**Description of utility-programs dealing with the configuration expansions in JJ-coupling (folder UTILS/CONF\_JJ)**

**Quick-references to the utilities**

|  |  |
| --- | --- |
| **genjconf** | prepares the list of configurations (without terms indication) from the list of electron occupations and allowed promotions |
| **genjterm** | prepares the list of CSF's from a list of the configurations |
| **cm\_j** | converts *cm*-file after RCI2 program from GRASP complex or *m*-file after RSCF2 program to *j*-file of DBSR\_CI format |
| **jcfile** | extracts the state expansion from DBSR\_CI j-file |
| **jj\_order** | ordering the CSFs according their weights |
| **jfile** | find the maximum contributions for given configurations from the list of solutions in j-file |
| **jj\_list** | creates list of states from one or set of j-files |
|  |  |

**G E N J C O N F**

|  |  |
| --- | --- |
| Description: | prepares the list of possible configurations (without terms indication) from the list of electron occupations and allowed promotions. |
| Input files: | **nlj.inp** (default) or define by parameter **inp** |
| Output files: | **conf.inp** (default) ordefine by parameter **out** |
| Call as: | **genjconf inp=... out=...** or **atom=...** |

All arguments are optional. If input file is absent, it will be created for the user to fill it in. Example of input file with comments can be created for the given atom using the parameter **atom**.

**Core subshells:**

**1s 2s 2p- 2p 3s 3p- 3p**

**Peel subshells:**

**3d- 3d 4s**

**Occupation limits:**

**0 2 2**

**4 6 2**

**n\_orbitals = 3 ! number of peel subshels**

**n\_electrons = 8 ! number of peel electrons**

**parity = 1 ! +1 or -1**

**k\_ref = 3 ! reference orbitals**

**k\_min = 0 ! min. promotion from the ref. orbitals**

**k\_max = 2 ! max. promotion from the ref. orbitals**

**Figure** **1.** Example of the **nlj.inp** file.

**Core subshells:**

**1s 2s 2p- 2p 3s 3p- 3p**

**Peel subshells:**

**3d- 3d 4s**

**CSF(s):**

**3d-( 4) 3d ( 4)**

**3d-( 4) 3d ( 2) 4s ( 2)**

**3d-( 3) 3d ( 5) 4s ( 1)**

**3d-( 3) 3d ( 3) 4s ( 2)**

**3d-( 2) 3d ( 6) 4s ( 1)**

**3d-( 2) 3d ( 4) 4s ( 2)**

**3d-( 1) 3d ( 5) 4s ( 2)**

**3d ( 6) 4s ( 2)**

**\*\*\***

**Figure** **2.** Example of the **conf.inp** file obtained on base of the information in the **nlj.inp, Fig**.**1.**

**G E N J T E R M**

|  |  |
| --- | --- |
| Description: | prepares the list of CSF's from a list of the configurations |
| Input files: | **conf.inp** (default) or define by parameter **inp** |
| Output files: | **cfg.inp** (default)ordefine by parameter **out** |
| Call as: | **genjterm inp=... out=... jmin=… jmax=…** or  **genjterm name jmin=… jmax=…** |

All arguments except **jmin** are optional (if jmax < jmin, jmax = jmin). If name is given, input file is **name.conf** and output file is **name.c**.

**Core subshells:**

**1s 2s 2p- 2p 3s 3p- 3p**

**Peel subshells:**

**3d- 3d 4s**

**CSF(s):**

**3d-( 4) 3d ( 4)**

**0**

**0+**

**3d-( 4) 3d ( 2) 4s ( 2)**

**0**

**0+**

**• • • • • • • • • • • • • • • • • • • • • • • • • • • • • • • • •**

**3d-( 2) 3d ( 4) 4s ( 2)**

**2 2**

**0 0+**

**3d ( 6) 4s ( 2)**

**0+**

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**3d-( 3) 3d ( 3) 4s ( 2)**

**3/2 5/2**

**1 1+**

**• • • • • • • • • • • • • • • • • • • • • • • • • • • • • • • • •**

**3d-( 1) 3d ( 5) 4s ( 2)**

**3/2 5/2**

**1 1+**

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**3d-( 4) 3d ( 4)**

**2**

**2+**

**• • • • • • • • • • • • • • • • • • • • • • • • • • • • • • • • •**

**3d-( 1) 3d ( 5) 4s ( 2)**

**3/2 5/2**

**2 2+**

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**Figure** **3.** Example of the **conf.inp** file obtained on base of the information in the **nlj.inp,** Fig.1.

**C M \_ J**

|  |  |
| --- | --- |
| Description: | convert *cm*-file after RCI2 program from GRASP complex or *m*-file after RSCF2 program to *j*-file of DBSR\_CI format. |
| Input files: | **name.cm** (or **name.m**), **name.c** |
| Output files: | **name.j** |
| Call as: | **cm\_j name.cm (or name.m)** |

**J C F I L E**

|  |  |
| --- | --- |
| Description: | extracts the state expansion from DBSR\_CI j-file |
| Input files: | **name.j, name.c** |
| Output files: | **result.c, result.bsw** |
| Call as: | **jcfile name.j nn result eps\_c** |

In the DBSR complex, each target state is described by a pair **name.c** and **name.bsw**. The DBSR\_CI program produces the results in the j-files as a list of states with their expansions. The JCFILE utility allows one to extract the expansion coefficients for a given state and create the corresponding *c*- and bsw-files. The user should indicate in the command line the name of the input *j*-file, the index of the needed state, **nn**, the name for the output *c*-file, and the tolerance for the expansion coefficients, **eps\_c**. When **eps\_c** > 0, configurations in result c-file are ordered according their weights.

**O R D E R \_ J J**

|  |  |
| --- | --- |
| Description: | ordering the configurations according their weights |
| Input files: | **name.c** |
| Output files: | **name.cc** |
| Call as: | **order\_jj name.c [eps\_c]**  **eps\_c** [0] - optional cut-off parameter |

**J F I L E**

|  |  |
| --- | --- |
| Description: | finds the maximum contributions for given configurations from the list of solutions in j-file. |
| Input files: | **name.j, name.c** |
| Output files: | **name.cc** |
| Call as: | **jcfile name [eps\_c]**  **eps\_c** [0] - optional cut-off parameter |

Example: **jfile 1 sol=1-5 eps\_c=0.0001**

In this case, program analyses the first 5 solutions in 1.j and outputs (in 1.cc) all configurations in order of importance. Now we may delete all configurations with small coefficients and used this file for another CI calculations.

**J J \_ L I S T**

|  |  |
| --- | --- |
| Description: | creates list of states in one j-file (given as argument) or in set of j-files |
| Input files: | **name.j, name.c** |
| Output files: | **name.list**  (can be redefined by parameter **out)** |
| Call as: | **jj\_list name.j** [**unit**=**…**  **shift**=**… Z=… awt=… eps\_c=…**  ]  Optional key-words parameters:    **unit** - au, Ry, eV, cm [au]  **shift** - overall energy shift [0.d0]  **msol** -max.number of solutions [0 -> all]  **Z** - nuclear charge  **awt** - atomic weight  **eps\_c** - tolerance for configuration weights [0.2]  **AFi -** input file with list of j-files and parameters [**jj\_list.inp**]  **AFr -** output file **[jj\_list]** |

List of j-files under consideration are defined as not key-words arguments. This list (F1.j, F2.j, ...), along with other parameters, can also be given in input file defined through **inp**=..., with one filename per line. The order of parameters or merging file does not matter. Parameters **Z, awt** are used for more accurate conversion factor from atomic units to eV. If **shift**=1.d0, the reference point will be the lowest state.

**R S A V E**

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| --- | --- |
| Description: | script file to save results of an GRASP calculations under specific name |

**cp rwfn.out %1.w**

**cp rcsl.inp %1.c**

**mv rmix.out %1.m**

**mv rscf.sum %1.sum**