ADF56: general ionisation promotional rules

Each data set of promotional rules provides a rule specification for all possible ground states of ionising ions of elements and an associated set of singly excited states based on a parent. The central ADAS data base has generic samples for small, medium and large computer systems. In practice the rules might be customised for a particular computer system.

Data mnemonic:
Data root: **/home/adas/adas/adf56/**
Last update: Jan 09, 2009
Utilising subroutines: **xxdata_56.py, read_adf56.pro**

Data lines:

Data lines	Format
nmax, nel	31x,1i3,5x,1i2
do i=0 to n_index-1	
do j=0 to nel-1	
index(i*nel+j), config(i*nel+j)	1i5,1a*
enddo	
index[nel*i:(nel*(i+1))-1]	16x,10i5
n_el[nel*i:(nel*(i+1))-1]	16x,10i5
no_v_shl[nel*i:(nel*(i+1))-1]	16x,10i5
v1_shl[nel*i:(nel*(i+1))-1]	16x,10i5
v2_shl[nel*i:(nel*(i+1))-1]	16x,10i5
drct_eval_v[nel*i:(nel*(i+1))-1]	16x,10i5
drct_eval_cl[nel*i:(nel*(i+1))-1]	16x,10i5
min_shl_cl[nel*i:(nel*(i+1))-1]	16x,10i5
exca_eval_v2[nel*i:(nel*(i+1))-1]	16x,10i5
max_dn_v2[nel*i:(nel*(i+1))-1]	16x,10i5
min_dn_v2[nel*i:(nel*(i+1))-1]	16x,10i5
max_dl_v2[nel*i:(nel*(i+1))-1]	16x,10i5
min_dl_v2[nel*i:(nel*(i+1))-1]	16x,10i5
exca_eval_cl[nel*i:(nel*(i+1))-1]	16x,10i5
max_dn_cl[nel*i:(nel*(i+1))-1]	16x,10i5
min_dn_cl[nel*i:(nel*(i+1))-1]	16x,10i5
max_dl_cl[nel*i:(nel*(i+1))-1]	16x,10i5
min_dl_cl[nel*i:(nel*(i+1))-1]	16x,10i5
exst_eval [nel*i:(nel*(i+1))-1]	16x,10i5
exst_adf00_prt[nel*i:(nel*(i+1))-1]	16x,10i5
exst_prt_hole_shl[nel*i:(nel*(i+1))-1]	16x,10i5
max_n_exst[nel*i:(nel*(i+1))-1]	16x,10i5
max_l_exst[nel*i:(nel*(i+1))-1]	16x,10i5
drct_eval_exst_v[nel*i:(nel*(i+1))-1]	16x,10i5
drct_eval_exst_cl[nel*i:(nel*(i+1))-1]	16x,10i5
exca_eval_exst_v[nel*i:(nel*(i+1))-1]	16x,10i5
exca_eval_exst_cl[nel*i:(nel*(i+1))-1]	16x,10i5
repeat	

Variable identification:

Name	Meaning	Comment
nmax	number of ground configs.	
nel	number of ground configs per block	
n_index	number of blocks (= nmax/nel)	
index[]	ground config. index	
config[]	ground config. strings	Cowan form
n_el[]	number of electrons	
no_v_shl[]	number of shells to treat as valence shells. Max. 2 relevant to relating ion and parent	
v1_shl[]	first valence shell position in adf56 configuration specifications.	
v2_shl[]	second valence shell position in adf56 configuration specifications. zero if none defined.	
drct_eval_v[]	evaluate direct ionisation from the valence shell(s).	
drct_eval_cl[]	evaluate direct ionisation from other non-valence (closed) shells.	
min_shl_cl[]	lowest closed shell to include (position in adf56 configuration specifications).	
exca_eval_v2[]	evaluate excitation/autoionisation from second valence shell if identified.	
max_dn_v2[]	maximum change in v2 n-shell to be included.	
min_dn_v2[]	minimum change in v2 n-shell to be include.	
max_dl_v2[]	maximum change in v2 l-shell to be included.	
min_dl_v2[]	minimum change in v2 l-shell to be include.	
exca_eval_cl[]	evaluate excitation/autoionisation from other non-valence (closed) shells.	
max_dn_cl[]	maximum change in closed n-shell to be included.	
min_dn_cl[]	minimum change in closed n-shell to be included.	
max_dl_cl[]	maximum change in closed l-shell to be included.	
min_dl_cl[]	minimum change in closed l-shell to be included.	
exst_eval[]	evaluate ionisation from excited states.	
exst_adf00_prt[]	assume parent for building excited states is as present in the adf00 data set for the ion.	
exst_prt_hole_shl[]	specify position of shell in ground configuration to form parent if not from adf00 above.	
max_n_exst[]	maximum n-shell for excited states to be included.	
max_l_exst[]	maximum l-shell for excited states to be included.	
drct_eval_exst_v[]	evaluate direct ionisation from excited state valence shells.	
drct_eval_exst_cl[]	evaluate direct ionisation from excited state non-valence (closed) shells.	
exca_eval_exst_v[]	evaluate excitation/autoionisation for excited states from valence shells (v1 and v2 above).	
exca_eval_exst_cl[]	evaluate excitation/autoionisation for excited states from non-valence (closed) shells.	

Sample:

```
/ADF56    /PROMOTION RULES    /180    /10
index    config
    0    1s2  2s2  2p6  3s2  3p6  3d10 4s2  4p6  4d10 4f14 5s2  5p6  5d10 5f0  5g0  6s2  6p6
    1    1s2  2s2  2p6  3s2  3p6  3d10 4s2  4p6  4d10 4f14 5s2  5p6  5d10 5f0  5g0  6s2  6p5
    2    1s2  2s2  2p6  3s2  3p6  3d10 4s2  4p6  4d10 4f14 5s2  5p6  5d10 5f0  5g0  6s2  6p4
    3    1s2  2s2  2p6  3s2  3p6  3d10 4s2  4p6  4d10 4f14 5s2  5p6  5d10 5f0  5g0  6s2  6p3
    4    1s2  2s2  2p6  3s2  3p6  3d10 4s2  4p6  4d10 4f14 5s2  5p6  5d10 5f0  5g0  6s2  6p2
    5    1s2  2s2  2p6  3s2  3p6  3d10 4s2  4p6  4d10 4f14 5s2  5p6  5d10 5f0  5g0  6s2  6p1
    6    1s2  2s2  2p6  3s2  3p6  3d10 4s2  4p6  4d10 4f14 5s2  5p6  5d10 5f0  5g0  6s2
    7    1s2  2s2  2p6  3s2  3p6  3d10 4s2  4p6  4d10 4f14 5s2  5p6  5d10 5f0  5g0  6s1
    8    1s2  2s2  2p6  3s2  3p6  3d10 4s2  4p6  4d10 4f14 5s2  5p6  5d10
    9    1s2  2s2  2p6  3s2  3p6  3d10 4s2  4p6  4d10 4f14 5s2  5p6  5d9  5f0  5g0  6s1

index             0     1     2     3     4     5     6     7     8     9
n_el             86    85    84    83    82    81    80    79    78    78
no_v_shl          2     2     2     2     2     2     1     1     1     2
v1_shl           17    17    17    17    17    17    16    16    13    16
v2_shl           16    16    16    16    16    16     0     0     0    13
drct_eval_v       1     1     1     1     1     1     1     1     1     1
drct_eval_cl      1     1     1     1     1     1     1     1     1     1
min_shl_cl       11    11    11    11    11    11    11    11    11    11
exca_eval_v2      1     1     1     1     1     1     1     1     1     1
max_dn_v2         0     0     0     0     0     0     0     0     0     1
min_dn_v2        -1    -1    -1    -1    -1    -1     0     0     0     0
max_dl_v2         3     3     3     3     3     3     0     0     0     2
min_dl_v2        -1    -1    -1    -1    -1    -1     0     0     0    -2
exca_eval_cl      1     1     1     1     1     1     1     1     1     1
max_dn_cl         1     1     1     1     1     1     1     1     1     1
min_dn_cl         0     0     0     0     0     0     0     0     0     0
max_dl_cl         4     4     4     4     4     4     4     4     4     4
min_dl_cl        -3    -3    -3    -3    -3    -3    -3    -3    -3    -3
exst_eval         1     1     1     1     1     1     1     1     1     1
exst_adf00_prt    1     1     1     1     1     1     1     1     1     1
exst_prt_hole_shl 0     0     0     0     0     0     0     0     0     0
max_n_exst        0     0     0     0     0     0     0     0     0     0
max_l_exst        0     0     0     0     0     0     0     0     0     0
drct_eval_exst_v  1     1     1     1     1     1     1     1     1     1
drct_eval_exst_cl 1     1     1     1     1     1     1     1     1     1
exca_eval_exst_v  1     1     1     1     1     1     1     1     1     1
exca_eval_exst_cl 1     1     1     1     1     1     1     1     1     1

         .     .     .

index    config
  170    1s2  2s2  2p6
  171    1s2  2s2  2p5
  172    1s2  2s2  2p4
  173    1s2  2s2  2p3
  174    1s2  2s2  2p2
  175    1s2  2s2  2p1
  176    1s2  2s2
  177    1s2  2s1
  178    1s2
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  179    1s1

index           170   171   172   173   174   175   176   177   178   179
n_el             10     9     8     7     6     5     4     3     2     1
no_v_shl          1     1     1     1     1     1     1     1     1     1
v1_shl           17    17    17    17    17    17    16    16    13    16
v2_shl           16    16    16    16    16    16     0     0     0    13
drct_eval_v       1     1     1     1     1     1     1     1     1     1
drct_eval_cl      1     1     1     1     1     1     1     1     1     1
min_shl_cl       11    11    11    11    11    11    11    11    11    11
exca_eval_v2      1     1     1     1     1     1     1     1     1     1
max_dn_v2         0     0     0     0     0     0     0     0     0     1
min_dn_v2        -1    -1    -1    -1    -1    -1     0     0     0     0
max_dl_v2         3     3     3     3     3     3     0     0     0     2
min_dl_v2        -1    -1    -1    -1    -1    -1     0     0     0    -2
exca_eval_cl      1     1     1     1     1     1     1     1     1     1
max_dn_cl         1     1     1     1     1     1     1     1     1     1
min_dn_cl         0     0     0     0     0     0     0     0     0     0
max_dl_cl         4     4     4     4     4     4     4     4     4     4
min_dl_cl        -3    -3    -3    -3    -3    -3    -3    -3    -3    -3
exst_eval         1     1     1     1     1     1     1     1     1     1
exst_adf00_prt    1     1     1     1     1     1     1     1     1     1
exst_prt_hole_shl 0     0     0     0     0     0     0     0     0     0
max_n_exst        0     0     0     0     0     0     0     0     0     0
max_l_exst        0     0     0     0     0     0     0     0     0     0
drct_eval_exst_v  1     1     1     1     1     1     1     1     1     1
drct_eval_exst_cl 1     1     1     1     1     1     1     1     1     1
exca_eval_exst_v  1     1     1     1     1     1     1     1     1     1
exca_eval_exst_cl 1     1     1     1     1     1     1     1     1     1

C-----------------------------------------------------------------------
C This is a hand  selected set of rules chosen by H. Summers.
C
C User:  Hugh Summers
C Date:  09/01/09
C-----------------------------------------------------------------------
```