ATOMCI

Input & Output Documentation

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Acknowledgments

The first version of ATOMCI was prepared in 1972 at the IBM Research Center in San Jose. In the present version of ATOMCI the routines for the generation of the energy expression have been completely rewritten to increase the speed and decrease the disk space requirements of the code. Routines for the perturbative selection of the configurations have been implemented, and high performance code for the diagonalization, written by N. Kosugi, has been used. Dr. Nagashima helped in preparing the ATGEN utility.

Introduction

ATOMCI is a Configuration Integration, CI, program for atoms in the Russell-Saunders coupling scheme. The method for the calculation of the matrix elements is based on the vacuum expectation value of tensor operators and on the recoupling transformation coefficients (F. Sasaki, IJQC, **8**, 605, (1974); F. Sasaki, M. Sekiya, T. Noro, K. Ohtsuki and Y. Osanai, in "Methods and Techniques in Computational Chemistry: METECC-94", E. Clementi ed., STEF, Cagliari, 1993, pp 163-219). A conventional formula tape approach is used for the construction of the Hamiltonian matrix.

The reader should refer to the "Overall Installation Guide" which came with the MOTECC tape for specific instructions on how to load the ATOMCI package on RS/6000. The package inserted in METECC-94 includes the actual ATOMCI program, FPL (Fortran Preprocessing Language) program, and two utilities which allow to prepare the coefficients of fractional parentage (CFP) table and the configuration state functions (CSF) input data for a Singles and Doubles CI, SD-CI, calculation.

The contents of directory (See README in the directory atomci)

seed	Shell script for making ATOMCI, ATGEN, CFP table and FPL.
root	Makefiles, shell scripts, manual of FPL and some sample input.
source	Source files for ATOMCI, ATGEN, CFPA, CFPB, and FPL.
include	Include files for ATOMCI.
utility	utility files.
fplincl	Include files for FPL.
output	output files of the sample input.

Overview of ATOMCI

Features

The following features are available in the present version of the program :

1. Full exploitation of the atomic symmetry.
2. Use of Slater Type Functions with azimuthal quantum number l up to 9 or of Gaussian Type Functions with l up to 7.
3. Doing SCF calculation or MCSCF calculation with restrictions: different CSF's must differ by an even shell occupation number in each other.
4. Possibility of doing either a general CI calculation or a SD-CI calculation.
5. Perturbative selection of the most important configurations and estimate of the contribution to the energy from the rejected CSF.
6. Analysis of the contribution to the total energy from individual CSF.
7. Determination of the Natural Orbitals, NO's, with estimation of the contribution from each NO to the total energy.
8. Determination of the first order density matrices.

Limits

This version of the code can handle up to 150 basis functions. The table of coefficient of fractional parentage (CFP table) computed through the CFPA and CFPB utilities is extended up to the m shell. ATOMCI cannot handle configurations with an occupation number greater than two in each single shell having $l > 3$ (beyond the f shell), i.e. for instance a configuration including a $5g^3$ shell is not allowed, but a combination of shells including more than two shells with $l > 3$ is permitted provided that the total number of open shells in the resulting configuration does not exceed 10. The program has been conceived as "open ended", with eight independent steps each one connected to the others through I/O files, and thus any other limitation is dictated in principle by the memory size requirements.

Memory management and memory size requirements

The core memory is dynamically allocated at the time of execution. The dimensions in the main codes are defined so that ATGEN can run with 8Mbytes and ATOMCI with 32Mbytes of allocated core memory. Should the memory be insufficient to run a specific case, the program will stop and in most cases a warning message indicating the required amount of core memory will be printed. The user should then change to the appropriate value the constant MCORE, in the include/PARAM file, MCORE gives the size of the work memory in single precision words. The source codes require an average of 2 to 4 Megabytes of memory to load, exclusive of the dynamically allocated part. Thus for the version provided here an approximate 12Mbytes and 36Mbytes of memory are sufficient for ATGEN and ATOMCI respectively. ATOMCI will not be able to run if the dynamically allocated

memory is less than 8Mbytes. ATGEN requires a minimum of 2Mbytes of dynamically allocated memory.

Restart capabilities for ATOMCI

The program being structured in eight separate steps connected through I/O files, it can be stopped and restarted by enabling the run options for the appropriate steps (see &CNTL NAMELIST) and by providing all the necessary file informations. The user should refer to the 'I/O files description' section of this documentation for a list of the files allocated in an ATOMCI run and their use and contents.

If the program stops within the AIMAIN, MCMAIN, or WFMAIN routines, it should be restarted from the beginning. Actually, when RULE=1 and the program stops within WFMAIN, it is possible to restart from EXMAIN with RETRY=1 (i.e. set NRNFG(3)=0, NRNFG(6)=1 in the &CNTL NAMELIST and RETRY=1 in the &EX NAMELIST). Refer to the description of the &CNTL , &WF and &EX NAMELIST for a description of NRNFG, RULE and RETRY variables respectively.

A restart within TRMAIN requires the existence of the atomic orbitals integrals file (unit NFAII, usually number 18).

To restart the execution within the PTMAIN module, units NFWFP (energy expression for the Perturbative Selection, usually number 14) and NFTRI (transformed integrals, usually number 16) should be supplied.

When the user wants to continue the execution with the EXMAIN routines, it has to furnish units NFPTB (selected CSF, usually number 11) if RULE=2 or unit NFWFB0 (CSF list for general CI, usually number 11) if RULE=0. For informations on how to restart after an abort occurred within EXMAIN the user is referred to the paragraph on the description of the &EX NAMELIST.

Restarting after an abort occurred within the CIMAIN step implies supplying several files, i.e. units NFTRI, NFTRC1 (the transformation coefficients, usually number 27), NFWFE (the energy expression file, usually number 15), NFCIV (the CI vector, usually number 37), NFCIH1, NFCIH2 (the Hamiltonian matrix, usually numbers 38 and 39). By supplying the necessary file informations, the user should be able to restart from any of the sections of the CIMAIN step (see NRNFG input data in the discussion of the &CI NAMELIST).

Finally, the execution can restart from within RSMAIN if units NFCIS (CI summary file, usually number 71), NFPTB and NFPTH1 and NFPTH2 exist.

Input

No input data are required for CFP. The user will use this utility when installing the ATOMCI package, to create the CFP table, and rerun it only to regenerate the table should it be necessary. In the following a detailed description of the input which should be supplied by the user for ATGEN and ATOMCI is given.

Input for FDOPEN

This UNIX versions have file allocatiton routine, FDOPEN.

1. KEYWORD (Uppercase only)

   UNIT= unit number
   FILE= file-name STATUS={UNKNOWN,OLD,NEW}
   OPEN
   CLOSE
   BINARY
   SCRATCH
   END

2. Typical usage

   You should set input of FDOPEN at the top of the standard input file. If you put the command of "OPEN UNIT=5", the present input file is automatically closed without END keyword and all the data after the command of "OPEN UNIT=5" in this input file are ignored. The data will be read from the file given by UNIT=5. If you do not put "OPEN UNIT=5", you should put the keyword "END" at the end of OPEN file definitions. The data of atomci should be followed.

   If you set the symbol of " at the top of columns, this line is recognized as the comment card and it is skipped.

   a) Formatted, OLD files(STATUS=UNKNOWN is default)
   OPEN UNIT=2 FILE=f.orb STATUS=OLD

   b) Unformatted binary files
   OPEN UNIT=10 FILE=/home/user/etc/CFPTBL BINARY

   c) Unformatted SCRATCH files
   OPEN UNIT=14 SCRATCH

3. Example

   OPEN UNIT=7 FILE=HISTORY STATUS=UNKNOWN
   " Comment line
   OPEN UNIT=10 FILE=/home/user/etc/CFPTBL BINARY
   OPEN UNIT=11 SCRATCH
   OPEN UNIT=15 FILE=EE01 BINARY
   END
   " atomci or atgen input

4. Example

   OPEN UNIT=7 FILE=HISTORY STATUS=UNKNOWN
   OPEN UNIT=10 FILE=/home/user/etc/CFPTBL BINARY
   OPEN UNIT=11 SCRATCH
   OPEN UNIT=15 FILE=EE01 BINARY
   OPEN UNIT=5 FILE=ATOMCI.INPUT STATUS=OLD

" ATOMCI.INPUT is swiched by new INPUT file

ATGEN is an utility program which should be used to generate the input

Input for ATGEN

ATGEN is an utility program which should be used to generate the input data of the CSF for a SD-CI calculation. In general the list of CSF in a CI run needs to be keyed in by the user and inserted after the &WF NAMELIST set of data in the ATOMCI input file. The reader is referred to the discussion of the 'Input data for the CSF' section for a description of the input conventions. For the case of SD-CI calculation the list may be much more conveniently generated by using ATGEN. The user needs only to supply informations on the characteristics of the occupied and of the correlating orbitals, on the reference configurations and on the order of coupling. ATGEN will provide in output the full list of CSF, in the correct format to be used in input for the subsequent run of ATOMCI. All the possible configurations which may be obtained by single or double excitations from the occupied orbitals in the reference to all correlating orbitals are generated. A check is done on the correct parity of the resulting CSF, but no check is done on the correct spin or spatial symmetries. The list will thus be in general larger than necessary, including configurations giving rise to CSF of all possible spin and spatial symmetry types. CSF of the wrong spin-spatial symmetry are discarded by ATOMCI in the WFMAIN step, and thus the appearance of unnecessary configurations in the ATGEN output file is not harmful.

The input to ATGEN consists in series of cards in free format. Lines with the '"' character in the first column are treated as comment lines. Lines with a blank on the first column are considered as valid input cards. Each input card ends with a ')))' sequence.

As an example we will refer to the ATGEN input file supplied with the ATOMCI package.

CARDS

CARD 1 Number and symmetries of the correlating orbitals.

List here the number of correlating orbitals for each symmetry and the corresponding symmetry label. The orbitals must be listed in ascending quantum orbital momentum number (i.e. *s, p, d, f* ... etc.) and in order to be able to include orbitals with quantum angular momentum l at least one correlating orbital for each quantum number from 0 to l-1 has to be included (i.e. one cannot include *g* orbitals in the correlating space without including at least one correlating orbital for each of the *s, p, d* and *f* symmetries). Limit the number of correlating orbitals in each symmetry type to less than 40.

A valid input is for example

2S 2P 2D 2F)))

which indicates that two orbitals on each of the *s, p, d* and *f* symmetries constitute the

correlating space. All single and double excitations from the reference orbitals to these orbitals will be generated.

CARD 2 Occupied orbitals in the reference configurations.

Input here the orbitals which are used to specify the reference configurations. Arrange the orbitals with ascending order of principal quantum number and angular momentum. Do not list frozen core orbitals. Since, as previously specified, shells with $l > 3$ cannot have an occupation number > 2 in ATOMCI, orbitals with azimuthal quantum number > 3 should not be occupied in the reference configurations.

In ATGEN, for example:

2S 2P 3P)))

which indicates that the 2s, 2p and 3s orbitals will be included in the reference configurations listed in the following input cards.

CARD 3 Reference state configurations.

The reference configurations are input using the following conventions

1. The orbitals must be arranged in ascending order of principal quantum number and angular momentum.
2. The occupation of each orbital (say n) is indicated by typing '*n' after the orbital label.
3. Each shell is separated from the other by a ')' character.
4. An extra ')' separates two configurations.
5. A ')))' sequence ends the list of configurations.

The frozen core orbitals should not be included.

For example

2S*2) 2P*4) 3P*0))
2S*2) 2P*3) 3P*1))
)))

is the correct input for a reference including the $(2s)^2$ $(2p)^4$ and the $(2s)^2$ $(2p)^3$ (3p) configurations.

CARD 4 Order of coupling.

Input here the order in which the shells in the reference configurations will be coupled (in the Russell-Saunders scheme). Use the same input conventions of CARD 2. If the coupling order is the same as the one used in CARD 2, simply type ')'.

In our example, for instance,

2S 2P 3P)))

or

)

could be used equivalently to indicate that the 2s shell should be first coupled to the 2p, and the resulting multiplet should then be coupled to the 3p. Notice that, while the order in CARD 2 is fixed (ascending order in principal and azimuthal quantum numbers), the user is free to choose his own coupling order in CARD 4, i.e.

2P 2S 3P)))

is another valid choice for our example. Notice also that the order chosen at this moment must be maintained and reproduced in the ATOMCI input (see &TR NAMELIST).

CARD 5 Frozen Core.

List here the orbitals which will be maintained frozen (no excitations allowed from them). For this and the next card no termination symbol is needed.

Example

1S

which states that the 1s orbital will be doubly occupied in each excited configuration.

CARD 6 End of Input

The ATGEN input ends with either a -1 or 0 in CARD 6. ATGEN will insert a ')' between the reference state configurations and the singly and doubly excited configurations if -1 is entered in CARD 6. The parenthesis is required by ATOMCI when RULE > 0 in the &WF NAMELIST input data (see &WF NAMELIST). No extra ')' will be inserted when 0 is input in CARD 6. The resulting list of configurations in this case could be used either as part of an input for a general CI (RULE=0) or for another run of ATGEN, for instance to generate triple and/or quadruple excitations from the initial reference state.

Input for ATOMCI

Free format NAMELIST are used to input the data to ATOMCI. Lines beginning with '"' are treated as comment lines. Informations on the run are contained in the initial &CNTL NAMELIST. Each one of the eight steps requires a NAMELIST input data. A description of all the NAMELIST follows. Special attention will be given to the conventions used to supply the list of configurations, the basis set and the orbital coefficients.

The user will probably notice by looking at the code that the list of variables included in each NAMELIST instruction is much larger than it appears from the contents of these documentation notes. Only those variables which will be used in normal, problem-free applications shall be documented here. The remaining variables are intended for debug purposes, or in some cases for the

purpose of rearranging sizes and structure of the arrays in the dynamically allocated memory. The default values in the present version of the program should be sufficient to handle all possible cases. The user should contact us if problems arise.

The eight steps of ATOMCI being independent from each other, options are provided to change the unit number for each of the relevant I/O files at each step in the execution. A list of the unit names, numbers and file contents is given in a following section of this documentation. Of course for a normal run the default values for the unit numbers are more than appropriate, and the user should not have reasons to modify them. Changing the unit number for a file at the time of execution implies changing correspondingly the file allocations. The user might find this option of some utility in restart procedures.

&CNTL NAMELIST

Function

This NAMELIST sets the input for the control of the execution of the different steps in ATOMCI.

Parameters

NRNFG(8) Integer*4. Run flags (default: 0,0,0,0,0,0,0,0).

Each element of the vector controls the execution of a step in ATOMCI. Enter 1 to execute the corresponding step and 0 to skip.

NRNFG(1) ··· Module AIMAIN. Atomic orbitals integrals.
NRNFG(2) ··· Module MCMAIN. MCSCF calculation.
NRNFG(3) ··· Module WFMAIN. Definition of CSF and Energy Expression (EE).
NRNFG(4) ··· Module TRMAIN. Integral transformation.
NRNFG(5) ··· Module PTMAIN. Perturbative selection of the CSF.
NRNFG(6) ··· Module EXMAIN. Construction of the EE file.
NRNFG(7) ··· Module CIMAIN. Diagonalization, NO's, density matrices.
NRNFG(8) ··· Module RSMAIN. Analysis of the CI vector and summary.

Note that in the present version the routines for the SCF calculation (Module MCMAIN) was included and the order of modules was rearranged.

TITLE Character*72. A title for the run (default: none).

Up to 72 characters.

Example

&CNTL TITLE='CARBON TRIPLET EVEN', NPFLG= 0,1,1,1,0,0,1,1, &END

instructs the program to proceed through the WFMAIN, AIMAIN, TRMAIN, CIMAIN and RS-

MAIN steps for a calculation on the ^3P_e state of C.

&AI NAMELIST

Function This NAMELIST sets the input for the control of the execution of the AIMAIN step in ATOMCI (atomic integrals generation).

Parameters

NAME(33) Integer*4. A title for the AIMAIN step (default: copy of TITLE, see &CNTL NAMELIST).

Up to 132 characters.

NWT Integer*4. Number of basis functions (default: none).

The program checks only if NWT is greater than the maximum allowed (150 in the present version). If the actual number of functions entered is different from the value assigned to NWT a warning message is printed and the execution continues.

Z Real*8. Nuclear charge (default: none).

NTYPE Integer*4. Type of basis set (default: 1).

1 ... Slater type orbitals.
2 ... Spherical Gaussian type orbitals.

NPFLG Integer*4. Debug print flag (default: 0).

Any value > 0 is intended for debug purposes.

IDPRNT Integer*4. Print flag (default: 0).

0 ... No echo of input.
1 ... Echo of input.

IUNIT Integer*4. Unit number for the list of basis functions (default: 5).

By default the input data for the basis set should go in a file assigned to unit 5. In this case the basis should follow the &AI NAMELIST. It may be convenient to assign the file to another unit. In the sample 2 supplied with the package, for instance, the basis input data are supposed to be included in a file associated with unit number 3 (i.e., IUNIT=3 in the

&AI NAMELIST should be used).

LOEI Integer*4. Length of write buffer. (default: 448).

The user will probably never need to modify the default value.

Example

```
&AI IUNIT=5, NWT=47, Z=5.D0, NTYPE=2, &END
```

indicates that a set of 47 GTO's (NWT=47, NTYPE=2) follows in input (IUNIT=5). The nuclear charge for the system is 5 (Z=5.D0).

Input data for the Basis set

The basis set is entered in free format from unit IUNIT specified in the &AI NAMELIST.

For STO's:

Enter orbital type (4P, 5F, etc.) and orbital exponent in sequence. End with '))'. Example

1S 15.3745 1S 8.3863 2S 10.6875
2S 7.1933 2P 9.6868
...
))

For GTO's:

Enter orbital type (P, F, etc.), number of terms in the contraction, scaling factor, list of orbital exponents and list of contraction coefficients in sequence. End with '))'. Example

S 3 1.0
10.0 5.0 2.5
0.20 0.50 0.30
S 1 1.0 1.5 1.0
S 1 1.0 0.5 1.0
...
))

&MC NAMELIST

Function

This NAMELIST sets the input for the control of the execution of the MCMAIN step (definition of the CSF and of the EE).

Parameters

NAME(30) Integer*4. A title for the MCMAIN step (default: copy of TITLE, see &CNTL NAMELIST).

Up to 120 characters.

RULE Integer*4. Should set to 0 (default: 0).

ITNEL Integer*4. Number of electrons in the system (default: none).

ISPIN Integer*4. Spin multiplicity (default: none).

Spin multiplicity 2S+1 (1 for singlet, 2 for doublet, ...).

IORB Integer*4. Orbital angular momentum (default: none).

Spatial angular momentum 2L+1 (1 for S, 3 for P, 5 for D, ...).

IPAR Integer*4. Parity of the system.

0 ... even 1 ... odd

NPFLG Integer*4. Debug print flag (default: 0).

Any value > 2 is intended for debug purposes, and should not be used. NPFLG > 3 in particular will cause an I/O error.

IVCS Integer*4. The unit number of the coefficients save file (default: 27).

The coefficient save file (see I/O File Description) is structured in subsequent records. The records are written according to the directives given by the user via the NSET variable within the &MC NAMELIST. The user is referred to the discussion of the &GET NAMELIST for a description of the use of the initial vectors of transformation coefficients. In general each record after the first in unit IVCS contains a set of NO's, obtained at a given time by running ATOMCI with the appropriate save directives.

NSET Integer*4. Flag controlling write operation for converged SCF orbitals on unit IVCS (default: 0).

NSET controls the write operations by enabling or disabling the write option and by establishing where to write. Values given to NSET have are interpreted as follows:

-1 ... Do not write on the save file.
0 ... Write in append mode (after the last existing record).
n ... Write on record n (all records following record n will be destroyed).

IND(4,100) Criteria of selection for inital orbitals (default: 4*0).

A series of NIND quartets (columns)
a_1, l_1, c_1, d_1,
a_2, l_2, c_2, d_2,
...
specifying that the next c_j through d_j orbital coefficients of symmetry type l_j should be taken from the record number a_j of the save file. The data in this array should be such that all the needed orbital coefficient are accounted for.

If you don't specify this entry or set to 0, program automaticaly generate initial orbitals.

CLOSED Character*80 Closed shells.

The orbitals which are treated as closed shells in SCF configurations should be listed here.

Following the same example

1S 2S)

indicating a doubly occupancy for the 1s and 2s shell in SCF configurations.

CSFS(20) Character*80. List of SCF configurations.

A general format for the configuration specification is:
The reference configurations are input using the following conventions

1. The orbitals must be arranged in ascending order of principal quantum number and angular momentum.
2. The occupation of each orbital (say n) is indicated by typing '*n' after the orbital label.
3. Each shell is separated from the other by a ')' character.
4. An extra ')' separates two configurations.
5. Each SCF configuration must be put on just one card (each Array).
6. A '))))' sequence ends the list of configurations.

Example:
CSFS= ' 2S*2) 2P*3) 3P*1)) ',
')))',

Example

```
&MC RULE=0, ISPIN=3, IPAR=0, IORB=3, ITNEL=6,
    NAME=' C TRIPLET EVEN', NPFLG=1,
    CLOSED= ' 1S) ',
    CSFS= ' 2S*2) 2P*2)) ',' )))',     &END
```

is the appropriate input for a SCF calculation on, for instance, Carbon (ITNEL=6), ^3P_o (ISPIN=3, IORB=3, IPAR=1).

&WF NAMELIST

Function

This NAMELIST sets the input for the control of the execution of the WFMAIN step (definition of the CSF and of the EE).

Parameters

NAME(30) Integer*4. A title for the WFMAIN step (default: copy of TITLE, see &CNTL NAMELIST).

Up to 120 characters.

RULE Integer*4. Type of CI calculation (default: 1).

0 ... general CI (no reference).
1 ... SD-CI (Single or Multi Reference).
2 ... Perturbative selection of the relevant CSF.

The choice of RULE influences the selection of the NRNFG execution flags in the &CNTL NAMELIST. A standard input for NRNFG is

RULE=0, ... NRNFG= 1, 1, 1, 1, 0, 1, 1, 1,
RULE=1, ... NRNFG= 1, 1, 1, 1, 0, 0, 1, 1,
RULE=2, ... NRNFG= 1, 1, 1, 1, 1, 1, 1, 1,

for calculations starting from scratch. Refer to the 'Restart Capabilities' section for restarts with preexisting files.

ITNEL Integer*4. Number of electrons in the system (default: none).

ISPIN Integer*4. Spin multiplicity (default: none).

Spin multiplicity 2S+1 (1 for singlet, 2 for doublet, ...).

IORB Integer*4. Orbital angular momentum (default: none).

Spatial angular momentum 2L+1 (1 for S, 3 for P, 5 for D, ...).

IPAR Integer*4. Parity of the system.

0 ... even 1 ... odd

ISMAX Integer*4. Maximum spin multiplicity of the intermediate state (default: 21).

Gives the maximum spin multiplicity allowed in the intermediate coupling. All configurations which will result from a sequence of coupling steps giving rise to intermediate states with spin multiplicity grater than ISMAX will not be included in the CSF list.

IRMAX Integer*4. Maximum spatial multiplicity of the intermediate state (default: 31).

Gives the maximum spatial multiplicity allowed in the intermediate coupling. All configurations which will result from a sequence of coupling steps giving rise to intermediate states with orbital angular momentum multiplicity grater than IRMAX will not be included in the CSF list.

NPFLG Integer*4. Debug print flag (default: 0).

Any value > 2 is intended for debug purposes, and should not be used. NPFLG > 3 in particular will cause an I/O error.

0 ... prints reference informations only (RULE=1 or 2).
1 ... prints type of configurations.
2 ... prints the whole list of CSF and echoes the input.

IUNIT Integer*4. Unit number for the list of configurations (default: 5).

By default the input data for the configurations follow the &WF NAMELIST. It may be convenient anyway to include the data in a file assigned to another unit. In the sample 2 supplied with the package for instance, the CSF input data are supposed to be in a file associated with unit number 2 (i.e., IUNIT=2 in the &WF NAMELIST should be used).

A list of less used variables, mainly controlling buffers sizes, and which the user is less likely to modify, follows. In most cases the program will print a warning message instructing to change a specific variable and will stop with return code $\neq 0$ into WFMAIN. Notice that these variables specify the amount of space reserved to the buffer, and do not correspond in general to the actual amount of space, generally much smaller, used by the program.

LRPS Integer*4. Length of write buffer. (default: 10000).
LTRI Integer*4. Length of write buffer. (default: 100000).
LWFL Integer*4. Length of write buffer. (default:2000).
LCFC Integer*4. Length of write buffer (work file). (default:300).
LISL Integer*4. Length of integral address buffer. (default: 1000).
LIJB Integer*4. Length of the integral indexes buffer. (default:2000).

Example

```
 &WF RULE=1, ISPIN=3, IPAR=0, IORB=3, ITNEL=6,
      NAME=' C TRIPLET EVEN', NPFLG=1, IUNIT=2, &END
```

is the appropriate input for a SD-CI (RULE=1) calculation on, for instance, Carbon (ITNEL=6), ^3P_o (ISPIN=3, IORB=3, IPAR=1). The file with the CSF is on unit 2 (IUNIT=2) and a list of the configuration types will be provided in output (NPFLG=1).

Input data for the CSF

The list of CSF should follow the &WF NAMELIST if IUNIT=5 (default). It will be included in a separate file assigned to unit n if IUNIT=n. The ATGEN utility was designed to prepare the input data for the configuration state functions in a SD-CI calculation (RULE=1 or RULE=2). The user should thus need to type the list only when attempting a general CI calculation (RULE=0) or when planning to include restrictions to the intermediate couplings (see below). For a better understanding of the input conventions it might help to look at a CSF output file from ATGEN.

CARDS

CARD 1 List of the atomic orbitals.

Input here the orbitals which will be used in defining the configurations (including frozen core). End the list with a ')'. The usual ordering is: virtuals (in ascending order of azimuthal quantum number), valence (again in ascending order of azimuthal quantum number), closed shells. The principal quantum numbers for the virtuals serve only to order the orbitals between their respective sets and have nothing to do with the functional form of the radial functions.

Let's look at the f.csf output file obtained by running ATGEN with the f.atg input data. ATGEN labels the virtual orbitals arbitrarily by assigning them principal quantum numbers starting from 11 upward. CARD 1 is then

12S 11S 12P 11P 12D 11D 12F 11F 2S 2P 3P 1S)

CARD 2 Closed shells.

The orbitals which are treated as closed shells in all configurations should be listed here. The user does not need to include these shells in the configuration input (CARD 5). If a shell is open though, it must be explicitly included in the list of configurations, even if no excitation is allowed from that shell. Again, end with ')'. The user should set at least one closed shell.

Following the same example (see f.csf)

1S)

indicating a doubly occupancy for the 1s shell in all CSF.

CARD 3 Order of coupling.

The order in which the shells should be coupled will be entered here. If the order is the same of the definition of the orbitals given in CARD 1, input only '))'.

For our example

12S 11S 12P 11P 12D 11D 12F 11F 2S 2P 3P 1S)

or

))

can be used equivalently.

CARD 4 Symbolic definition of the occupancy numbers.

It may be useful to define here symbolic occupancy numbers, to be used in the input of the configurations. This proves to be handy when running with the same choice of orbitals on systems with different orbital occupancies. The user will have then to change the symbolic definitions in CARD 4 without having to change each configuration. Use alphabetic characters. In the input of configurations (CARD 5) a combination of symbols and numbers is allowed (i.e., 'A-1', 'B+2' for instance are accepted, provided that the A and B symbols are defined in CARD 4).

By including after CARD 3 in sample 1 the following line

A=2, B=4,

The reference configurations (see CARD 5) could then be input as

2S*A) 2P*B))
2S*A) 2P*B-1) 3P*A-1))

See also the boron.stdin sample file included in the package and discussed in the 'Sample 1' section of this Documentation.

CARD 5 Input of configurations.

A general format for the configuration specification is:

<orbital list>, LS-range) <orbital list>, LS-range) ...
<orbital list>, LS-range))

where

<orbital list> ... list of orbitals of the same angular symmetry, followed by an occupancy designation of the form '*n' (or also '*A', if A has been defined in CARD 4), n and A giving the number of electron in the shell.

Valid examples:
1S*2 ... two electrons in orbital 1s
3 4 5P*1 ... one electron in the 3p or 4p or 5p orbitals
2S*0 ... zero occupancy in the 2s orbital
3 4 5 6D*A ... two electrons in 3d or 4d or 5d or 6d (A=2 given in CARD 4)
5F*7 ... seven electrons in orbital 5f.

LS-range ... ranges of spin multiplicities and spatial angular momentum values to be retained in building the CSF. Give the lower limit first. Upper and lower limits must be separated by a '-', the S-range by the L-range by a comma. Ranges in S are given by numbers (multiplicities). Ranges in L by symmetry symbols (S, P, D ...). The ranges are optional, and do not have to be specified if all possible CSF generated by a given configuration are desired. ATOMCI retains at each intermediate coupling step only those states which fall within the ranges and are consistent with Pauli's principle.

Valid examples:
1-1,S-P ... Keep only S and P singlet states at this stage of coupling.
1-3,S-S ... Keep only singlet and triplet S states.
1-3,S-G ... Keep all singlet and triplet S, P, D, F and G states.

while the following specification, as an alternative to 3S*2), is not allowed (null coupling):

3S*1) 3S*1, 1-1,S-S)

Each shell ends with a ')'. A '))' sequence ends a configuration. The list of configurations ends with ')))'.

When RULE > 0 (see &WF NAMELIST), the reference configurations should be separated from the following configurations by an extra ')'.

One input statement cannot generate more than 800 CSF.

The system does not check for duplication of CSF at this stage, but it will eventually provoke an abort of the run at the WFMAIN or EXMAIN steps, with a corresponding warning message.

By typing 'DISPLAY' at the beginning of the list a printout of the available type of spin states (Shell states in the LSQ scheme, see F.Sasaki et al., in "Methods and Techniques in Computational Chemistry: METECC-94", cited above) will be obtained.

In our example, corresponding to a RULE=1 situation, the reference state configurations are first entered

```
2S*2) 2P*4))
2S*2) 2P*3) 3P*1))
)
```

Notice that blank characters within a shell are neglected, that shells have to be separated from each other by at least one blank (and by ')') and that lines starting with '"' are consider as comment lines. ATGEN puts extra blank characters within a shell and between the configurations and thus the output looks slightly different from what is printed above. After the reference configurations, the singly and doubly excited configurations within the valence orbitals are input (labeled for convenience 'SINGLE AND DOUBLE EXCITATIONS WITHIN GROUP 1' by ATGEN)

```
2S*2) 2P*2) 3P*2))
2P*6))
...
```

followed by the single and double excitations to the virtual orbitals (labeled 'FIRST ORDER SPACE' and 'SECOND ORDER SPACE' respectively by ATGEN)

```
12 11S*1) 2S*1) 2P*4))
...
12 11S*2) 2P*4))
...
```

There are several ways to generate the same list of CSF. In the following two examples identical sets are generated, but with the second input arrangement the generation is faster.

```
2 3 4 5 6S*1) 2 3 4P*1))
1S*1) 2 3 4 5 6S*2) 2 3 4P*1))
1S*0) 2 3 4 5 6S*2) 2 3 4 5 6S*1) 2 3 4P*1))
1S*1) 2 3 4 5 6S*1) 2 3 4 5 6S*1) 2 3 4P*1))
1S*1) 2 3 4P*2) 2 3 4P*1))
1S*1) 2 3 4P*1) 2 3 4P*2))
1S*0) 2 3 4 5 6S*1) 2 3 4P*2) 2 3 4P*1))
1S*0) 2 3 4 5 6S*1) 2 3 4P*1) 2 3 4P*2))
)))
```

```
1 2 3 4 5 6S*2) 2 3 4 5 6S*1) 2 3 4P*1))
1 2 3 4 5 6S*1) 2 3 4 5 6S*2) 2 3 4P*1))
1 2 3 4 5 6S*1) 2 3 4 5 6S*1) 3 4 5 6S*1) 2 3 4P*1))
1 2 3 4 5 6S*1) 2 3 4P*2) 3 4P*1))
1 2 3 4 5 6S*1) 2 3 4P*1) 3 4P*2))
)))
```

Finally, two examples of use of restriction ranges in intermediate coupling. In the following case ranges are specified, though needlessly since it is assumed that the final state is a ^1S_e for a four electron system, and thus all other possible intermediate state couplings are incompatible

with the final target symmetry:

3 4 5D*1) 3 4 5D*1, 1-1,S-S) 2S*2))

a d electron (^{2}D) is coupled to a d electron (^{2}D) but out of the several possible resulting intermediate state symmetries only ^{1}S states are retained, and then coupled with the ^{1}S state arising from the $(2s)^2$ shell. Notice however that giving ranges even when not really needed could result in saving CPU time by reducing the amount of work done by the EE generation routine.

In the following example on the other hand the restrictions are effective (same four electron system and ^{1}S final state symmetry).

3 4 5S*1) 3 4 5S*1, 1-1,S-S) 1S*1) 2S*1))

Only three CSF are generated, corresponding to three singlet-singlet couplings of the first two electrons to the second electron pair. CSF coming from possible intermediate triplet S states are excluded.

&TR NAMELIST

Function

This NAMELIST sets the input for the control of the execution of the TRMAIN step in ATOMCI (integral transformation).

Parameters

NAME(33) Integer*4. A title for the TRMAIN step (default: copy of TITLE, see &CNTL NAMELIST).

Up to 132 characters.

NSYM Integer*4. Number of symmetries (default: none).

Is also the dimension of the NOB and NBF vectors.

NOB() Integer*4. A vector containing the number of orbitals in each symmetry (default: none).

Number of rows in each symmetry block of the transformation coefficients matrix.

NBF() Integer*4. A vector containing the number of basis functions in each symmetry (default: none).

Number of columns in each symmetry block of the transformation coefficients matrix.

MPOB() Integer*4. Correspondence table (default: none).

Correspondence table between the orbitals defined in the input of CSF and the transformation coefficients. A vector with TNOB elements, TNOB being the total number of orbitals. Input one symmetry at a time. See example at the end of this section.

NPFLG Integer*4. Debug print flag (default: 0).

Any value > 0 is intended for debug purposes.

ITVCI Integer*4. Input mode for transformation coefficients.

0 ... input from the user.
1 ... input from a previous ATOMCI run.

If ITVCI=0 the &BASVC NAMELIST is needed in input and the transformation coefficients will be read in from the file in unit IUNIT (see &BASVC NAMELIST).
If ITVCI=1 the &GET NAMELIST is needed and the transformation coefficients will be read in from the file in unit IVCS (see &GET NAMELIST).

Example

Referring to the example used in documenting the input conventions for ATGEN and for the list of CSF, a possible form for the &TR NAMELIST might be

```
&TR NSYM=4, NBF= 4,4,2,2,  NOB= 4,4,2,2,
    MPOB= 4,3,2,1,
          4,3,1,2,
              2,1,
              2,1,
      ITVCI=0, &END
```

A total of 12 orbitals (NOB=4,4,2,2) projected on 12 basis functions (NBF=4,4,2,2) are used, involving 4 symmetries (NSYM=4). The order of the atomic orbitals given in CARD 1 in the input data for the CSF was

12S 11S 12P 11P 12D 11D 12F 11F 2S 2P 3P 1S

The 12S orbital corresponds to the fourth orbital of symmetry s in the following list of transformation coefficients (MPOB(1)=4); the 11S orbital corresponds to the third s orbital in the following list; the 2S orbital to the second; the 1S to the first. The 12P orbital corresponds to the fourth p orbital in the list and so on. The transformation coefficient matrix will be supplied by the user (ITVCI=0) and the &BASVC NAMELIST will follow.

&BASVC NAMELIST

Function

Needed when the transformation coefficients are supplied by the user.

Parameters

IUNIT Integer*4. The unit number of the file containing the coefficients (default: 5).

By default the transformation matrix follows the &BASVC NAMELIST.

IDPRNT Integer*4. Print flag. (default: 0)

0 ... Echo of input.
1 ... No echo of input.

The transformation coefficients are input in free format. The input sequence follows a sort of triple nested loop scheme:

```
Loop over the symmetry types.
     Loop over the orbitals of a given symmetry type.
          Loop over the basis functions for the symmetry in object.
               Input transformation coefficients matrix element.
               End loop.
          End loop.
     Input ')'
     End loop.
Input ')))'
```

As indicated above, each symmetry block ends with a ')' character. The whole list ends with the usual ')))' sequence. The number of coefficients is obviously equal to the dot product of the NOB and NBF vectors. The ordering must be in agreement with the one established with the MPOB vector in the &TR NAMELIST.

Example

An example of &BASVC NAMELIST:

```
&BASVC IDPRNT=0, IUNIT=4, &END
```

The transformations coefficients are in unit 4 (IUNIT=4). No echo of input is requested (IDPRNT=0). An arbitrary set (for example an identity transformation matrix) of coefficients for NBF=4,4,2,2, NOB=4,4,2,2, could be arranged as follows

```
1, 0, 0, 0,
0, 1, 0, 0,
0, 0, 1, 0,
0, 0, 0, 1,  )
```

```
1, 0, 0, 0,
0, 1, 0, 0,
0, 0, 1, 0,
0, 0, 0, 1,  )
1, 0,
0, 1,  )
1, 0,
0, 1,  )
)))
```

&GET NAMELIST

Function

To be used when the transformation coefficients are extracted from the orbital save file of previous ATOMCI runs.

Parameters

IVCS Integer*4. The unit number of the coefficients save file (default: 27).

By default the coefficient save file is assigned to unit 27, and the sample data supplied with the package assumes the use of the default value. The coefficient save file (Unit NFCIC, see I/O File Description) is structured in subsequent records. When created by ATOMCI, the first record is used to save the original transformation coefficients matrix. The following records are written according to the directives given by the user via the IOFLG variable within the &CI NAMELIST. The user is referred to the discussion of the &CI NAMELIST for a description of the use of the IOFLG input data. In general each record after the first in unit IVCS contains a set of NO's, obtained at a given time by running ATOMCI with the appropriate save directives.

NIND Integer*4. Number of columns in the array IND (default: none).

IND(4,100) Criteria of selection for thetransformation coefficients (default: none).

A series of NIND quartets (columns)
a_1, l_1, c_1, d_1,
a_2, l_2, c_2, d_2,
...
specifying that the next c_j through d_j orbital coefficients of symmetry type l_j should be taken from the record number a_j of the save file. The data in this array should be such that all the needed orbital coefficient are accounted for.

Example

An example of &GET NAMELIST:

```
 &GET IVCS=27, NIND=6,
  IND= 1,0,1,2,
       2,0,3,4,
       1,1,1,2,
       2,1,3,4,
       2,2,3,4,
       2,3,3,4,
  &END
```

The transformations coefficients are read in from unit 27 (IVCS=27). The first and second orbitals (IND(3,1)=1, IND(4,1)=2) of the s symmetry type (IND(2,1)=0) are taken from the first record of the save file (original input) (IND(1,1)=1). The third and fourth orbitals (IND(3,2)=3, IND(4,2)=4) of the s symmetry type (IND(2,2)=0) are taken from the second record of the save file (natural orbitals) (IND(1,2)=2). The first and second orbitals (IND(3,3)=1, IND(4,3)=2) of the p symmetry type (IND(2,3)=1) are taken from the first record of the save file (original input) (IND(1,3)=1), and so on.

&PT NAMELIST

Function

This NAMELIST sets the input for the control of the execution of the PTMAIN step (perturbative selection of the relevant CSF). Normally invoked by setting RULE=2 in the &WF NAMELIST and correspondingly NRNFG(5)=1 in the &CNTL NAMELIST.

Parameters

NAME(30) Integer*4. A title for the PTMAIN step (default: copy of TITLE, see &CNTL NAMELIST).

Up to 120 characters.

NRNFG(3) Integer*4. Run flags (default: 1,1,1).

Each flag controls the execution of one of the three sections in the PTMAIN step. Type 1 to execute and 0 to skip.

NRNFG(1) ... Construction of the effective Hamiltonian.
NRNFG(2) ... Diagonalization.
NRNFG(3) ... Analysis of the contribution to the energy.

HOW Integer*4. Selection scheme (default: 2)

Specifies how to select the relevant CSF.

0 ... Contribution to solution number ISTATE (see below).
1 ... Average contribution among NSOLVE solutions (see below).
2 ... Maximum contribution among NSOLVE solutions (see below).

ISTATE Integer*4. Index of the solution of the eigenvalue problem (default: 1).

Specifies the index of a single root in the diagonalization of the effective Hamiltonian. Needed when HOW=0. Must always be $\leq$ NSOLVE.

NSOLVE Integer*4. Number of solutions of the eigenvalue problem (default: 1).

Specifies how many roots are requested in the diagonalization of the effective Hamiltonian.

IPS Integer*4. Threshold for the diagonalization (default: 5).

Norm of the correction vector in the Davidson diagonalization routine. The actual threshold will be 10^{-IPS}.

ETHR Real*8. Threshold for the selection of the CSF (default: 1.0D-04).

The program will compute the contribution to the energy from each configuration state function and will then arrange the CSF accordingly. A cumulative energy is defined by summing all contributions (smaller in absolute value than CTHR, see below) along the list, starting from the smallest. When the cumulative energy reaches the value of ETHR all the CSF which were taken into account for the summation are rejected. Those remaining are automatically selected. Note however that CSF corresponding to single excitations from a reference configurations are always selected.

CTHR Real*8. Threshold for the contribution of a single CSF (default: 1.0D-03).

A configuration state function is automatically included if the absolute value of the coefficient is larger that CTHR. It is advisable to choose for CTHR a value at most one order of magnitude larger than ETHR not to affect the accuracy of the result.

PTHR Real*8. Print flag for the list of selected CSF (default: -1.0D00).

1.0d0 ... Do not print the list.
-1.0d0 ... Print the whole list.

NPFLG(3) Integer*4. Debug print flag (default: 0,0,0).

Each section of PTMAIN (see NRNFG) has its debug print flag. Set to 1 for debug informa-

tions.

LTRI Integer*4. Length of write buffer. (default: 100000).

Should be equal or greater than the dimensions actually used in WFMAIN. The user should make sure, by looking at the output of the WFMAIN step, that the this write buffer length in both the PTMAIN and CIMAIN steps is adequate.

Example

A typical choice of input data for the &PT NAMELIST:

```
&PT NAME=' PERTURBATIVE SELECTION WITH THRESHOLD=1.D-05 ',
    HOW=0, ISTATE=1, IPS=7, ETHR=1.D-05,
    CTHR=1.0D-04, PTHR=1.D0, &END
```

ATOMCI will go through the construction of the effective Hamiltonian, the solution of the eigenvalue problem for the lowest state (ISTATE=1) with a diagonalization threshold of 10^{-7} (IPS=7) and the analysis of the contribution to the energy of state number ISTATE (HOW=0), rejecting all CSF giving rise to a cumulative energy of 1.D-05 a.u. (ETHR=1.D-05). A CSF whose contribution exceeds 1.D-04 a.u. will be automatically selected (CTHR=1.D-04). The printout of the selected CSF is disabled (PTHR=1.D0).

&EX NAMELIST

Function

This NAMELIST sets the input for the control of the execution of the EXMAIN step (Construction of the energy expression). Set NRNFG(6)=1 in the &CNTL NAMELIST when doing a general CI (RULE=0) or a perturbative selection (RULE=2).

Parameters

NAME(30) Integer*4. A title for the EXMAIN step (default: copy of TITLE, see &CNTL NAMELIST).

Up to 120 characters.

RETRY Integer*4. Restart run flag (default: 0).

0 ... Normal execution.
1 ... Restart.

The construction of the energy expression is generally the most expensive step of the CI calculation. The RETRY flag is provided for restart operations after an abort occurred

within the EXMAIN step. When RETRY=1, the user should provide the incomplete EE file (unit NFEXW, see below).

NFEXE Integer*4. Unit number of the EE file (default: 15).

Normally (RETRY=0) it should not be modified, unless by modifying accordingly the input file and the unit number in all other steps using this file. In a restart, setting NFEXE to the same value of NFEXW (the incomplete EE file, see below) will result in the EE file being updated.

NFEXW Integer*4. Unit number of the incomplete EE file (default: 0).

The incomplete EE file (resulting for an aborted ATOMCI run) should be assigned to unit number NFEXW.

NPFLG Integer*4. Debug print flag (default: 0).

Should be used only for debug. Setting NPFLG > 3 will generate an error in input.

Among the less used variables in the &EX NAMELIST we should mention LWFL, LCFC, LIJB, and LISL, already briefly discussed within the &WF NAMELIST documentation. They have here the same meaning and default values, and the user should refer to the &WF NAMELIST section in the quite remote occurrence of necessity of their modification.

Example

A normal form for the &EX NAMELIST:

```
&EX RETRY=0 &END
```

while for a restart after an abort within the EXMAIN module

```
&EX RETRY=1, NFEXW=14, NFEXE=15, &END
```

with the incomplete EE file assigned to unit 14 (NFEXW=14) and the complete EE file resulting in unit 15 (NFEXE=15). Notice that only the RETRY=1 input is essential, the selected unit numbers corresponding to the default values.

&CI NAMELIST

Function

This NAMELIST sets the input for the control of the execution of the CIMAIN step (Construction and diagonalization of the CI Hamiltonian, density matrices, natural orbitals).

Parameters

NAME(30) Integer*4. A title for the CIMAIN step (default: copy of TITLE, see &CNTL NAMELIST).

Up to 120 characters.

NRNFG(6) Integer*4. Run flags (default: 1,1,1,0,1,1).

The CIMAIN step is divided in six sections, whose execution is controlled by the NRNFG flag. Set to 1 to execute and to 0 to skip a particular section.

NRNFG(1) ... Construction of the Hamiltonian (energy matrix).
NRNFG(2) ... Diagonalization of the Hamiltonian.
NRNFG(3) ... Density matrices.
NRNFG(4) ... Not used. Set always to 0.
NRNFG(5) ... Natural orbitals.
NRNFG(6) ... Preparation of the interface (summary) file for the RSMAIN step.

NSTATE Integer*4. Number of solutions requested (default: 1).

Number of solutions requested in the diagonalization of the Hamiltonian.

MAXIT Integer*4. Maximum number of iterations in the diagonalization (default: 1000).

NSDIM Integer*4. Initial expansion vector for the diagonalization (default: 400).

0 ... unit vector.
> 0 ... dimension of the trial submatrix.

The initial trial vector can be either a unit vector (NSDIM=0) or the eigenvector of a block of dimension NSDIM (NSDIM > 0) of the energy matrix.

IPS Integer*4. Threshold for the diagonalization (default: 6).

Norm of the correction vector in the Davidson diagonalization routine. The actual threshold will be $10^{-\mathbf{IPS}}$.

NPFLG(6) Integer*4. Debug print flag for each section (default: 0,0,0,0,0,0).

Should be used only for debug.

NFIV Integer*4. Unit number for the CI vector file (default: 0).

A preexisting CI vector file can be used to furnish the initial trial vector for the diagonalization. Use NFIV to indicate its unit number (usually 37). Useful when restarting after

missing convergence. Overrides NSDIM.

NFTE Integer*4. Unit number for the EE file (default: 15).

IOFLG(6) Integer*4. Flag controlling write operations (default: 0,-1,-1,0,0,0).

IOFLG(1) ... Not used.
IOFLG(2) ... Write mode for the CI vectors.
IOFLG(3) ... Write mode for the density matrices.
IOFLG(4) ... Not used.
IOFLG(5) ... Write Mode for the natural orbitals.
IOFLG(6) ... Not used.

The CI vectors, the density matrices and the natural orbitals can be saved on file. CI vectors and density matrices can be written on unit NFCIW (default: 28). Natural orbitals can be saved on unit NFCIC (default: 27). It is possible to modify the default unit numbers. The files may be preexisting and already storing data from old ATOMCI runs. IOFLG controls the write operations by enabling or disabling the write option and by establishing where to write. Values given to IOFLG have are interpreted as follows:

-1 ... Do not write on the save file.
0 ... Write in append mode (after the last existing record).
n ... Write on record n (all records following record n will be destroyed).

By default, the NO's are saved on unit 27 after each ATOMCI run (provided of course that NRNFG(5)=1), while CI vectors and density matrices are not saved on unit 28. Since those last two arrays are transferred to the same file, the values given to IOFLG(2) and IOFLG(3) must be consistent, i.e. one cannot specify different records in the same write operation for the CI vectors and the density matrices. Thus

IOFLG(2)= n ... IOFLG(3)= n
IOFLG(2)= n ... IOFLG(3)= 0
IOFLG(2)= 0 ... IOFLG(3)= n

are invalid choices of options.

LTRI Integer*4. Length of write buffer. (default: 100000).

See &PT NAMELIST.

Example

A valid &CI NAMELIST input could be the following:

```
 &CI NAME=' CI STEP ', NRNFG= 1,1,1,0,1,1,
     NSTATE= 1, MAXIT= 500, IPS= 7, NFIV= 37,
```

```
IOFLG= 0,-1,0,0,0,0, &END
```

ATOMCI will go through all five implemented sections of CIMAIN (NRNFG= 1,1,1,0,1,1), attempting to solve the eigenvalue problem for the lowest root (NSTATE=1) in a maximum of 500 iterations (MAXIT=500), with a threshold at 10^{-7} (IPS=7). The initial trial CI vector will be read in from the save file on unit 37 (NFIV=37). This file was assigned to unit number NFCIV (default: 37) on a preceding run of ATOMCI (see I/O file description') The final CI vector will not be saved on unit 28 (IOFLG(2)=-1), while the density matrix will be written after the last record on unit 28 (IOFLG(3)=0) and the natural orbitals will be saved after the last record in unit 27 (IOFLG(5)=0).

&RS NAMELIST

Function

This NAMELIST sets the input for the control of the execution of the RSMAIN step (Analysis of the CI vectors and summary).

Parameters

NAME(30) Integer*4. A title for the RSMAIN step (default: copy of TITLE, see &CNTL NAMELIST).

Up to 120 characters.

NRNFG Integer*4. Run flag (default: 0).

0 ... General CI or SD-CI.
> 0 ... Perturbative selection.

Set NRNFG=0 when RULE=0 or RULE=1 in the &WF NAMELIST. Set NRNFG > 0 when RULE=2 in the &WF NAMELIST; in this case an estimate of the correction to the energy from the rejected CSF will be computed. Notice that the RSMAIN step will be executed only if the summary files from the CIMAIN step (unit number NFCIS, default:71) exists.

RULE Integer*4. Method of estimation of the CSF contribution (default: 2).

1 ... Bunge method.
2 ... Brown's formula.

The Bunge method cannot be applied when the reference is not defined. In this case the system automatically selects RULE=2. See R.E. Brown, Ph.D. thesis, Indiana University, Bloomington, Indiana, (1967) and C.F. Bunge, Phys. Rev. **168**, 92, (1968) for details on the two methods.

PTHR Real*8. Print threshold (default: 0.001)

Threshold for the value of the contributions to the eigenvector. Set PTHR > 0 to print everything. Set PTHR < 0 to print only contributions exceeding PTHR.

NPFLG Integer*4. Debug print flag (default: 0).

Should be used only for debug purposes.

Example

```
&RS RULE=2, PTHR= -0.001, &END
```

for a non perturbative calculation (NRNFG=0, default) where the analysis of the contributions to the CI eigenvectors is done using the Brown's formula (RULE=2) and only contributions exceeding -0.001 are printed on unit 6 (PTHR=-0.001).

I/O File description

The list of units used within ATOMCI follows. For each unit a brief description and the default value for the unit number are given. The names assigned in the control routine (&CNTL NAMELIST) are employed to organize the list. Alternative unit names, assigned within the seven steps of ATOMCI, are also reported. The user will find this list of essential help in restart procedures.

FILES default: 7

Summary file, containing informations on the return codes of the run and on the consumed CPU time.

NFAII default: 18

Atomic orbital integrals file. Generated in AIMAIN and used in TRMAIN.

NFCIC default: 27

Natural orbitals file. Generated and modified in section 5 of CIMAIN (unit NFTV).

NFCID default: 24

One electron expression. Generated in section 1 of CIMAIN and used in section 3 (unit NFTD).

NFCIH default: 22

Density matrices. Temporary file (unit NFTH) in CIMAIN, is then copied to unit NFCIW. Used within section 3 of CIMAIN.

NFCIH1 default: 38

Diagonal Hamiltonian matrix elements. Generated in section 1 of CIMAIN (unit NFHD) and used in section 2.

NFCIH2 default: 39

Off-diagonal Hamiltonian matrix elements. Generated in section 1 of CIMAIN (unit NFHO) and used in sections 2 and 6.

NFCII default: 0

Initial CI vector, unit NFIV in CIMAIN. Supplied by the user in section 2.

NFCIS default: 71

File containing CI summary informations passed from CIMAIN, section 6 (unit NFCI), to RSMAIN.

NFCIV default: 37

CI vectors. Generated within section 2 of CIMAIN (unit NFCV) and used in sections 3 and 6.

NFCIW default: 28

Density matrices and CI vectors. Generated and modified within section 3 of CIMAIN (unit NFTW).

NFEXE default: 15

Energy expression file. Generated in EXMAIN (see NFWFP, NFWFE) and used in CIMAIN, sections 1 and 6, (unit NFTE).

NFEXW default: 0

Incomplete energy expression file. Generated in EXMAIN and supplied when restarting with RETRY=1 (see &EX NAMELIST). Defaulted at 14 in EXMAIN (unit NFEXW).

NFPTB default: 11

Selected CSF. Generated within PTMAIN and used in EXMAIN and RSMAIN.

NFPTH1 default: 32

Diagonal effective Hamiltonian Matrix elements. Generated and used within PTMAIN, section 2 (unit NFPTD).

NFPTH2 default: 33

Off-diagonal effective Hamiltonian Matrix elements. Generated and used within PTMAIN, section 2 (unit NFPTO).

NFPTL default: 35

Work file generated and used sometimes within PTMAIN.

NFPTV default: 31

CI vectors in Perturbative CI. Generated and used in PTMAIN (section 3).

NFTBL default: 88

Work file. Used sometimes in WFMAIN and EXMAIN. Contains temporary data on the CFP.

NFTF default: 10

Coefficients of Fraction Parentage, CFP, tables. Used in WFMAIN, PTMAIN, EXMAIN and RSMAIN.

NFTD default: 20

Direct access work file. Unit NFTRD in TRMAIN. Usually not used, will be necessary only if the programs finds impossible to perform the transformation wholly in core.

NFTRC1 default: 27

Transformation coefficients (NO's or original). Permanent file generated in CIMAIN, section 5 (unit NFTV), and used in TRMAIN (unit NFTRN).

NFTRC2 default: 21

Transformation coefficients (NO's or original). Temporary file generated in TRMAIN as a copy of NFTRC1 (and named NFTRC) and used in CIMAIN, sections 3 and 6 (unit NFTT).

NFTRI default: 16

Transformed integrals file. Generated in TRMAIN and used in CIMAIN (unit NFTA) and PTMAIN.

NFWFB0 default: 11

CSF list for general CI. Generated in WFMAIN (unit NFWFA) and used in EXMAIN.

NFWFB1 default: 12

CSF list for SD-CI. Generated and used in WFMAIN (unit NFWFB).

NFWFE default: 15

Energy expression in the CI calculation. Generated in WFMAIN, used in CIMAIN and in EXMAIN (units NFEXE for the complete and NFEXW for the uncompleted EE files).

NFWFP default: 14

Energy expression in the perturbative selection. Generated in WFMAIN, and used in PTMAIN.

NFWFW default: 9

Work file.

How to Install

Step 1

Change a directory which you want to install and type in tar xvf ... .

It creates the following directories

source
root
seed
include
fplincl
output
samples
bin
doc

and file create.ibm in the main directory.

Step 2

Type in create.ibm. All files in the subdirectory *source* and *root* are copied in the current directory and you will get

CFPTBL ... cfp table
atgen ... csf generator
atomci ... atomci program
fpl ... FPL preprocessor
fpl90lib.o ... FPL link library.

The three files, – CFPTBL, atgen and atomci – are all you need for production run of ATOMCI. You should keep at least these three files.

It also runs test jobs

boron .stdin (Sample 1)
f.atg and f.stdin (Sample 2)
fpt.atg and fpt.stdin (Sample 3)

These jobs creates boron.output f.NO etc in the main directory.

Sample outputs are stored in *output*. Timin data are also recorded in *output*.

Tue May 31 12:10:48 1994
========== atomci installation starts =====
Tue May 31 12:10:49 1994

```
========================================== make all =====
Tue May 31 12:10:50 1994
========================== atomci installation ends =====
Tue May 31 12:10:51 1994
================================== test run starts =====
Tue May 31 12:10:51 1994
============================================== boron =====
Tue May 31 12:14:30 1994
================================== fluorin mc and sd =====
Tue May 31 12:34:34 1994
======================================== fluorin pt =====
Tue May 31 12:37:43 1994
======================================== test run ends =====
```

Utilities

THe atomdiff script compares newly generated outputs to those in the subdirectory output. To get the difference files, type in.

```
atomdiff boron
atomdiff f
atomdiff fpt
```

In the subdirectory root, there are documentation for FPL, fpl90.doc and brief descriptions about file management of ATOMCI systems, README file,

SAMPLE 1: CI calculations on the ground state of Boron.

The **boron.stdin** file included in the package is a sample input file for General CI on the ground ^2P_o state of the Boron atom. For sake of brevity we do not reproduce here the whole input list as it appears in the actual file.

Run by typing

atomci < boron.stdin > boron.output &

The results are in the directory *output*.

SAMPLE 2: CI calculations on the ground state of Fluorine

The **f.stdin** file included in the package is a sample input file which allows to perform a SD-CI calculation on the ground ^2P_o state of Fluorine using a set of 35 Spherical GTO's (13s,11p,6d,5f)

and neglecting single and double excitations from the 1s core orbital. The natural orbitals are determined and then used to repeat the calculation. Notice the use of the &GET NAMELIST to select the NO's from the first calculation.

The first step will be the generation of the f.csf input.

atgen < f.atg

Proceed then to perform the actual CI calculation

atomci < f.stdin > f.output &

The results are in the directory *output*.

Notice that the WFMAIN and AIMAIN steps are not repeated in the second run, since all the necessary files (EE, AO integrals) do not depend on the actual orbitals, and thus do not need to be regenerated. ITVCI=1 in the natural orbitals iteration. In this case the transformation coefficients are taken from the second record on unit 27 (f.NO), i.e. are the natural orbitals generated in the first run (cfr. IOFLG=0,-1,-1,0,0, in both the first and second run). Notice also that the first 16 elements of the IND array could be reduced equivalently to 8, i.e.

IND= 2,0,1,2, 2,0,3,13, 2,1,1,1, 2,1,2,11, ...

is equivalent to

IND= 2,0,1,13, 2,1,1,11, ...

SAMPLE 3: PT-CI calculations on the ground state of Fluorine

The last example is a perturbative selection CI calculation on the ground ^2P_o state of Fluorine using a set of 35 Spherical GTO's (13s,11p,6d,5f) and neglecting single and double excitations from the 1s core orbital (**fpt.stdin**) . The natural orbitals are selected from the previous calculation.

Run by typing

atgen < fpt.atg
atomci < fpt.stdin > fpt.output

The results are in the directory *output*.

Appendix: Error Codes.

In normal runs the return code for each of the eight steps of ATOMCI should be 0. Very often when an error occurs ATOMCI will stop and return a non zero error code. The following is a list of error codes which may be observed. It is not intended to be complete, and it gives only a brief general description of the type of error which occurred. Most of the error codes arise when trying

to read or write to one of the several I/O files, and the user should then check the status of that particular file. Some error codes report inconsistencies between data read in from a particular unit and current data. In that case the user should check the consistency of input data for the different steps of ATOMCI. Finally, some errors may be related with the dimensions of the working space and/or of some buffer sizes. The user should keep an eye on the informations printed in output on the reserved space for some variables or buffers and on the space actually used or needed.

Error codes:

1 to 9	Dynamic allocation failed.

Error codes in WFMAIN:

2000	Cannot find NAMELIST in input.
2010	Error in reading from unit NFWFB0.
2011	Error in reading from unit NFWFB0.
2012	Inconsistency: value of RULE and input from unit NFWFB0.
2021	Error in writing on unit NFWFB1.
2022	Error in writing on unit NFWFB1.
2071	End of File detected in reading CFP table (unit NFTF).
2072	Error detected in reading CFP table (unit NFTF).
2100	Error in reading from unit NFWFB0.
2101	Input data error: Reference CSF.
2102	Input data error: No Reference CSF.
2110	EOF detected in reading unit NFWFB0.
2112	Input data error: Format of Reference CSF.
2210	Duplication of configuration in input.
2211	Storage overflow in reading wavefunction (NFWFB0).
2212	EOF detected in reading unit NFWFB0.
2215	Error in constructing the EE file.
2321	Error in writing on the EE file (unit NFWFE or NFWFP).
2322	Error in writing on the EE file (unit NFWFE or NFWFP).
2323	Error in writing on the EE file (unit NFWFE or NFWFP).
2325	Error in reading from unit NFWFW.
2330	Severe error: Cannot prepare the EE file.
9611	IO buffer overflow: LIJB is too small.
9613	IO buffer overflow: LTRI is too small.
9614	IO buffer overflow: LTRI is too small.
9620	Error in writing on the EE file (unit NFWFE or NFWFP).

Error codes in AIMAIN:

3000	Cannot find NAMELIST in input.
3999	Basis set too large.

Error codes in TRMAIN:

4000 Cannot find NAMELIST in input.
4001 Cannot find unit NFAII.
4101 Input data error: NSYM.
4300 Error in reading from unit NFAII.
4320 Error in writing on unit NFTRI.
4321 Error in reading from unit NFTRC2.
4322 Error in reading from unit NFAII.
4323 Norm too small.
4324 Error in writing on unit NFTRC2.
4400 Cannot transform basis integral.

Error codes in PTMAIN:

5000 Cannot find NAMELIST in input.
5001 Inconsistency in assigning number to unit NFWFP.
5002 Inconsistency in assigning number to unit NFTRI.
5003 Inconsistency: Number of selected CSF from unit NFPTH2.
5011 Error in reading from unit NFWFP.
5012 EOF detected in reading from unit NFWFP.
5020 Error in reading from unit NFPTV.
5021 NSOLVE $>$ number of selected CSF.
5022 NSOLVE=0.
5023 ISTATE=0 when HOW=0.
5024 ISTATE $>$ NSOLVE.
5025 NSOLVE $<$ 0.
5201 No reference CSF.
5211 Inconsistency: number of CSF.
5310 Error in reading from unit NFPTL.
5311 Error in reading from unit NFPTL.
5312 Error in reading from unit NFPTL.
5313 Error in reading from unit NFPTL.
5314 Error in reading from unit NFPTL.
5315 Error in reading from unit NFPTL.
5321 Error in writing on unit NFPTL.
5331 Inconsistency: data read in from unit NFPTL.
5332 Inconsistency: data read in from unit NFPTL.
5333 Error in sorting records read from unit NFPTL.
5401 Error in reading reference CSF from unit NFWFP.
5601 Sorting failed.
5711 Error in reading from unit NFWFP.
5712 Error in reading from unit NFWFP.
5721 Error in reading from unit NFWFP.
5722 EOF detected in reading from unit NFWFP.
5731 Error in reading from unit NFWFP.
5811 EOF detected in reading from unit NFPTH1.
5812 Error in reading from unit NFPTH1.
5821 Inconsistency: data read in from unit NFPTH1.

5831 EOF detected in reading from unit NFPTV.
5832 Error in reading from unit NFPTV.
5841 Inconsistency: data read in from unit NFPTV.
5842 Inconsistency: data read in from unit NFPTV.
5911 Error in writing on unit NFPTB.
5912 Error in writing on unit NFPTB.
5988 Error in selection (sorting contributions).
5999 Error in selection of CSF. Number of selected CSF.

Error codes in EXMAIN:

6000 Cannot find NAMELIST in input.
6001 Inconsistency in assigning number to unit NFPTB.
6101 Error in reading from unit NFWFB0 or NFPTB.
6110 Error in reading from unit NFWFB0, NFWFB1, or NFPTB.
6111 Error in reading from unit NFWFB0, NFWFB1, or NFPTB.
6112 Error in reading from unit NFWFB0, NFWFB1, or NFPTB.
6113 Error in reading from unit NFWFB0, NFWFB1, or NFPTB.
6121 Error in reading from unit NFEXW.
6201 Error in writing on unit NFEXE.
6202 Error in writing on unit NFEXE.
6203 Error in writing on unit NFEXE.
6210 Duplication of configuration in input.
6211 Error in reading from unit NFEXE.
6212 Error copying from unit NFEXW to unit NFEXE.
6221 Inconsistency: data read in from unit NFEXE.
6222 Inconsistency: error in reading from unit NFEXW.
6223 Error copying from unit NFEXW to unit NFEXE.
6231 Inconsistency: data read in from unit NFEXE.
6232 Inconsistency in copying from unit NFEXW to unit NFEXE.
6233 Error copying from unit NFEXW to unit NFEXE.
6301 Error in reading wavefunction from unit NFEXW.
6399 Error in restart.
9095 Orbital too large.
9611 IO buffer overflow: LIJB is too small.
9613 IO buffer overflow: LTRI is too small.
9614 IO buffer overflow: LTRI is too small.
9620 Error in writing on the EE file (unit NFEXE)

Error codes in CIMAIN:

7000 Cannot find NAMELIST in input.
7011 Error in reading from the EE file (unit NFEXE or NFWFE).
7110 Error in reading from unit NFTRI
7111 Error in reading from unit NFTRI
7120 Storage overflow in reading integrals (NFTRI).

7121 Error in reading from unit NFTRI
7122 Error in reading from unit NFTRI
7131 Storage overflow: Extend LTRI or change MCORE.
7132 Storage overflow: Extend LTRI or change MCORE.
7134 Inconsistency: number of orbitals (NFEXE (or NFWFE) and NFTRI).
7135 Inconsistency: number of Symmetries (NFEXE (or NFWFE) and NFTRI).
7201 Inconsistency: number of CSF, unit NFCIW.
7211 Error in reading from unit NFCIH1 or NFCIH2.
7212 Error in reading from unit NFCIH1 or NFCIH2.
7230 Storage overflow: extend MCORE.
7231 Storage overflow: extend MCORE.
7250 Error: Cannot obtain the eigenvectors.
7310 Storage overflow: extend MCORE.
7321 Error in reading from unit NFCID.
7322 EOF in reading from unit NFCID.
7331 Error in writing on unit NFCIH.
7341 Error in reading from unit NFCIW.
7342 EOF in reading from unit NFCIW.
7343 Error in reading from unit NFCIW.
7344 Input data error: cannot get CI vectors.
7351 Error in reading/writing on unit NFCIW.
7352 Error in reading/writing on unit NFCIW.
7353 Error in writing on unit NFCIW.
7360 Input data error: IOFLG(2) or IOFLG(3) in &CI NAMELIST
7361 Error in reading from unit NFCIH.
7501 Error in reading from unit NFTRC2
7502 Error in writing on unit NFTRC2
7511 Error in reading from unit NFTRC2
7512 Error in writing on unit NFTRC2
7513 Error in writing on unit NFTRC2
7521 Error in reading from unit NFCIH.
7531 Error in constructing the natural orbitals (JACOBI).
7540 Storage overflow in obtaining the natural orbitals.
7551 Error in reading/writing on unit NFCIW.
7552 Error in reading/writing on unit NFCIW.
7611 Error in reading from the EE file (unit NFTE).
7612 Error in reading from the EE file (unit NFTE).
7613 EOF detected in reading from the EE file (unit NFTE).
7614 Error in writing on unit NFCIS.
7615 Error in writing on unit NFCIS.
7616 Error in writing on unit NFCIS.
7617 Error in copying from the EE file (unit NFTE) to unit NFCIS.
7618 EOF detected in copying from the EE file (unit NFTE) to unit NFCIS.
7621 Error in reading from unit NFCIH1.
7622 EOF detected in reading from unit NFCIH1.
7623 Error in writing on unit NFCIS.
7631 Error in reading from unit NFCIH2.

7632 EOF detected in reading from unit NFCIH2.
7633 Error in reading from unit NFCIH2.
7634 Error in writing on unit NFCIS.
7641 EOF detected in reading from unit NFCIV.
7642 Error in reading from unit NFCIV.
7643 EOF detected in reading from unit NFCIV.
7644 Error in reading from unit NFCIV.
7645 Error in writing on unit NFCIS.
7681 Inconsistency: number of reference (reading from the EE file (unit NFTE) or NFWFE)
7682 Inconsistency: number of CSF (reading from NFCIH1)
7683 Inconsistency: number of CSF (reading from NFCIV)
7684 Inconsistency: number of solutions (reading from NFCIV)

Error codes in RSMAIN:

8000 Cannot find NAMELIST in input.
8001 Inconsistency in assigning number to unit NFCIS.
8111 Error in reading from unit NFCIS.
8112 Error in reading from unit NFCIS.
8113 Error in reading from unit NFCIS.
8114 Error in reading from unit NFCIS.
8115 Error in reading from unit NFCIS.
8121 EOF detected in reading from unit NFCIS.
8122 EOF detected in reading from unit NFCIS.
8123 EOF detected in reading from unit NFCIS.
8124 EOF detected in reading from unit NFCIS.
8125 EOF detected in reading from unit NFCIS.
8131 Error in number of types of configurations in reference.
8132 Inconsistency: number of CSF, unit NFCIS.
8201 Inconsistency: data read in unit NFPTB and NFCIS.
8202 Inconsistency: number of CSF, unit NFPTB and NFCIS.
8203 Inconsistency: orbital informations, unit NFPTB and NFCIS.
8211 Error in reading from unit NFPTB.
8301 Inconsistency: data read in unit NFPTB and NFCIS.
8302 Inconsistency: data read in unit NFPTB and NFCIS.
8303 Inconsistency: data read in unit NFPTB and NFCIS.
8304 Inconsistency: number of CSF, unit NFPTB and NFCIS.
8305 Inconsistency: number of CSF, unit NFPTB and NFCIS.
8311 Error in reading from unit NFPTB.
8312 Error in reading from unit NFPTB.
8313 Error in reading from unit NFPTB.
8321 Inconsistency: Energy matrix, unit NFPTH1.
8322 Inconsistency: number of CSF, unit NFPTH2.
8323 Inconsistency: number of selected CSF, unit NFPTB.
8330 Error in reading from unit NFPTH1.
8331 Error in reading from unit NFPTH2.
8332 Error in reading from unit NFPTH2.

8333 Error in reading from unit NFPTH2.