MODULE 2
Complex species in the core and edge of the fusion plasma. Describing and calculating their characteristics - the current state.

Demonstration script

Hugh Summers, Martin O'Mullane and Alessandra Giunta

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Contents

1 Demo (a) Identifying metastables

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DEMO A: Identifying metastables
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PURPOSE: Identify the metastable terms or levels using population calculations
and from adf00 file, which contains ionisation potentials and normalised
energies for ground and metastable terms (ls-resolution) or levels
(ic-resolution).

EXAMPLE: For demo a1 see also Module 1 Demo d1.
The input file is the following  adf04 for neutral helium:
/home/adas/adas/adf04/adas#2/mom97_ls#he0.dat
The temperature chosen is 8.6 eV.

The element chosen for Demo a2 is silicon. There are 3 adf00 files for this
element:
1. unresolved adf00:  /home/adas/adas/adf00/si.dat
2. ls resolved adf00: /home/adas/adas/adf00/si_ls.dat
3. ic resolved adf00: /home/adas/adas/adf00/si_ic.dat


DEMO a1: Examine an ADAS205 graph
1. Use ADAS205 interactively (see Module 1 Demo d1 - demo_d1.ps)
2. Look at the behaviour of the population of different terms.
Sample of output file: demo_a_1.ps


DEMO a2: Interrogate adf00 '_ls' and '_ic' forms
1. Look at the 3 adf00 data files for Silicon.
2. Read the 3 adf00 using read-adf00.pro.
3. Plot ionisation potential as a function of ionisation stage
   for the unresolved case.
4. List metastable states in the different resolutions.

Program: demo_a_2.pro
Sample of output file: demo_a_2.ps,demo_a_2.txt
```

1.1 Demo (a) Figures

1.1.1 Demo (a-1) demo_a/demo_a_1pdf

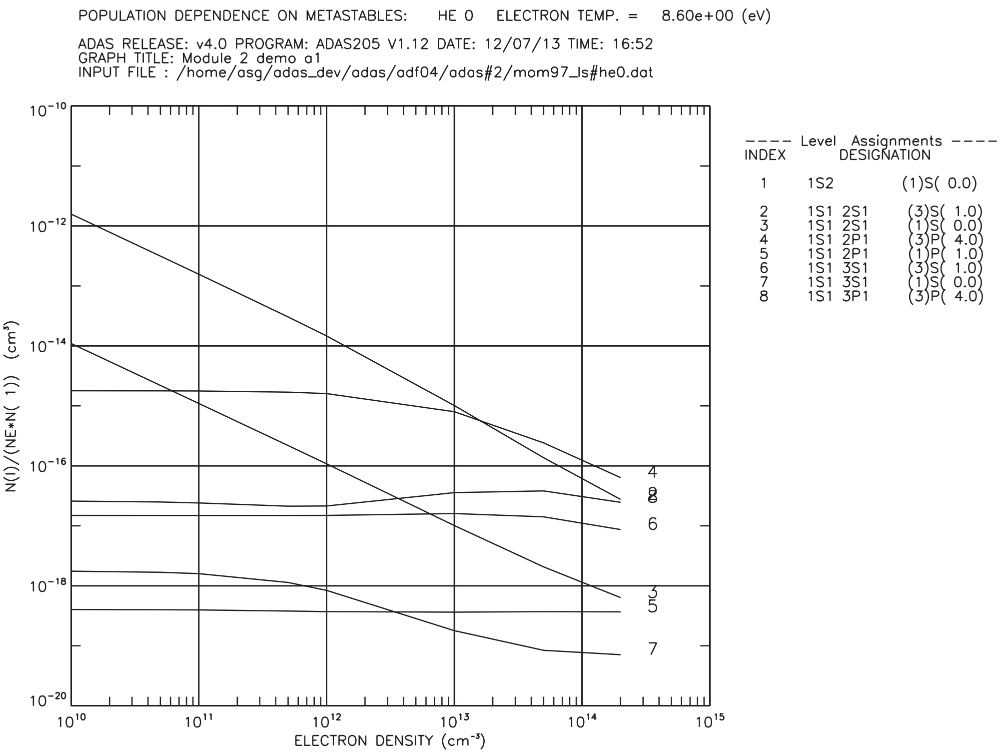

Figure 1: demo_a/demo_a_1.pdf

1.2 Demo (a) IDL procedures

1.2.1 Demo (a-2) demo_a_2.pro

Demonstration IDL procedure using *read_adf00*.

```
pro demo_a_2

;Define file paths
file_unres='/home/adas/adas/adf00/si.dat'
file_ls='/home/adas/adas/adf00/si_ls.dat'
file_ic='/home/adas/adas/adf00/si_ic.dat'


;Use read_adf00.pro in the unresolved case and using ls and ic resolutions
read_adf00,file=file_unres,z1=z1,$
           ionpot=ionpot_unres,nmeta=nmeta_unres,config=config_unres,/all
read_adf00,file=file_ls,z1=z1,$
           ionpot=ionpot_ls,nmeta=nmeta_ls,config=config_ls,isa=isa_ls,$
           ila=ila_ls,xja=xja_ls,/all,/ls
read_adf00,file=file_ic,z1=z1,$
           ionpot=ionpot_ic,nmeta=nmeta_ic,config=config_ic,isa=isa_ic,$
           ila=ila_ic,xja=xja_ic,/all,/ic

;plot ionisation potential as a function of ionisation stage

set_plot,'ps'
device, /isolatin1, font_index=8
device, bits=8, filename='demo_a_2.ps',         $
        font_size = 14, xsize=18.0, ysize=16.0, $
        yoffset=7.0, /color
device, /helvetica
plot_io,z1,ionpot_unres,title='Silicon',$
                     xtitle='Ionisation stage',$
                     ytitle='Ionisation potential'

device,/close
set_plot,'x'

;Print the number of metastables in each resolution in a file
openw,lun,'demo_a_2.txt',/get_lun
printf, lun,' ion.stage   unres   ls      ic'
for j = 0, 13 do printf,lun, ' Si+' + string(j,format='(i2.2)'),  $
                 nmeta_unres[j], nmeta_ls[j], nmeta_ic[j]

;For Si+9 identify the metastables

printf,lun, ''
printf,lun, 'Unresolved : ' + config_unres[9]
printf,lun, ''
printf,lun, 'LS resolution'
```

```
for j = 1, nmeta_ls[9] do printf,lun, strtrim(strmid(config_ls[9,j],4),2),'  ',$
                                      strtrim(string(isa_ls[9,j]),2),$
                                      '('+strtrim(string(ila_ls[9,j]),2)+')',  $
                                      strtrim(string(xja_ls[9,j]),2)
printf,lun, ''
printf,lun, 'IC resolution'
for j = 1, nmeta_ic[9] do printf,lun, strtrim(strmid(config_ic[9,j],4),2),'  ',$
                                      strtrim(string(isa_ic[9,j]),2),$
                                      '('+strtrim(string(ila_ic[9,j]),2)+')',  $
                                      strtrim(string(xja_ic[9,j]),2)

close,lun
free_lun,lun

end
```

2 Demo (b) Computing 'bn' and 'ca'/'ls'/'ic' populations

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DEMO B: Computing 'bn' and 'ca'/'ls'/'ic' populations
------------------------------
PURPOSE: To evaluate the populations at different resolutions. Furthermore,
this demo shows how to create and locate the projection file and the effect
on the low levels.

This is required in the Generalised Collisional-Radiative (GCR) modelling
for the solution of the whole population structure.
In ADAS the GCR model is implemented as "ls resolution", that is to say  the
population structure is evaluated for LS terms.
This is appropriate for light element ions for which the fine structure
separation of levels is small. Although fine structure separation may be
observable through distinct components in high resolution spectroscopy, the
levels are in relative statistical proportion.

As one moves to heavier species and more highly ionised ions, the fine
structure separations become larger  and the relative population deviates
from relative statistical.  This is called "ic resolution".  On the other
hand, in finite density plasma, as one moves to higher quantum shells
collisional redistribution becomes more efficient and populations move
progressively towards the LTE regime. Firstly, terms of the same nl-shell
move into relative statistical proportions. This is called "ca resolution".
Finally l-subshells of the same n-shell move into relative statistical
populations. This is referred to as "bn resolution". This mnemonics indicate
that at bn resolution it is only necessary to work with whole n-shell
population whereas at ic resolution it is necessary to work with individual
level population.

A high precision study must deal with all the levels of an atom, but it is
only required to treat the low levels, particularly which are observed
spectroscopically in high resolution, higher level population may be treated
in coarser resolution. This leads to a sequence of condensation and
projection extended down to the low levels (See Module 2 notes).

EXAMPLE: The input file for ADAS316, which shows the behaviour of bn
resolution as a function of representative n-shell, is adf25_bn#14_si3.dat.

For producing the projection file, Si3+ is used as example. The input for
ADAS204 is   bns96#na_si3.dat. The output is adas204_adf17.pass in the adf17
format.

The data file exp96#na_si3ls.dat in the adf18 format is a mapping file which
relate the adf17 produced by ADAS204 to the adf04.
The populations of excited states are calculated by ADAS208 (run_adas208.pro
from the command line). Demo b4 uses run_adas208.pro to compute the
```

populations of excited states for Si3+ including the projection file and without it.
The input are the following:
- adf04: asg09_lgy09_ls#si3.dat
- adf18: exp96#na_si3ls.dat

COMMENTS: The file used as driver for ADAS316 and ADAS204 have been copied from central ADAS and changed according to the purpose (e.g. adding the correct paths etc.).

DEMO b1: 'bn' population with ADAS316
1. Run ADAS316 interactively.
Sample of output file: adas316_plot.ps

DEMO b2: Using ADAS204 to produce a projection file
1. Run ADAS204 interactively to produce the projection file of the adf17 format.
Sample of output file: adas204_adf17.pass

DEMO b3: Locating projection/expasion matrices of type adf17
1. Look at the projection file produced bu ADAS204 and build up the mapping file in the adf18 format.
Sample of output file: exp96#na_si3ls.dat

DEMO b4: Use run_adas208.pro with and without projection file
1. define the input file in the adf04 and adf18 formats.
2. Use run_adas208.pro including the adf18 data file (projection mapping file).
3. Use run_adas208.pro without the adf18 data file.
4. Plot the populations as a function of excited states in case 2. and 3.
Program: demo_b_4.pro
Output files: demo_b_4.ps

2.1 Demo (b) Figures

2.1.1 Demo (b-1) demo_b/adas316_plot.pdf

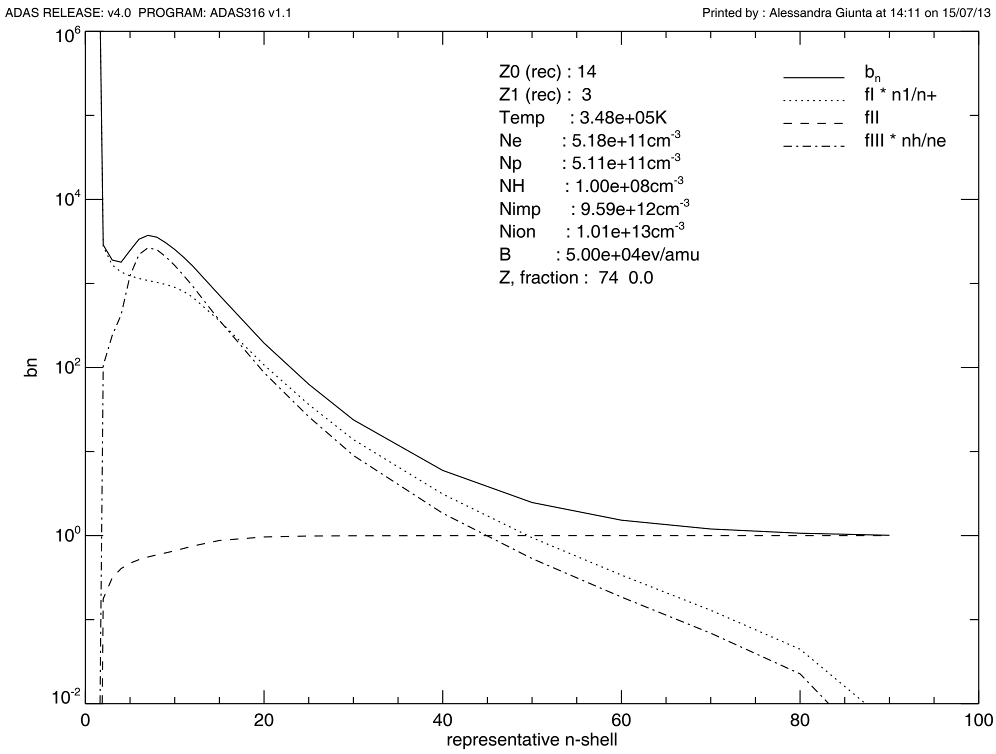

Figure 2: GTe-function plot vs Te for and O^{+4} transition

2.1.2 Demo (b-4) demo_b/demo_b_4.pdf

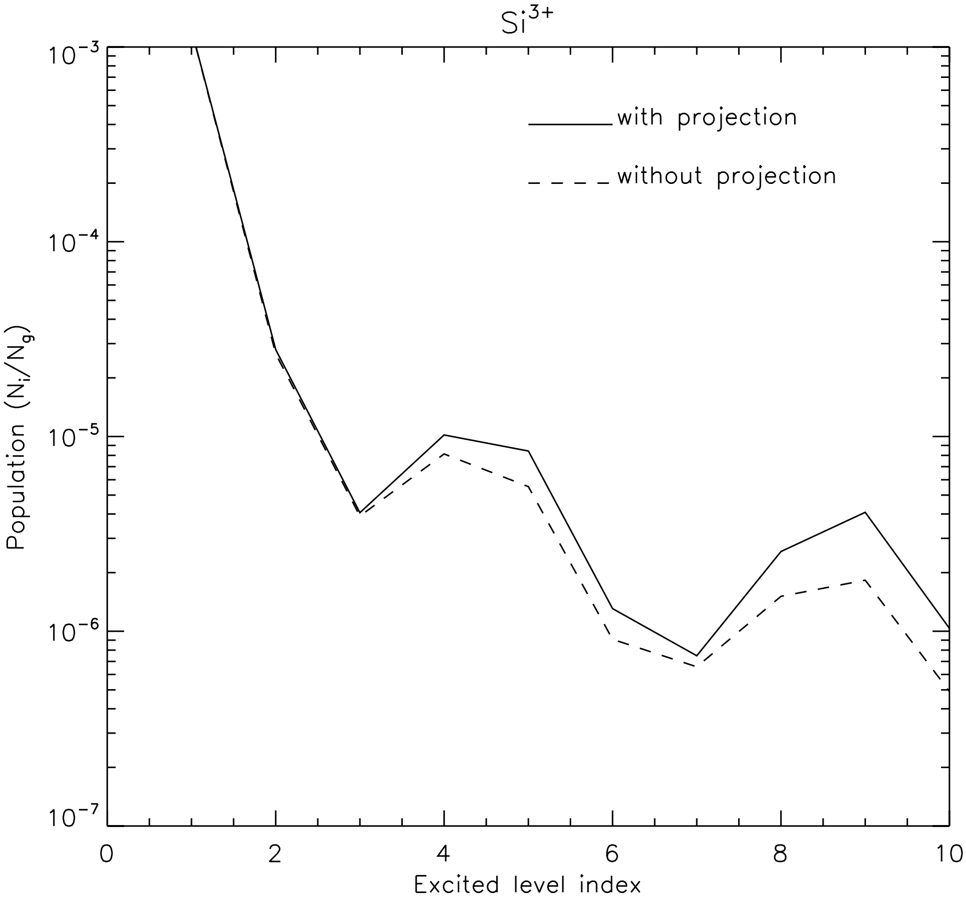

Figure 3: demo_b/demo_b_4.pdf

2.2 Demo (b) Procedures

2.2.1 Demo (b-4) demo_b/demo_b_4.pro

```
pro demo_b_4
;to compare the population obtained from the adf04 for Si3+ using the projection
;file and without it


te        = 13.0
dens      = 1e13
unit_te   = 'ev'
unid_dens = 'cm-3'
meta_list = [1]


adf04 = 'asg09_lgy09_ls#si3.dat'
adf18 = 'exp96#na_si3ls.dat'

;use run_adas208.pro to calculate the populations with the projection file
run_adas208, adf04=adf04, adf18=adf18,                                  $
             te=te,dens=dens, unit_te=unit_te,unit_dens=unit_dens,      $
             meta=meta_list,                                            $
             pass_dir='.', pop=pop_pju, log='paper.txt'

;use run_adas208.pro without the projection file
run_adas208, adf04=adf04,                                               $
             te=te,dens=dens, unit_te=unit_te,unit_dens=unit_dens,      $
             meta=meta_list,                                            $
             pass_dir='.', pop=pop_llu



;-----------------
; Plot populations
;-----------------

index     = indgen(pop_pju.numlev) + 1
dep_pju   = pop_pju.dependence
dep_llu   = pop_llu.dependence

xmin = 1
xmax = 10
ymin = 1e-7
ymax = 1e-3

set_plot,'ps'
device, /isolatin1, font_index=8
device, bits=8, filename='demo_b_4.ps',  $
        font_size = 14, xsize=18.0, ysize=16.0, $
```

```
        yoffset=7.0, /color
device, /helvetica
plot_io, [xmin, xmax], [ymin, ymax], /nodata, ystyle=1,$
         title='Si!u3+!n', $
         xtitle = 'Excited level index', $
         ytitle = 'Population (N!di!n/N!dg!n)'

oplot, index, dep_pju, thick=3
oplot, index, dep_llu, line=2, thick=3

plots,[5.,6.],[4.e-4,4.e-4], thick=3
xyouts,6.05,4.e-4,'with projection'
plots,[5.,6.],[2.e-4,2.e-4], thick=3,line=2
xyouts,6.05,2.e-4,'without projection'


device, /close
set_plot,'X'
!p.font=-1

end
```

2.3 Demo (b) Tables and datasets

2.3.1 Demo (b-2) demo_b/adas204_adf17.pass

```
 SEQUENCE = na   NUCCHG =14   NPARNT = 2   MAXD =24   MAXT =24

 IEDMAT = 0   IECION = 0   IETREC = 0   IEDREC = 0   IERREC = 0   IEXREC = 0   IERSYS = 0

 NE(CM-3) =   1.64D+05  1.64D+06  1.64D+07  1.64D+08  1.64D+09  1.64D+10  4.92D+10  1.64D+11
              4.92D+13  1.64D+14  4.92D+14  1.64D+15  4.92D+15  1.64D+16  4.92D+16  1.64D+17
 TE(K)    =   8.00D+03  1.12D+04  1.60D+04  2.40D+04  3.20D+04  4.80D+04  8.00D+04  1.12D+05
              8.00D+05  1.12D+06  1.60D+06  2.40D+06  3.20D+06  4.80D+06  8.00D+06  1.12D+07

 IPRT =  1     TRMPRT = (1S)     SPNPRT =  1.
 --------------------------------------------
                                                  SPNSYS =  2.     NSHEL =  3
                                                  ---------------------------
 ID= 1 IT= 1 N= 3   9.3737513787D-13-2.5881195019D+09-6.2892858578D+08
             N= 4  -9.3732071464D-13 2.5881195019D+09-7.2243053977D+08
             N= 5  -5.4423231613D-17-5.8160151830D-06 1.3513591255D+09
       (DIR) N= 3   9.3737489303D-13-2.5881195019D+09-6.2892858578D+08
             N= 4  -9.3732060783D-13 2.5881195019D+09-7.2243053977D+08
             N= 5  -5.4285198554D-17-5.8031868604D-06 1.3513591255D+09
       (PRB)        4.2567599516D-22

 ID= 1 IT= 2 N= 3   6.6555125989D-10-2.5881195019D+09-6.2892858578D+08
             N= 4  -6.6509918273D-10 2.5881195019D+09-7.2243053977D+08
             N= 5  -4.5207702277D-13-6.0327599846D-05 1.3513591255D+09
       (DIR) N= 3   6.6554400139D-10-2.5881195019D+09-6.2892858578D+08
             N= 4  -6.6509599877D-10 2.5881195019D+09-7.2243053977D+08
             N= 5  -4.4800261554D-13-5.9867220145D-05 1.3513591255D+09
       (PRB)        3.3778496536D-22
       .        .       .
                                                                          0.0000000000D+00

 ID=24 IT=24 N= 3   1.9035247633D+11-8.5202879688D+10-1.0056202220D+10
             N= 4  -1.4628947181D+11 1.1544201549D+12-5.3447206624D+11
             N= 5  -2.5724447421D+10-8.3267586993D+11 3.9016749836D+12
       (DIR) N= 3   1.6895371708D+11-8.5163410268D+10-8.8547709432D+09
             N= 4  -1.4622619208D+11 8.8410431550D+11-5.1277901425D+11
```

```
          N= 5  -2.2727524999D+10-7.9894090523D+11 5.2163378519D+11
      (PRB)        1.4013878323D-22

---------------------------------------------------------------------------------------------
```

2.3.2 Demo (b-3) demo_b/exp96#na_si3ls.dat

```
 &SEQINF SEQ='Na',
         DSNREF='asg09_lgy09_ls#si3.dat',
         DSNCPM='/home/asg/adas_modules/module_2/demo_b/adas204_adf17.pass ',
         NPARNT=2,
         NSHEL=5,
         NLEV= 12,
 &END

       PARENT      :(1S)       :(3P)       :
       SPINPRT     :1          :3          :
       NSPNSYS     :1          :1          :

    PARENT =  1
    -----------
       SPINSYS     :2          :
       LOWESTN     :3          :
       IMAX        :1          :
       LOWESTP     :1.0000     :
       FRPARNT     :0.2500     :

    PARENT =  2
    -----------
       SPINSYS     :2          :
       LOWESTN     :3          :
       IMAX        :1          :
       LOWESTP     :1.0000     :
       FRPARNT     :0.7500     :

 RESOLVED NL  <-- BUNDLE-N               N:1     N:2     N:3     N:4     N:5

INDX CODE                 SZD SP SH PT   N-SHELL NORMALISED WEIGHTS
---- ----                 --- -- -- --   -------------------------
  1 3S        (2)0( 0.5)   0  2  3  1  :       :       : 0.1111:       :
  1 3S        (2)0( 0.5)   0  2  3  2  :       :       : 1.0000:       :
  2 3P        (2)1( 2.5)   0  2  3  1  :       :       : 0.3333:       :
  3 3D        (2)2( 4.5)   0  2  3  1  :       :       : 0.5556:       :
  4 4S        (2)0( 0.5)   0  2  4  1  :       :       :       : 0.0625:
  5 4P        (2)1( 2.5)   0  2  4  1  :       :       :       : 0.1875:
  6 4D        (2)2( 4.5)   0  2  4  1  :       :       :       : 0.3125:
  7 4F        (2)3( 6.5)   0  2  4  1  :       :       :       : 0.4375:
  8 5S        (2)0( 0.5)   0  2  5  1  :       :       :       :       : 0.0400
  9 5P        (2)1( 2.5)   0  2  5  1  :       :       :       :       : 0.1200
 10 5D        (2)2( 4.5)   0  2  5  1  :       :       :       :       : 0.2000
 11 5F        (2)3( 6.5)   0  2  5  1  :       :       :       :       : 0.2800
 12 5G        (2)4( 8.5)   0  2  5  1  :       :       :       :       : 0.3600

C-----------------------------------------------------------------
C
C  ADF04 FILE FOR PARENT ION:
C  adf04/ada#14/asg09_ls#si4.dat
C
C  ADF04 FILE FOR RECOMBINED ION:
C  adf04/ada#14/asg09_lgy09_ls#si3.dat
C
C  Code     : ADAS807
C  Producer : Alessandra Giunta
C  Date     : 22/10/10
C
C-----------------------------------------------------------------
```

3 Demo (c) Producing and examining a mapping file

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DEMO C: Producing and examining a mapping file
------------------------------
PURPOSE: Create a mapping file to connect the specific ion file in the adf04
format to the dielectronuc data in the af09 format.

EXAMPLE: Li0+ is used as example. The input file for the ADAS807 running are the
following:
- adf04:  /home/adas/adas/adas#3/cpb02_ls#li0.dat
- adf09: /home/adas/adas/adf09/nrb93#he/nrb93#he_li1ls12.dat
         /home/adas/adas/adf09/nrb93#he/nrb93#he_li1ls22.dat


DEMO c1: Using ADAS807 to produce a mapping file
1. Run ADAS807 interactively to produce a mapping file for Li0+.
2. Examine the mapping file.
Sample of output files: adas807_a09_a04.pass
```

3.1 Demo (c) Tables and datasets

3.1.1 Demo (c-1) demo_c/adas807_a09_a04.pass

```
Specific ion input file
-----------------------
"ADASCENT"/adf04/adas#3/cpb02_ls#li0.dat   : specific ion file

Badnell dielectronic files
--------------------------
/home/adas/adas/adf09/nrb93#he/nrb93#he_li1ls12.dat : 1st. Badnell file
/home/adas/adas/adf09/nrb93#he/nrb93#he_li1ls22.dat : 2nd. Badnell file

Output files
------------
"ADASUSER"/pass/postllev.pass       : supplemented spec. ion file
"ADASUSER"/pass/postllev.pass1      : dielectronic data for MAINCL codes

Level cross-reference lists for specific ion and badnell files
---------------------------------------------------------------

    sp.        bd1.        bd2.        bd3.        bd4.        bd5.        bd6.
    ---        ----        ----        ----        ----        ----        ----
     1           1           1
     2          34          34
     3           2           2
     4           3           3
     5           4           4
     6           5           5
     7           6           6
     8           8           8
     9           7           7

C-------------------------------------------------------------------
C  #  specific ion                    Badnell 1                    Badnell 2
C   1      2S1              2S 1/2-->   2S1              2S 1/2 |    2S1              2S 1/2 |
C   2      2P1              2P 5/2-->   2P1              2P 5/2 |    2P1              2P 5/2 |
C   3      3S1              2S 1/2-->   3S1              2S 1/2 |    3S1              2S 1/2 |
C   4      3P1              2P 5/2-->   3P1              2P 5/2 |    3P1              2P 5/2 |
C   5      3D1              2D 9/2-->   3D1              2D 9/2 |    3D1              2D 9/2 |
C   6      4S1              2S 1/2-->   4S1              2S 1/2 |    4S1              2S 1/2 |
C   7      4P1              2P 5/2-->   4P1              2P 5/2 |    4P1              2P 5/2 |
C   8      4D1              2D 9/2-->   4D1              2D 9/2 |    4D1              2D 9/2 |
C   9      4F1              2F13/2-->   4F1              2F13/2 |    4F1              2F13/2 |
```

```
C-------------------------------------------------------------------

C----------------------------------------------------------------
C
C  ADF04 FILE  :
C     /home/asg/adas_dev/adas/adf04/adas#3/cpb02_ls#li0.dat
C
C  ADF09 FILE(S) FOR RECOMBINED ION:
C     /home/adas/adas/adf09/nrb93#he/nrb93#he_li1ls12.dat
C     /home/adas/adas/adf09/nrb93#he/nrb93#he_li1ls22.dat
C
C
C  Code     : ADAS807
C  Producer : Alessandra Giunta
C  Date     : 19/06/13
C
C----------------------------------------------------------------
```

4 Demo (d)Evaluating metastable pathways for ionisation cross-sections

```
------------------------------
DEMO D: Evaluating metastable pathways for ionisation cross-sections
------------------------------
PURPOSE: Convert an unresolved adf07 data file in a ls resolved adf07.
The adf07 data files provide electron impact ionisation rate coefficients for
each ion of an element. The baseline within ADAS is calculated using the offline
ADAS8#2 using the Configuration Average Distorted Wave  (CADW) method, which
guves stage to stage ionisation rates. The GCR picture requires metastable
resolved ionisation rates and so a resolved adf07.
This can be produced using the following idl routines, stored
in /home/adas/adas/idl/adaslib/proc_adf/:
- pathways_adf07.pro
- fractionate_adf07.pro
- split_adf07.pro.

EXAMPLE: For this demo Boron is considered. The resolved ionisation rates for
B1+->B2+ are derived.
The input files are the following:
- input adf04 for B1+:/home/adas/adas/adf04/belike/belike_nrb03#b1.dat
- input adf04 for B2+:/home/adas/adas/adf04/lilike/lilike_dvb02#b2.dat
- unresolved adf07 for B: /home/adas/adas/adf07/szd93#b/szd93#b_b.dat

DEMO d1:Convert adf07 from unresolved to resolved
1. Create the pathway file from the adf04 data files.
2. Generate an ionisation pathway spreadsheet.
3. Produce the resolved adf07.
4. Compare the resolved and unresolved adf07.
Program: demo_d.pro
Sample of output files: pathways_b1_b2.dat, fractionation_b.csv (use oocalc to
view), boron_adf07.dat
```

4.1 Demo (d) Tables and datasets

4.1.1 Demo (d-1) demo_d/pathways_b1_b2.dat

```
B+1
  B+1 Metastable Number:   2
  B+2 Metastable Number:   1
        Orbital Number:   3
       Pathway Numbers:   2   2
----------------------------------
Orbital      Energy(Ryd)
----------------------------------
1s              16.418
2s               1.919
2p               1.462

B+1 -> B+2
-------------------------------------------------------------------------------------
Pathways                                                    I.P.(cm-1)      I.P.(Ryd)
-------------------------------------------------------------------------------------
                1s2 2s2   1S   ->
                                    2s        1s2 2s1  2S       202888.0        1.84885
```

```
                              1s       1s1 2s2  2S           -1.0       -1.00000
          1s2 2s1 2p1   3P   ->
                              2p       1s2 2s1  2S       165544.0        1.50855
                              2s       1s2 2p1  2P       213916.0        1.94935
-----------------------------------------------------------------------------------
```

4.1.2 Demo (d-1) demo_d/fractionation_b.csv

```
"Transition","Metastable","Index","Purpose","Formula","Shell 1",,"Shell 2",,"Shell 3",
,"Shell 4",,"Shell 5",,"Shell 6",,"Shell 7",,"Scale factor"
,,,,,"I(1s) (Ryd)","z(1s)","I(2s) (Ryd)","z(2s)","I(2p) (Ryd)","z(2p)","I(3s)(Ryd)",
"z(3s)","I(3p)(Ryd)","z(3p)","I(4s)(Ryd)","z(4s)","I(3d)(Ryd)","z(3d)",
"B+1 -> B+2",,"f1",,,    14.4990,    2.00000,    1.84885,    2.00000,,,,,,,,,,1.000
,,,"RATE comparison","ratio=RATE/f1",,,,,,,,,,,,,,
,"1s2 2s2(1S)","f2","2s  via  2S  direct",,,,      1.84885,      2.00000,,,,,,,,,,1.00000
,,"f3","1s +auto",,      14.4990,      2.00000,,,,,,,,,,,,1.00000
,,"f4","1s direct",,      16.4180,      2.00000,,,,,,,,,,,,1.00000
,,,"1s2 2s2(1S) total","(f2+f3)*ratio",,,,,,,,,,,,,,
,"#",,"1s2 2s2(1S)->1s2 2s1(2S)","(f2+f3)*ratio",,,,,,,,,,,,,,
,"1s2 2s1 2p1(3P)","f5","2p  via  2S  direct",,,,,,      1.50855,      1.00000,,,,,,,,1.00000
,,"f6","2s  via  2P  +auto",,,,1.50855,      1.00000,,,,,,,,,,1.00000
,,"f7","1s +auto",,      14.4990,      2.00000,,,,,,,,,,,,1.00000
,,"f8","1s direct",,      16.4180,      2.00000,,,,,,,,,,,,1.00000
,,,"1s2 2s1 2p1(3P) total","(f5+f6+f7)*ratio",,,,,,,,,,,,,,
,"#",,"1s2 2s1 2p1(3P)->1s2 2s1(2S)","(f5+f6+f7)*ratio",,,,,,,,,,,,,,
```

4.1.3 Demo (d-1) demo_d/boron_adf07.dat

```
    4    /B   IONISATION RATE COEFFICIENTS   /
B + 1/B + 2/   24/I.P. =          202887.2/ICODE =  1/FCODE =  0/ISEL =   1
 1.000E+00 2.000E+00 3.000E+00 4.000E+00 5.000E+00 7.000E+00
 1.000E+01 1.500E+01 2.000E+01 3.000E+01 4.000E+01 5.000E+01
 7.000E+01 1.000E+02 1.500E+02 2.000E+02 3.000E+02 4.000E+02
 5.000E+02 7.000E+02 1.000E+03 2.000E+03 5.000E+03 1.000E+04
 2.629E-12 3.189E-10 1.803E-09 4.520E-09 8.059E-09 1.618E-08
 2.832E-08 4.526E-08 5.807E-08 7.539E-08 8.620E-08 9.339E-08
 1.019E-07 1.079E-07 1.110E-07 1.111E-07 1.088E-07 1.058E-07
 1.028E-07 9.758E-08 9.128E-08 7.803E-08 6.079E-08 4.915E-08
B + 1/B + 2/   24/I.P. =          202887.2/ICODE =  1/FCODE =  1/ISEL =   2
 1.000E+00 2.000E+00 3.000E+00 4.000E+00 5.000E+00 7.000E+00
 1.000E+01 1.500E+01 2.000E+01 3.000E+01 4.000E+01 5.000E+01
 7.000E+01 1.000E+02 1.500E+02 2.000E+02 3.000E+02 4.000E+02
 5.000E+02 7.000E+02 1.000E+03 2.000E+03 5.000E+03 1.000E+04
 2.629E-12 3.189E-10 1.803E-09 4.520E-09 8.059E-09 1.618E-08
 2.832E-08 4.526E-08 5.807E-08 7.539E-08 8.620E-08 9.339E-08
 1.019E-07 1.079E-07 1.110E-07 1.111E-07 1.088E-07 1.058E-07
 1.028E-07 9.758E-08 9.128E-08 7.803E-08 6.079E-08 4.915E-08
B + 1/B + 2/   24/I.P. =          165543.8/ICODE =  2/FCODE =  0/ISEL =   3
 1.000E+00 2.000E+00 3.000E+00 4.000E+00 5.000E+00 7.000E+00
 1.000E+01 1.500E+01 2.000E+01 3.000E+01 4.000E+01 5.000E+01
 7.000E+01 1.000E+02 1.500E+02 2.000E+02 3.000E+02 4.000E+02
 5.000E+02 7.000E+02 1.000E+03 2.000E+03 5.000E+03 1.000E+04
 4.047E-10 4.817E-09 1.252E-08 2.123E-08 2.990E-08 4.574E-08
 6.504E-08 8.806E-08 1.037E-07 1.231E-07 1.342E-07 1.411E-07
 1.485E-07 1.526E-07 1.529E-07 1.507E-07 1.450E-07 1.396E-07
 1.347E-07 1.267E-07 1.176E-07 9.936E-08 7.655E-08 6.151E-08
B + 1/B + 2/   24/I.P. =          165543.8/ICODE =  2/FCODE =  1/ISEL =   4
 1.000E+00 2.000E+00 3.000E+00 4.000E+00 5.000E+00 7.000E+00
 1.000E+01 1.500E+01 2.000E+01 3.000E+01 4.000E+01 5.000E+01
 7.000E+01 1.000E+02 1.500E+02 2.000E+02 3.000E+02 4.000E+02
 5.000E+02 7.000E+02 1.000E+03 2.000E+03 5.000E+03 1.000E+04
 4.047E-10 4.817E-09 1.252E-08 2.123E-08 2.990E-08 4.574E-08
 6.504E-08 8.806E-08 1.037E-07 1.231E-07 1.342E-07 1.411E-07
 1.485E-07 1.526E-07 1.529E-07 1.507E-07 1.450E-07 1.396E-07
 1.347E-07 1.267E-07 1.176E-07 9.936E-08 7.655E-08 6.151E-08
C-------------------------------------------------------------------------
C
C
C
C  Resolved adf07 :  /home/adas/adas/adf07/szd93#b/szd93#b_b.dat
C
C
```

```
C
C
C
C   ISEL  INITIAL MET.    DESIG.                     FINAL  MET.    DESIG.
C           ION   CODE                                ION   CODE
C   ----  ------- ---- ---------------              ------- ---- ---------------
C     1   B + 1    1     1s2 2s2 (1S)                B + 2    0     Total
C     2   B + 1    1     1s2 2s2 (1S)                B + 2    1     1s2 2s1 (2S)
C     3   B + 1    2     1s2 2s1 2p1 (3P)            B + 2    0     Total
C     4   B + 1    2     1s2 2s1 2p1 (3P)            B + 2    1     1s2 2s1 (2S)
C
C
C
C  Code   : split_adf07.pro
C  Author : Alessandra Giunta
C  Date   : 16/07/13
C
C----------------------------------------------------------------------------
```

5 Demo (e)Making up partitions and executing superstage compression

```
------------------------------
DEMO E: Making up partitions and executing superstage compression
------------------------------
PURPOSE: To build up a partition and execute a superstage compression.
In the GCR picture, each element is decribed by the fractional abundances of
every ionisation stage, derived by the effective ionisation and recombination
coefficients. From a dynamic point of view the whole set of populations may be
tracked in transport modelling. However, for heavy species, the complete set of
populations is large. Since not all populations are of equal importance,
grouping of populations may be appropriate and reduces the problem od dealing
with a too large number of ionisation stages. The specification of grouping is
called "partition", while the members of partition are called "superstages".

EXAMPLE: Tungsten is used fo this demo. The input file for the ADAS416 run is
w_partition_7groups.dat. The output provide the whole set of effective
coefficients for the superstages. These files can be read by read_adf11.pro to
shoe the effective coefficients.

COMMENTS: In demo_e_3.pro, the paths which define the adf11 produced by ADAS416
depend on the user.


DEMO e1: Examine a natural partition
1.Use preview_natural_partition.pro to show the
  - fractional ionisation otential change
  - partition fractional abundance
  - fractional abundances for all 74 W ionisation stages
  - fractional abundances for 35 partitions of W
Programs: demo_e_1.pro
Sample of output files: demo_e_1.ps


DEMO e2: Apply superstage compression with ADAS416
1. Use ADAS416 interactively.
Samples of ouput files: adas416_plot.ps
All set of adf11 data files: acd50  ccd50  ecd50  plt50  prb50
                             prc50  scd50  ycd50  zcd50

DEMO e3: Show the superstage coefficient behaviour.
1. Define input files.
2. Use read_adf1.pro to read:
   - recombination rates
   - effective charge
Program: demo_e_3.pro
Sample of output files: demo_e_3_acd.ps, demo_e_3_zeff.ps
```

5.1 Demo (e) Figures

5.1.1 Demo (e-1) demo_e/demo_e_1.pdf

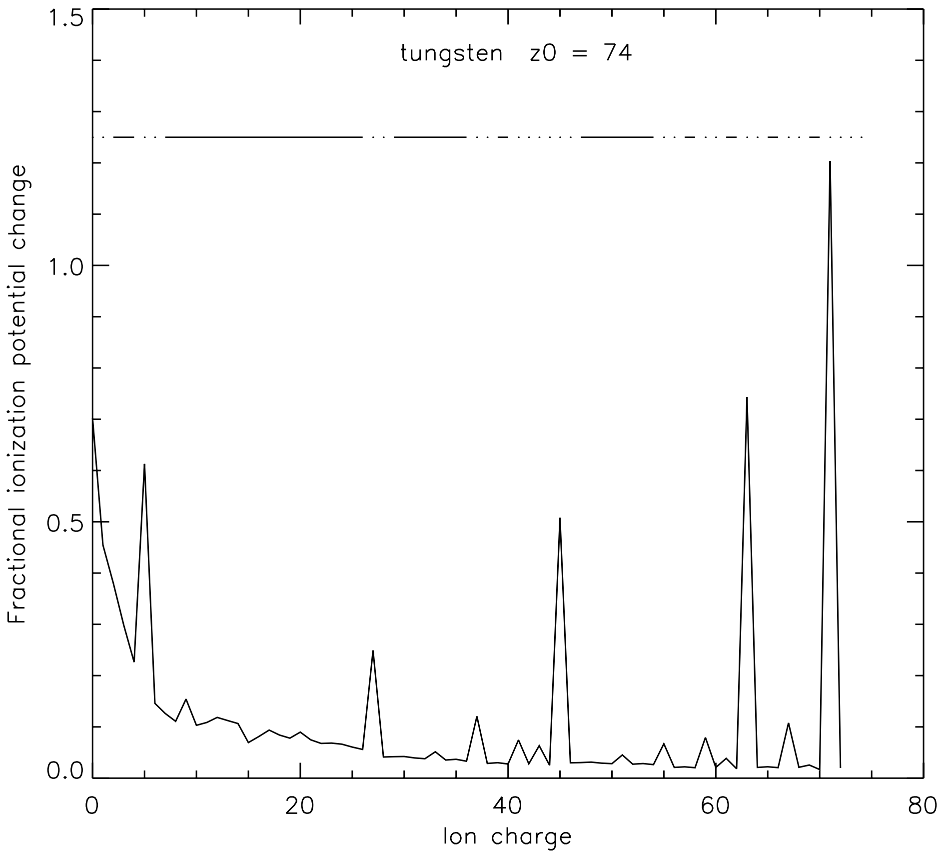

Figure 4: Natural partition for tungsten

5.1.2 Demo (e-2) demo_e/adas416_plot.pdf

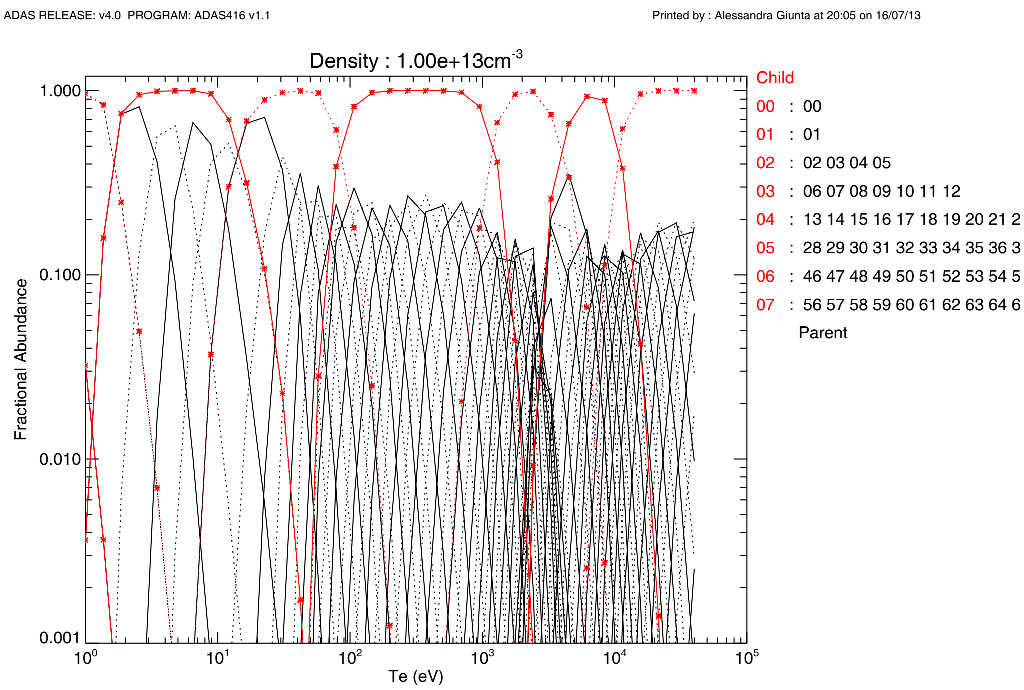

Figure 5: Superstage ionisation balance for tungsten

5.1.3 Demo (e-3) demo_e/demo_e_3_acd.pdf

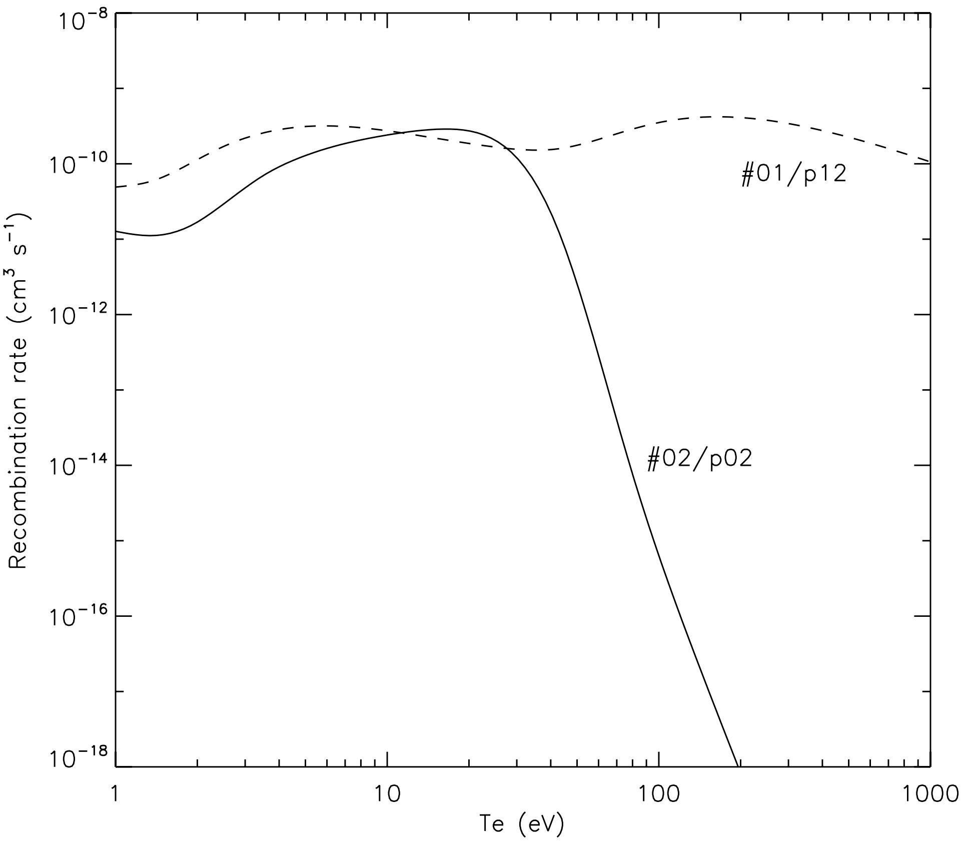

Figure 6: Superstage recombination coeffients for tungsten

5.1.4 Demo (e-3) demo_e/demo_e_3_zeff.pdf

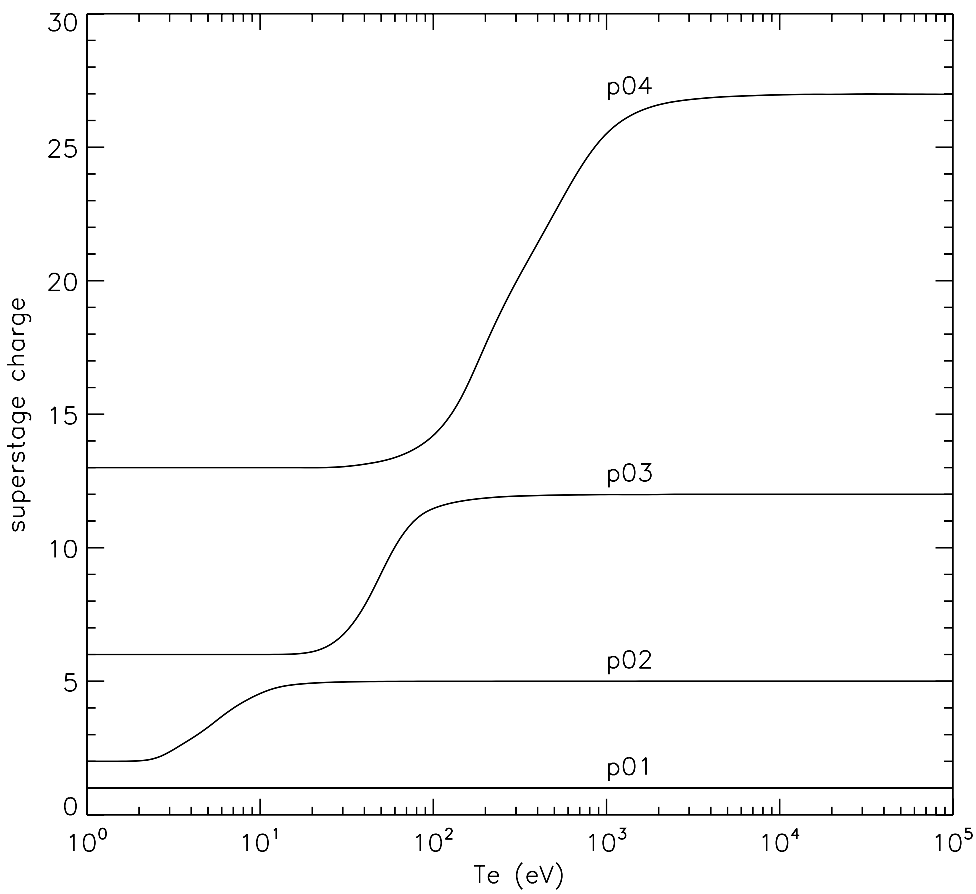

Figure 7: Superstage charges for tungsten

5.2 Demo (e) Procedures

5.2.1 Demo (e-1 demo_e_1.pro

Demonstration IDL procedure for preliminary examination of supestage partitions.

```
pro demo_e_1
;to identify the natural partition for W and plot the superstages

set_plot,'ps'
device, /isolatin1, font_index=8
device, bits=8, filename='demo_e_1.ps',  $
        font_size = 14, xsize=18.0, ysize=16.0, $
        yoffset=7.0, /color
device, /helvetica

preview_natural_partition, z0=74, te_min=10, te_max=50000, plot_type=1

preview_natural_partition, z0=74, te_min=10, te_max=50000, plot_type=2

preview_natural_partition, z0=74, te_min=10, te_max=50000, plot_type=3

preview_natural_partition, z0=74, te_min=10, te_max=50000, plot_type=4

device, /close
set_plot,'X'
!p.font=-1

end
```

5.2.2 Demo (e-3 demo_e_3.pro

To show the effective coefficients for W after a superstage compression.

```
pro demo_e_3
;To show the effective coefficients for W after a superstage compression has been
applied.

; Conditions

itval = 200
te    = adas_vector(low=1, high=1e5, num=itval)
dens  = fltarr(itval) + 1e13

; files

files    =  $
     { acd : '/home/asg/adas_modules/module_2/demo_e/adf11/acd50/acd50_w.dat', $
       scd : '/home/asg/adas_modules/module_2/demo_e/adf11/scd50/scd50_w.dat', $
       plt : '/home/asg/adas_modules/module_2/demo_e/adf11/plt50/plt50_w.dat', $
       prb : '/home/asg/adas_modules/module_2/demo_e/adf11/prb50/prb50_w.dat'  }
```

```
files_ss =
     { acd : '/home/asg/adas_modules/module_2/demo_e/adf11/acd50/acd50_w_02.dat', $
       scd : '/home/asg/adas_modules/module_2/demo_e/adf11/scd50/scd50_w_02.dat', $
       plt : '/home/asg/adas_modules/module_2/demo_e/adf11/plt50/plt50_w_02.dat', $
       prb : '/home/asg/adas_modules/module_2/demo_e/adf11/prb50/prb50_w_02.dat'  }


; Recombination rates


read_adf11, file=files_ss.acd, class='acd', iz0=74, iz1=3, $
            te=te, dens=dens, data=acd_ss

read_adf11, file=files.acd, class='acd', iz0=74, iz1=13, $
            te=te, dens=dens, data=acd


xmin = min(te, max=xmax)
xmax = 1e3
ymin = 1e-18
ymax = 1e-8


set_plot,'ps'
device, /isolatin1, font_index=8
device, bits=8, filename='demo_e_3_acd.ps',  $
        font_size = 14, xsize=18.0, ysize=16.0, $
        yoffset=7.0, /color
device, /helvetica

plot_oo, [xmin, xmax], [ymin, ymax], /nodata, ystyle=1,  $
         xtitle = 'Te (eV)', $
         ytitle = 'Recombination rate (cm!u3!n s!u-1!n)'

oplot, te, acd_ss, thick=3

oplot, te, acd, thick=3, line=2

xyouts, 90, 1e-14, '#02/p02'
xyouts, 200, 6e-11, '#01/p12'

device, /close
set_plot,'X'
!p.font=-1

; Effective charge

file = '/home/asg/adas_modules/module_2/demo_e/adf11/zcd50/zcd50_w_02.dat'

read_adf11, file=file, class='zcd', iz0=74, iz1=1, $
```

```
            te=te, dens=dens, data=zcd_p0
read_adf11, file=file, class='zcd', iz0=74, iz1=2, $
            te=te, dens=dens, data=zcd_p1
read_adf11, file=file, class='zcd', iz0=74, iz1=3, $
            te=te, dens=dens, data=zcd_p2
read_adf11, file=file, class='zcd', iz0=74, iz1=4, $
            te=te, dens=dens, data=zcd_p3
read_adf11, file=file, class='zcd', iz0=74, iz1=5, $
            te=te, dens=dens, data=zcd_p4


xmin = min(te, max=xmax)
ymin = min(zcd_p0)
ymax = max(zcd_p4)

set_plot,'ps'
device, /isolatin1, font_index=8
device, bits=8, filename='demo_e_3_zeff.ps',  $
        font_size = 14, xsize=18.0, ysize=16.0, $
        yoffset=7.0, /color
device, /helvetica

plot_oi, [xmin, xmax], [ymin, ymax], /nodata, ystyle=0,  $
         xtitle = 'Te (eV)', $
         ytitle = 'superstage charge'

oplot, te, zcd_p0, thick=3
oplot, te, zcd_p1, thick=3
oplot, te, zcd_p2, thick=3
oplot, te, zcd_p3, thick=3
oplot, te, zcd_p4, thick=3

xyouts, 1000, 1.5, 'p01'
xyouts, 1000, 5.5, 'p02'
xyouts, 1000, 12.5, 'p03'
xyouts, 1000, 27, 'p04'

device, /close
set_plot,'X'
!p.font=-1



end
```

5.3 Demo (e) Tables and datasets

5.3.1 Demo (e-2) demo_d/adf11/acd50/acd50_w_02.dat

```
   74    5   35    1    7     /TUNGSTEN              /ACD /GCR PROJECT     ADF11
--------------------------------------------------------------------------------
//#02/p00/ 00 /
      p01/ 01/
      p02/ 02 03 04 05/
      p03/ 06 07 08 09 10 11 12/
      p04/ 13 14 15 16 17 18 19 20 21 22 23 24 25 26 27/
      p05/ 28 29 30 31 32 33 34 35 36 37 38 39 40 41 42 43 44 45/
      p06/ 46 47 48 49 50 51 52 53 54 55/
      p07/ 56 57 58 59 60 61 62 63 64 65 66 67 68 69 70 71 72 73 74/
//#01/p00/ 00/p01/ 01/p02/ 02/p03/ 03/p04/ 04/p05/ 05/p06/ 06/p07/ 07/
      p08/ 08/p09/ 09/p10/ 10/p11/ 11/p12/ 12/p13/ 13/p14/ 14/p15/ 15/
      p16/ 16/p17/ 17/p18/ 18/p19/ 19/p20/ 20/p21/ 21/p22/ 22/p23/ 23/
      p24/ 24/p25/ 25/p26/ 26/p27/ 27/p28/ 28/p29/ 29/p30/ 30/p31/ 31/
      p32/ 32/p33/ 33/p34/ 34/p35/ 35/p36/ 36/p37/ 37/p38/ 38/p39/ 39/
      p40/ 40/p41/ 41/p42/ 42/p43/ 43/p44/ 44/p45/ 45/p46/ 46/p47/ 47/
      p48/ 48/p49/ 49/p50/ 50/p51/ 51/p52/ 52/p53/ 53/p54/ 54/p55/ 55/
      p56/ 56/p57/ 57/p58/ 58/p59/ 59/p60/ 60/p61/ 61/p62/ 62/p63/ 63/
      p64/ 64/p65/ 65/p66/ 66/p67/ 67/p68/ 68/p69/ 69/p70/ 70/p71/ 71/
      p72/ 72/p73/ 73/p74/ 74/
--------------------------------------------------------------------------------
  11.00000  12.00000  13.00000  14.00000  15.00000
   0.00000   0.13535   0.27071   0.40606   0.54142   0.67677   0.81213   0.94748
   1.08284   1.21819   1.35355   1.48890   1.62426   1.75961   1.89497   2.03032
   2.16568   2.30103   2.43638   2.57174   2.70709   2.84245   2.97780   3.11316
   3.24851   3.38387   3.51922   3.65458   3.78993   3.92529   4.06064   4.19600
   4.33135   4.46671   4.60206
---------------------/ ISPP= 1  / ISPB= 1  /--------/ S1= 1   / DATE= 16:07:13
 -11.66843 -11.68984 -11.70588 -11.71774 -11.72646
 -11.52151 -11.59021 -11.64720 -11.69306 -11.72901
 -11.29994 -11.40750 -11.50442 -11.58920 -11.66132
 -11.08599 -11.21833 -11.34420 -11.46009 -11.56388
 -10.92868 -11.07716 -11.22298 -11.36081 -11.48740
 -10.81161 -10.97420 -11.13840 -11.29643 -11.44335
 -10.73620 -10.90971 -11.08948 -11.26557 -11.43106
 -10.70565 -10.88643 -11.07782 -11.26838 -11.44958
 -10.71961 -10.90458 -11.10375 -11.30484 -11.49815
 -10.77329 -10.96022 -11.16421 -11.37247 -11.57451
 -10.85983 -11.04725 -11.25397 -11.46690 -11.67499
 -10.97215 -11.15911 -11.36714 -11.58301 -11.79516
 -11.10252 -11.28845 -11.49694 -11.71464 -11.92959
 -11.24088 -11.42552 -11.63416 -11.85333 -12.07072
 -11.37526 -11.55864 -11.76761 -11.98862 -12.20907
 -11.49888 -11.68110 -11.89069 -12.11414 -12.33859
 -11.61440 -11.79538 -12.00557 -12.23161 -12.46047
 -11.73011 -11.90957 -12.11998 -12.34815 -12.58100
 -11.85346 -12.03106 -12.24114 -12.47069 -12.70664
 -11.98796 -12.16341 -12.37263 -12.60283 -12.84091
 -12.13402 -12.30708 -12.51502 -12.74527 -12.98467
 -12.29040 -12.46091 -12.66726 -12.89709 -13.13718
 -12.45533 -12.62316 -12.82769 -13.05675 -13.29708
 -12.62709 -12.79215 -12.99467 -13.22270 -13.46292
 -12.80421 -12.96643 -13.16680 -13.39362 -13.63347
 -12.98548 -13.14483 -13.34294 -13.56838 -13.80769
 -13.16999 -13.32642 -13.52218 -13.74612 -13.98473
 -13.35701 -13.51048 -13.70382 -13.92617 -14.16397
 -13.54599 -13.69649 -13.88733 -14.10800 -14.34490
 -13.73647 -13.88399 -14.07228 -14.29119 -14.52713
 -13.92813 -14.07267 -14.25835 -14.47543 -14.71032
 -14.12074 -14.26228 -14.44531 -14.66051 -14.89431
 -14.31410 -14.45263 -14.63298 -14.84623 -15.07889
 -14.50804 -14.64358 -14.82119 -15.03245 -15.26390
 -14.70251 -14.83506 -15.00991 -15.21910 -15.44931
---------------------/ ISPP= 1  / ISPB= 1  /--------/ S1= 2   / DATE= 16:07:13
 -11.43897 -11.45854 -11.47317 -11.48398 -11.49191
 -11.22838 -11.30461 -11.36954 -11.42320 -11.46625
 -10.91068 -11.02587 -11.13353 -11.23227 -11.32061
 -10.64807 -10.78941 -10.93270 -11.07665 -11.21821
 -10.65524 -10.84518 -11.04928 -11.26819 -11.49887
 -11.02404 -11.26858 -11.53654 -11.83362 -12.16029
```

```
 -11.74823 -12.04148 -12.36408 -12.72787 -13.13952
        .       .       .
C-------------------------------------------------------------------------------
C
C    Rate coefficients: adf11 class acd
C    Units            : cm3 s-1
C    Status           : partition applied
C    Parent dataset   :  /home/asg/adas_modules/module_2/demo_e/adf11/acd50/acd50_w.dat
C
C    Code             : adas416
C    Producer         : Alessandra Giunta
C    Date             : 16/07/13
C
C-------------------------------------------------------------------------------
```