

TAURUS_{mix}: Manual for the input files

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1 Structure of the standard input file

The input file is read by the code as STDIN and therefore has no fixed naming convention. On the other hand, the format of the file is fixed. We describe in this manual how to write a proper input file for TAURUS_{mix} and the different options that the code offers. We will present the different section of the input file separately (but remember that they are all part of the same file).

Before going further, a few remark are in order:

- We use here the Fortran convention for the format of variables, e.g. 1i5 or 1a30, assuming that the reader know their meaning. If it is not the case, we encourage the reader to search for a tutorial somewhere else. There is a large body of Fortran documentation available online therefore it should not be too difficult.
- All lines starts with the reading of an element of an array, `input_names` or `input_spec`, made of `character(30)` variables. These variables only play a cosmetic/descriptive role when reading or printing the input parameters and can be set to any desired value by the user. Therefore, we are not going to comment them further.
- The number of lines in the input files depends on the number of “specific” cut-offs used. Here, we will give the line numbers considering two specific cut-offs.

1.1 Section about the general parameters

Description

Line	Format	Data
1	1a	<code>input_names(1)</code>
2	1a	<code>input_names(2)</code>
3	1a30, 1i1	<code>input_names(3), hwg_phys</code>
4	1a30, 1i1	<code>input_names(4), hwg_algo</code>
5	1a30, 1i1	<code>input_names(5), hwg_norm</code>
6	1a30, 1i1	<code>input_names(6), hwg_rmev</code>
7	1a30, 1i1	<code>input_names(7), hwg_conv</code>
8	1a30, 1i3	<code>input_names(8), hwg_Edis</code>
9	1a	<code>input_names(9)</code>

where

- **hwg_phys**: physical case studied.
= 0 excitation spectrum and γ spectroscopy (ELM transiions: E0-3, M1-2).
- **hwg_algo**: algorithm used to solve the HWG equation.
= 0 reduction to a standard eigenvalue problem through the calculation of the square root of the norm matrix.
= 1 QZ algorithm (as implemented in LAPACK).
- **hwg_norm**: option to normalize the projected matrix elements before solving the HWG equation.
= 0 no normalization is performed.
= 1 normalization using the projected overlaps.

- **hwg_rmev**: option to remove the projected states giving large negative eigenvalues, i.e. smaller than **-cutoff_algo**, determined from incremental diagonalization of the norm. Only referenced for **hwg_algo** = 0.
 = 0 no removal is performed.
 = 1 removes the projected states.
- **hwg_conv**: option to perform an anlysis of the convergence as a function of the number of norm eigenvalues considered. Only referenced for **hwg_algo** = 0.
 = 0 no analysis is performed.
 = 1 For each J^P block, the HWG equation is solved several times incrementally adding more norm eigenvalues. The results
- **hwg_Edis**: Maximum exictation energy displayed in the final tables containing the information on the spectrum and transitions. Note that separate files are created that contain the spectrum/transitions up to much higher excitation energy.

Example

```

General parameters
-----
Physics case studied           0
Algorithm to solve HWG eq.    0
Normalization of matrices     1
Remove states giving ev<0     1
Convergence analysis (norm)   0
Max(E_exc) displayed (Mev)    10

```

1.2 Section about the quantum numbers

Description

Line	Format	Data
10	1a	input_names(10)
11	1a	input_names(11)
12	1a30, 1i3	input_names(12), hwg_Z
13	1a30, 1i3	input_names(13), hwg_N
14	1a30, 1i3	input_names(14), hwg_Zc
15	1a30, 1i3	input_names(15), hwg_Nc
16	1a30, 1i3	input_names(16), hwg_2jmax
17	1a30, 1i3	input_names(17), hwg_2jmin
18	1a30, 1i3	input_names(18), hwg_pmin
19	1a30, 1i3	input_names(19), hwg_pmax
20	1a30, 1f5.2	input_names(20), hwg_echp
21	1a30, 1f5.2	input_names(21), hwg_echn
22	1a	input_names(22)

where

- **hwg_Z**: number of active protons (after particle-number projection on the ket).

- `hwg_N`: number of active neutrons (same as above).
- `hwg_Zc`: number of core protons.
- `hwg_Nc`: number of core neutrons.
- `hwg_2jmin`: minimum value of the angular momentum $2J$ considered.
- `hwg_2jmax`: maximum value of the angular momentum $2J$ considered.
- `hwg_pmin`: minimum value of the parity P considered.
- `hwg_pmax`: maximum value of the parity P considered.
- `hwg_echp`: electric charge for the protons.
- `hwg_echn`: electric charge for the neutrons.

Example

Quantum numbers	

Number of active protons Z	20
Number of active neutrons N	28
Number of core protons Zc	0
Number of core neutrons Nc	0
Angular momentum min($2J$)	0
Angular momentum max($2J$)	8
Parity min(P)	1
Parity max(P)	1
Electric charge protons (*e)	1.00
Electric charge neutrons (*e)	0.00

1.3 Section about the cut-offs

Description

Line	Format	Data
23	1a	input_names(23)
24	1a	input_names(24)
25	1a30, 1i5	input_names(25), cutoff_ldim
26	1a30, 1es10.3	input_names(26), cutoff_over
27	1a30, 1es10.3	input_names(27), cutoff_algo
28	1a30, 1es10.3	input_names(28), cutoff_negev
29	1a30, 1es10.3	input_names(29), cutoff_J
30	1a30, 1es10.3	input_names(30), cutoff_A
31	1a30, 1i5	input_names(31), cutoff_spec_dim
		do i=1, cutoff_spec_dim
	1a30, 1a1,	input_spec(i), cutoff_spec_type(i),
	2i3,	cutoff_spec_2j(i), cutoff_spec_p(i),
	1x, 1es10.3	cutoff_spec_value(i)
		(if cutoff_spec_type(i) \neq 'L')
	OR	OR
	1a30, 1a1,	input_spec(i), cutoff_spec_type(i),
	2i3,	cutoff_spec_2j(i), cutoff_spec_p(i),
	1i19,1i3	cutoff_spec_label(i), cutoff_spec_lab2k(i)
		(if cutoff_spec_type(i) = 'L')
		enddo

where

- **cutoff_ldim**: Maximum number of reference states considered in the mixing.
- **cutoff_over**: Default cut-off value for the projected overlap. The projected states with an overlap $< \text{cutoff_over}$ will be discarded when reading the projected matrix elements.
- **cutoff_algo**: Default cut-off value for the norm eigenvalues. For **hwg_algo** = 0, the norm eigenstates with an eigenvalue $< \text{cutoff_algo}$ will be discarded when building the natural basis. For **hwg_algo** = 1, the generalized eigenvalues (α, β) , with $\beta < \text{cutoff_algo}$ will be discarded.
- **cutoff_negev**: Default cut-off value for the negative eigenvalues. For **hwg_rmev** = 1, the projected states giving a negative eigenvalue $< -\text{cutoff_negev}$ will be discarded before solving the HWG equation.
- **cutoff_J**: Default cut-off value for the expectation values of J_z and J^2 . The projected states with an expectation value $|\langle J_z/J^2 \rangle - K/J^2| > \text{cutoff_J}$ will be discarded when reading the projected matrix elements.
- **cutoff_A**: Default cut-off value for the expectation values of N , Z and A . The projected states with an expectation value $|\langle N/Z/A \rangle - N/Z/A| > \text{cutoff_A}$ will be discarded when reading the projected matrix elements.
- **cutoff_spec_dim**: Number of specific cut-offs, i.e. cut-offs that are specific to a given angular momentum/parity block.

- `cutoff_spec_type`: Type of specific cut-off.
 = O overlap cut-off.
 = S small norm eigenstate cut-off.
 = N negative eigenvalue cut-off.
 = J J_z and J^2 cut-off.
 = A N , Z and A cut-off.
 = L label cut-off.
- `cutoff_spec_2j`: $2*J$ of the block considered.
- `cutoff_spec_p`: P of the block considered.
- `cutoff_spec_value`: Value of the cut-off (if 'O', 'S', 'N', 'J' or 'A').
- `cutoff_spec_label`: Label of the state (if 'L').
- `cutoff_spec_lab2k`: $2*K$ of the state (if 'L').

Example

Cut-offs	

Maximum number of states	0
Cut-off projected overlap	1.000E-06
Cut-off norm eigenvalues	1.000E-06
Cut-off expect. val. J_z/J^2	1.000E-02
Cut-off expect. val. $N/Z/A$	1.000E+01
No. of specialized cut offs	2
Example of label cut-off	L 0 1 1234567891234567891 0
Example of overlap cut-off	0 0 1 1.000E-05

2 Other input files

The code `TAURUSmix` takes in entry several binary input files produced by `TAURUSpav`:

- `projmatelem_states.bin`: contains the information about the projected states (e.g. expectation values for the Hamiltonian, quantum numbers and radii).
- `projmatelem_Q1.bin` ($Q1=E1,E2,E3,M1,M2$): contains the informations about the electromagnetic transitions. These files are not necessary and the code will skip the calculations of a given multipole if its associated file is missing.

To gather all the files coming from different runs of `TAURUSpav`, we recommend using the “cat” command. For example:

```
touch projmatelem_states.bin
cat state1_projmatelem_states.bin » projmatelem_states.bin
cat state2_projmatelem_states.bin » projmatelem_states.bin
...
```

The files can be gathered in any arbitrary order.