwn.inp                                               *
*****
```

```
>>erwf
```

```
ERWF: Execution begins ...
Estimating Relativistic Wave Functions: Output file = rwn.inp
Default settings ?
```

```
>>y
```

```
Loading CSL file ... Header only
There are/is          4 relativistic subshells;
The following subshell radial wavefunctions remain to be estimated:
1s 2s 2p- 2p
```

```
Read subshell radial wavefunctions. Choose one below
  1 -- GRASP92 File
  2 -- Thomas-Fermi
  3 -- Screened Hydrogenic
```

```
>>2
```

```
Enter the list of relativistic subshells:
>>*
```

All required subshell radial wavefunctions have been estimated:

| Shell | e | p0 | gamma | P(2) | Q(2) | MTP | SRC |
|-------|------------|------------|------------|------------|-------------|-----|-----|
| 1s | 0.2476D+01 | 0.9246D+01 | 0.1000D+01 | 0.9481D-06 | -0.3767D-10 | 310 | T-F |
| 2s | 0.2895D+00 | 0.2308D+01 | 0.1000D+01 | 0.2366D-06 | -0.9404D-11 | 333 | T-F |
| 2p- | 0.2173D+00 | 0.1444D-03 | 0.1000D+01 | 0.7276D-13 | 0.1353D-08 | 336 | T-F |
| 2p | 0.2173D+00 | 0.1204D+01 | 0.2000D+01 | 0.1266D-13 | -0.5029D-18 | 336 | T-F |

ERWF: Execution complete.

```
*****
*          RUN RSCF2 TO OBTAIN SELF CONSISTENT SOLUTIONS          *
*          OUTPUT FILES: rwn.out, rmix.out, rscf.sum              *
*                                                                    *
*          NOTE: ORBITALS BUILDING REFERENCE STATES ARE REQUIRED TO HAVE *
*          THE CORRECT NUMBER OF NODES. THEY ARE REFERRED TO AS SPECTROSCOPIC *
*          ORBITALS. IN THIS RUN WE VARY 1s, 2s, 2p AND THEY ARE ALL *
*          SPECTROSCOPIC. WE CAN USE WILD CARDS FOR SPECIFYING ORBITALS *
*****
```

>>rscf2

```
=====
          RSCF2: Execution Begins ...
=====

Date and Time:
  Date: 20070603  Time: 161709.150  Zone: +0200

Default settings? (y/n)
>>y
Loading CSL file ... Header only
There are/is          4 relativistic subshells;
Loading CSL File for ALL blocks
There are          3 relativistic CSFs... load complete;
Loading Radial WaveFunction File ...
(E)OL type calculation? (y/n)
>>y
There are          3 blocks (block  J/Parity  NCF):
  1  1/2+    1      2  1/2-    1      3  3/2-    1

Enter ASF serial numbers for each block
Block          1    ncf =          1 id =  1/2+
>>1
Block          2    ncf =          1 id =  1/2-
>>1
Block          3    ncf =          1 id =  3/2-
>>1
level weights (1 equal;  5 standard;  9 user)
>>5
Radial functions
  1s 2s 2p- 2p
Enter orbitals to be varied (Updating order)
>>*
Which of these are spectroscopic orbitals?
>>*
Enter the maximum number of SCF cycles:
```

```
>>100
```

```
.....
```

```
Generalised occupation numbers:
```

```
2.0000D+00 2.5000D-01 2.5000D-01 5.0000D-01
```

```
=====
```

```
RSCF2: Execution Finished ...
```

```
=====
```

```
Wall time:
```

```
21 seconds
```

```
Finish Date and Time:
```

```
Date (Yr/Mon/Day): 2011/09/20
```

```
Time (Hr/Min/Sec): 23/57/51.642
```

```
Zone: +0200
```

```
RSCF2: Execution complete.
```

```
*****
*          RUN RSAVE TO SAVE OUTPUT FILES          *
*****
```

```
>>rsave 2s_2p_DF
```

```
Created 2s_2p_DF.w, 2s_2p_DF.c, 2s_2p_DF.m and 2s_2p_DF.sum
```

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

```
>>jjgen
```

```
Version 2
```

```
* : new list
```

```
e : expand existing list
```

```
q : quit
```

```
>>
```

```
Default, reverse, symmetry or user specified ordering? (*r/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
```

```
Predefine open, closed or no core? (o/c/*)
```

```
>>
```

```

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 2*J-number? lower, higher (J=1 -> 2*J=2 etc.)
>>1,1
Number of excitations = ? (0..3)
>>3
79 configuration states have been generated.
79 configuration states in the final list.

```

```

You have the possibility to generate another list
This list must have the same 2*J values as
previous lists of the same parity
Generate another list? (y/*)
>>
The merged file is called clist.out.

```

```

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

```

```

>>cp clist.log 2s_3.log
>>cp clist.out rcs1.inp

```

```

*****
*          RUN JSPLIT          *
*      OUTPUT FILE: rcs1.out   *
*****

```

```

>>jsplit
Perform duplicate check and remove them ?
>>n
      1 blocks were found
nb  J/P  ncf

```

```

      1  1/2+          79

```

```

*****
*          COPY FILES          *
*****

```

```

>>cp rcs1.out rcs1.inp

```

```

*****
*          RUN MCP3 TO GENERATE ENERGY EXPRESSION          *
*      OUTPUT FILES: mcp.xxx          *
*****

```

```

>>mcp3

```

```

=====
MCP3: Execution Begins ...
=====
Date and Time:
  Date: 20070603  Time: 162634.101  Zone: +0200

Default settings? (y/n)
>>y
Block          1 ,  ncf =          79
Loading CSL file ... Header only
There are/is          9  relativistic subshells;

.....

=====
MCP3: Execution Finished ...
=====
Wall time:
  9 seconds

Finish Date and Time:
  Date (Yr/Mon/Day): 2011/09/21
  Time (Hr/Min/Sec): 00/00/46.466
  Zone: +0200

MCP3: Execution complete.

*****
*          RUN ERWF TO GENERATE INITIAL ESTIMATES FOR RADIAL FUNCTIONS          *
*          OUTPUT FILE: rwn.inp                                                *
*****

>>erwf
ERWF: Execution begins ...
Estimating Relativistic Wave Functions:  Output file = rwn.inp
Default settings ?
>>y
Loading CSL file ... Header only
There are/is          9  relativistic subshells;
The following subshell radial wavefunctions remain to be estimated:
1s 2s 2p- 2p 3s 3p- 3p 3d- 3d

Read subshell radial wavefunctions. Choose one below
  1 -- GRASP92 File
  2 -- Thomas-Fermi
  3 -- Screened Hydrogenic
>>1
Enter the file name (Null then "rwn.out")
>>2s_2p_DF.w
Enter the list of relativistic subshells:
>>*

```

The following subshell radial wavefunctions remain to be estimated:

3s 3p- 3p 3d- 3d

Read subshell radial wavefunctions. Choose one below

- 1 -- GRASP92 File
- 2 -- Thomas-Fermi
- 3 -- Screened Hydrogenic

>>2

Enter the list of relativistic subshells:

>>*

All required subshell radial wavefunctions have been estimated:

| Shell | e | p0 | gamma | P(2) | Q(2) | MTP | SRC |
|-------|------------|------------|------------|------------|-------------|-----|-----|
| 1s | 0.2518D+01 | 0.9281D+01 | 0.1000D+01 | 0.9517D-06 | -0.3781D-10 | 333 | 2s_ |
| 2s | 0.1963D+00 | 0.1453D+01 | 0.1000D+01 | 0.1489D-06 | -0.5918D-11 | 339 | 2s_ |
| 2p- | 0.1287D+00 | 0.5116D-04 | 0.1000D+01 | 0.2578D-13 | 0.4793D-09 | 344 | 2s_ |
| 2p | 0.1287D+00 | 0.4265D+00 | 0.2000D+01 | 0.4485D-14 | -0.1782D-18 | 344 | 2s_ |
| 3s | 0.9128D-01 | 0.9784D+00 | 0.1000D+01 | 0.1003D-06 | -0.3987D-11 | 347 | T-F |
| 3p- | 0.7531D-01 | 0.6592D-04 | 0.1000D+01 | 0.3321D-13 | 0.6175D-09 | 349 | T-F |
| 3p | 0.7531D-01 | 0.5495D+00 | 0.2000D+01 | 0.5777D-14 | -0.2296D-18 | 349 | T-F |
| 3d- | 0.6228D-01 | 0.3234D-05 | 0.2000D+01 | 0.3342D-21 | 0.6213D-17 | 351 | T-F |
| 3d | 0.6228D-01 | 0.3237D-01 | 0.3000D+01 | 0.3491D-22 | -0.1387D-26 | 351 | T-F |

ERWF: Execution complete.

```
*****
*          RUN RSCF2 TO OBTAIN SELF CONSISTENT SOLUTIONS          *
*          OUTPUT FILES: rwn.out, rmix.out, rscf.sum              *
*                                                                *
*          NOTE: FOR CORRELATION ORBITALS THERE ARE NO RESTRICTIONS ON THE *
*          NUMBER OF NODES, I.E. THEY ARE NOT SPECTROSCOPIC. IN THIS RUN WE *
*          VARY THE CORRELATION ORBITALS 3s,3p, 3d. NONE OF THESE ARE *
*          SPECTROSCOPIC. WE CAN USE WILD CARDS FOR SPECIFYING ORBITALS *
*****
```

>>rscf2

```
=====
RSCF2: Execution Begins ...
=====
```

Date and Time:

Date: 20070603 Time: 162752.521 Zone: +0200

Default settings? (y/n)

>>y

Loading CSL file ... Header only

There are/is 9 relativistic subshells;

Loading CSL File for ALL blocks

There are 79 relativistic CSFs... load complete;

Loading Radial WaveFunction File ...

(E)OL type calculation? (y/n)

>>y

There are 1 blocks (block J/Parity NCF):

1 1/2+ 79

Enter ASF serial numbers for each block


```

Block          1      ncf =          79 id = 1/2+
>>1
  Radial functions
  1s 2s 2p- 2p 3s 3p- 3p 3d- 3d
  Enter orbitals to be varied (Updating order)
>>3*
  Which of these are spectroscopic orbitals?
>>
  Enter the maximum number of SCF cycles:
>>100

  .....

Generalised occupation numbers:

  1.9940D+00  9.9996D-01  3.8609D-05  7.7191D-05  2.5018D-03  1.1036D-03
  2.2074D-03  5.9745D-05  8.9702D-05
=====
          RSCF2: Execution Finished ...
=====

Wall time:
      18 seconds

Finish Date and Time:
  Date (Yr/Mon/Day): 2011/09/21
  Time (Hr/Min/Sec): 00/02/42.794
  Zone: +0200

RSCF2: Execution complete.

*****
*          RUN RSAVE TO SAVE OUTPUT FILES          *
*****

>>rsave 2s_3
  Created 2s_3.w, 2s_3.c, 2s_3.m and 2s_3.sum

*****
*          RUN RCI3 TO INCLUDE BREIT AND QED EFFECTS          *
*          OUTPUT FILE: 2s_3.cm, 2s_3.csum                    *
*
*          THE TRANSVERSE PHOTON FREQUENCIES CAN BE SET TO THE LOW FREQUENCY *
*          LIMIT. RECOMMENDED IN CASES WHERE YOU HAVE CORRELATION ORBITALS *
*          THE SELF ENERGY CORRECTION MAY FAIL FOR CORRELATION ORBITALS WITH *
*          HIGH N.                                             *
*****

>>rci3
=====
          RCI3: Execution Begins ...
=====

Default settings?

```

```

>>y
  Name of state:
>>2s_3
  isofile = isodata
  name = 2s_3
  Calling CHKPLT...
  Calling SETDBG...
  Calling SETMC...
  Calling SETCON...
  Calling SETSUM...
  Calling setcsl...
  Block          1 , ncf =          79
  Loading CSL file ... Header only
  There are/is          9 relativistic subshells;
  Calling SETRES...
  Calling SETISO ...
  Include contribution of H (Transverse)?
>>y
  Modify all transverse photon frequencies?
>>y
  Enter the scale factor:
>>1d-6
  Include H (Vacuum Polarisation)?
>>y
  Include H (Normal Mass Shift)?
>>n
  Include H (Specific Mass Shift)?
>>n
  Estimate self-energy?
>>y
  Largest n quantum number for including self-energy for orbital
  n should be less or equal 8
>>3
  Loading Radial WaveFunction File ...
  Calling SETMIX...
  There are          1 blocks (block  J/Parity  NCF):
  1  1/2+  79

  Enter ASF serial numbers for each block
  Block          1  ncf =          79  id =  1/2+
>>1

  .....

  Finish time, Statistics

=====
                RCI3: Execution Finished ...
=====

Wall time:
      79 seconds

Finish Date and Time:
  Date (Yr/Mon/Day): 2011/09/21

```

Time (Hr/Min/Sec): 00/04/56.426
 Zone: +0200

RCI3: Execution complete.

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

>>jjgen

Version 2

```
* : new list
e : expand existing list
q : quit
```

>>

Default, reverse, symmetry or user specified ordering? (*r/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

Predefine open, closed or no core? (o/c/*)

>>

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 2*J-number? lower, higher (J=1 -> 2*J=2 etc.)

>>1,3

Number of excitations = ? (0..3)

>>3

186 configuration states have been generated.

186 configuration states in the final list.

You have the possibility to generate another list

This list must have the same 2*J values as

previous lists of the same parity

Generate another list? (y/*)

>>

The merged file is called clist.out.

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

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

```
>>cp clist.log 2p_3.log
>>cp clist.out rcs1.inp
```

```
*****
*          RUN JSPLIT          *
*          OUTPUT FILE: rcs1.out          *
*****
```

```
>>jsplit
Perform duplicate check and remove them ?
>>n
```

```
          2 blocks were found
nb  J/P  ncf

          1  1/2-          76
          2  3/2-          110
```

```
*****
*          COPY FILES          *
*****
```

```
>>cp rcs1.out rcs1.inp
```

```
*****
*          RUN MCP3 TO GENERATE ENERGY EXPRESSION          *
*          OUTPUT FILES: mcp.xxx          *
*****
```

```
>>mcp3
```

```
=====
MCP3: Execution Begins ...
=====
```

```
Default settings? (y/n)
>>y
Block          1 ,  ncf =          76
Block          2 ,  ncf =          110
Loading CSL file ... Header only
There are/is          9 relativistic subshells;
```

```
.....
```

```
=====
MCP3: Execution Finished ...
=====
```

```
Wall time:
          12 seconds
```

```
Finish Date and Time:
Date (Yr/Mon/Day): 2011/09/21
Time (Hr/Min/Sec): 00/07/01.366
```

Zone: +0200

MCP3: Execution complete.

```
*****
*          RUN ERWF TO GENERATE INITIAL ESTIMATES FOR RADIAL FUNCTIONS          *
*          OUTPUT FILE: rwn.inp                                                *
*****
```

>>erwf

ERWF: Execution begins ...

Estimating Relativistic Wave Functions: Output file = rwn.inp

Default settings ?

>>y

Loading CSL file ... Header only

There are/is 9 relativistic subshells;

The following subshell radial wavefunctions remain to be estimated:

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

Read subshell radial wavefunctions. Choose one below

- 1 -- GRASP92 File
- 2 -- Thomas-Fermi
- 3 -- Screened Hydrogenic

>>1

Enter the file name (Null then "rwn.out")

>>2s_2p_DF.w

Enter the list of relativistic subshells:

>>*

The following subshell radial wavefunctions remain to be estimated:

3s 3p- 3p 3d- 3d

Read subshell radial wavefunctions. Choose one below

- 1 -- GRASP92 File
- 2 -- Thomas-Fermi
- 3 -- Screened Hydrogenic

>>2

Enter the list of relativistic subshells:

>>*

All required subshell radial wavefunctions have been estimated:

| Shell | e | p0 | gamma | P(2) | Q(2) | MTP | SRC |
|-------|------------|------------|------------|------------|-------------|-----|-----|
| 1s | 0.2518D+01 | 0.9281D+01 | 0.1000D+01 | 0.9517D-06 | -0.3781D-10 | 333 | 2s_ |
| 2s | 0.1963D+00 | 0.1453D+01 | 0.1000D+01 | 0.1489D-06 | -0.5918D-11 | 339 | 2s_ |
| 2p- | 0.1287D+00 | 0.5116D-04 | 0.1000D+01 | 0.2578D-13 | 0.4793D-09 | 344 | 2s_ |
| 2p | 0.1287D+00 | 0.4265D+00 | 0.2000D+01 | 0.4485D-14 | -0.1782D-18 | 344 | 2s_ |
| 3s | 0.9128D-01 | 0.9784D+00 | 0.1000D+01 | 0.1003D-06 | -0.3987D-11 | 347 | T-F |
| 3p- | 0.7531D-01 | 0.6592D-04 | 0.1000D+01 | 0.3321D-13 | 0.6175D-09 | 349 | T-F |
| 3p | 0.7531D-01 | 0.5495D+00 | 0.2000D+01 | 0.5777D-14 | -0.2296D-18 | 349 | T-F |
| 3d- | 0.6228D-01 | 0.3234D-05 | 0.2000D+01 | 0.3342D-21 | 0.6213D-17 | 351 | T-F |
| 3d | 0.6228D-01 | 0.3237D-01 | 0.3000D+01 | 0.3491D-22 | -0.1387D-26 | 351 | T-F |

ERWF: Execution complete.

```
*****
*          RUN RSCF2 TO OBTAIN SELF CONSISTENT SOLUTIONS          *
*****
```

```

*          OUTPUT FILES: rwn.out, rmix.out, rscf.sum          *
*
*          NOTE: FOR CORRELATION ORBITALS THERE ARE NO RESTRICTIONS ON THE *
*          NUMBER OF NODES, I.E. THEY ARE NOT SPECTROSCOPIC. IN THIS RUN WE *
*          VARY THE CORRELATION ORBITALS 3s,3p, 3d. NON OF THESE ARE *
*          SPECTROSCOPIC. WE CAN USE WILD CARDS FOR SPECIFYING ORBITALS *
*****

```

```
>>rscf2
```

```

=====
RSCF2: Execution Begins ...
=====

```

```

Default settings? (y/n)
>>y
Loading CSL file ... Header only
There are/is          9 relativistic subshells;
Loading CSL File for ALL blocks
There are          186 relativistic CSFs... load complete;
Loading Radial WaveFunction File ...
(E)OL type calculation? (y/n)
>>y
There are          2 blocks (block J/Parity NCF):
  1 1/2-   76      2 3/2-  110

Enter ASF serial numbers for each block
Block          1   ncf =          76 id = 1/2-
>>1
Block          2   ncf =          110 id = 3/2-
>>1
level weights (1 equal; 5 standard; 9 user)
>>5
Radial functions
1s 2s 2p- 2p 3s 3p- 3p 3d- 3d
Enter orbitals to be varied (Updating order)
>>3*
Which of these are spectroscopic orbitals?
>>
Enter the maximum number of SCF cycles:
>>100

```

```
.....
```

```
Generalised occupation numbers:
```

```

1.9939D+00 2.0158D-04 3.3333D-01 6.6667D-01 2.5203D-03 1.0853D-03
2.1709D-03 6.4805D-05 9.7285D-05

```

```

=====
RSCF2: Execution Finished ...
=====

```

```

Wall time:
38 seconds

```

```
Finish Date and Time:
```

Date (Yr/Mon/Day): 2011/09/21
 Time (Hr/Min/Sec): 00/08/57.582
 Zone: +0200

RSCF2: Execution complete.

```
*****
*          RUN RSAVE TO SAVE OUTPUT FILES          *
*****
```

```
>>rsave 2p_3
Created 2p_3.w, 2p_3.c, 2p_3.m and 2p_3.sum
```

```
*****
*          RUN RCI3 TO INCLUDE BREIT AND QED EFFECTS          *
*          OUTPUT FILE: 2p_3.cm, 2p_3.csum              *
*
*          THE TRANSVERSE PHOTON FREQUENCIES CAN BE SET TO THE LOW FREQUENCY *
*          LIMIT. RECOMMENDED IN CASES WHERE YOU HAVE CORRELATION ORBITALS *
*          THE SELF ENERGY CORRECTION MAY FAIL FOR CORRELATION ORBITALS WITH *
*          HIGH N.                                         *
*****
```

```
>>rci3
```

```
=====
RCI3: Execution Begins ...
=====
```

```
Default settings?
>>y
Name of state:
>>2p_3
isofile = isodata
name = 2p_3
Calling CHKPLT...
Calling SETDBG...
Calling SETMC...
Calling SETCON...
Calling SETSUM...
Calling setcsl...
Block          1 , ncf =          76
Block          2 , ncf =          110
Loading CSL file ... Header only
There are/is          9 relativistic subshells;
Calling SETRES...
Calling SETISO ...
Include contribution of H (Transverse)?
>>y
Modify all transverse photon frequencies?
>>y
Enter the scale factor:
>>1.d-6
Include H (Vacuum Polarisation)?
>>y
```

```

Include H (Normal Mass Shift)?
>>n
Include H (Specific Mass Shift)?
>>n
Estimate self-energy?
>>y
Largest n quantum number for including self-energy for orbital
n should be less or equal 8
>>3
Loading Radial WaveFunction File ...
Calling SETMIX...
There are      2 blocks (block  J/Parity  NCF):
  1  1/2-   76      2  3/2-   110

Enter ASF serial numbers for each block
Block          1   ncf =           76  id =  1/2-
>>1
Block          2   ncf =           110  id =  3/2-
>>1

.....

=====
                RCI3: Execution Finished ...
=====

Wall time:
      60 seconds

Finish Date and Time:
Date (Yr/Mon/Day): 2011/09/21
Time (Hr/Min/Sec): 00/10/55.223
Zone: +0200

RCI3: Execution complete.

*****
*          RUN RLEVELS TO VIEW ENERGIES AND ENERGY SEPARATIONS          *
*****

>> rlevels
You can also use command-line option:
  %rlevels file1 file2 (wild cards allowed)...
Now, carry on

Type the input file name, one for each line (NULL to terminate)

File name ?
>>2s_3.cm
File name ?
>>2p_3.cm
File name ?
>>
nblock =          1   ncftot =          79   nw =          9   nelec =          3
nblock =          2   ncftot =         186   nw =          9   nelec =          3

```


Energy levels for ...

Rydberg constant is 109737.31534

No - Serial number of the state; Pos - Position of the state within the J/P block; Splitting is the energy difference with the lower neighbor

| No | Pos | J Parity | Energy Total (a.u.) | Levels (cm ⁻¹) | Splitting (cm ⁻¹) |
|----|-----|----------|------------------------|-------------------------------|----------------------------------|
| 1 | 1 | 1/2 + | -7.4719740 | 0.00 | 0.00 |
| 2 | 1 | 1/2 - | -7.4042610 | 14861.28 | 14861.28 |
| 3 | 1 | 3/2 - | -7.4042597 | 14861.57 | 0.29 |

```
*****
*          RUN SMS2 FOR 2s_3          *
*          OUTPUT FILE: 2s_3.ci      *
*****
```

>>sms2

```
=====
SMS2: Execution Begins ...
=====
```

Default settings?

>>y

Name of state

>>2s_3

Mixing coefficients from a CI calc.?

>>y

Loading Configuration Symmetry List File ...

There are 9 relativistic subshells;

There are 79 relativistic CSFs;

... load complete;

Loading Radial WaveFunction File ...

.....

```
=====
SMS2: Execution Finished ...
=====
```

Wall time:

50 seconds

Finish Date and Time:

Date (Yr/Mon/Day): 2011/09/21

Time (Hr/Min/Sec): 00/12/13.537

Zone: +0200

SMS2: Execution complete.

```
*****
*          RUN SMS2 FOR 2p_3                      *
*          OUTPUT FILE: 2p_3.ci                  *
*****
```

```
>>sms2
```

```
=====
SMS2: Execution Begins ...
=====
```

```
Default settings?
```

```
>>y
```

```
Name of state
```

```
>>2p_3
```

```
Mixing coefficients from a CI calc.?
```

```
>>y
```

```
Loading Configuration Symmetry List File ...
```

```
There are 9 relativistic subshells;
```

```
There are 186 relativistic CSFs;
```

```
... load complete;
```

```
Loading Radial WaveFunction File ...
```

```
.....
```

```
=====
SMS2: Execution Finished ...
=====
```

```
Wall time:
```

```
26 seconds
```

```
Finish Date and Time:
```

```
Date (Yr/Mon/Day): 2011/09/21
```

```
Time (Hr/Min/Sec): 00/13/08.567
```

```
Zone: +0200
```

```
SMS2: Execution complete.
```

```
*****
*          RUN RHFS2 FOR 2s_3                      *
*          OUTPUT FILE: 2s_3.ch, 2s_3.choffd      *
*****
```

```
>>rhfs3
```

```
=====
RHFS2: Execution Begins ...
=====
```

```
THIS VERSION COMPUTES GJ FACTORS
ANGULAR DATA, IF AVAILABLE, ARE READ FROM FILE
```

```
Default settings?
```



```

Mixing coefficients from a CI calc.?
>>y
NPLANTS:          215          590          214          54
Loading Configuration Symmetry List File ...
There are 9 relativistic subshells;
There are 186 relativistic CSFs;
... load complete;
Loading Radial WaveFunction File ...

      nelec =          3
      ncftot =        186
      nw      =          9
      nblock =          2

      block   ncf      nev   2j+1  parity
          1     76       1     2     -1
          2    110       1     4     -1
Column 100 complete;

=====
                RHFS2: Execution Finished ...
=====

Wall time:
          5 seconds

Finish Date and Time:
Date (Yr/Mon/Day): 2011/09/21
Time (Hr/Min/Sec): 00/15/42.608
Zone: +0200

RHFS2: Execution complete.

*****
*          RUN BIOTRA3 FOR 2s_3 AND 2p_3 TO TRANSFORM WAVE FUNCTIONS          *
*          OUTPUT FILES: 2s_3.cbm, 2s_3.bw, 2p_3.cbm, 2p_3.bw                *
*****

>>biotra3
=====
                BIOTRA3: Execution Begins ...
=====

Default settings?
>>y

Input from a CI calculation?
>>y

Name of the Initial state
>>2s_3
Name of the Final state
>>2p_3
Transformation of all J symmetries?
>>y

```

```

Loading Configuration Symmetry List File ...
There are 9 relativistic subshells;
There are 79 relativistic CSFs;
... load complete;
Loading Configuration Symmetry List File ...
There are 9 relativistic subshells;
There are 186 relativistic CSFs;
... load complete;

.....

=====
      BIOTRA3: Execution Finished ...
=====

Wall time:
      31 seconds

Finish Date and Time:
      Date (Yr/Mon/Day): 2011/09/21
      Time (Hr/Min/Sec): 00/17/00.136
      Zone: +0200

BIOTRA3: Execution complete.

*****
*          RUN BIOSCL3 FOR 2s_3 and 2p_3 TO COMPUTE TRANSITION PARAMETERS          *
*          OUTPUT FILE: 2s_3.2p_3.ct                                             *
*****

>>bioscl3

=====
      BIOSCL3: Execution Begins ...
=====

Input from a CI calculation?
>>y

Generate debug output?
>>n

Name of the Initial state
>>2s_3
Name of the Final state
>>2p_3

MRGCSL: Execution begins ...
Loading Configuration Symmetry List File ...
There are 9 relativistic subshells;
There are 79 relativistic CSFs;
... load complete;
Loading Configuration Symmetry List File ...
There are 9 relativistic subshells;

```

```

There are 186 relativistic CSFs;
... load complete;
  1 s
  2 s
  2 p-
  2 p
  3 s
  3 p-
  3 p
  3 d-
  3 d
  1
  79
  2
  76          186
Loading Configuration Symmetry List File ...
there are 9 relativistic subshells;
there are 265 relativistic CSFs;
... load complete;
Enter the list of transition specifications
e.g., E1,M2 or E1 M2 or E1;M2 :
>>E1

```

.....

```

=====
      BIOSCL3: Execution Finished ...
=====

```

```

Wall time:
      54 seconds

```

```

Finish Date and Time:
  Date (Yr/Mon/Day): 2011/09/21
  Time (Hr/Min/Sec): 00/18/45.036
  Zone: +0200

```

```

BIOSCL3: Execution complete.

```

2.2 Second example: $1s^22s2p\ ^3P_{0,1,2},\ ^1P_1$ in B II

The second example is $1s^22s2p\ ^3P_{0,1,2},\ ^1P_1$ in B II.

Overview

1. Define nuclear data
2. Generate configuration list containing 4 CSFs belonging to $1s^22s2p\ ^1,^3P$
3. Perform angular integration
4. Perform HF calculation
5. Convert HF orbitals to relativistic orbitals. We do not need to run `erwf` since all orbitals have been estimated

6. Perform self-consistent field calculation on the weighted average (EOL) on the state belonging to $1s^22s2p^1, ^3P$
7. Save output to 2s2p_DF
8. Transform from *jj*- to *LSJ*-coupling
9. Run rlevels to view energy separations.

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 ISO TO GENERATE NUCLEAR DATA          *
*          OUTPUT FILE: isodata                       *
*****

>>iso
  Enter the atomic number:
>>5
  Enter the mass number (0 if the nucleus is to be modelled as a point source):
>>11
  The default root mean squared radius is      2.42924735571595      fm;
  the default nuclear skin thickness is      2.30000000000000      fm;
  Revise these values?
>>n
  Enter the mass of the neutral atom (in amu) (0 if the nucleus is to be static):
>>10.81
  Enter the nuclear spin quantum number (I) (in units of h / 2 pi):
>>1.5
  Enter the nuclear dipole moment (in nuclear magnetons):
>>2.6886489
  Enter the nuclear quadrupole moment (in barns):
>>1

*****
*          RUN JJGEN TO GENERATE CONFIGURATION LIST FOR 1P_1 AND 3P_0,1,2          *
*          WITH FOUR CSFs: 2s2p- J=0, 2s2p- J=1, 2s2p J=1, 2s2p J = 2          *
*          OUTPUT FILES: clist.out, clist.log                                       *
*****

>>jjgen
  Version 2
    * : new list
    e : expand existing list
    q : quit
>>
  Default, reverse, symmetry or user specified ordering? (* / r / s / u)
>>
  Highest principal quantum number, n? (1..15)
>>2
  Highest orbital angular momentum, l? (s..p)
```

```

>>p
  Are all these nl-subshells active? (n/*)
>>
  Limitations on population of n-subshells? (y/*)
>>
  Highest n-number in reference configuration? (1..2)
>>2
  Predefine open, closed or no core? (o/c/*)
>>
  Number of electrons in 1s? (0..2)
>>2
  Number of electrons in 2s? (0..2)
>>1
  Number of electrons in 2p? (0..6)
>>1
  Resulting 2*J-number? lower, higher (J=1 -> 2*J=2 etc.)
>>0,4
  Number of excitations = ? (0..4)
>>0
  4 configuration states have been generated.
  4 configuration states in the final list.

```

```

You have the possibility to generate another list
This list must have the same 2*J values as
previous lists of the same parity
Generate another list? (y/*)
>>
  The merged file is called clist.out.

```

```

*****
*          COPY FILES          *
*****

```

```

>>cp clist.log 2s2p_DF.log
>>cp clist.out rcsl.inp

```

```

*****
*          RUN JSPLIT          *
*          OUTPUT FILE: rcsl.out          *
*****

```

```

>>jsplit
  Perform duplicate check and remove them ?
>>n
      3 blocks were found
nb  J/P  ncf
    1  0-      1
    2  1-      2
    3  2-      1

```

```

*****
*          COPY FILES          *
*****

```



```
>>cp rcs1.out rcs1.inp
```

```
*****
*          RUN MCP3 TO GENERATE ENERGY EXPRESSION          *
*          OUTPUT FILES: mcp.xxx                            *
*****
```

```
>>mcp3
```

```
=====
MCP3: Execution Begins ...
=====
```

```
Default settings? (y/n)
```

```
>>y
```

```
Block          1 , ncf =          1
Block          2 , ncf =          2
Block          3 , ncf =          1
Loading CSL file ... Header only
There are/is          4 relativistic subshells;
```

```
.....
```

```
=====
MCP3: Execution Finished ...
=====
```

```
Wall time:
    9 seconds
```

```
Finish Date and Time:
  Date (Yr/Mon/Day): 2011/09/21
  Time (Hr/Min/Sec): 00/28/23.256
  Zone: +0200
```

```
MCP3: Execution complete.
```

```
*****
*          RUN HF PROGRAM TO GENERATE NON-RELATIVISTIC RADIAL ORBITALS          *
*          THAT CAN BE CONVERTED TO RELATIVISTIC ORBITALS                      *
*          OUTPUT FILE: wfn.out                                                *
*****
```

```
>>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.

>>B,AV,5.

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

... .. etc.

>> 1s (Note that the closed shells should be entered right-centered with respect to the dots on the line above!!!)

Enter electrons outside CLOSED shells (blank line if none)

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

>>2s(1)2p(1)

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

.....

ITERATION NUMBER 6

SCF CONVERGENCE CRITERIA (SCFTOL*SQRT(Z*NWF)) = 1.2D-06

```
C( 1s 2s) = 0.00000 V( 1s 2s) = -7.06535 EPS = 0.000000
E( 2s 1s) = 0.02654 E( 1s 2s) = 0.01327
```

| EL | ED | AZ | NORM | DPM |
|----|------------|------------|-----------|----------|
| 1s | 16.3418222 | 20.8332819 | 1.0000000 | 1.93D-08 |
| 2s | 1.8579695 | 4.7336947 | 1.0000000 | 1.38D-08 |
| 2p | 1.4015370 | 4.0799511 | 1.0000000 | 1.74D-08 |

< 1s | 2s > = 8.0D-09

TOTAL ENERGY (a.u.)

| | | | |
|--------------------|--------------|-----------|--------------|
| Non-Relativistic | -24.06678870 | Kinetic | 24.06678852 |
| Relativistic Shift | -0.00587815 | Potential | -48.13357722 |
| Relativistic | -24.07266685 | Ratio | -2.000000008 |

Additional parameters ? (Y/N/H)

>>n

Do you wish to continue along the sequence ?

>>n

END OF CASE

=====

```
*****
*          COPY FILES          *
*****
```

>>cp wfn.out wfn.inp

```
*****
*          RUN MCHFCDF TO CONVERT NON-RELATIVISTIC RADIAL ORBITALS TO          *
*          RELATIVISTIC ONES          *
*          OUTPUT FILE: rwn.out          *
*****
```

>>mchfmcdf

```
=====
MCHF to MCDF
=====
```

Input: wfn.inp

Output: rwn.out

```
*****
*          COPY FILES          *
*          WE DONT NEED TO INVOKE ERWF SINCE ALL ORBIATALS HAVE BEEN ESTIMATED *
*****
```

>>cp rwn.out rwn.inp

```
*****
*          RUN RSCF2 TO OBTAIN SELF CONSISTENT SOLUTIONS          *
*          OUTPUT FILES: rwn.out, rmix.out, rscf.sum          *
*****
```

```

*          NOTE: ORBITALS BUILDING REFERENCE STATES ARE REQUIRED TO HAVE          *
*          THE CORRECT NUMBER OF NODES. THEY ARE REFERRED TO AS SPECTROSCOPIC    *
*          ORBITALS. IN THIS RUN WE VARY 1s, 2s, 2p AND THEY ARE ALL             *
*          SPECTROSCOPIC. WE CAN USE WILD CARDS FOR SPECIFYING ORBITALS          *
*****

```

```
>>rscf2
```

```
=====
RSCF2: Execution Begins ...
=====
```

```
Default settings? (y/n)
```

```
>>y
```

```
Loading CSL file ... Header only
There are/is          4 relativistic subshells;
Loading CSL File for ALL blocks
There are          4 relativistic CSFs... load complete;
Loading Radial WaveFunction File ...
(E)OL type calculation? (y/n)
```

```
>>y
```

```
There are          3 blocks (block  J/Parity  NCF):
  1  0-    1      2  1-    2      3  2-    1
```

```
Enter ASF serial numbers for each block
```

```
Block          1  ncf =          1 id =  0-
```

```
>>1
```

```
Block          2  ncf =          2 id =  1-
```

```
>>1,2
```

```
Block          3  ncf =          1 id =  2-
```

```
>>1
```

```
level weights (1 equal; 5 standard; 9 user)
```

```
>>5
```

```
Radial functions
```

```
1s 2s 2p- 2p
```

```
Enter orbitals to be varied (Updating order)
```

```
>>*
```

```
Which of these are spectroscopic orbitals?
```

```
>>*
```

```
Enter the maximum number of SCF cycles:
```

```
>>100
```

```
.....
```

```
Generalised occupation numbers:
```

```
2.0000D+00 1.0000D+00 3.3333D-01 6.6667D-01
```

```
=====
RSCF2: Execution Finished ...
=====
```

```
Wall time:
```

```
8 seconds
```

```
Finish Date and Time:
```

Date (Yr/Mon/Day): 2011/09/21
 Time (Hr/Min/Sec): 00/32/20.913
 Zone: +0200

RSCF2: Execution complete.

```
*****
*          RUN RSAVE TO SAVE OUTPUT FILES          *
*****
```

```
>>rsave 2s2p_DF
Created 2s2p_DF.w, 2s2p_DF.c, 2s2p_DF.m and 2s2p_DF.sum
```

```
*****
*          RUN JJ2LSJ TO GET THE LSJ-COMPOSITION    *
*          OUTPUT FILE: 2s2p_DF.lsj.lbl            *
*****
```

```
>>jj2lsj
```

```
=====
jj2lsj: Execution Begins ...
=====
```

```
jj2lsj: Transformation of ASFs from a jj-coupled CSF basis
into an LS-coupled CSF basis (Fortran 95 version)
(C) Copyright by G. Gaigalas and Ch. F. Fischer,
NIST (2011).
```

```
Name of state
>>2s2p_DF
Loading Configuration Symmetry List File ...
There are 4 relativistic subshells;
There are 4 relativistic CSFs;
... load complete;
```

```
Mixing coefficients from a CI calc.?
```

```
>>n
nelec =          4
ncftot =         4
nw     =          4
nblock =          3

block   ncf   nev   2j+1  parity
   1     1     1     1     -1
   2     2     2     3     -1
   3     1     1     5     -1
```

```
Default settings? (y/n)
```

```
>>y
```

```
.....
```

```
=====
jj2lsj: Execution Finished ...
=====
```

```

=====
Wall time:
      7 seconds

Finish Date and Time:
  Date (Yr/Mon/Day): 2012/07/17
  Time (Hr/Min/Sec): 08/58/10.774
  Zone: +0200

jj2lsj: Execution complete.

*****
*          RUN RLEVELS TO VIEW ENERGIES AND ENERGY SEPARATIONS          *
*          NOTE: SINCE LSJ-INFORMATION NOW IS AVAILABLE OUTPUT LABELS     *
*          WILL BE IN LSJ-COUPLING                                       *
*****

>> rlevels
  You can also use command-line option:
    %rlevels file1 file2 (wild cards allowed)...
  Now, carry on

Type the input file name, one for each line (NULL to terminate)

File name ?
>>2s2p_DF.m
File name ?
>>
nblock =          3  ncftot =          4  nw =          4  nelec =          4

Energy levels for ...
Rydberg constant is 109737.31534
Splitting is the energy difference with the lower neighbor
-----
No Pos  J Parity Energy Total    Levels    Splitting    Configuration
          (a.u.)    (cm^-1)    (cm^-1)
-----
  1  1  0  -   -24.1270877      0.00      0.00  1s(2).2s_2S.2p_3P
  2  1  1  -   -24.1270404     10.39     10.39  1s(2).2s_2S.2p_3P
  3  1  2  -   -24.1269457     31.17     20.79  1s(2).2s_2S.2p_3P
  4  2  1  -   -23.9154061    46458.75   46427.58  1s(2).2s_2S.2p_1P
-----

```

2.3 Third example: $2s^22p^3$ and $2p^5$ in Si VIII

The third example is $2s^22p^3$ and $2p^5$ in Si VIII.

Overview

1. Define nuclear data
2. Generate configuration list belonging to $2s^22p^3$ and $2p^5$
3. Perform angular integration

4. Generate initial estimates of radial orbitals
5. Perform self-consistent field calculation on the weighted average (EOL) of all states belonging to $2s^22p^3$ and $2p^5$ (there are 2 states with $J = 1/2$, 4 states with $J = 3/2$ and 1 state with $J = 5/2$, see NIST Tables)
6. Save output to `2s22p3_2p5_DF`
7. Generate CSF list from SD-excitations from $2s^22p^3$ and $2p^5$ to $n = 3$
8. Run `jjreduce3` to extract CSFs that interacts with CSFs belonging to $2s^22p^3$ and $2p^5$
9. Perform angular integration
10. Generate initial estimates of radial orbitals
11. Perform self-consistent field calculation on the weighted average (EOL) of all states belonging to $2s^22p^3$ and $2p^5$
12. Save output to `2s22p3_2p5_3`
13. Perform CI calculations in which Breit and QED effects are added.
14. Transform from *jj*- to *LSJ*-coupling
15. Run `rlevels` to view energy separations.
16. Compute the M1 transition rates from the CI wave functions. Biorthogonal transformation not needed in this case since the states are described using the same orthogonal orbital set. Copy files and run the transition program.

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 ISO TO GENERATE NUCLEAR DATA          *
*          OUTPUT FILE: isodata                       *
*****
>>iso
  Enter the atomic number:
>>14
  Enter the mass number (0 if the nucleus is to be modelled as a point source):
>>28
  The default root mean squared radius is      3.1085883804880532      fm;
  the default nuclear skin thickness is      2.2999999999999998      fm;
  Revise these values?
>>n
  Enter the mass of the neutral atom (in amu) (0 if the nucleus is to be static):
>>27.9769271
  Enter the nuclear spin quantum number (I) (in units of h / 2 pi):
>>0
  Enter the nuclear dipole moment (in nuclear magnetons):
>>0
  Enter the nuclear quadrupole moment (in barns):
>>0
```

```

*****
*          RUN JJGEN TO GENERATE CONFIGURATION LIST FOR ALL STATES OF          *
*          2s(2)2p(3) + 2p(5)                                                *
*          OUTPUT FILES: clist.out, clist.log                                  *
*****
>>jjgen
  Version 2
    * : new list
    e : expand existing list
    q : quit
>>
  Default, reverse, symmetry or user specified ordering? (*r/s/u)
>>
  Highest principal quantum number, n? (1..15)
>>2
  Highest orbital angular momentum, l? (s..p)
>>p
  Are all these nl-subshells active? (n/*)
>>
  Limitations on population of n-subshells? (y/*)
>>
  Highest n-number in reference configuration? (1..2)
>>2
  Predefine open, closed or no core? (o/c/*)
>>
  Number of electrons in 1s? (0..2)
>>2
  Number of electrons in 2s? (0..2)
>>2
  Number of electrons in 2p? (0..6)
>>3
  Resulting 2*J-number? lower, higher (J=1 -> 2*J=2 etc.)
>>1,5
  Number of excitations = ? (0..7)
>>0
  5 configuration states have been generated.
  5 configuration states in the final list.

  You have the possibility to generate another list
  This list must have the same 2*J values as
  previous lists of the same parity
  Generate another list? (y/*)
>>y
  Highest n-number? (1..15)
>>2
  Highest l-number? (s..p)
>>p
  Are all these nl-subshells active? (n/*)
>>
  Limitations on population of n-subshells? (y/*)
>>
  Highest n-number in reference configuration? (1..2)
>>2

```



```

Number of electrons in 1s? (0..2)
>>2
Number of electrons in 2s? (0..2)
>>0
Number of electrons in 2p? (0..6)
>>5
Resulting 2*J-number? lower, higher (J=1 -> 2*J=2 etc.)
>>1,5
Number of excitations = ? (0..7)
>>0
2 configuration states have been generated.
7 configuration states in the final list.

```

```

You have the possibility to generate another list
This list must have the same 2*J values as
previous lists of the same parity
Generate another list? (y/*)
>>
The merged file is called clist.out.

```

```

*****
*          COPY FILES                                *
*          NOTE THAT WE COPY AN UNSPLIT FILE TO MRLIST FOR FUTURE USE          *
*          TOGETHER WITH JJREDUCE                                *
*****

```

```

>>cp clist.log 2s22p3_2p5_DF.log
>>cp clist.out rcs1.inp
>>cp clist.out mrlist

```

```

*****
*          RUN JSPLIT                                    *
*          OUTPUT FILE: rcs1.out                                *
*****

```

```

>>jsplit
Perform duplicate check and remove them ?
>>n

```

```

          3 blocks were found
nb  J/P  ncf
  1  1/2-      2
  2  3/2-      4
  3  5/2-      1

```

```

*****
*          COPY FILES                                *
*****

```

```

>>cp rcs1.out rcs1.inp

```

```

*****
*          RUN MCP3 TO GENERATE ENERGY EXPRESSION          *
*          OUTPUT FILES: mcp.xxx                                *
*****

```

```

>>mcp3

=====
                MCP3: Execution Begins ...
=====

Default settings? (y/n)
>>y
Block           1 , ncf =           2
Block           2 , ncf =           4
Block           3 , ncf =           1
Loading CSL file ... Header only
There are/is           4 relativistic subshells;

=====
                MCP3: Execution Finished ...
=====

Wall time:
          0 seconds

Finish Date and Time:
  Date (Yr/Mon/Day): 2012/07/17
  Time (Hr/Min/Sec): 09/15/43.865
  Zone: +0200

MCP3: Execution complete.

*****
*          RUN ERWF TO GENERATE INITIAL ESTIMATES FOR RADIAL FUNCTIONS          *
*          OUTPUT FILE: rwfn.inp                                             *
*****

>>erwf
ERWF: Execution begins ...
Estimating Relativistic Wave Functions: Output file = rwfn.inp
Default settings ?
>>y
Loading CSL file ... Header only
There are/is           4 relativistic subshells;
The following subshell radial wavefunctions remain to be estimated:
1s 2s 2p- 2p

Read subshell radial wavefunctions. Choose one below
  1 -- GRASP92 File
  2 -- Thomas-Fermi
  3 -- Screened Hydrogenic
>>3
Enter the list of relativistic subshells:
*

***** Screening parameters *****
1s          0.00
2s          0.00

```

```

2p-      0.00
2p        0.00
All required subshell radial wavefunctions have been estimated:
Shell      e          p0          gamma          P(2)          Q(2)          MTP  SRC
1s  0.9826D+02  0.1033D+03  0.1000D+01  0.1153D-04  -0.5903D-06  275  Hyd
2s  0.2458D+02  0.3670D+02  0.1000D+01  0.4094D-05  -0.2097D-06  291  Hyd
2p- 0.2458D+02  0.8338D-01  0.1000D+01  0.9303D-08  0.1816D-06  291  Hyd
2p  0.2452D+02  0.1492D+03  0.2000D+01  0.1636D-11  -0.4182D-13  291  Hyd
ERWF: Execution complete.

```

```

*****
*          RUN RSCF2 TO OBTAIN SELF CONSISTENT SOLUTIONS          *
*          OUTPUT FILES: rwn.out, rmix.out, rscf.sum              *
*                                                                *
*          NOTE: FOR CORRELATION ORBITALS THERE ARE NO RESTRICTIONS ON THE *
*          NUMBER OF NODES, I.E. THEY ARE NOT SPECTROSCOPIC. IN THIS RUN WE *
*          VARY 1s,2s,2p ALL OF THESE ARE SPECTROSCOPIC. WE CAN USE WILD CARDS *
*          FOR SPECIFYING ORBITALS                                *
*****

```

```
>>rscf2
```

```

=====
RSCF2: Execution Begins ...
=====

```

```

Default settings? (y/n)
>>y
Loading CSL file ... Header only
There are/is          4 relativistic subshells;
Loading CSL File for ALL blocks
There are          7 relativistic CSFs... load complete;
Loading Radial WaveFunction File ...
(E)OL type calculation? (y/n)
>>y
There are          3 blocks (block  J/Parity  NCF):
  1  1/2-    2          2  3/2-    4          3  5/2-    1

Enter ASF serial numbers for each block
Block          1  ncf =          2  id =  1/2-
>>1,2
Block          2  ncf =          4  id =  3/2-
>>1,2,3,4
Block          3  ncf =          1  id =  5/2-
>>1
level weights (1 equal;  5 standard;  9 user)
>>5
Radial functions
1s 2s 2p- 2p
Enter orbitals to be varied (Updating order)
>>*
Which of these are spectroscopic orbitals?
>>*

```

Enter the maximum number of SCF cycles:

>>100

.....

Generalised occupation numbers:

2.0000D+00 1.5385D+00 1.1538D+00 2.3077D+00

=====

RSCF2: Execution Finished ...

=====

Wall time:

53 seconds

Finish Date and Time:

Date (Yr/Mon/Day): 2012/07/17

Time (Hr/Min/Sec): 09/20/21.495

Zone: +0200

RSCF2: Execution complete.

```
*****
*          RUN RSAVE TO SAVE OUTPUT FILES          *
*****
```

>>rsave 2s22p3_2p5_DF

Created 2s22p3_2p5_DF.w, 2s22p3_2p5_DF.c, 2s22p3_2p5_DF.m and 2s22p3_2p5_DF.sum

```
*****
*          RUN JJGEN TO GENERATE LIST OBTAINED BY SD EXCITATIONS FROM          *
*          2s(2)2p(3) + 2p(5) TO n = 3                                          *
*          OUTPUT FILES: clist.out, clist.log                                    *
*****
```

>>jjgen

Version 2

* : new list

e : expand existing list

q : quit

>>

Default, reverse, symmetry or user specified ordering? (*r/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

Predefine open, closed or no core? (o/c/*)

>>

```

Number of electrons in 1s? (0..2)
>>2
Number of electrons in 2s? (0..2)
>>2
Number of electrons in 2p? (0..6)
>>3
Resulting 2*J-number? lower, higher (J=1 -> 2*J=2 etc.)
>>1,5
Number of excitations = ? (0..7)
>>2
1968 configuration states have been generated.
1968 configuration states in the final list.

```

```

You have the possibility to generate another list
This list must have the same 2*J values as
previous lists of the same parity
Generate another list? (y/*)

```

```

>>y
Highest n-number? (1..15)
>>3
Highest l-number? (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)
>>5
Resulting 2*J-number? lower, higher (J=1 -> 2*J=2 etc.)
>>1,5
Number of excitations = ? (0..7)
>>2
751 configuration states have been generated.
2356 configuration states in the final list.

```

```

You have the possibility to generate another list
This list must have the same 2*J values as
previous lists of the same parity
Generate another list? (y/*)

```

```

>>
The merged file is called clist.out.

```

```

*****
*          COPY FILES          *
*****

```

```

>>cp clist.out rcs1.inp

```

```
*****
*      RUN JJREDUCE3 PROGRAM TO DETERMINE WHICH OF THE CSFs IN THE LIST      *
*      rcsl.inp LIST THAT INTERACTS WITH THE CSFs IN THE mrlist             *
*      THE INTERACTING CSFs ARE WRITTEN TO rcsl.out                         *
*      OUTPUT FILE: rcsl.out                                                *
*****
```

```
>>jjreduce3
```

```
JJREDUCE: Execution begins ...
```

```
Default settings?
```

```
>>y
```

```
Loading Configuration Symmetry List File ...
```

```
There are 9 relativistic subshells;
```

```
There are 2356 relativistic CSFs;
```

```
... load complete;
```

```
JJREDUCE: Execution complete.
```

```
The reduced list is in rcsl.out
```

```
*****
*      COPY FILES                                                            *
*****
```

```
>>cp rcsl.out rcsl.inp
```

```
*****
*      RUN JSPLIT                                                            *
*      OUTPUT FILE: rcsl.out                                                *
*****
```

```
>>jsplit
```

```
Perform duplicate check and remove them ?
```

```
>>n
```

```
3 blocks were found
```

| nb | J/P | ncf | |
|----|------|-----|-----|
| 1 | 1/2- | | 274 |
| 2 | 3/2- | | 590 |
| 3 | 5/2- | | 300 |

```
*****
*      COPY FILES                                                            *
*****
```

```
>>cp rcsl.out rcsl.inp
```

```
*****
*      RUN MCP3 TO GENERATE ENERGY EXPRESSION                             *
*      OUTPUT FILES: mcp.xxx                                                *
*****
```

```
>>mcp3
```

```

=====
MCP3: Execution Begins ...
=====

Default settings? (y/n)
>>y
Block          1 , ncf =          274
Block          2 , ncf =          590
Block          3 , ncf =          300

.....

=====
MCP3: Execution Finished ...
=====

Wall time:
    1 seconds

Finish Date and Time:
    Date (Yr/Mon/Day): 2012/07/17
    Time (Hr/Min/Sec): 09/38/08.109
    Zone: +0200

MCP3: Execution complete.

*****
*          RUN ERWF TO GENERATE INITIAL ESTIMATES FOR RADIAL FUNCTIONS          *
*          OUTPUT FILE: rwfn.inp                                             *
*****

>>erwf

ERWF: Execution begins ...
Estimating Relativistic Wave Functions: Output file = rwfn.inp
Default settings ?
>>y
Loading CSL file ... Header only
There are/is          9 relativistic subshells;
The following subshell radial wavefunctions remain to be estimated:
1s 2s 2p- 2p 3s 3p- 3p 3d- 3d

Read subshell radial wavefunctions. Choose one below
    1 -- GRASP92 File
    2 -- Thomas-Fermi
    3 -- Screened Hydrogenic
>>1
Enter the file name (Null then "rwfn.out")
>>2s22p3_2p5_DF.w
Enter the list of relativistic subshells:
>>*
The following subshell radial wavefunctions remain to be estimated:
3s 3p- 3p 3d- 3d

```

```

Read subshell radial wavefunctions. Choose one below
  1 -- GRASP92 File
  2 -- Thomas-Fermi
  3 -- Screened Hydrogenic
>>3
Enter the list of relativistic subshells:
>>*

**** Screening parameters ****
3s      0.00
3p-     0.00
3p      0.00
3d-     0.00
3d      0.00
All required subshell radial wavefunctions have been estimated:
Shell   e          p0          gamma          P(2)          Q(2)          MTP  SRC
1s    0.7698D+02  0.1056D+03  0.1000D+01  0.1082D-04  -0.9224D-09  294  2s2
2s    0.1236D+02  0.3088D+02  0.1000D+01  0.3167D-05  -0.3599D-09  298  2s2
2p-   0.1089D+02  0.5761D-01  0.1000D+01  0.1477D-10  0.1157D-06  299  2s2
2p    0.1086D+02  0.1007D+03  0.2000D+01  0.1059D-11  -0.1204D-15  300  2s2
3s    0.1092D+02  0.1998D+02  0.1000D+01  0.2229D-05  -0.1142D-06  301  Hyd
3p-   0.1092D+02  0.4942D-01  0.1000D+01  0.5514D-08  0.1076D-06  301  Hyd
3p    0.1090D+02  0.8855D+02  0.2000D+01  0.9710D-12  -0.2482D-13  301  Hyd
3d-   0.1090D+02  0.4311D-01  0.2000D+01  0.4729D-15  0.1850D-13  300  Hyd
3d    0.1089D+02  0.9250D+02  0.3000D+01  0.1026D-18  -0.1747D-20  300  Hyd
ERWF: Execution complete.

*****
*          RUN RSCF2 TO OBTAIN SELF CONSISTENT SOLUTIONS          *
*          OUTPUT FILES: rwn.out, rmix.out, rscf.sum              *
*                                                                 *
*          NOTE: FOR CORRELATION ORBITALS THERE ARE NO RESTRICTIONS ON THE *
*          NUMBER OF NODES, I.E. THEY ARE NOT SPECTROSCOPIC. IN THIS RUN WE *
*          VARY THE CORRELATION ORBITALS 3s, 3p, 3d. NONE OF THESE ARE *
*          SPECTROSCOPIC. WE CAN USE WILD CARDS FOR SPECIFYING ORBITALS *
*****

>>rscf2

=====
RSCF2: Execution Begins ...
=====

Default settings? (y/n)
>>y
Loading CSL file ... Header only
There are/is          9 relativistic subshells;
Loading CSL File for ALL blocks
There are          1164 relativistic CSFs... load complete;
Loading Radial WaveFunction File ...
(E)OL type calculation? (y/n)
>>y
There are          3 blocks (block J/Parity NCF):

```


1 1/2- 274 2 3/2- 590 3 5/2- 300

```

Enter ASF serial numbers for each block
Block          1    ncf =          274 id = 1/2-
>>1,2
Block          2    ncf =          590 id = 3/2-
>>1,2,3,4
Block          3    ncf =          300 id = 5/2-
>>1
level weights (1 equal; 5 standard; 9 user)
>>5
Radial functions
1s 2s 2p- 2p 3s 3p- 3p 3d- 3d
Enter orbitals to be varied (Updating order)
>>3*
Which of these are spectroscopic orbitals?
>>
Enter the maximum number of SCF cycles:
>>100

```

.....

Generalised occupation numbers:

```

1.9998D+00 1.5371D+00 1.1513D+00 2.3027D+00 5.8239D-04 4.8570D-04
9.6735D-04 2.8070D-03 4.2144D-03

```

```

=====
RSCF2: Execution Finished ...
=====

```

```

Wall time:
195 seconds

```

```

Finish Date and Time:
Date (Yr/Mon/Day): 2012/07/17
Time (Hr/Min/Sec): 09/44/11.007
Zone: +0200

```

RSCF2: Execution complete.

```

*****
*          RUN RSAVE TO SAVE OUTPUT FILES          *
*****

```

```

>>rsave 2s22p3_2p5_3
Created 2s22p3_2p5_3.w, 2s22p3_2p5_3.c, 2s22p3_2p5_3.m and 2s22p3_2p5_3.sum

```

```

*****
*          RUN RCI3 TO INCLUDE BREIT AND QED EFFECTS          *
*          OUTPUT FILE: 2s22p3_2p5_3.cm, 2s22p3_2p5_3.csum    *
*          *                                                    *
*          THE TRANSVERSE PHOTON FREQUENCIES CAN BE SET TO THE LOW FREQUENCY *
*          LIMIT. RECOMMENDED IN CASES WHERE YOU HAVE CORRELATION ORBITALS *
*          THE SELF ENERGY CORRECTION MAY FAIL FOR CORRELATION ORBITALS WITH *
*          HIGH N.                                             *
*****

```

```
>>rci3
=====
                RCI3: Execution Begins ...
=====
Default settings?
>>y
Name of state:
>>2s22p3_2p5_3
isofile = isodata
name = 2s22p3_2p5_3
Calling CHKPLT...
Calling SETDBG...
Calling SETMC...
Calling SETCON...
Calling SETSUM...
Calling setcsl...
Block          1 , ncf =          274
Block          2 , ncf =          590
Block          3 , ncf =          300
Loading CSL file ... Header only
There are/is          9 relativistic subshells;
Calling SETRES...
Calling SETISO ...
Include contribution of H (Transverse)?
>>y
Modify all transverse photon frequencies?
>>y
Enter the scale factor:
>>1.d-6
Include H (Vacuum Polarisation)?
>>y
Include H (Normal Mass Shift)?
>>n
Include H (Specific Mass Shift)?
>>n
Estimate self-energy?
>>y
Largest n quantum number for including self-energy for orbital
n should be less or equal 8
>>3
Loading Radial WaveFunction File ...
Calling SETMIX...
There are          3 blocks (block  J/Parity  NCF):
  1  1/2-   274      2  3/2-   590      3  5/2-   300

Enter ASF serial numbers for each block
Block          1   ncf =          274  id =  1/2-
>>1,2
Block          2   ncf =          590  id =  3/2-
>>1,2,3,4
Block          3   ncf =          300  id =  5/2-
>1
```

.....

Finish time, Statistics

```
=====
                RCI3: Execution Finished ...
=====
```

Wall time:
233 seconds

Finish Date and Time:
Date (Yr/Mon/Day): 2012/07/18
Time (Hr/Min/Sec): 17/13/28.331
Zone: +0200

RCI3: Execution complete.

```
*****
*          RUN JJ2LSJ TO GET THE LSJ-COMPOSITION          *
*          OUTPUT FILE: 2s22p3_2p5_3.lsj.lbl             *
*****
```

>>jj2lsj

```
=====
                jj2lsj: Execution Begins ...
=====
```

jj2lsj: Transformation of ASFs from a jj-coupled CSF basis
into an LS-coupled CSF basis (Fortran 95 version)
(C) Copyright by G. Gaigalas and Ch. F. Fischer,
NIST (2011).

Name of state
>>2s22p3_2p5_3
Loading Configuration Symmetry List File ...
There are 9 relativistic subshells;
There are 1164 relativistic CSFs;
... load complete;

Mixing coefficients from a CI calc.?
>>y

```
nelec =          7
ncftot =        1164
nw     =          9
nblock =          3
```

| block | ncf | nev | 2j+1 | parity |
|-------|-----|-----|------|--------|
| 1 | 274 | 2 | 2 | -1 |
| 2 | 590 | 4 | 4 | -1 |
| 3 | 300 | 1 | 6 | -1 |

Default settings? (y/n)

>>y

.....

```
=====
                jj2lsj: Execution Finished ...
=====
```

```
Wall time:
    58 seconds
```

```
Finish Date and Time:
  Date (Yr/Mon/Day): 2012/07/17
  Time (Hr/Min/Sec): 09/52/21.594
  Zone: +0200
```

jj2lsj: Execution complete.

```
*****
*          RUN RLEVELS TO VIEW ENERGIES AND ENERGY SEPARATIONS          *
*          NOTE: SINCE LSJ-INFORMATION NOW IS AVAILABLE OUTPUT LABELS      *
*          WILL BE IN LSJ-COUPLING                                         *
*****
```

>>rlevels

```
You can also use command-line option:
  %rlevels file1 file2 (wild cards allowed)...
Now, carry on
```

Type the input file name, one for each line (NULL to terminate)

```
File name ?
>>2s22p3_2p5_3.cm
File name ?
>>
```

```
nblock =          3   ncftot =      1164   nw =          9   nelec =          7
```

```
Energy levels for ...
Rydberg constant is 109737.31534
Splitting is the energy difference with the lower neighbor
```

| No | Pos | J | Parity | Energy Total (a.u.) | Levels (cm ⁻¹) | Splitting (cm ⁻¹) | Configuration |
|----|-----|-----|--------|------------------------|-------------------------------|----------------------------------|-------------------------|
| 1 | 1 | 3/2 | - | -263.2797816 | 0.00 | 0.00 | 1s(2).2s(2).2p(3)4S3_4S |
| 2 | 2 | 3/2 | - | -262.9550531 | 71269.67 | 71269.67 | 1s(2).2s(2).2p(3)2D3_2D |
| 3 | 1 | 5/2 | - | -262.9538181 | 71540.71 | 271.04 | 1s(2).2s(2).2p(3)2D3_2D |
| 4 | 1 | 1/2 | - | -262.7906314 | 107356.05 | 35815.34 | 1s(2).2s(2).2p(3)2P1_2P |
| 5 | 3 | 3/2 | - | -262.7882718 | 107873.93 | 517.89 | 1s(2).2s(2).2p(3)2P1_2P |
| 6 | 4 | 3/2 | - | -259.5241162 | 824273.28 | 716399.35 | 1s(2).2p(5)_2P |
| 7 | 2 | 1/2 | - | -259.4979382 | 830018.67 | 5745.39 | 1s(2).2p(5)_2P |

```

*           WE WILL NOW COMPUTE THE M1 TRANSITION RATES           *
*           IN THIS CASE THE INITIAL AND FINAL STATE FILES ARE THE SAME *
*           AND WE DO NOT NEED TO PERFORM A BIORTHOGONAL TRANSFORMATION *
*           USING BIOTRA. JUST COPY FILES TO NAME.bw AND NAME.cbm      *
*****

```

```

>>cp 2s22p3_2p5_3.w 2s22p3_2p5_3.bw
>>cp 2s22p3_2p5_3.cm 2s22p3_2p5_3.cbm

```

```

*****
*           RUN BIOSCL3 FOR 2s22p3_2p5_3 TO COMPUTE M1 TRANSITION PARAMETERS *
*           OUTPUT FILE: 2s22p3_2p5_3.2s22p3_2p5_3.ct,                *
*                               2s22p3_2p5_3.2s22p3_2p5_3.ct.lsj      *
*                                                                           *
*           NOTE THAT THE LATTER OUTPUT FILE HAS ALL THE LABELS IN LSJ- *
*           COUPLING WHICH IS VERY CONVENIENT                            *
*                                                                           *
*           PLEASE OBSERVE!! IF WE ARE GOING TO RUN BIOSCL FOR AN RCI WAVE *
*           FUNCTIONS THEN THE LSJ-INFORMATION SHOULD BE AVAILABLE FOR THE SAME *
*           WAVE FUNCTION. IF FOR EXAMPLE THE LSJ-INFORMATION FROM JJ2LSJ IS *
*           IS AVAILABLE FROM AN RSCF RUN AND WE RUN BIOSCL ON THE RCI WAVE *
*           FUNCTION THEN BIOSCL3 WILL STOP. In THIS CASE JUST RERUN JJ2LSJ *
*           FOR THE RCI WAVE FUNCTION AND START BIOSCL AGAIN FOR THE SAME *
*           WAVE FUNCTION. IN OUR EXAMPLE JJ2LJS AND BIOSCL3 ARE RUN FOR RCI *
*           WAVE FUNCTIONS AND EVERYTHING IS OK.                        *
*****

```

```

>>bioscl3

```

```

=====
          BIOSCL3: Execution Begins ...
=====

```

```

Input from a CI calculation?
>>y

```

```

Generate debug output?
>>n

```

```

Name of the Initial state
>>2s22p3_2p5_3
Name of the Final state
>>2s22p3_2p5_3

```

```

MRGCSL: Execution begins ...
Loading Configuration Symmetry List File ...
There are 9 relativistic subshells;
There are 1164 relativistic CSFs;
... load complete;
Loading Configuration Symmetry List File ...
There are 9 relativistic subshells;
There are 1164 relativistic CSFs;
... load complete;
      1 s

```

```

2 s
2 p-
2 p
3 s
3 p-
3 p
3 d-
3 d
3
274      864      1164
3
274      864      1164
Loading Configuration Symmetry List File ...
there are 9 relativistic subshells;
  1
  2      2
there are 2328 relativistic CSFs;
... load complete;
Enter the list of transition specifications
e.g., E1,M2 or E1 M2 or E1;M2 :
>>M1
M1 transitions only between levels with different J?
>>n

.....

=====
      BIOSCL3: Execution Finished ...
=====

Wall time:
      88 seconds

Finish Date and Time:
Date (Yr/Mon/Day): 2012/07/17
Time (Hr/Min/Sec): 10/02/34.969
Zone: +0200

BIOSCL3: Execution complete.
```

Chapter 3

Running the tools

3.1 Extracting and condensing

We first demonstrate how to extract mixing coefficients from a wave functions and also how to condense an expansion.

Overview

1. Extract mixing coefficients for the CI wave function 2p_3
2. Condense the CI wave function 2p_3. The files containing the condensed configuration list and the mixing coefficients will have letter D appended in their names.

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 EXTMIX TO EXTRACT MIXING COEFFICIENTS FOR 2p_3          *
*          OUTPUT FILE: rcsl.out                                       *
*****
```

```
>>extmix
```

```
extmix - Extract mixing coefficients and CSF
Files to be read :
    <name>.c, <name>.m / <name>.cm
Files to be written :
    rcsl.out, screen output
Enter the file <name>
>>2p_3
Mixing coefficients from CI or RSCF calc. ?
    a -- CI ;      b -- RSCF
>>a
Enter the cut-off value for the coefficients [0--1]
>>0.01
Sort the eigen vector components ? (y/n)
>>y
```

nblock = 2 ncfatot = 186 nw = 9 nelec = 3

```
=====
nb = 1  ncfblk = 76  nevblk = 1  2J+1 = 2  parity = -1
nb = 1  ncfblk = 76  nevblk = 1  2J+1 = 2  parity = -1
=====
```

Average Energy = 8.4326214447012884 ncf_reduced = 5

Energy = -7.4042610306325809 Coefficients and CSF :

```
1 0.99844919818571742
1s ( 2) 2p-( 1)
          1/2
          1/2-
2 -3.43284268055015288E-002
2p-( 1) 3s ( 2)
          1/2
          1/2-
3 3.25958079398396758E-002
2p-( 1) 3p ( 2)
          1/2
          0
          1/2-
4 2.30630117289014891E-002
2p-( 1) 3p-( 2)
          1/2
          1/2-
5 1.07509560347749163E-002
2s ( 1) 2p-( 1) 3s ( 1)
          1/2   1/2   1/2
          1   1/2-
```

```
=====
nb = 2  ncfblk = 110  nevblk = 1  2J+1 = 4  parity = -1
nb = 2  ncfblk = 110  nevblk = 1  2J+1 = 4  parity = -1
=====
```

Average Energy = 9.6081891369267218 ncf_reduced = 4

Energy = -7.4042597183271539 Coefficients and CSF :

```
1 0.99844920108615898
1s ( 2) 2p ( 1)
          3/2
          3/2-
2 -3.43284268104856322E-002
2p ( 1) 3s ( 2)
          3/2
          3/2-
3 3.25895578847494038E-002
2p ( 1) 3p ( 2)
          3/2
          0
          3/2-
4 2.30718743933811983E-002
2p ( 1) 3p-( 2)
          3/2
          3/2-
```


STOP Successful

```
*****
*          RUN CNDENS2 TO CONDENSE THE 2p_3 EXPANSION          *
*          OUTPUT FILES 2p_3D.c, 2P_3D.cm                    *
*                                                                *
*          NOTE THAT THE LETTER D INDICATES THAT CSFs HAVE BEEN DELETED *
*          (WHICH AMOUNTS TO A CONDENSATION)                  *
*****
```

>>cndens2

Default settings?
>>y

Name of state
>>2p_3
2p_3

Mixing coefficients from a CI calc.?
>>y
2p_3.c

```
                filnam2p_3
Loading Configuration Symmetry List File ...
There are 9 relativistic subshells;
There are 186 relativistic CSFs;
... load complete;
```

```
      2
     76      186
What is the value below which an
eigenvector component is to be
neglected?
```

```
>>0.001
nelec  =          3
ncftoti =         186
nwi    =           9
nblocki =          2
```

```
9 relativistic subshells;
22 relativistic CSFs.
```

CNDENS: Execution complete.

3.2 Extract radial orbitals for printing

The program `plotmcd` extracts a specified orbital from the binary radial orbital file and prints in ASCII format, in three columns, the grid, the large component, and the small component of the orbital. The input file containing the radial orbital should have the name `mcd.f.w`. The ASCII output file has the name `mcd.f.w.dat`. In this example we extract the $1s$ and $2p$ orbitals from

2p_3.w. In the input the orbitals are labeled by n and l . In addition the user should supply a number that is 1 or -1 depending whether $nl(j = l + 1/2)$ or $nl(j = l - 1/2)$ is to be extracted. To extract the $2p_{3/2}$ orbital the input string is 2,1,1. To extract the $2p_{1/2}$ orbital the input string is 2,1,-1.

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.

```
*****
*          COPY 2p_3.w TO mcdf.w WHICH IS THE INPUT FILE TO PLOTMCDF          *
*****

>>cp 2p_3.w mcdf.w

*****
*          RUN PLOTMCDF TO EXTRACT THE 1s ORBITAL                            *
*          OUTPUT: mcdf.w.dat                                                *
*****

>>plotmcd

***** PLOTMCDF *****
Convert one orbital to ASCII form for plotting

Enter the n, l, J(1 or -1)
>>1,0,1

          1          -1  2.5177395462822258          333

*****
*          COPY mcdf.w.dat TO plot_1s.dat                                    *
*****

>>cp mcdf.w.dat plot_1s.dat

*****
*          RUN PLOTMCDF TO EXTRACT THE 2p ORBITAL                            *
*          OUTPUT: mcdf.w.dat                                                *
*****

>>plotmcd

***** PLOTMCDF *****
Convert one orbital to ASCII form for plotting

Enter the n, l, J(1 or -1)
>>2,1,1

          1          -1  2.5177395462822258          333
          2          -1  0.19634308440517523          339
          2           1  0.12867248391836894          344
```

```
2          -2  0.12866992751269327          344
```

```
*****  
*          COPY mcdf.w.dat TO plot_2p.dat          *  
*****
```

```
>>cp mcdf.w.dat plot_2p.dat
```

Given the two ASCII files it is easy to invoke a program, e.g. MATLAB, for plotting, see figure 3.1.

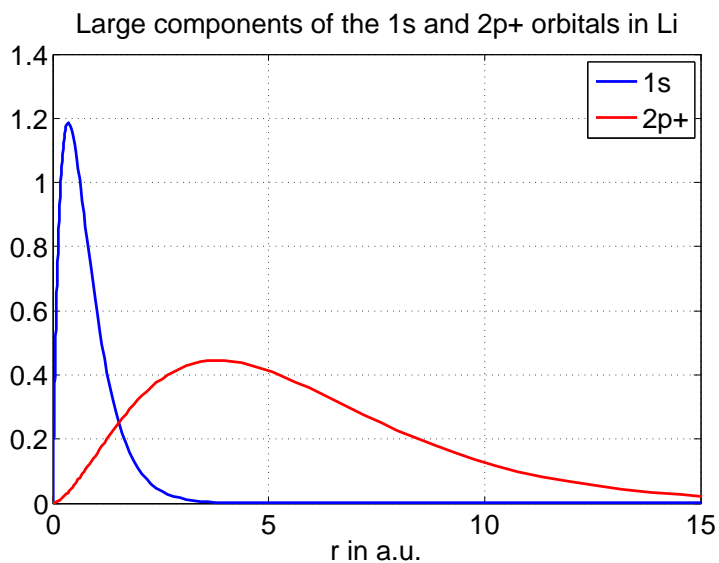


Figure 3.1: Plot of the large components of the 1s and $2p_{3/2}$ orbitals in Li I. The plot has been produced by editing the ASCII files.

Chapter 4

Description of output files

In this chapter we describe in detail what information can be found in the different output files and how this information should be interpreted.

4.1 Output files from the first example

The isodata file

Below is the `isodata` file for the Li example.

```
Atomic number:
  3.0000000000000000
Mass number (integer) :
  7.0000000000000000
Fermi distribution parameter a:
  0.52338755531043146
Fermi distribution parameter c:
  1.2520789669753825
Mass of nucleus (in amu):
  6.9393542602910001
Nuclear spin (I) (in units of h / 2 pi):
  1.5000000000000000
Nuclear dipole moment (in nuclear magnetons):
  3.2564267999999998
Nuclear quadrupole moment (in barns):
 -4.00000000000000008E-002
```

The calculation was for ${}^7\text{Li}$ with $Z = 3$ and $M = 7$. The nuclear charge distribution $\rho(r)$ was modeled as an extended Fermi distribution with

$$\rho(r) = \frac{\rho_0}{1 + e^{(r-b)/a}} \quad (4.1)$$

The parameters a and b are set by default and depend on the mass of the isotope. In this case we have $a = 0.52338755531043146$ fm and $c = 1.2520789669753825$ fm. At the end of the `isodata` file the nuclear spin I is displayed along with the nuclear magnetic dipole moment μ in nuclear magnetons and the nuclear quadrupole moment Q in barns.

The `jjgen` log file

After each `jjgen` run there is a log file displaying the response to the different questions. Below is the log file `2p_3.log` from the $n = 3$ complete active space expansion for $1s^2 2p^2 P_{1/2,3/2}$.

```

Option :
Standard ordering.
    3 Highest principal quantum number.
    2 Highest orbital angular momentum.
T all subshells active.
F limitations on population of n-subshells.
    2 highest n-number.
Predefined core:
    2 number of electrons in          1 s
    0 number of electrons in          2 s
    1 number of electrons in          2 p
    1 to          3 is the resulting term.
    3 number of excitations.
F Generate another list.

```

We see that the highest principal quantum number for the active set was $n = 3$. The highest orbital quantum number was $l = 2$. This corresponds to an active set of orbitals $\{1s, 2s, 2p, 3s, 3p, 3d\}$ in non-relativistic notation. All subshells are active and there is no limitations on the population of the subshells (see write-up of the `jjgen` program). The highest principal quantum number for orbitals in the reference configuration was $n = 2$. The reference configuration contains 2 electrons in $1s$ and 1 electron in $2p$, i.e. the reference configuration is $1s^2 2p$. The resulting values of $2J$ range from 1 to 3, i.e. we generate CSFs that have $J = 1/2$ and $J = 3/2$. The number of excitations from the reference configuration $1s^2 2p$ to the active set of orbitals is 3, i.e. we allow SDT-excitations.

The configuration state list file

The `jjgen` program produces a configuration state list file. The file has a header with information about the radial orbitals and the closed shells (core shells). After this information there is a list of configuration state functions (CSFs). After running `jsplit` the configuration state functions are ordered in blocks with specified value of J . Each block is separated by a line with asterisk. Below is the file `2p_3.c`.

Core subshells:

Peel subshells:

```

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

```

CSF(s):

```

1s ( 2) 2p-( 1)
           1/2
           1/2-
1s ( 2) 3p-( 1)
           1/2
           1/2-
1s ( 1) 2s ( 1) 2p ( 1)
           1/2           1/2           3/2
                   1           1/2-

```

.....

```

3p-( 1) 3d-( 1) 3d ( 1)
           1/2           3/2           5/2
                   2           1/2-
3p-( 1) 3d-( 2)

```

```

      1/2      0
              1/2-
*
1s ( 2) 2p ( 1)
              3/2
              3/2-
1s ( 2) 3p ( 1)
              3/2
              3/2-
1s ( 1) 2s ( 1) 2p ( 1)
      1/2      1/2      3/2
              0      3/2-
.....

3p-( 1) 3d-( 1) 3d ( 1)
      1/2      3/2      5/2
              2      3/2-
3p-( 1) 3d-( 2)
      1/2      2
              3/2-

```

The line with core subshells is empty and in this case we have no closed core. The radial orbitals are $1s, 2s, 2p-, 2p, 3s, 3p-, 3p, 3d-, 3d$. After the radial orbitals there are lists of CSFs arranged in blocks. The first block of CSFs has $J = 1/2$. The second block has $J = 3/2$. An asterisk is separating the blocks. In the file each CSF occupies three lines. On the first line the subshells and their occupations are listed in a linear form where, for example, $1s^2$ becomes $1s (2)$. The second line shows the coupling of each subshell to a J quantum number and the third line shows how the J quantum numbers of each subshell are coupled from left to right to a final J .

The rscf2 summary file

The self-consistent field program `rscf2` produces a summary file. After running `rsave` this file is saved in `name.sum`. Below is the summary file `2p_3.sum` from the run on weighted average (EOL) of the $1s^2 2p^2 P_{1/2,3/2}$ states.

```

There are 3 electrons in the cloud
in 186 relativistic CSFs
based on 9 relativistic subshells.

The atomic number is 3.0000000000;
the mass of the nucleus is 1.264966897439D+04 electron masses;
Fermi nucleus:
c = 2.366086344330D-05 Bohr radii,
a = 9.890591408973D-06 Bohr radii;
there are 53 tabulation points in the nucleus.

Speed of light = 137.0359990840D+00 atomic units.

Radial grid: R(I) = RNT*(exp((I-1)*H)-1), I = 1, ..., N;

RNT = 2.000000000000D-06 Bohr radii;
H   = 5.000000000000D-02 Bohr radii;
N   = 590;

```

R(1) = 0.000000000000D+00 Bohr radii;
 R(2) = 1.025421927520D-07 Bohr radii;
 R(N) = 1.233111896689D+07 Bohr radii.

EOL calculation.
 2 levels will be optimised;
 their indices are: 1, 1.
 Each is assigned its statistical weight;

Radial wavefunction summary:

| Subshell | e | p0 | gamma | P(2) | Q(2) | Self Consistency | MTP |
|----------|------------------|-----------|-------|-----------|------------|------------------|-----|
| 1s | 2.5177395463D+00 | 9.281D+00 | 1.00 | 9.517D-07 | -3.781D-11 | 0.000D+00 | 333 |
| 2s | 1.9634308441D-01 | 1.453D+00 | 1.00 | 1.489D-07 | -5.918D-12 | 0.000D+00 | 339 |
| 2p- | 1.2867248392D-01 | 5.116D-05 | 1.00 | 2.578D-14 | 4.793D-10 | 0.000D+00 | 344 |
| 2p | 1.2866992751D-01 | 4.265D-01 | 2.00 | 4.485D-15 | -1.782D-19 | 0.000D+00 | 344 |
| 3s | 8.0600845411D+00 | 1.179D+01 | 1.00 | 1.507D-06 | -8.686D-12 | 8.965D-08 | 338 |
| 3p- | 8.7786094243D+00 | 2.853D-03 | 1.00 | 2.042D-12 | 2.677D-08 | 8.942D-07 | 342 |
| 3p | 8.7823538492D+00 | 2.381D+01 | 2.00 | 2.508D-13 | -3.787D-17 | 1.303D-06 | 342 |
| 3d- | 1.6298092508D+01 | 8.146D-03 | 2.00 | 8.417D-19 | 1.565D-14 | 6.785D-06 | 336 |
| 3d | 1.6306599830D+01 | 8.170D+01 | 3.00 | 8.809D-20 | -3.503D-24 | 8.699D-06 | 336 |

| Subshell | < r > ⁻³ | < r > ⁻¹ | < r > | < r > ² | < r > ⁴ | Generalised occupation |
|----------|---------------------|---------------------|-------------|--------------------|--------------------|------------------------|
| 1s | 0.00000D+00 | 2.68556D+00 | 5.73199D-01 | 4.47081D-01 | 5.33751D-01 | 1.99386D+00 |
| 2s | 0.00000D+00 | 3.45596D-01 | 3.87317D+00 | 1.77347D+01 | 5.65669D+02 | 2.01584D-04 |
| 2p- | 0.00000D+00 | 2.65023D-01 | 4.79564D+00 | 2.78265D+01 | 1.47509D+03 | 3.33335D-01 |
| 2p | 5.85643D-02 | 2.65011D-01 | 4.79578D+00 | 2.78280D+01 | 1.47522D+03 | 6.66669D-01 |
| 3s | 0.00000D+00 | 3.09463D+00 | 8.79428D-01 | 1.76019D+00 | 3.83411D+01 | 2.52035D-03 |
| 3p- | 0.00000D+00 | 1.94750D+00 | 6.74894D-01 | 8.40900D-01 | 2.20221D+01 | 1.08534D-03 |
| 3p | 1.72790D+01 | 1.94712D+00 | 6.74750D-01 | 8.40046D-01 | 2.19775D+01 | 2.17087D-03 |
| 3d- | 1.01792D+01 | 1.82956D+00 | 6.31485D-01 | 4.57970D-01 | 4.14736D-01 | 6.48046D-05 |
| 3d | 1.01575D+01 | 1.82935D+00 | 6.31441D-01 | 4.57852D-01 | 4.14179D-01 | 9.72851D-05 |

Eigenenergies:

| Level | J Parity | Hartrees | Kaysers | eV |
|-------|----------|---------------------|---------------------|---------------------|
| 1 | 1/2 - | -7.404577002212D+00 | -1.625116808015D+06 | -2.014887871281D+02 |
| 1 | 3/2 - | -7.404574142856D+00 | -1.625116180459D+06 | -2.014887093211D+02 |

Weights of major contributors to ASF:

| Block | Level | J Parity | CSF contributions | | | | |
|-------|-------|----------|-------------------|---------|--------|--------|--------|
| 1 | 1 | 1/2 - | 0.9985 | -0.0343 | 0.0326 | 0.0230 | 0.0107 |
| | | | 1 | 56 | 58 | 60 | 30 |
| 2 | 1 | 3/2 - | 0.9985 | -0.0343 | 0.0326 | 0.0230 | 0.0099 |
| | | | 1 | 62 | 67 | 71 | 32 |

The first lines of the file tell us that the calculation was for a three electron system and that there were in total 186 CSFs built on 9 relativistic radial orbitals. After this there is information about the nucleus. In this case the nucleus has $Z = 3$ and a mass of $1.264966897439 \times 10^4$ electron masses. The nuclear charge distribution is modeled by a Fermi distribution with $c = 2.366086344330 \times 10^{-5}$ Bohr radii, and $a = 9.890591408973 \times 10^{-6}$ Bohr radii. There is information about the radial grid used in the calculation. The grid is given by

$$R(I) = RNT(\exp((I-1)H) - 1), \quad I = 1, \dots, N$$

with $RNT = 2 \times 10^{-6}$ Bohr radii and $H = 5 \times 10^{-2}$ Bohr radii. There are $N = 590$ grid points.

We see that it is an EOL calculation and that the calculation was on the lowest state (first eigenvalue) of each block ($J = 1/2$ and $J = 3/2$). In the optimization each state is weighted according to the statistical weight $2J + 1$.

The information on optimization is followed by a radial orbital summary. Important characteristics of a radial orbital are the orbital energy eigenvalue and parameters that determine the behavior near $r = 0$. The radial amplitudes

$$u(r) = \begin{pmatrix} P(r) \\ Q(r) \end{pmatrix},$$

can be expanded in power series

$$u(r) = r^\gamma [u_0 + u_1 r + u_2 r^2 + \dots], \quad u_k = \begin{pmatrix} p_k \\ q_k \end{pmatrix}$$

near the origin where the index γ , p_k , and q_k are constants that depend on the nuclear potential model. In the radial orbital summary **e** is orbital energy eigenvalue, **p0** is a parameter related to the leading expansion coefficients of the radial amplitudes and **gamma** is the exponent γ , for details see I.P. Grant, *Relativistic Quantum Theory of Atoms and Molecules*, Springer 2007, p 272 - 273 and also the subroutine **start** in **lib92**. **P(2)** and **Q(2)** are the values of the radial amplitudes at the first grid point **R(2)** away from zero. Then the self consistency (weighted change of an orbital during an iteration) is given for each orbital. In this case the orbitals $1s, 2s, 2p-, 2p$ were kept frozen and they thus have a self consistency of zero. The orbitals $3s, 3p-, 3p, 3d-, 3d$ were optimized and the self consistency is between 8.699×10^{-6} for $3d$ and 8.965×10^{-8} for $3s$. Finally, the value **MTP** gives the number of the outermost grid point used for representing the radial amplitudes of the orbital. At remaining grid points the radial amplitudes of the orbital are set to zero. Around 340 of the available 590 grid points are utilized.

Different radial expectation values

$$\langle r^k \rangle = \langle nlj | r^{-k} | nlj \rangle$$

of the orbitals are given along with the generalized occupation numbers. The generalized occupation number $\bar{q}(nlj)$ of an orbital nlj is defined as

$$\bar{q}(nlj) = \sum_{r=1}^{NCSF} d_r^2 q_r(nlj),$$

where $q_r(nlj)$ is the number of electrons in subshell nlj in CSF r and d_r^2 is the generalized weight

$$d_r^2 = \frac{\sum_{i=1}^{nL} (2J_i + 1) c_{ri}^2}{\sum_{i=1}^{nL} (2J_i + 1)}.$$

In the expression for the generalized weight the sum is over all levels in the EOL calculation. c_{ri} , $r = 1, \dots, NCSF$ are the mixing coefficients of level i in the basis of the CSFs. An orbital with a small generalized occupation number is associated with CSFs that have small expansion coefficients.

At the end of the summary file the eigenenergies for the states are displayed in different energy units. The weights of the major CSF contributors are also given. Note that the CSFs in this case are counted blockwise.

The specific mass shift file

The `sms2` program computes isotope shift data. Below is the output file `2p_3.ci` from the `sms2` run of the relativistic CI wave function, given in the `2p_3.c`, `2p_3.w` and `2p_3.cm` files, of the $1s^2 2p^2 P_{1/2,3/2}$ states.

Level J Parity Specific mass shift (au)

| | | |
|---|-------|------------------|
| 1 | 1/2 - | 0.2425644705D+00 |
| 1 | 3/2 - | 0.2425741117D+00 |

Electron density in atomic units

Level J Parity DENS (a.u.)

| | | |
|---|-------|------------------|
| 1 | 1/2 - | 0.1372387504D+02 |
| 1 | 3/2 - | 0.1372387755D+02 |

Kinetic energy

Level J Parity T (a.u.)

| | | |
|---|-------|------------------|
| 1 | 1/2 - | 0.7405495457D+01 |
| 1 | 3/2 - | 0.7405486537D+01 |

Radial expectationvalue

Level J Parity <r> (a.u.)

| | | |
|---|-------|------------------|
| 1 | 1/2 - | 0.5942052019D+01 |
| 1 | 3/2 - | 0.5942191269D+01 |

Radial expectationvalue

Level J Parity <r2> (a.u.)

| | | |
|---|-------|------------------|
| 1 | 1/2 - | 0.2871844755D+02 |
| 1 | 3/2 - | 0.2871990038D+02 |

Radial expectationvalue

Level J Parity <r-1> (a.u.)

| | | |
|---|-------|------------------|
| 1 | 1/2 - | 0.5636518702D+01 |
| 1 | 3/2 - | 0.5636507661D+01 |

Radial expectationvalue

Level J Parity <r-2> (a.u.)

| | | |
|---|-------|------------------|
| 1 | 1/2 - | 0.2991265967D+02 |
| 1 | 3/2 - | 0.2991265070D+02 |

Presented in the file is, for each level or state, the specific mass shift parameter

$$S_{sms} = \langle \Gamma P J M_J | \sum_{i < j}^N \mathbf{p}_i \cdot \mathbf{p}_j | \Gamma P J M_J \rangle$$

the electron density at the nucleus

$$\rho(\mathbf{0}) = \langle \Gamma P J M_J | \sum_{i=1}^N \delta(\mathbf{r}_i) | \Gamma P J M_J \rangle$$

and the kinetic energy T parameter, or S_{nms} parameter,

$$T = S_{nms} = \langle \Gamma P J M_J | \sum_{i=1}^N [c\alpha_i \cdot \mathbf{p}_i + (\beta_i - 1)c^2] | \Gamma P J M_J \rangle$$

The mass and field shift corrected energy for an isotope of mass M is then

$$E_M = E_0 + \frac{1}{M} S_{nms} + \frac{1}{M} S_{sms} + \frac{2}{3} \pi Z \rho(\mathbf{0}) \langle r_M^2 \rangle,$$

where $\langle r_M^2 \rangle$ is the mean square radius of the nuclear charge density.

At the end of the file different radial expectation values are given

$$\langle r^k \rangle = \langle \Gamma P J M_J | \sum_{i=1}^N r_i^k | \Gamma P J M_J \rangle$$

See the original write-up by P. Jönsson and C. Froese Fischer *Comput. Phys. Commun.* 94, 249 (1997) for details.

The hyperfine structure files

The `rhfs3` program computes hyperfine structure data. In addition the Landé g_J factor is computed. Below is the output file `2p_3.ch` from the `rhfs3` run for the relativistic CI wave function, given in the `2p_3.c`, `2p_3.w` and `2p_3.cm` files, of the $1s^2 2p^2 P_{1/2,3/2}$ states.

```
Nuclear spin                1.5000000000000000D+00 au
Nuclear magnetic dipole moment 3.2564268000000000D+00 n.m.
Nuclear electric quadrupole moment -4.0000000000000000D-02 barns
```

Interaction constants:

| Level1 | J Parity | A (MHz) | B (MHz) | g_J |
|--------|----------|-------------------|-------------------|------------------|
| 1 | 1/2 - | 4.4822178884D+01 | -0.0000000000D+00 | 6.6588395646D-01 |
| 1 | 3/2 - | -3.5381701048D+00 | -1.7729096404D-01 | 1.3340987050D+00 |

At the top the nuclear spin and moments are displayed. Then, for each level, the A and B hyperfine interaction constants are given in MHz along with the Landé g_J factor.

The `rhfs3` program gives another file `2p_3.choffd` which contains off-diagonal hyperfine data

```
Nuclear spin                1.5000000000000000D+00 au
Nuclear magnetic dipole moment 3.2564268000000000D+00 n.m.
Nuclear electric quadrupole moment -4.0000000000000000D-02 barns
```

Interaction constants:

| Level1 | J Parity | Level2 | J Parity | A (MHz) | B (MHz) |
|--------|----------|--------|----------|-------------------|-------------------|
| 1 | 1/2 - | 1 | 1/2 - | 4.4822178884D+01 | -0.0000000000D+00 |
| 1 | 3/2 - | 1 | 1/2 - | 1.1768858007D+01 | -3.8388220252D-02 |
| 1 | 3/2 - | 1 | 3/2 - | -3.5381701048D+00 | -1.7729096404D-01 |

Matrix elements:

| Level1 | J Parity | Level2 | J Parity | F | Matrix element (a.u.) |
|--------|----------|--------|----------|---|-----------------------|
| 1 | 1/2 - | 1 | 1/2 - | 1 | -8.5152606539D-09 |
| 1 | 1/2 - | 1 | 1/2 - | 2 | 5.1091563924D-09 |

Matrix elements:

| Level1 | J Parity | Level2 | J Parity | F | Matrix element (a.u.) |
|--------|----------|--------|----------|---|-----------------------|
| 1 | 3/2 - | 1 | 1/2 - | 1 | 4.0297076210D-09 |
| 1 | 3/2 - | 1 | 1/2 - | 2 | 5.3525246272D-09 |

Matrix elements:

| Level1 | J Parity | Level2 | J Parity | F | Matrix element (a.u.) |
|--------|----------|--------|----------|---|-----------------------|
| 1 | 3/2 - | 1 | 3/2 - | 0 | 1.9828496847D-09 |
| 1 | 3/2 - | 1 | 3/2 - | 1 | 1.4720532420D-09 |
| 1 | 3/2 - | 1 | 3/2 - | 2 | 4.2351514680D-10 |
| 1 | 3/2 - | 1 | 3/2 - | 3 | -1.2166550207D-09 |

Given are diagonal and off-diagonal hyperfine interaction constants A and B in MHz and the F dependent hyperfine matrix elements in atomic units. The above quantities are defined in P. Jönsson F.A. Parpia and C. Froese Fischer Comput. Phys. Commun. 96, 301 (1996), Eq (13-17) and Eq (7-8).

The transition file

The bioscl3 program computes transition data. Below is the output file 2s_4.2p_3.ct from the bioscl3 electric dipole E1 run for the relativistic CI wave functions given in the 2s_3.c, 2s_3.w, 2s_3.cm and 2p_3.c, 2p_3.w and 2p_3.cm files.

Transition between files:

f1 = 2s_3

f2 = 2p_3

Electric 2**(1)-pole transitions

=====

| Upper | Lower | | | | | | |
|--------------|--------------|----------|---------|----|---|--|--|
| File Lev J P | File Lev J P | E (Kays) | A (s-1) | gf | S | | |

```

f2  1  1/2 -  f1  1  1/2 +      14861.28 C  3.81311D+07  5.17671D-01  1.14676D+01
                                     B  3.74756D+07  5.08773D-01  1.12705D+01
f2  1  3/2 -  f1  1  1/2 +      14861.57 C  3.81334D+07  1.03537D+00  2.29353D+01
                                     B  3.74782D+07  1.01758D+00  2.25413D+01

```

The first lines of the file gives the name of the files defining the wave functions. Then data are given for the electric dipole transition E1. The first transition is from the upper level 1 with $J = 1/2$ and negative parity in file f2, i.e. $1s^2 2p^2 P_{1/2}$ to the lower level 1 with $J = 1/2$ and positive parity in file f1, i.e. $1s^2 2s^2 S_{1/2}$. The second transition is from the upper level 1 with $J = 3/2$ and negative parity in file f2, i.e. $1s^2 2p^2 P_{3/2}$ to the lower level 1 with $J = 1/2$ and positive parity in file f1, i.e. $1s^2 2s^2 S_{1/2}$. For each transition the transition energy E is given in Kays (cm^{-1}). Also the transition rate A , the weighted oscillator strength gf and the line strength S are given in Coulomb (velocity) and Babushkin (length) gauge.

4.2 Output files from the third example

The third example case was the extended optimal level (EOL) calculations of the states belonging to the $1s^2 2s^2 2p^3$ and $1s^2 2p^5$ configurations in Si VIII.

The jj2lsj file

The jj2lsj program transforms from jj - to LSJ -coupling and gives the LSJ -composition of the states. Below is the output file 2s22p3_2p5_3.lsj.lb1 from the jj2lsj run of the relativistic CI wave functions given in the 2s22p3_2p5_3.c, 2s22p3_2p5_3.w, 2s22p3_2p5_3.cm files. For each case, the first line gives the position (number) of the eigenstate in the interaction matrix, parity, total energy and the percentage of the atomic state function (ASF) that has been transformed. Thus 99.946 % implies that 0.054 % has not been transformed.

| Pos | J | Parity | Energy Total | Comp. of ASF |
|-----|-----|-------------|----------------|-------------------------------|
| 1 | 1/2 | - | -262.790631446 | 99.946% |
| | | 0.98656029 | 0.97330120 | 1s(2).2s(2).2p(3)2P1_2P |
| | | 0.15010909 | 0.02253274 | 1s(2).2p(5)_2P |
| | | -0.03364614 | 0.00113206 | 1s(2).2s_2S.2p(3)2P1_1P.3d_2P |
| 2 | 1/2 | - | -259.497938232 | 99.613% |
| | | 0.98251139 | 0.96532864 | 1s(2).2p(5)_2P |
| | | -0.14989839 | 0.02246953 | 1s(2).2s(2).2p(3)2P1_2P |
| | | -0.06893364 | 0.00475185 | 1s(2).2s_2S.2p(3)2D3_3D.3d_2P |
| | | -0.03674439 | 0.00135015 | 1s(2).2s_2S.2p(3)2D3_1D.3d_2P |
| | | 0.03527443 | 0.00124429 | 1s(2).2s_2S.2p(3)2P1_3P.3d_2P |
| 1 | 3/2 | - | -263.279781588 | 99.951% |
| | | 0.99652486 | 0.99306180 | 1s(2).2s(2).2p(3)4S3_4S |
| | | -0.06051742 | 0.00366236 | 1s(2).2s_2S.2p(3)2D3_3D.3d_4S |
| | | 0.03703206 | 0.00137137 | 1s(2).2s(2).2p(3)2P1_2P |
| 2 | 3/2 | - | -262.955053092 | 99.950% |
| | | 0.98954099 | 0.97919137 | 1s(2).2s(2).2p(3)2D3_2D |
| | | -0.12139915 | 0.01473775 | 1s(2).2s(2).2p(3)2P1_2P |
| | | 0.04260716 | 0.00181537 | 1s(2).2s_2S.2p(3)2D3_1D.3d_2D |
| | | -0.03690740 | 0.00136216 | 1s(2).2s_2S.2p(3)4S3_3S.3d_2D |
| 3 | 3/2 | - | -262.788271788 | 99.956% |
| | | 0.97818838 | 0.95685251 | 1s(2).2s(2).2p(3)2P1_2P |
| | | 0.15010555 | 0.02253168 | 1s(2).2p(5)_2P |
| | | 0.12276481 | 0.01507120 | 1s(2).2s(2).2p(3)2D3_2D |
| | | -0.03672209 | 0.00134851 | 1s(2).2s(2).2p(3)4S3_4S |

```

-0.03335975  0.00111287  1s(2).2s_2S.2p(3)2P1_1P.3d_2P
4  3/2  -      -259.524116164      99.612%
  0.98234136  0.96499454  1s(2).2p(5)_2P
-0.15102027  0.02280712  1s(2).2s(2).2p(3)2P1_2P
-0.06882345  0.00473667  1s(2).2s_2S.2p(3)2D3_3D.3d_2P
-0.03662955  0.00134172  1s(2).2s_2S.2p(3)2D3_1D.3d_2P
  0.03537697  0.00125153  1s(2).2s_2S.2p(3)2P1_3P.3d_2P

1  5/2  -      -262.953818133      99.429%
  0.99713868  0.99428554  1s(2).2s(2).2p(3)2D3_2D

```

There is a total of seven states. For each state the file gives the LSJ -composition. The lowest $J = 1/2$ state (pos 1) with negative parity and energy -262.790631446 a.u. has the LSJ -composition

```

0.98656029  1s(2).2s(2).2p(3)2P1_2P
0.15010909  1s(2).2p(5)_2P
-0.03364614  1s(2).2s_2S.2p(3)2P1_1P.3d_2P

```

The second lowest $J = 1/2$ state (pos 2) with negative parity and energy -259.497938232 a.u. has the LSJ -composition

```

0.98251139  1s(2).2p(5)_2P
-0.14989839  1s(2).2s(2).2p(3)2P1_2P
-0.06893364  1s(2).2s_2S.2p(3)2D3_3D.3d_2P
-0.03674439  1s(2).2s_2S.2p(3)2D3_1D.3d_2P
 0.03527443  1s(2).2s_2S.2p(3)2P1_3P.3d_2P

```

We see that the states are close to pure LSJ -coupling and the file provides meaningful labels that match labels given in, for example, the NIST data tables.

The transition file in LSJ -coupling

The bioscl3 program computes transition data. Below is the output file 2s22p3_2p5_3.2s22p3_2p5_3.ct from the bioscl3 magnetic dipole M1 run of the relativistic CI wave functions given in the 2s22p3_2p5_3.c, 2s22p3_2p5_3.w, 2s22p3_2p5_3.cm files giving the states belonging to the $1s^22s^22p^3$ and $1s^22p^5$ configurations

```

Transition in file:
f = 2s22p3_2p5_3

```

```

Magnetic 2*( 1)-pole transitions
=====

```

| Upper | | | Lower | | | E (Kays) | A (s-1) | gf | S |
|-------|-----|-------|-------|-----|-------|-------------|-------------|-------------|-------------|
| File | Lev | J P | File | Lev | J P | | | | |
| f | 2 | 1/2 - | f | 1 | 1/2 - | 722662.63 M | 6.00625D-05 | 3.44842D-16 | 1.18002D-11 |
| f | 3 | 3/2 - | f | 1 | 1/2 - | 517.89 M | 1.22718D-03 | 2.74385D-08 | 1.31018D+00 |
| f | 4 | 3/2 - | f | 1 | 1/2 - | 716917.24 M | 4.29996D+00 | 5.01700D-11 | 1.73053D-06 |
| f | 1 | 1/2 - | f | 1 | 3/2 - | 107356.05 M | 3.11300D+01 | 8.09869D-09 | 1.86549D-03 |
| f | 2 | 1/2 - | f | 1 | 3/2 - | 830018.68 M | 4.56696D+00 | 1.98765D-11 | 5.92184D-07 |
| f | 1 | 1/2 - | f | 2 | 3/2 - | 36086.38 M | 1.27613D+01 | 2.93830D-08 | 2.01353D-02 |
| f | 2 | 1/2 - | f | 2 | 3/2 - | 758749.01 M | 4.24419D+00 | 2.21048D-11 | 7.20432D-07 |
| f | 2 | 1/2 - | f | 3 | 3/2 - | 722144.74 M | 1.09838D+01 | 6.31527D-11 | 2.16258D-06 |
| f | 2 | 1/2 - | f | 4 | 3/2 - | 5745.39 M | 3.40761D+00 | 3.09527D-07 | 1.33224D+00 |
| f | 2 | 3/2 - | f | 1 | 3/2 - | 71269.67 M | 1.41119D+00 | 1.66607D-09 | 5.78087D-04 |

| | | | | | | | | | | | | |
|---|---|-----|---|---|---|-----|---|-----------|---|-------------|-------------|-------------|
| f | 3 | 3/2 | - | f | 1 | 3/2 | - | 107873.93 | M | 7.52313D+01 | 3.87689D-08 | 8.88734D-03 |
| f | 4 | 3/2 | - | f | 1 | 3/2 | - | 824273.28 | M | 1.25265D+01 | 1.10562D-10 | 3.31695D-06 |
| f | 3 | 3/2 | - | f | 2 | 3/2 | - | 36604.27 | M | 2.11595D+01 | 9.47020D-08 | 6.39783D-02 |
| f | 4 | 3/2 | - | f | 2 | 3/2 | - | 753003.62 | M | 9.62936D+00 | 1.01841D-10 | 3.34448D-06 |
| f | 4 | 3/2 | - | f | 3 | 3/2 | - | 716399.35 | M | 7.21349D-02 | 8.42854D-13 | 2.90939D-08 |
| f | 1 | 5/2 | - | f | 1 | 3/2 | - | 71540.71 | M | 1.99972D-02 | 3.51456D-11 | 1.21485D-05 |
| f | 1 | 5/2 | - | f | 2 | 3/2 | - | 271.04 | M | 2.11530D-04 | 2.59004D-08 | 2.36306D+00 |
| f | 3 | 3/2 | - | f | 1 | 5/2 | - | 36333.22 | M | 1.17594D+01 | 5.34187D-08 | 3.63575D-02 |
| f | 4 | 3/2 | - | f | 1 | 5/2 | - | 752732.58 | M | 5.41425D+00 | 5.73026D-11 | 1.88252D-06 |

The structure of the file is the same as for the 2s_3_2p_3.ct file discussed above. If the information of *LSJ*-coupling is available from a jj2lsj run bioscl3 also produces a file 2s22p3_2p5_3.2s22p3_2p5_3.ct.lsj

Transition between files:

2s22p3_2p5_3

2s22p3_2p5_3

1 -262.79063145 1s(2).2s(2).2p(3)2P1_2P
 1 -259.49793823 1s(2).2p(5)_2P
 722662.63 CM-1 138.38 ANGS(VAC) 138.38 ANGS(AIR)
 M1 S = 1.18002D-11 GF = 3.44842D-16 AKI = 6.00625D-05

1 -262.79063145 1s(2).2s(2).2p(3)2P1_2P
 3 -262.78827179 1s(2).2s(2).2p(3)2P1_2P
 517.89 CM-1 193093.04 ANGS(VAC) 193073.07 ANGS(AIR)
 M1 S = 1.31018D+00 GF = 2.74385D-08 AKI = 1.22718D-03

1 -262.79063145 1s(2).2s(2).2p(3)2P1_2P
 3 -259.52411616 1s(2).2p(5)_2P
 716917.24 CM-1 139.49 ANGS(VAC) 139.49 ANGS(AIR)
 M1 S = 1.73053D-06 GF = 5.01700D-11 AKI = 4.29996D+00

3 -263.27978159 1s(2).2s(2).2p(3)4S3_4S
 1 -262.79063145 1s(2).2s(2).2p(3)2P1_2P
 107356.05 CM-1 931.48 ANGS(VAC) 931.48 ANGS(AIR)
 M1 S = 1.86549D-03 GF = 8.09869D-09 AKI = 3.11300D+01

3 -263.27978159 1s(2).2s(2).2p(3)4S3_4S
 1 -259.49793823 1s(2).2p(5)_2P
 830018.68 CM-1 120.48 ANGS(VAC) 120.48 ANGS(AIR)
 M1 S = 5.92184D-07 GF = 1.98765D-11 AKI = 4.56696D+00

3 -262.95505309 1s(2).2s(2).2p(3)2D3_2D
 1 -262.79063145 1s(2).2s(2).2p(3)2P1_2P
 36086.38 CM-1 2771.13 ANGS(VAC) 2770.83 ANGS(AIR)
 M1 S = 2.01353D-02 GF = 2.93830D-08 AKI = 1.27613D+01

3 -262.95505309 1s(2).2s(2).2p(3)2D3_2D
 1 -259.49793823 1s(2).2p(5)_2P
 758749.01 CM-1 131.80 ANGS(VAC) 131.80 ANGS(AIR)
 M1 S = 7.20432D-07 GF = 2.21048D-11 AKI = 4.24419D+00

3 -262.78827179 1s(2).2s(2).2p(3)2P1_2P

1 -259.49793823 1s(2).2p(5)_2P
 722144.74 CM-1 138.48 ANGS(VAC) 138.48 ANGS(AIR)
 M1 S = 2.16258D-06 GF = 6.31527D-11 AKI = 1.09838D+01

3 -259.52411616 1s(2).2p(5)_2P
 1 -259.49793823 1s(2).2p(5)_2P
 5745.39 CM-1 17405.25 ANGS(VAC) 17403.45 ANGS(AIR)
 M1 S = 1.33224D+00 GF = 3.09527D-07 AKI = 3.40761D+00

3 -263.27978159 1s(2).2s(2).2p(3)4S3_4S
 3 -262.95505309 1s(2).2s(2).2p(3)2D3_2D
 71269.67 CM-1 1403.12 ANGS(VAC) 1403.12 ANGS(AIR)
 M1 S = 5.78087D-04 GF = 1.66607D-09 AKI = 1.41119D+00

3 -263.27978159 1s(2).2s(2).2p(3)4S3_4S
 3 -262.78827179 1s(2).2s(2).2p(3)2P1_2P
 107873.93 CM-1 927.01 ANGS(VAC) 927.01 ANGS(AIR)
 M1 S = 8.88734D-03 GF = 3.87689D-08 AKI = 7.52313D+01

3 -263.27978159 1s(2).2s(2).2p(3)4S3_4S
 3 -259.52411616 1s(2).2p(5)_2P
 824273.28 CM-1 121.32 ANGS(VAC) 121.32 ANGS(AIR)
 M1 S = 3.31695D-06 GF = 1.10562D-10 AKI = 1.25265D+01

3 -262.95505309 1s(2).2s(2).2p(3)2D3_2D
 3 -262.78827179 1s(2).2s(2).2p(3)2P1_2P
 36604.27 CM-1 2731.92 ANGS(VAC) 2731.63 ANGS(AIR)
 M1 S = 6.39783D-02 GF = 9.47020D-08 AKI = 2.11595D+01

3 -262.95505309 1s(2).2s(2).2p(3)2D3_2D
 3 -259.52411616 1s(2).2p(5)_2P
 753003.62 CM-1 132.80 ANGS(VAC) 132.80 ANGS(AIR)
 M1 S = 3.34448D-06 GF = 1.01841D-10 AKI = 9.62936D+00

3 -262.78827179 1s(2).2s(2).2p(3)2P1_2P
 3 -259.52411616 1s(2).2p(5)_2P
 716399.35 CM-1 139.59 ANGS(VAC) 139.59 ANGS(AIR)
 M1 S = 2.90939D-08 GF = 8.42854D-13 AKI = 7.21349D-02

3 -263.27978159 1s(2).2s(2).2p(3)4S3_4S
 5 -262.95381813 1s(2).2s(2).2p(3)2D3_2D
 71540.71 CM-1 1397.81 ANGS(VAC) 1397.81 ANGS(AIR)
 M1 S = 1.21485D-05 GF = 3.51456D-11 AKI = 1.99972D-02

3 -262.95505309 1s(2).2s(2).2p(3)2D3_2D
 5 -262.95381813 1s(2).2s(2).2p(3)2D3_2D
 271.04 CM-1 368946.28 ANGS(VAC) 368908.14 ANGS(AIR)
 M1 S = 2.36306D+00 GF = 2.59004D-08 AKI = 2.11530D-04

5 -262.95381813 1s(2).2s(2).2p(3)2D3_2D
 3 -262.78827179 1s(2).2s(2).2p(3)2P1_2P
 36333.22 CM-1 2752.30 ANGS(VAC) 2752.01 ANGS(AIR)
 M1 S = 3.63575D-02 GF = 5.34187D-08 AKI = 1.17594D+01


```
5 -262.95381813 1s(2).2s(2).2p(3)2D3_2D
3 -259.52411616 1s(2).2p(5)_2P
752732.58 CM-1      132.85 ANGS(VAC)      132.85 ANGS(AIR)
M1 S = 1.88252D-06  GF = 5.73026D-11  AKI = 5.41425D+00
```

Here labels of the upper and lower states in the transition are in LSJ -notation. In addition to transition energies in cm^{-1} also the wave lengths (vacuum and air) are given in Angstrom. On the next line the line strength S , the weighted oscillator strength gf and the transition rate A are given. The format is the same as the one produced by the transition program of the ATSP2K package [C. Froese Fischer, G. Tachiev, G. Gaigalas, and M. R. Godefroid, *Comput. Phys. Commun.* 176, 559-579 (2007).]

Chapter 5

Case study: $2s^22p$, $2s2p^2$ in Mo XXXVIII using scripts

In this case study we use script files to perform systematic calculations for all the states of the $2s^22p$ and $2s2p^2$ configurations in Mo XXXVIII. The 10 states are as follows:

odd: $2s^22p^2P_{1/2,3/2}$

even: $2s2p^2^4P_{1/2,3/2,5/2}$, $2s2p^2^2D_{3/2,5/2}$, $2s2p^2^2P_{1/2,3/2}$, $2s2p^2^2S_{1/2}$

The script files can be found in `manual\casestudy`. Output files from the runs are available in the same directory.

In a real application a correlation model should be defined, i.e. some rule to generate the CSFs from an orbital set. The convergence of computed properties is then monitored as the orbital set is increased. For the odd state a reasonable correlation model is to start from the $\{1s^22s^22p, 1s^22p^3\}$ multireference and then generate all CSFs that can be obtained by single- and double- excitations from the multireference to an active set of orbitals. The active set of orbitals is then systematically increased. Following the normal conventions the orbital set is denoted by the highest principal quantum number. For example $n = 3$ means the orbital set $\{1s, 2s, 2p, 3s, 3p, 3d\}$. In this study we increase the active set of orbitals up to $n = 6$. For the even states we start from the $1s^22s2p^2$ reference and generate all CSFs that can be obtained by single- and double- excitations from the multireference to the active sets of orbitals. The correlation model can be easily be extended by adding CSFs to the multireference.

5.1 Running script files

To automate the calculations we use script files. For convenience we have a main script that calls subscripts to perform different tasks. The construction of the scripts is greatly simplified if the names of the files are chosen in a simple and systematic way. In the case study we use the names `odd2`, `odd3`, `odd4`, `odd5`, `odd6` and `even2`, `even3`, `even4`, `even5`, `even6` to denote files for the odd and even parity states, respectively. The digit indicates which orbital set has been used to generate the expansion.

Before starting please note that the scripts assume that the environment variable `GRASP` has been set. If you compiled GRASP2K with the gfortran compiler this is done by issuing the command

```
source ./make_environment_gfort
```

in the GRASP2K installation directory. Issue similar commands if you have compiled with the ifort or portland compiler.

The main script `sh_grasp2K_case` is shown below. This script controls the computational flow and calls several subscripts.

```
#!/bin/sh

set -x

#   Main script for 2s(2)2p and 2s2p(2)

# 1.   Generate the expansions
      ./sh_files_c

# 2.   Get the nuclear data
      ./sh_iso

# 3.   Get screened hydrogenic orbitals as initial estimates
      ./sh_initial

# 4.   Perform scf calculations and a final rci calculation that
#       includes the Breit correction and QED
      ./sh_scf

# 5.   Transform ASF from jj-coupling to LSJ-coupling
      ./sh_jj2lsj

# 6.   Perform a transition calculation
      ./sh_tr
```

Each of the subscripts are given below together with some comments.

If all script files are available with execute permission (use the command `chmod +x`) we start the computation by typing the name of the main script

```
./sh_grasp2K_case
```

Please note that these calculations will take several hours to finish!

1. Generate expansions

The expansions are generated by the script `sh_files_c`. This is by far the most complicated script. Once the scripts for the smallest expansions (odd2, odd3 and even2, even3) are tested and running the remaining part can be obtained by cut and paste with minor modifications.

```
#!/bin/sh
set -x

# 1.   Generate grasp2K expansions
#       1.1 HF for 2s(2)2p

$GRASP/bin/jjgen << EOF
*
*
2
p
*
*
```

```
2
*
2
2
1
1,3
0
y
2
p
*
*
2
2
0
3
1,3
0
*
EOF
```

```
mv clist.out rcsl.inp
$GRASP/bin/jsplit << EOF
n
EOF
```

```
mv rcsl.out odd2.c
```

```
#          1.2 SD-MR for n=3
```

```
$GRASP/bin/jjgen <<EOF
*
*
3
d
*
*
2
*
2
2
1
1,3
2
y
3
d
*
*
2
2
0
3
1,3
```

```
2
*
EOF
```

```
mv clist.out rcs1.inp
$GRASP/bin/jsplit <<EOF
n
EOF
```

```
mv rcs1.out odd3.c
```

```
#          1.3 SD-MR for n=4
```

```
$GRASP/bin/jjgen <<EOF
```

```
*
*
4
f
*
*
2
*
2
2
1
1,3
2
y
4
f
*
*
2
2
0
3
1,3
2
*
EOF
```

```
mv clist.out rcs1.inp
$GRASP/bin/jsplit <<EOF
n
EOF
```

```
mv rcs1.out odd4.c
```

```
#          1.4 SD-MR for n=5
```

```
$GRASP/bin/jjgen <<EOF
```

```
*
*
5
```

```
g
*
*
2
*
2
2
1
1,3
2
y
5
g
*
*
2
2
0
3
1,3
2
*
EOF
```

```
mv clist.out rcsl.inp
$GRASP/bin/jsplit <<EOF
n
EOF
```

```
mv rcsl.out odd5.c
```

```
#          1.5 SD-MR for n=6
```

```
$GRASP/bin/jjgen <<EOF
*
*
6
h
*
*
2
*
2
2
1
1,3
2
y
6
h
*
*
2
2
```

```
0
3
1,3
2
*
EOF
```

```
mv clist.out rcs1.inp
$GRASP/bin/jsplit <<EOF
n
EOF
```

```
mv rcs1.out odd6.c
```

```
# 1. Generate grasp2K expansions
# 1.6 HF for 2s2p(2)
```

```
$GRASP/bin/jjgen << EOF
*
*
2
P
*
*
2
*
2
1
2
1,5
0
*
EOF
```

```
mv clist.out rcs1.inp
$GRASP/bin/jsplit << EOF
n
EOF
```

```
mv rcs1.out even2.c
```

```
# 1.7 SD-MR for n=3
```

```
$GRASP/bin/jjgen <<EOF
*
*
3
d
*
*
2
*
2
1
```



```
2
1,5
2
*
EOF
```

```
mv clist.out rcs1.inp
$GRASP/bin/jsplit <<EOF
n
EOF
```

```
mv rcs1.out even3.c
```

```
#          1.8 SD-MR for n=4
```

```
$GRASP/bin/jjgen <<EOF
*
*
4
f
*
*
2
*
2
1
2
1,5
2
*
EOF
```

```
mv clist.out rcs1.inp
$GRASP/bin/jsplit <<EOF
n
EOF
```

```
mv rcs1.out even4.c
```

```
#          1.9 SD-MR for n=5
```

```
$GRASP/bin/jjgen <<EOF
*
*
5
g
*
*
2
*
2
1
2
1,5
```

```
2
*
EOF
```

```
mv clist.out rcsl.inp
$GRASP/bin/jsplit <<EOF
n
EOF
```

```
mv rcsl.out even5.c
```

```
# 1.10 SD-MR for n=6
```

```
$GRASP/bin/jjgen <<EOF
```

```
*
*
6
h
*
*
2
*
2
1
2
1,5
2
*
EOF
```

```
mv clist.out rcsl.inp
$GRASP/bin/jsplit <<EOF
n
EOF
```

```
mv rcsl.out even6.c
```

2. Get nuclear data

Nuclear data are defined by the script `sh_iso`. Since we are not interested in hyperfine structure the nuclear spin and moments have all been set to 1.

```
#!/bin/sh
set -x
```

```
# 2. Get isodata
$GRASP/bin/iso <<S1
42
96
n
96
1
1
1
```

```
S1
```

```
cat isodata
```

3. Get initial estimates

The script `sh_initial` performs angular integration, gets initial estimates and performs scf calculations for the odd and even reference states (odd2 and even2). As initial estimates we use screened hydrogenic functions. For the reference states all orbitals are required to be spectroscopic, i.e. they should have the correct number of nodes.

```
#!/bin/sh
set -x

# 3. For n=2, Get initial estimates for odd.

cp odd2.c rcs1.inp
$GRASP/bin/mcp3 <<S4
y
S4

# Get initial estimates of wave functions
$GRASP/bin/erwf <<S5
y
3
*
S5

# Perform self-consistent field calculations
$GRASP/bin/rscf2 <<S6
y
y
1
1
5
*
*
100
S6

# Save the result to odd2
$GRASP/bin/rsave odd2

# 3. For n=2, Get initial estimates for even

cp even2.c rcs1.inp
$GRASP/bin/mcp3 <<S4
y
S4

# Get initial estimates of wave functions
$GRASP/bin/erwf <<S5
y
3
```

```

*
S5

# Perform self-consistent field calculations
$GRASP/bin/rscf2 <<S6
y
y
1,2,3
1,2,3
1,2
5
*
*
100
S6

# Save the result to even2
$GRASP/bin/rsave even2

```

4. Scf calculations and rci

The script `sh_scf` performs angular integration, estimates the new radial functions and performs self-consistent field calculations for the odd and even states up to $n = 6$. At the end CI calculations are performed for the largest expansions. The CI calculations include Breit interaction and QED corrections. In the script, note how we loop over the digit n that indicates the size of the orbital set.

```

#!/bin/sh
set -x

# 4. Get results for odd n=3,4,5,6

for n in 3 4 5 6
do
  (cp odd${n}.c rcs1.inp

# Get angular data
$GRASP/bin/mcp3 <<S4
y
S4

# Get initial estimates of wave functions
m='expr $n - 1'
echo m=$m n=$n
$GRASP/bin/erwf <<S5
y
1
odd${m}.w
*
3
*
S5

# Perform self-consistent field calculations

```

```

$GRASP/bin/rscf2 > out_rscf2_${n} <<S6
y
y
1
1
5
${n}*

100
S6

$GRASP/bin/rsave odd${n}

    echo)
done

# Perform Breit-correction using CI for n=6

n=6
$GRASP/bin/rci3 <<S7
y
odd${n}
y
y
1.d-6
y
n
n
y
4
1
1
S7

# 4. Get results for even n=3,4,5,6

for n in 3 4 5 6
do
    (cp even${n}.c rcs1.inp

# Get angular data
$GRASP/bin/mcp3 <<S4
y
S4

# Get initial estimates of wave functions
m='expr $n - 1'
echo m=$m n=$n
$GRASP/bin/erwf <<S5
y
1
even${m}.w
*
3

```

```

*
S5

# Perform self-consistent field calculations
$GRASP/bin/rscf2 > out_rscf2_${n} <<S6
y
y
1,2,3
1,2,3
1,2
5
${n}*

100
S6

$GRASP/bin/rsave even${n}

    echo)
done

# Perform Breit-correction using CI for n=6

n=6
$GRASP/bin/rci3 <<S7
y
even${n}
y
y
1.d-6
y
n
n
y
4
1,2,3
1,2,3
1,2
S7

```

5. Transform to LSJ-coupling

The script `sh_jj2lsj` transforms from *jj*- to *LSJ*-coupling.

```

#!/bin/sh
set -x

# 5. Get LSJ coupling

n=6
$GRASP/bin/jj2lsj > out_jj2lsj_odd${n} <<S1
odd${n}
y
y

```

S1

```
$GRASP/bin/rlevels odd${n}.cm > out_rlevels_odd${n} <<S2
S2
```

```
n=6
$GRASP/bin/jj2lsj > out_jj2lsj_even${n} <<S1
even${n}
y
y
S1
```

```
$GRASP/bin/rlevels even${n}.cm > out_rlevels_even${n} <<S2
S2
```

6. Perform a transition calculation

The script `sh_tr` computes the E1 transition rates between the odd and even states. First we perform a biorthogonal transformation and then we perform the transition calculation itself.

```
#!/bin/sh
set -x

# 6. Perform transition calculation for the n=6 CI results

n=6

# First the biorthogonal rotations

$GRASP/bin/biotra3 > out_biotra <<EOF
y
y
odd$n
even$n
y
EOF

# Then the transition calculations

$GRASP/bin/bioscl3 > out_bioscl <<EOF
y
n
odd$n
even$n
E1
EOF
```

5.2 Comparison with experiment

To display the computed energies we give the command

```
rlevels odd6.cm even6.cm
```

The computer returns the energies together with labels in *LSJ*-coupling for all the states.

```

nblock =          2   ncftot =          20641   nw =          36   nelec =          5
nblock =          3   ncftot =          36290   nw =          36   nelec =          5

```

Energy levels for ...

Rydberg constant is 109737.31534

Splitting is the energy difference with the lower neighbor

| No | Pos | J | Parity | Energy Total (a.u.) | Levels (cm ⁻¹) | Splitting (cm ⁻¹) | Configuration |
|----|-----|-----|--------|------------------------|-------------------------------|----------------------------------|-------------------------|
| 1 | 1 | 1/2 | - | -2386.3192492 | 0.00 | 0.00 | 1s(2).2s(2).2p_2P |
| 2 | 1 | 1/2 | + | -2382.2384104 | 895640.59 | 895640.59 | 1s(2).2s_2S.2p(2)3P2_4P |
| 3 | 1 | 3/2 | - | -2381.9234302 | 964770.76 | 69130.17 | 1s(2).2s(2).2p_2P |
| 4 | 1 | 3/2 | + | -2378.9978407 | 1606863.43 | 642092.67 | 1s(2).2s_2S.2p(2)3P2_4P |
| 5 | 1 | 5/2 | + | -2378.1468367 | 1793637.20 | 186773.77 | 1s(2).2s_2S.2p(2)3P2_4P |
| 6 | 2 | 3/2 | + | -2376.7262038 | 2105430.10 | 311792.89 | 1s(2).2s_2S.2p(2)1D2_2D |
| 7 | 2 | 1/2 | + | -2376.5304790 | 2148386.73 | 42956.63 | 1s(2).2s_2S.2p(2)3P2_2P |
| 8 | 2 | 5/2 | + | -2373.9005645 | 2725586.24 | 577199.51 | 1s(2).2s_2S.2p(2)1D2_2D |
| 9 | 3 | 1/2 | + | -2371.8997599 | 3164712.08 | 439125.84 | 1s(2).2s_2S.2p(2)1S0_2S |
| 10 | 3 | 3/2 | + | -2371.8553153 | 3174466.55 | 9754.47 | 1s(2).2s_2S.2p(2)3P2_2P |

The Mo XXXVIII transitions have been observed in the JET Tokamak, Myrnäs *et al.* 1993 <http://www.iop.org/Jet/fulltext/JETP93072.pdf>. In the table below the experimental transition energies are compared with the calculated energies. Please note that the quantum labels for the $2s2p^2\ ^2P_{1/2}$ and $2s2p^2\ ^2S_{1/2}$ seem to have been swapped in the experimental paper, i.e. the highest $J = 1/2$ state should be $2s2p^2\ ^2S_{1/2}$ and not $2s2p^2\ ^2P_{1/2}$. We see that the odd states are somewhat too high. This is due to an imbalance in the multireference. As discussed in the beginning of the chapter the correlation model can be refined by extending the multireference. Adopting the multireferences $\{2s^22p, 2p^3, 2s2p3d, 2p^33d\}$ and $\{2s^22p, 2p^23d, 2s^23d, 2s3d^2\}$ for, respectively, the odd and even parity states improves the energy separations considerably [P. Rynkun, P. Jönsson, and G. Gaigalas, Atomic Data and Nuclear Data Tables, **98** 481 (2012)]. A careful investigation of the effects of increasing the multireference is part of any systematic calculation.

| State | Experiment | Calculation |
|---------------------|------------------|-------------|
| $2s^22p\ ^2P_{1/2}$ | 0 | 0 |
| $2s2p^2\ ^4P_{1/2}$ | 894 050 ± 400 | 895 848 |
| $2s^22p\ ^2P_{3/2}$ | 964 050 ± 90 | 964 715 |
| $2s2p^2\ ^4P_{3/2}$ | | 1 606 863 |
| $2s2p^2\ ^4P_{5/2}$ | 1 790 130 ± 200 | 1 793 682 |
| $2s2p^2\ ^2D_{3/2}$ | 2 102 900 ± 900 | 2 106 354 |
| $2s2p^2\ ^2P_{1/2}$ | 2 147 300 ± 900 | 2 149 456 |
| $2s2p^2\ ^2D_{5/2}$ | | 2 725 586 |
| $2s2p^2\ ^2S_{1/2}$ | 3 164 770 ± 1500 | 3 166 168 |
| $2s2p^2\ ^2P_{3/2}$ | 3 171 300 ± 1500 | 3 175 559 |

5.3 Transition rates

Below are the transition rates as given in the file `odd6.even6.ct.lsj`. The agreement between calculated values in the two gauges is quite good, specially for the strong transitions. Expansions based on a larger multireference will further improve the agreement.

Transition between files:

odd6

even6

1-2386.31924920 1s(2).2s(2).2p_2P
 1-2382.23841041 1s(2).2s_2S.2p(2)3P2_4P
 895640.59 CM-1 111.65 ANGS(VAC) 111.65 ANGS(AIR)
 E1 S = 4.42136D-03 GF = 1.20286D-02 AKI = 3.21806D+09 dT = 0.05151
 4.66146D-03 1.26818D-02 3.39281D+09

1-2386.31924920 1s(2).2s(2).2p_2P
 1-2376.53047897 1s(2).2s_2S.2p(2)3P2_2P
 2148386.74 CM-1 46.55 ANGS(VAC) 46.55 ANGS(AIR)
 E1 S = 1.87909D-02 GF = 1.22627D-01 AKI = 1.88766D+11 dT = 0.00414
 1.88691D-02 1.23137D-01 1.89551D+11

1-2386.31924920 1s(2).2s(2).2p_2P
 1-2371.89975994 1s(2).2s_2S.2p(2)1S0_2S
 3164712.09 CM-1 31.60 ANGS(VAC) 31.60 ANGS(AIR)
 E1 S = 1.51562D-05 GF = 1.45696D-04 AKI = 4.86664D+08 dT = 0.06894
 1.62784D-05 1.56485D-04 5.22700D+08

1-2386.31924920 1s(2).2s(2).2p_2P
 3-2378.99784066 1s(2).2s_2S.2p(2)3P2_4P
 1606863.44 CM-1 62.23 ANGS(VAC) 62.23 ANGS(AIR)
 E1 S = 1.11563D-04 GF = 5.44535D-04 AKI = 2.34458D+08 dT = 0.01688
 1.13479D-04 5.53886D-04 2.38485D+08

1-2386.31924920 1s(2).2s(2).2p_2P
 3-2376.72620380 1s(2).2s_2S.2p(2)1D2_2D
 2105430.10 CM-1 47.50 ANGS(VAC) 47.50 ANGS(AIR)
 E1 S = 2.45759D-02 GF = 1.57172D-01 AKI = 1.16182D+11 dT = 0.00643
 2.47350D-02 1.58190D-01 1.16934D+11

1-2386.31924920 1s(2).2s(2).2p_2P
 3-2371.85531532 1s(2).2s_2S.2p(2)3P2_2P
 3174466.55 CM-1 31.50 ANGS(VAC) 31.50 ANGS(AIR)
 E1 S = 6.34291D-04 GF = 6.11623D-03 AKI = 1.02780D+10 dT = 0.00528
 6.30940D-04 6.08392D-03 1.02237D+10

1-2382.23841041 1s(2).2s_2S.2p(2)3P2_4P
 3-2381.92343016 1s(2).2s(2).2p_2P
 69130.17 CM-1 1446.55 ANGS(VAC) 1446.55 ANGS(AIR)
 E1 S = 5.06276D-04 GF = 1.06311D-04 AKI = 8.47221D+04 dT = 0.18819
 4.11000D-04 8.63046D-05 6.87783D+04

3-2381.92343016 1s(2).2s(2).2p_2P
 1-2376.53047897 1s(2).2s_2S.2p(2)3P2_2P
 1183615.97 CM-1 84.49 ANGS(VAC) 84.49 ANGS(AIR)
 E1 S = 2.36462D-03 GF = 8.50151D-03 AKI = 3.97219D+09 dT = 0.05226
 2.49501D-03 8.97033D-03 4.19124D+09

3-2381.92343016 1s(2).2s(2).2p_2P
 1-2371.89975994 1s(2).2s_2S.2p(2)1S0_2S
 2199941.33 CM-1 45.46 ANGS(VAC) 45.46 ANGS(AIR)

```

E1 S = 1.48021D-02 GF = 9.89142D-02 AKI = 1.59659D+11 dT = 0.00260
      1.47635D-02      9.86566D-02      1.59243D+11

3-2381.92343016 1s(2).2s(2).2p_2P
3-2378.99784066 1s(2).2s_2S.2p(2)3P2_4P
642092.68 CM-1      155.74 ANGS(VAC)      155.74 ANGS(AIR)
E1 S = 1.00858D-03 GF = 1.96712D-03 AKI = 1.35241D+08 dT = 0.11530
      1.14003D-03      2.22350D-03      1.52867D+08

3-2381.92343016 1s(2).2s(2).2p_2P
3-2376.72620380 1s(2).2s_2S.2p(2)1D2_2D
1140659.34 CM-1      87.67 ANGS(VAC)      87.67 ANGS(AIR)
E1 S = 2.73256D-03 GF = 9.46782D-03 AKI = 2.05421D+09 dT = 0.04984
      2.87589D-03      9.96443D-03      2.16195D+09

3-2381.92343016 1s(2).2s(2).2p_2P
3-2371.85531532 1s(2).2s_2S.2p(2)3P2_2P
2209695.79 CM-1      45.26 ANGS(VAC)      45.26 ANGS(AIR)
E1 S = 4.49451D-02 GF = 3.01675D-01 AKI = 2.45633D+11 dT = 0.00388
      4.51204D-02      3.02851D-01      2.46591D+11

3-2381.92343016 1s(2).2s(2).2p_2P
5-2378.14683675 1s(2).2s_2S.2p(2)3P2_4P
828866.45 CM-1      120.65 ANGS(VAC)      120.65 ANGS(AIR)
E1 S = 9.97374D-03 GF = 2.51112D-02 AKI = 1.91790D+09 dT = 0.08157
      1.08596D-02      2.73415D-02      2.08825D+09

3-2381.92343016 1s(2).2s(2).2p_2P
5-2373.90056450 1s(2).2s_2S.2p(2)1D2_2D
1760815.48 CM-1      56.79 ANGS(VAC)      56.79 ANGS(AIR)
E1 S = 1.52579D-02 GF = 8.16083D-02 AKI = 2.81289D+10 dT = 0.01678
      1.55183D-02      8.30007D-02      2.86088D+10

```