University of Strathclyde Glasgow

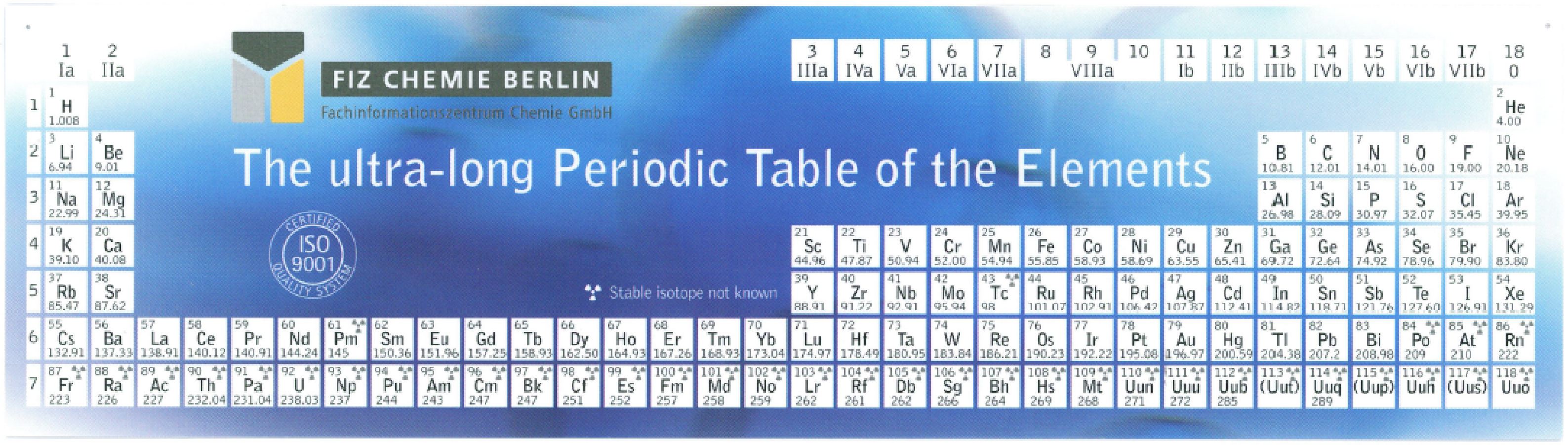
Heavy Species in ADAS

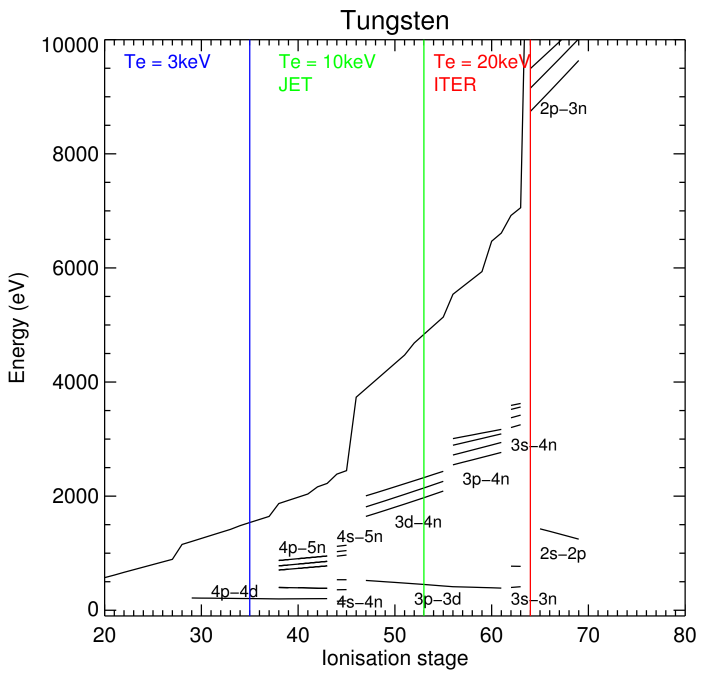
from the viewpoint of one lowly ion

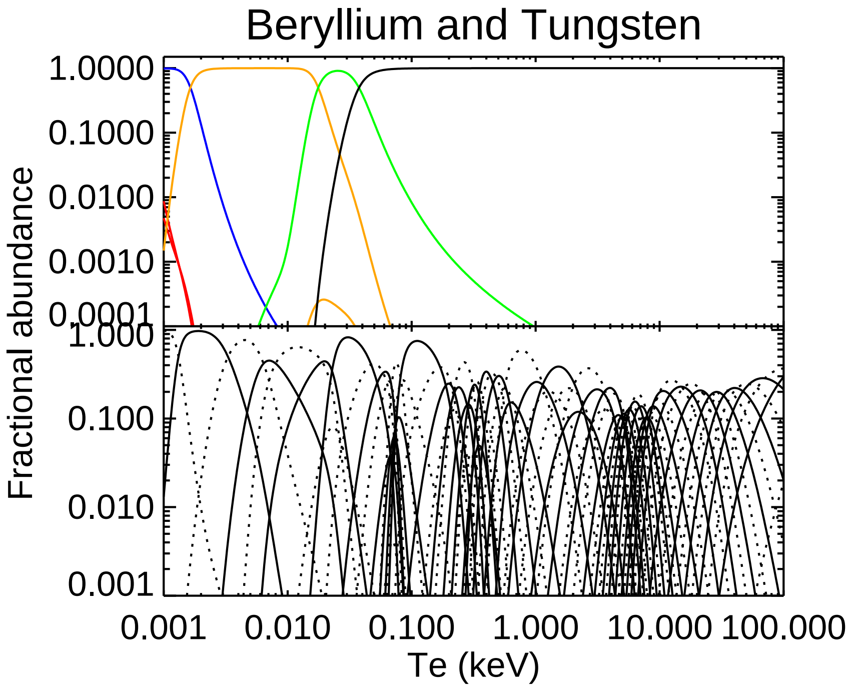
Martin O'Mullane

Department of Physics
University of Strathclyde

Atomic data requirements


FIZ CHEMIE BERLIN
Fachinformationszentrum Chemie GmbH
The ultra-long Periodic Table of the Elements
ISO 9001
Stable isotope not known





Three aspects of the heavy species question

The data we need

- Source functions — *adf11* acd, scd, ccd
- Power coefficients — *adf11* plt, prb
- Line emission — *adf15* pec
- Spectral feature emission — *adf40* f-pec

How to get it

- Scoping the problem
- Automated generation

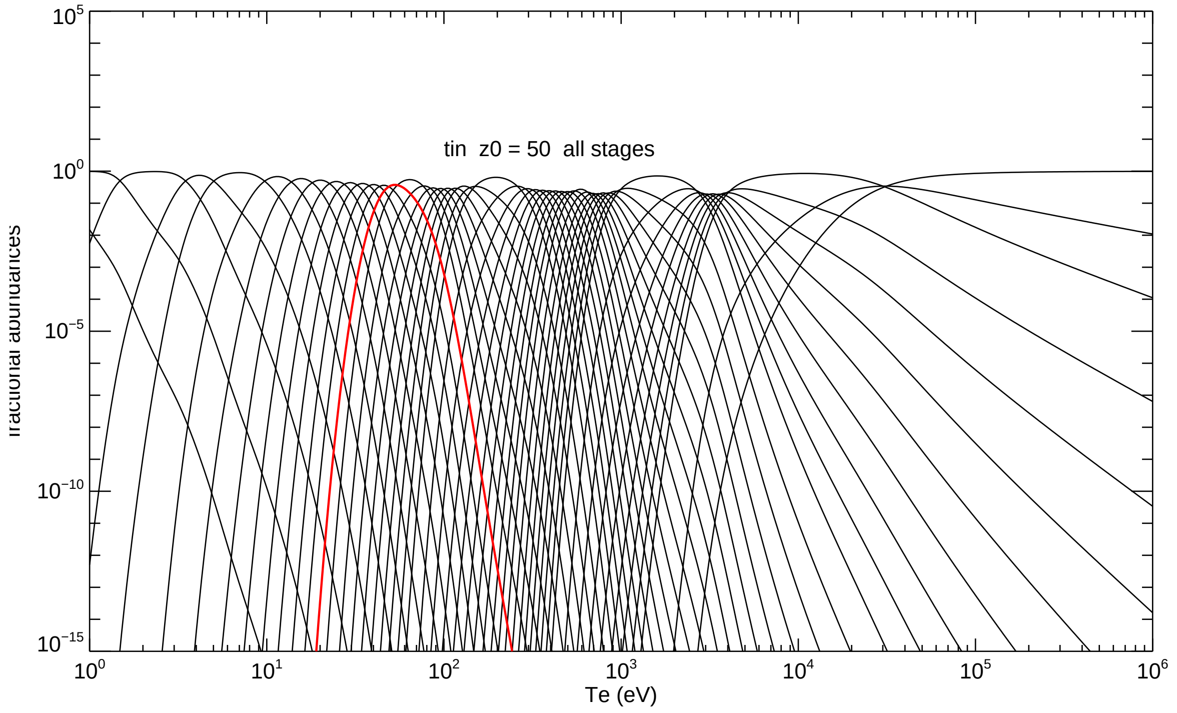
How to use it

- Potentially large datasets
- Partitioning and superstaging.

Let's choose tin (Z=50)

First questions: Where do its stages radiate? And what if there is no helpful ADAS *adf11* data?

```
preview_natural_partition, z0=50, plot_type=3,   $
                           te_min=1, te_max=1e6, $
                           te_plot=1000,         $
                           frac=frac
oplot, frac.te, frac.ion_all[13,*], color=5, thick=5
```



Now let’s narrow our focus to Sn^{13+}

- What is its ground state configuration?
- What configurations contribute to spectral emission?
- And to radiated power?
- How do we choose which ones to include?

The *adf00* set archives ionisation potential and ground configurations:

```
tin                 -50
 0 7.343d+00 1s2  2s2  2p6  3s2  3p6  3d10 4s2  4p6  4d10 4f0  5s2  5p2
 1 1.463d+01 1s2  2s2  2p6  3s2  3p6  3d10 4s2  4p6  4d10 4f0  5s2  5p1
                                ..
                                ..
12 2.744d+02 1s2  2s2  2p6  3s2  3p6  3d10 4s2  4p6  4d2
13 2.995d+02 1s2  2s2  2p6  3s2  3p6  3d10 4s2  4p6  4d1
14 3.959d+02 1s2  2s2  2p6  3s2  3p6  3d10 4s2  4p6
                                    ..
```

What configurations should be considered?

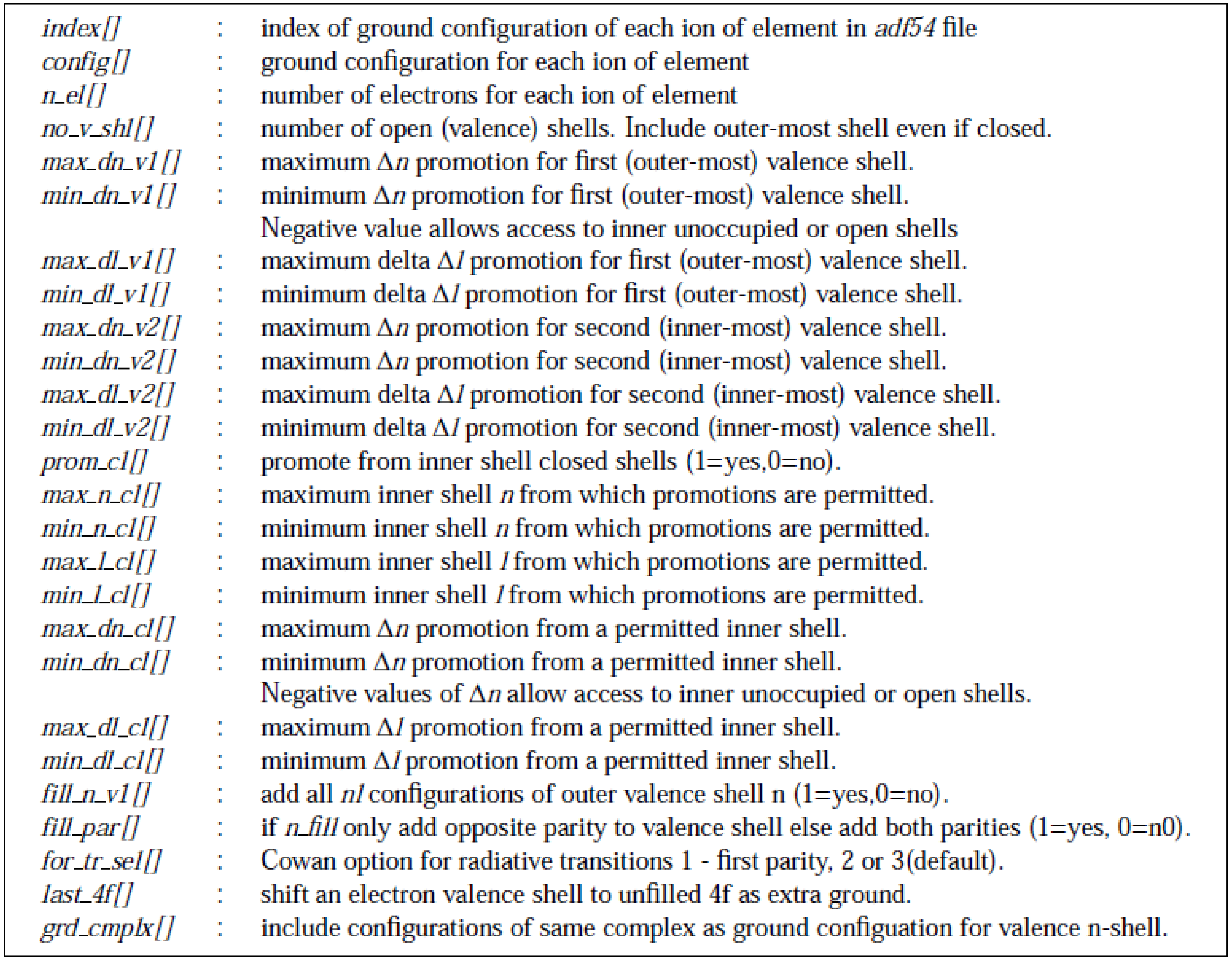
With a ground state of $3d^{10}4s^24p^64d^1$ we can

- promote the valence 4d electron to any higher *nl* shell
- allow 4s or 4p electrons to be excited
- or any other electron — from 2p perhaps?
- however where do we stop in Δn or Δl?
- and how many configurations should we consider?

There are 180 distinct ground configurations (for elements up to Radon)

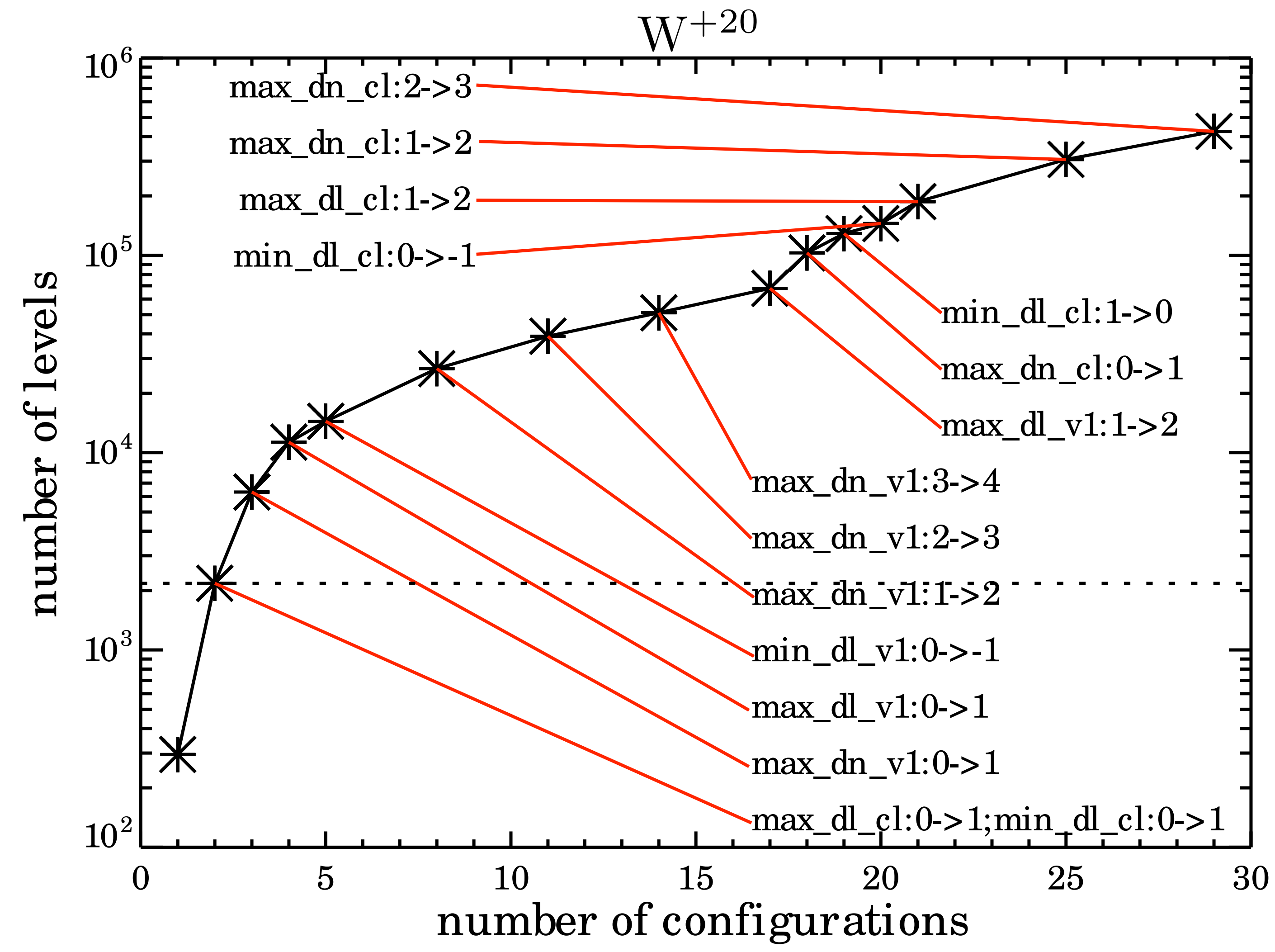
A rule based method is desirable (essential!)

ADAS rules for choosing where to promote electrons



index[]	:	index of ground configuration of each ion of element in *adf54* file
config[]	:	ground configuration for each ion of element
n_el[]	:	number of electrons for each ion of element
no_v_shl[]	:	number of open (valence) shells. Include outer-most shell even if closed.
max_dn_v1[]	:	maximum Δn promotion for first (outer-most) valence shell.
min_dn_v1[]	:	minimum Δn promotion for first (outer-most) valence shell.
		Negative value allows access to inner unoccupied or open shells
max_dl_v1[]	:	maximum delta Δl promotion for first (outer-most) valence shell.
min_dl_v1[]	:	minimum delta Δl promotion for first (outer-most) valence shell.
max_dn_v2[]	:	maximum Δn promotion for second (inner-most) valence shell.
min_dn_v2[]	:	maximum Δn promotion for second (inner-most) valence shell.
max_dl_v2[]	:	maximum delta Δl promotion for second (inner-most) valence shell.
min_dl_v2[]	:	minimum delta Δl promotion for second (inner-most) valence shell.
prom_cl[]	:	promote from inner shell closed shells (1=yes,0=no).
max_n_cl[]	:	maximum inner shell n from which promotions are permitted.
min_n_cl[]	:	minimum inner shell n from which promotions are permitted.
max_l_cl[]	:	maximum inner shell l from which promotions are permitted.
min_l_cl[]	:	minimum inner shell l from which promotions are permitted.
max_dn_cl[]	:	maximum Δn promotion from a permitted inner shell.
min_dn_cl[]	:	minimum Δn promotion from a permitted inner shell.
		Negative values of Δn allow access to inner unoccupied or open shells.
max_dl_cl[]	:	maximum Δl promotion from a permitted inner shell.
min_dl_cl[]	:	minimum Δl promotion from a permitted inner shell.
fill_n_v1[]	:	add all *nl* configurations of outer valence shell n (1=yes,0=no).
fill_par[]	:	if *n_fill* only add opposite parity to valence shell else add both parities (1=yes, 0=n0).
for_tr_sel[]	:	Cowan option for radiative transitions 1 - first parity, 2 or 3(default).
last_4f[]	:	shift an electron valence shell to unfilled 4f as extra ground.
grd_cmplx[]	:	include configurations of same complex as ground configuation for valence n-shell.

adf54 : rules for automatic data generation



Care needed!! resolved calculations (ic or LS) can overwhelm computers.

Work through Sn^{13+}

- Within ADAS the generation of heavy species data is almost exclusively a non-GUI activity.
- The outputs are standard *adf11*, *adf15* and *adf40* datasets which can be used and examined with the GUI interactive system.

At the IDL command line:

```
; Let's choose Sn13+

z_nuc = 50
z_ion = 13
tag   = xxesym(z_nuc, /lower) + string(z_ion, format='(i2.2)')

; Use promotion rules from W work

a54file = '/u/adas/adas/adf54/promotion_rules_w_adf54.dat'
```

```
adas8xx_promotion_rules, z0_nuc = z_nuc, z_ion = z_ion, ionpot = ip,  $
                         prom_rules=rules, a54file = file
help, rules, /st

** Structure <9b54e9c>, 25 tags, length=60, data length=60, refs=1:
   CONFIG          STRING '  1s2  2s2  2p6  3s2  3p6  3d10 4s2  4p6  4d1'
   INDEX           INT            129
   NO_V_SHL        INT              1
   MAX_DN_V1       INT              3
   MIN_DN_V1       INT              0
   MAX_DL_V1       INT              2
   MIN_DL_V1       INT             -2
   MAX_DN_V2       INT              0
   MIN_DN_V2       INT              0
   MAX_DL_V2       INT              0
   MIN_DL_V2       INT              0
   PROM_CL         INT              1
   MAX_N_CL        INT              4
   MIN_N_CL        INT              4
```

```
MAX_L_CL      INT             1
MIN_L_CL      INT             0
MAX_DN_CL     INT             1
MIN_DN_CL     INT             0
MAX_DL_CL     INT             2
MIN_DL_CL     INT             0
FILL_N_V1     INT             1
FILL_PAR      INT             0
FOR_TR_SEL    INT             3
LAST_4F       INT             0
GRD_CMPLX     INT             0
```

```
adas8xx_promotions, z0_nuc = z_nuc, z_ion = z_ion, ionpot = ip,  $
                    prom_rules        = rules,                    $
                    promotion_results = results

help, results, /st

** Structure <9b530dc>, 11 tags, length=2496, data length=2496, refs=1:
   GRD_CFG         STRING    '4d1  '
   GRD_OCC         INT       Array[36]
   EX_CFG          STRING    Array[25]
   GRD_PAR         INT              0
   EX_PAR          INT       Array[25]
   GRD_ZC_COW      LONG               -14
   EX_ZC_COW       LONG      Array[25]
   OC_STORE        INT       Array[36, 26]
   NO_CONFIGS      LONG      Array[7]
   NO_TERMS        LONG      Array[7]
   NO_LEVELS       LONG      Array[7]
```

```
print, results.grd_occ

       2      2      6      2      6     10      2      6      1      0
       0      0      0      0      0      0      0      0      0      0
       0      0      0      0      0      0      0      0      0      0
       0      0      0      0      0      0

print, results.oc_store[*,1]
       2      2      6      2      6     10      2      6      0      1
       0      0      0      0      0      0      0      0      0      0
       0      0      0      0      0      0      0      0      0      0
       0      0      0      0      0      0

print, results.oc_store[*,2]
       2      2      6      2      6     10      2      6      0      0
       1      0      0      0      0      0      0      0      0      0
       0      0      0      0      0      0      0      0      0      0
       0      0      0      0      0      0
```

```
; Write CA driver files for restricted plasma parameters

files = { adf34_file    : 'adf34_ca_' + tag + '.dat', $
          adf42_ca_file : 'adf42_ca_' + tag + '.dat', $
          adf04_ca_file : 'adf04_ca_' + tag + '.dat', $
          adf40_ca_file : 'adf40_ca_' + tag + '.dat', $
          adf15_ca_file : 'adf15_ca_' + tag + '.dat', $
          adf11_ca_file : 'adf11_ca_' + tag + '.dat'}

plasma = {theta         : [  1.0e3, 2.0e3, 5.0e3, 1.0e4, 1.5e4, $
                             2.0e4, 5.0e4, 1.0e5], $
          indx_theta    : indgen(8),
          rho           : [  1.0e8, 1.0e10, 1.0e12, 1.0e14],
          indx_rho      : indgen(4),
          npix          : [  128,   256],
          wvlmin        : [100.0,   1.0],
          wvlmax        : [150.0, 500.0],
          indx_wvl      : indgen(2),
          theta_noscale : 0,
          rho_scale     : 0
```

```
adas8xx_create_drivers, z0_nuc=z_nuc, z_ion=z_ion, ionpot=ip, $
                        promotion_results=results,            $
                        plasma=plasma, files=files
```

The driver file for ADAS801 (Cowan code):

```
2  -5    2   10  1.0    5.d-09    5.d-11-2  0130    1.0 0.65  0.0  0.5
   50  -14   Sn ground z1=13 0   4d1
   50  -14   Sn cfg 01       0   5s1
   50  -14   Sn cfg 02       0   5d1
   50  -14   Sn cfg 03       0   5g1
   50  -14   Sn cfg 04       0   6s1
   50  -14   Sn cfg 05       0   6d1
   50  -14   Sn cfg 06       0   6g1
   50  -14   Sn cfg 07       0   7s1
   50  -14   Sn cfg 08       0   7d1
   50  -14   Sn cfg 09       0   7g1
   50  -32   Sn cfg 10       0   3d10 4s1  4p6  4d2
   50  -32   Sn cfg 11       0   3d10 4s1  4p6  4d1  5s1
```

```
50  -32   Sn cfg 12       0   3d10 4s1  4p6  4d1  5d1
50  -32   Sn cfg 13       0   3d10 4s2  4p5  4d1  4f1
50  -32   Sn cfg 14       0   3d10 4s2  4p5  4d1  5p1
50  -32   Sn cfg 15       0   3d10 4s2  4p5  4d1  5f1
50  -14   Sn cfg 16       1   4f1
50  -14   Sn cfg 17       1   5p1
50  -14   Sn cfg 18       1   5f1
50  -14   Sn cfg 19       1   6p1
50  -14   Sn cfg 20       1   6f1
50  -14   Sn cfg 21       1   7p1
50  -14   Sn cfg 22       1   7f1
50  -32   Sn cfg 23       1   3d10 4s1  4p6  4d1  5p1
50  -32   Sn cfg 24       1   3d10 4s2  4p5  4d2
50  -32   Sn cfg 25       1   3d10 4s2  4p5  4d1  5d1
-1
```

Back to the IDL command line:

```
; Run the CA structure code

adas8xx_create_ca_adf04, z_ion,                                  $
                         z_nuc,                                  $
                         results.oc_store,                       $
                         ionpot          = ip,                   $
                         plasma          = plasma,               $
                         adf04_t3_file   = files.adf04_ca_file
```

adf04 file for Sn^{13+}

```
Sn+13        50        14        2415630.6
    1 19                  (0)0(    4.5)           0.0
    2 606527558529        (0)0(  134.5)      604454.8
    3 1B                  (0)0(    0.5)      656865.3
    4 1A                  (0)0(    6.5)      664371.3
    5 1C                  (0)0(    2.5)      810958.4
    6 1D                  (0)0(    4.5)     1048671.2
    7 606517568529        (0)0(   44.5)     1052972.9
    8 60652755851951A     (0)0(  419.0)     1259268.0
    9 1E                  (0)0(    6.5)     1290521.2
   10 1G                  (0)0(    0.5)     1291113.7
   11 1H                  (0)0(    2.5)     1366810.5
   12 1F                  (0)0(    8.5)     1400752.2
   13 60652755851951C     (0)0(  179.5)     1412966.0
   14 1I                  (0)0(    4.5)     1485688.9
   15 1J                  (0)0(    6.5)     1609362.8
   16 1M                  (0)0(    0.5)     1611744.1
   17 60652755851951D     (0)0(  299.5)     1649394.9
   18 1N                  (0)0(    2.5)     1654541.6
   19 1K                  (0)0(    8.5)     1668939.1
   20 60651756851951B     (0)0(   19.5)     1715621.3
   21 1O                  (0)0(    4.5)     1722798.2
   22 1P                  (0)0(    6.5)     1795180.9
   23 1Q                  (0)0(    8.5)     1831229.6
   24 60651756851951C     (0)0(   59.5)     1867168.5
   25 60652755851951E     (0)0(  419.0)     1891442.4
   26 60651756851951D     (0)0(   98.5)     2103915.7
   -1
  14.0    3          1.96+05 3.92+05 9.80+05 1.96+06 2.94+06 3.92+06 9.80+06 1.96+07
    4     1 1.92+11 7.92+00 8.17+00 8.96+00 1.02+01 1.12+01 1.20+01 1.54+01 1.87+01
    3     1 7.69+06 1.99-01 2.02-01 2.09-01 2.17-01 2.23-01 2.27-01 2.39-01 2.47-01
    5     1 1.07+11 3.89-01 4.07-01 4.70-01 5.77-01 6.73-01 7.59-01 1.13+00 1.50+00
    6     1 1.17+07 7.21-01 7.29-01 7.54-01 7.91-01 8.20-01 8.42-01 9.17-01 9.69-01
    9     1 2.22+10 1.34-01 1.35-01 1.35-01 1.37-01 1.39-01 1.41-01 1.59-01 1.83-01
   12     1 1.21+08 5.57-01 5.62-01 5.81-01 6.11-01 6.36-01 6.57-01 7.33-01 7.89-01
   10     1 2.97+06 2.19-02 2.19-02 2.22-02 2.25-02 2.27-02 2.29-02 2.35-02 2.39-02
```

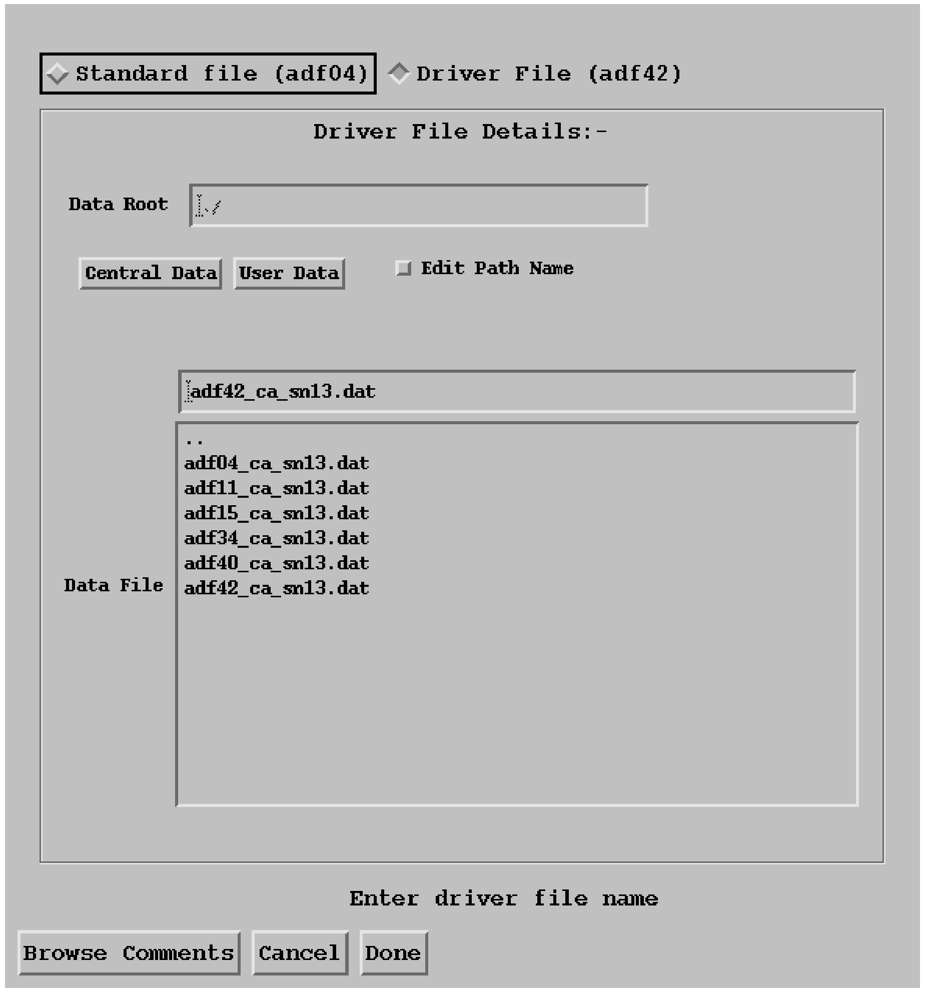
Eissner notation — quick recap

Each occupation/orbital-list pair is separated from the next by 5 (or 6)

```
1s
1

2s  2p
2   3

3s  3p  3d
4   5   6

4s  4p  4d  4f
7   8   9   A

5s  5p  5d  5f  5g
B   C   D   E   F

etc.
```

Generating spectral and power data — ADAS810

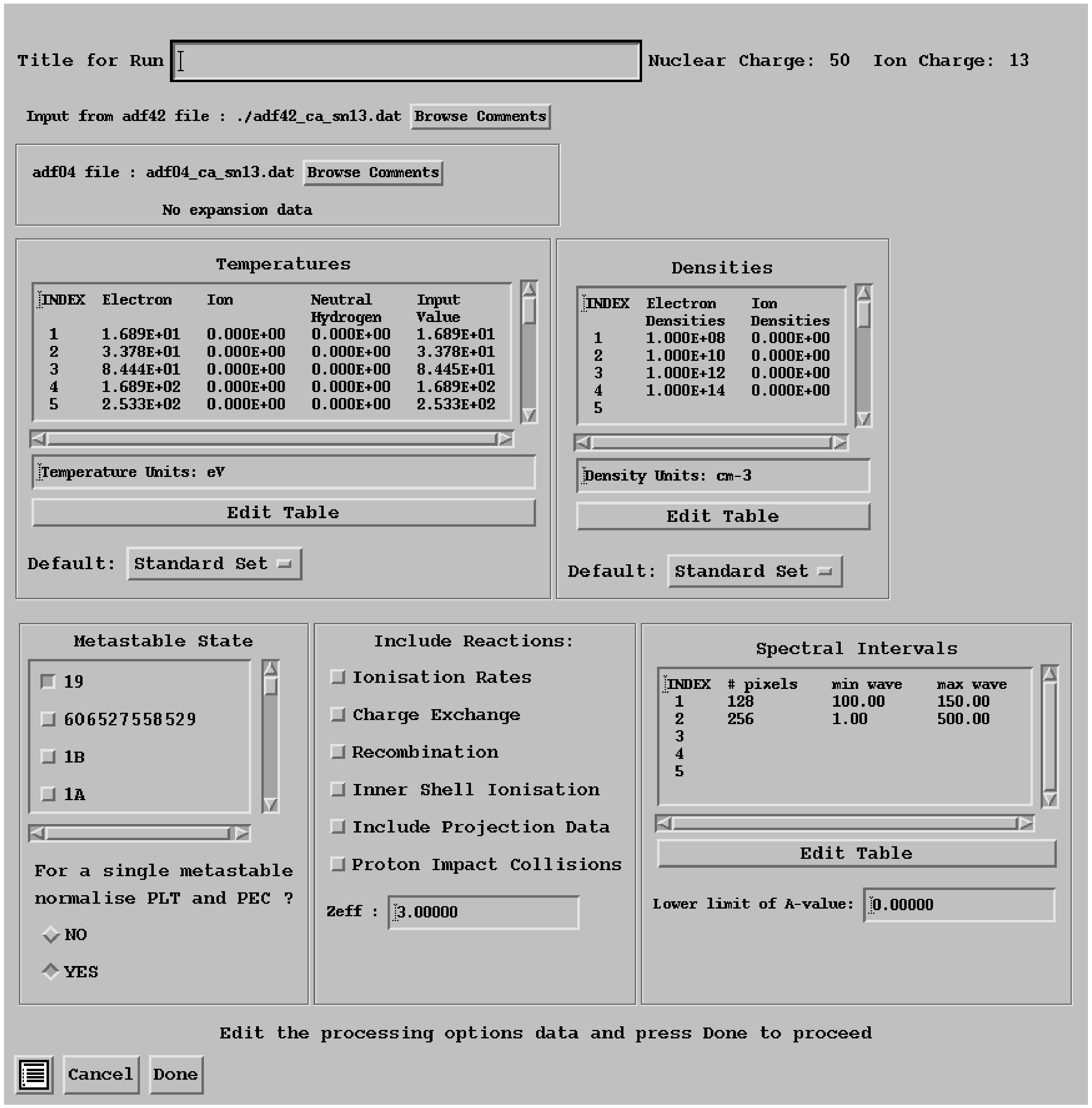
Process the *adf42* file made by `adas8xx_create_drivers` with ADAS810 to generate *adf11*/plt, *adf15* and *adf40* datasets.



Data Root: ./

Data File: adf42_ca_sn13.dat

```
..
adf04_ca_sn13.dat
adf11_ca_sn13.dat
adf15_ca_sn13.dat
adf34_ca_sn13.dat
adf40_ca_sn13.dat
adf42_ca_sn13.dat
```



Title for Run

Nuclear Charge: 50 Ion Charge: 13

Input from adf42 file : ./adf42_ca_sn13.dat Browse Comments

adf04 file : adf04_ca_sn13.dat Browse Comments

No expansion data

Temperatures

INDEX	Electron	Ion	Neutral Hydrogen	Input Value
1	1.689E+01	0.000E+00	0.000E+00	1.689E+01
2	3.378E+01	0.000E+00	0.000E+00	3.378E+01
3	8.444E+01	0.000E+00	0.000E+00	8.445E+01
4	1.689E+02	0.000E+00	0.000E+00	1.689E+02
5	2.533E+02	0.000E+00	0.000E+00	2.533E+02

Temperature Units: eV

Edit Table

Default: Standard Set

Densities

INDEX	Electron Densities	Ion Densities
1	1.000E+08	0.000E+00
2	1.000E+10	0.000E+00
3	1.000E+12	0.000E+00
4	1.000E+14	0.000E+00
5		

Density Units: cm-3

Edit Table

Default: Standard Set

Metastable State

- ☐ 19
- ☐ 606527558529
- ☐ 1B
- ☐ 1A

For a single metastable normalise PLT and PEC ?

◇ NO

◆ YES

Include Reactions:

- ☐ Ionisation Rates
- ☐ Charge Exchange
- ☐ Recombination
- ☐ Inner Shell Ionisation
- ☐ Include Projection Data
- ☐ Proton Impact Collisions

Zeff : 3.00000

Spectral Intervals

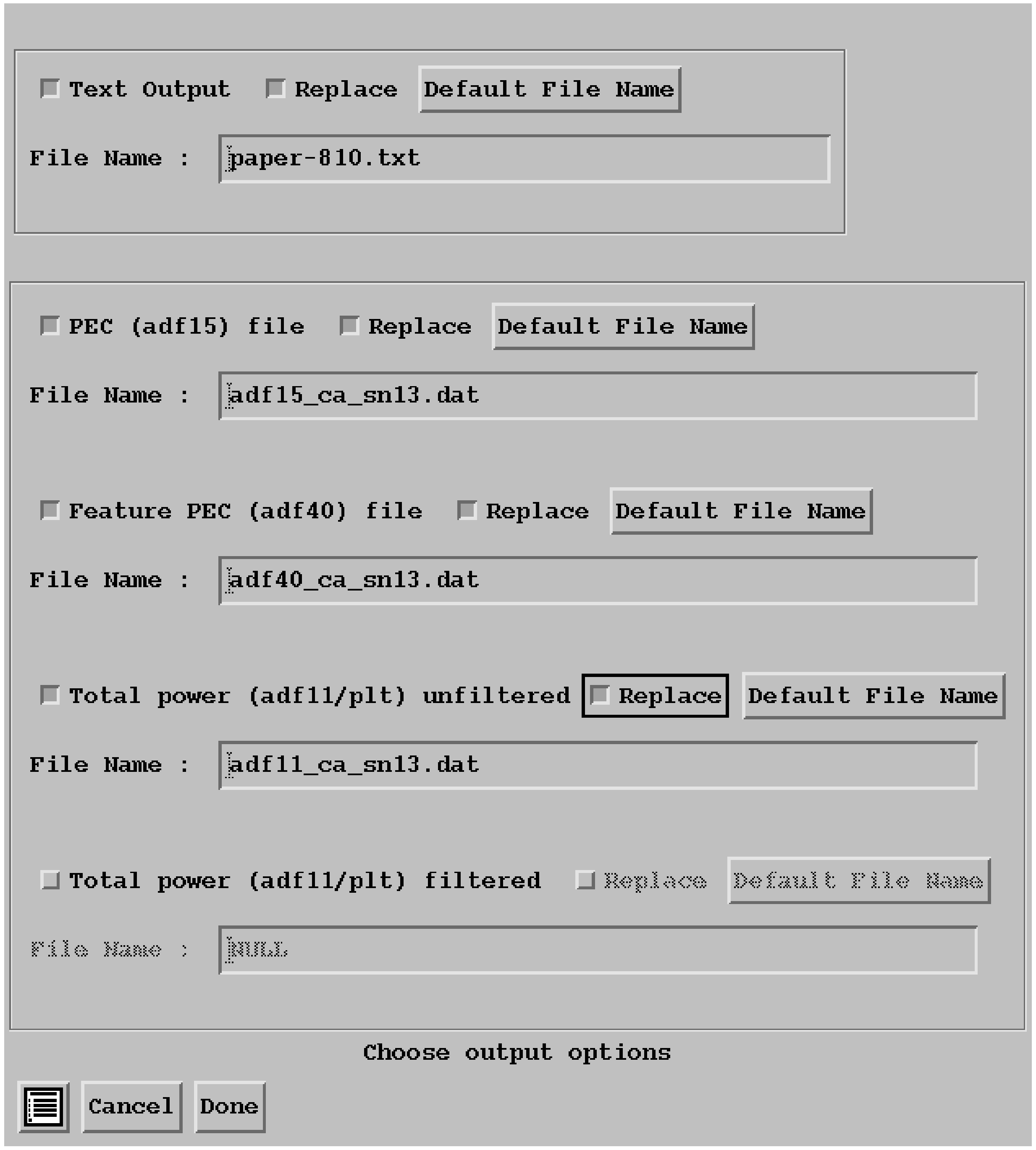
INDEX	# pixels	min wave	max wave
1	128	100.00	150.00
2	256	1.00	500.00
3			
4			
5			

Edit Table

Lower limit of A-value: 0.00000

Edit the processing options data and press Done to proceed

Cancel Done



Text Output Replace Default File Name

File Name : paper-810.txt

PEC (adf15) file Replace Default File Name

File Name : adf15_ca_sn13.dat

Feature PEC (adf40) file Replace Default File Name

File Name : adf40_ca_sn13.dat

Total power (adf11/plt) unfiltered Replace Default File Name

File Name : adf11_ca_sn13.dat

Total power (adf11/plt) filtered Replace Default File Name

File Name : NULL

Choose output options

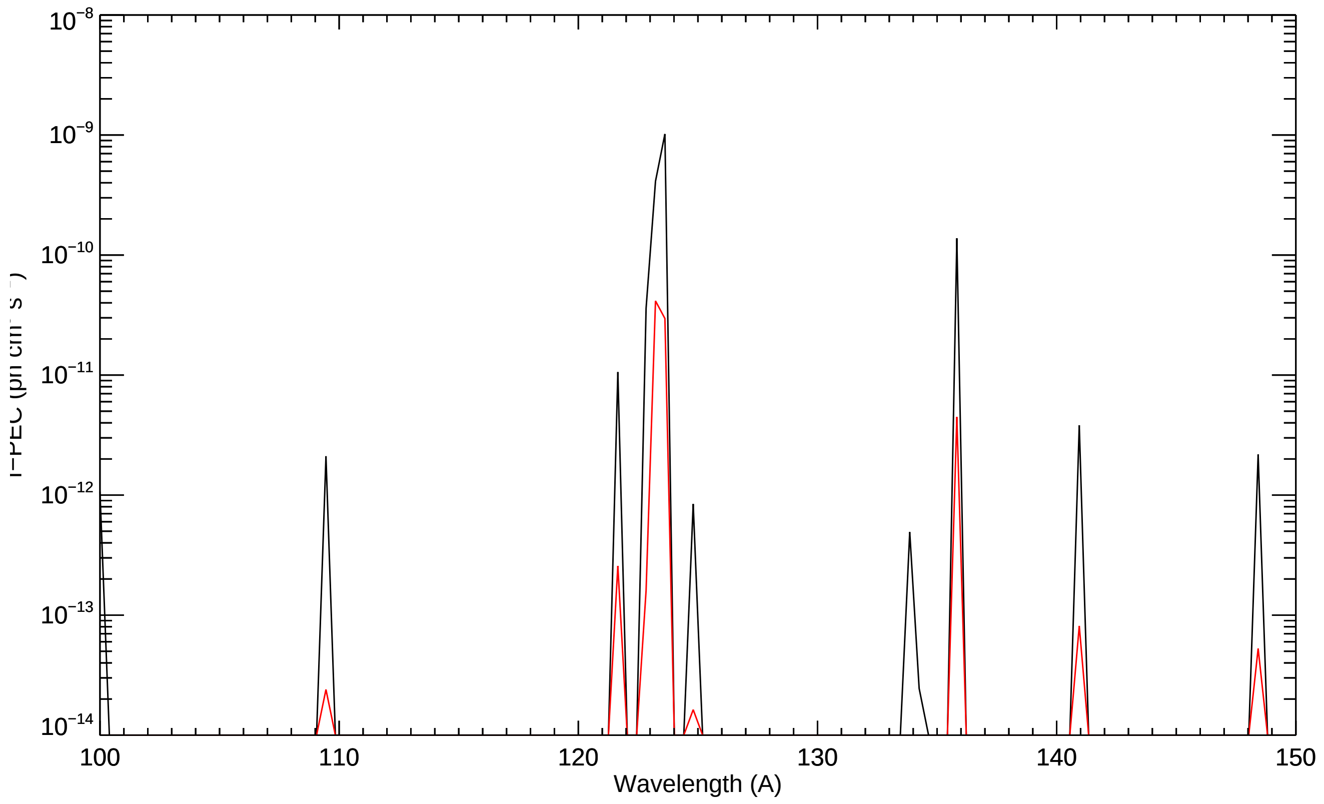
Cancel Done

Where lies the emission?

Back to the IDL command line!

```
read_adf40,file='adf40_ca_sn13.dat', fulldata=all

help, all, /st
   ESYM            STRING    'Sn'
   IZO             LONG                50
   IS              LONG                13
   IS1             LONG                14
   NBLOCK          LONG                 2
   NPIX            LONG      Array[2]
   WAVE_MIN        DOUBLE    Array[2]
   WAVE_MAX        DOUBLE    Array[2]
   NTE             LONG      Array[2]
   TE              DOUBLE    Array[8, 2]
   NDENS           LONG      Array[2]
   DENS            DOUBLE    Array[4, 2]
   FPEC            DOUBLE    Array[256, 8, 4, 2]
   TYPE            STRING    Array[2]
```

```
wave=adas_vector(low=all.wave_min[0], high=all.wave_max[0], $
                 num=all.npix[0], /linear)

plot_io, wave, all.fpec[*, 7, 2, 0] > 1e-14, $
         xtitle='Wavelength (A)', ytitle = 'f-PEC (ph cm!u3!n s!u-1!n)'
oplot, wave, all.fpec[*, 1, 2, 0] > 1e-14, color=5
```



How to identify contributing configurations

It depends of the width of the spectral region of interest

```
C
C   lv      configuration      (2S+1)L(w-1/2)       energy (cm^-1)
C  ---   ------------------- --------------       --------------
C    1   19                       (0)0(  4.5)             0.0
C    2   606527558529             (0)0(134.5)        604454.8
C    3   1B                       (0)0(  0.5)        656865.3
C    4   1A                       (0)0(  6.5)        664371.3
C    5   1C                       (0)0(  2.5)        810958.4
C    6   1D                       (0)0(  4.5)       1048671.2
C    7   606517568529             (0)0( 44.5)       1052972.9
                               -
                               -
C   20   60651756851951B          (0)0( 19.5)       1715621.3
C   21   10                       (0)0(  4.5)       1722798.2
C   22   1P                       (0)0(  6.5)       1795180.9
                               -
                               -
C     12    94.9692    7(0)0( 44.5)-  1(0)0(  4.5)       excit   1    1  13    17  48  12
C     13    99.5453   19(0)0(  8.5)-  4(0)0(  6.5)       excit   1    1  13    33  14  13
C     14    100.233   18(0)0(  2.5)-  3(0)0(  0.5)       excit   1    1  13    44  43  14
C     15    109.668   21(0)0(  4.5)-  5(0)0(  2.5)       excit   1    1  13    54  39  15
C     16    121.756   14(0)0(  4.5)-  4(0)0(  6.5)       excit   1    1  13    31  28  16
C     17    122.821   24(0)0( 59.5)-  7(0)0( 44.5)       excit   1    1  13   117  18  17
C     18    123.311    5(0)0(  2.5)-  1(0)0(  4.5)       excit   1    1  13     3   6  18
C     19    123.684   13(0)0(179.5)-  2(0)0(134.5)       excit   1    1  13   124   5  19
C     20    124.877   16(0)0(  0.5)-  5(0)0(  2.5)       excit   1    1  13    52  44  20
```

- Overplot/look at PEC *adf15* data.
- Refine promotion rules or adf34 driver to home-in
- Note that structure codes are not spectroscopically accurate.

Where next?

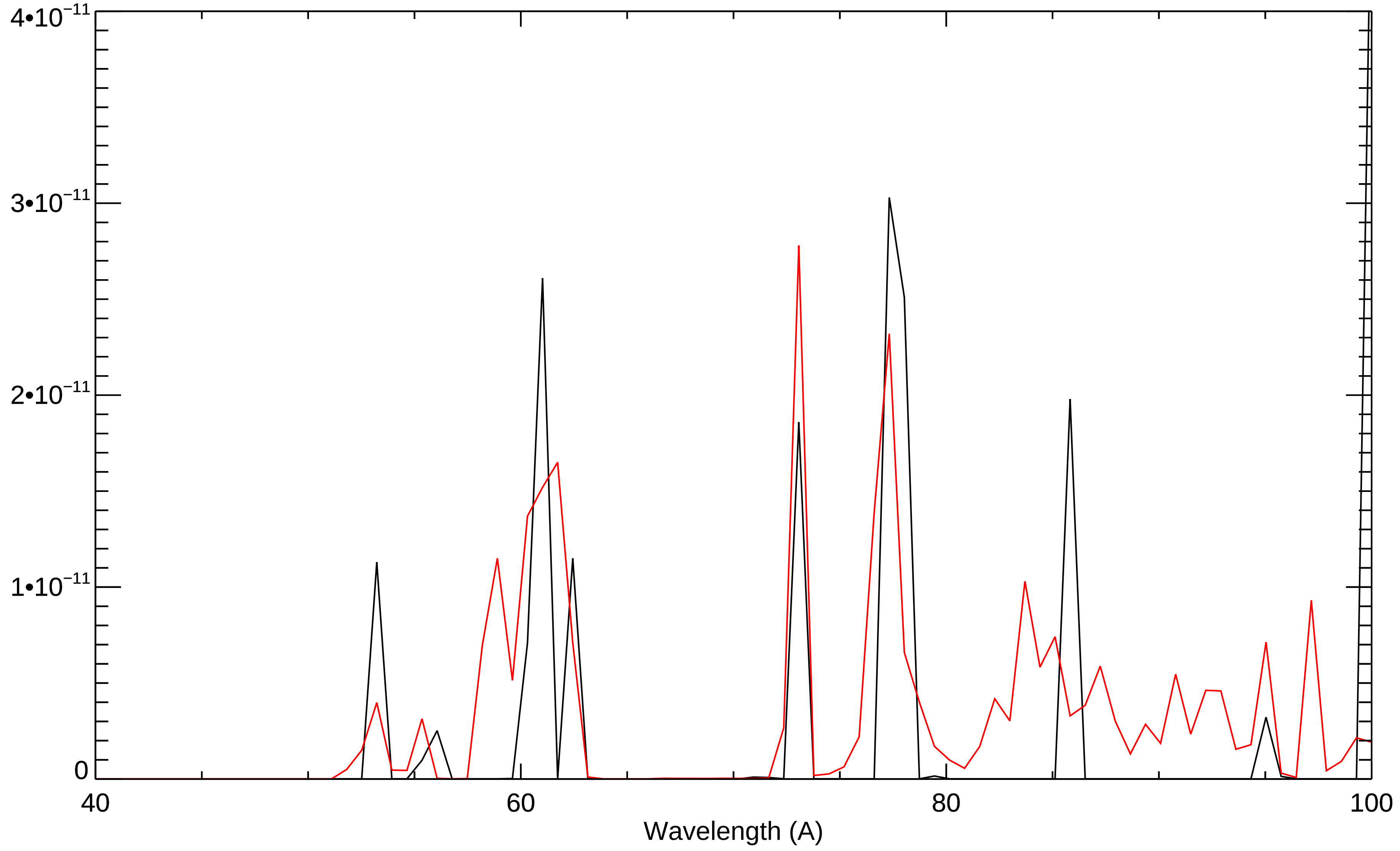
Identify emission region of interest — treat these in intermediate coupling.

For Sn^{13+} :

- 26 configurations, 226 terms, 554 levels

```
read_adf40,file='fpec40#sn_ca#sn13.dat', fulldata=all_ca
read_adf40,file='fpec40#sn_ic#sn13.dat', fulldata=all_ic

wave=adas_vector(low=all_ca.wave_min[1], high=all_ca.wave_max[1], $
                 num=all_ca.npix[1], /linear)

plot, wave, all_ca.fpec[*, 7, 2, 1] > 1e-14,      $
      xtitle = 'Wavelength (A)',                  $
      ytitle = 'f-PEC (ph cm!u3!n s!u-1!n)',      $
      xrange = [40, 100], yrange = [1e-12, 4e-11]

oplot, wave, all_ic.fpec[*, 7, 2, 1] > 1e-14, color=5
```

Configuration average (CA) *vs* intermediate coupling (ic)

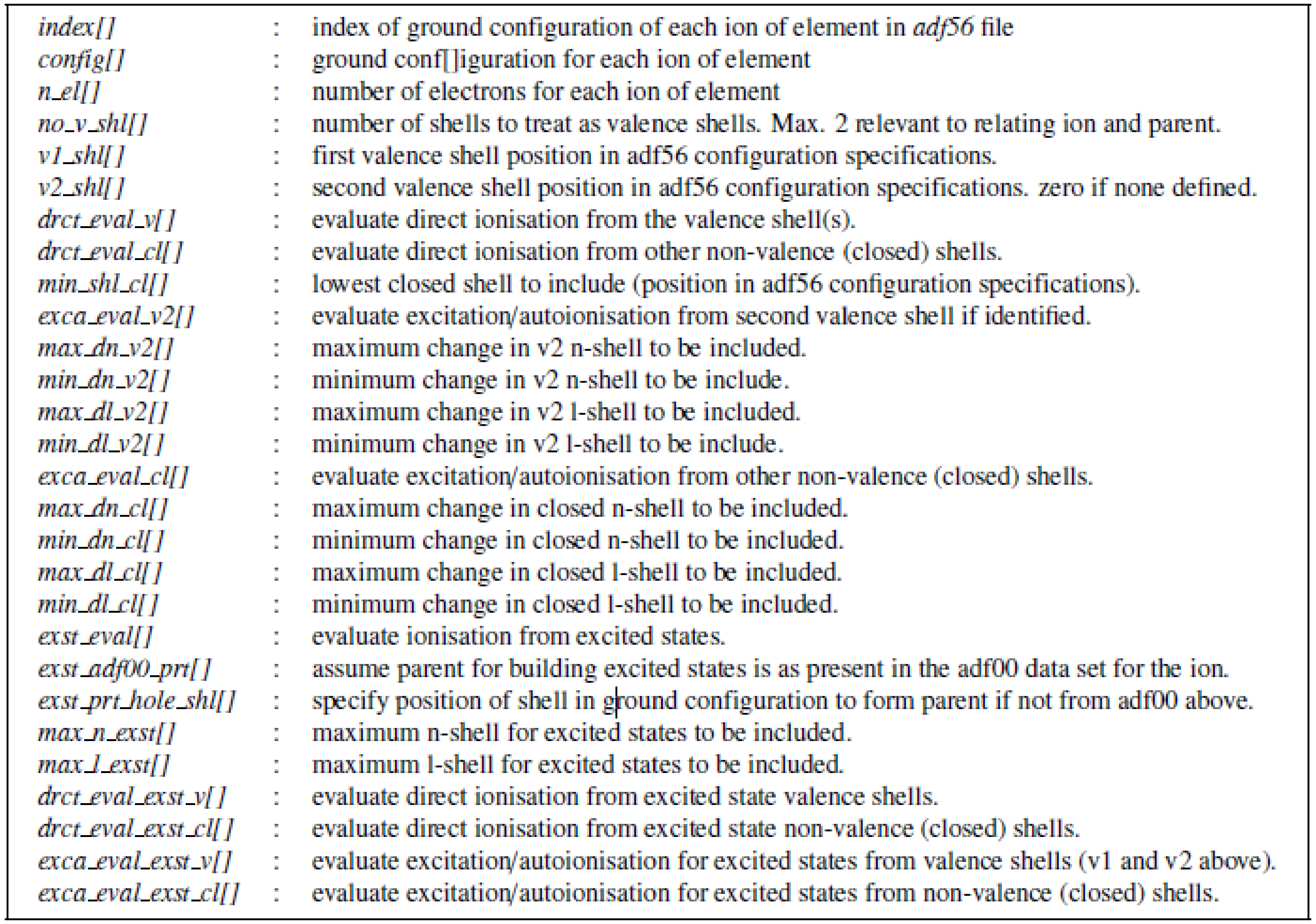


In Reality

- Do not consider each stage by hand — by element is preferable.
- Many scripts available within ADAS to aid this task.
- These impose a directory structure.
- Baseline data identified by the year ‘40’ tag.
- Full instructions in forthcoming ADAS technical report.

Ionisation

Very similar to excitation — driven by *adf56* collection of rules



index[]	:	index of ground configuration of each ion of element in *adf56* file
config[]	:	ground conf[]iguration for each ion of element
n_el[]	:	number of electrons for each ion of element
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.

adf32 is the driver file for CADW ionisation code from the Auburn group.

Once again to the IDL command line!

```
; Add offline-ADAS IDL library to the path

!path = expand_path('/u/adas/offline_adas/adas8#2/idl') + ':' + !path

; Promotion rules - compiled by Adam Foster (arf)

a56file = '/u/adas/adas/adf56/large_arf09.dat'

; Sn13+ !!

adas8xx_ionis_promotion_rules, z_nuc    = 50,                     $
                               z_ion    = 13,                     $
                               a56file  = a56file,                $
                               adf32    = 'adf32_ca_sn13.dat',    $
                               comments = ['C-------------------', $
                                           'C  I made this!',      $
                                           'C-------------------'  ]
```

```
elem   = Sn
stage  = 13
ip_z   =    3193147.3
ip_z1  =    2415629.2
seq    = rb
--------------------------------------------------------------------------------
Type = Direct /number=3/
#
200-51 1 2  01.   1.   5.0E-08   1.0E-11-2  0130 0 1.00 0.65   71.  0.5        0.70
   50   14  sn+13 ground     4d1                                     4d
   50   15  sn+14 from 4d    3d10 4s2  4p6
   -1
#
200-51 1 2  01.   1.   5.0E-08   1.0E-11-2  0130 0 1.00 0.65   73.  0.5        0.70
   50   14  sn+13 ground     4d1                                     4s
   50   15  sn+14 from 4s    3d10 4s1  4p6  4d1
   -1
#
200-51 1 2  01.   1.   5.0E-08   1.0E-11-2  0130 0 1.00 0.65   72.  0.5        0.70
   50   14  sn+13 ground     4d1                                     4p
   50   15  sn+14 from 4p    3d10 4s2  4p5  4d1
   -1
--------------------------------------------------------------------------------
Type = InDirect /number=2/
#
20 -51 0 2   10  1.0    5.e-08    1.e-11-2   130    1.0 0.65   66.   0.5        0.7
   50   14  sn+13 ground     4d1                                     4s
   50   14  sn+13 via  4d    3d10 4s1  4p6  4d2                      4d
   50   14  sn+13 via  4f    3d10 4s1  4p6  4d1  4f1                 4f
   50   14  sn+13 via  5s    3d10 4s1  4p6  4d1  5s1                 5s
                               -
                               -
   50   14  sn+13 via  7h    3d10 4s1  4p6  4d1  7h1                 7h
   50   14  sn+13 via  7i    3d10 4s1  4p6  4d1  7i1                 7i
   -1
#
20 -51 0 2   10  1.0    5.e-08    1.e-11-2   130    1.0 0.65   66.   0.5        0.7
   50   14  sn+13 ground     4d1                                     4p
   50   14  sn+13 via  4d    3d10 4s2  4p5  4d2                      4d
   50   14  sn+13 via  4f    3d10 4s2  4p5  4d1  4f1                 4f
                               -
                               -
   50   14  sn+13 via  7h    3d10 4s2  4p5  4d1  7h1                 7h
   50   14  sn+13 via  7i    3d10 4s2  4p5  4d1  7i1                 7i
   -1
--------------------------------------------------------------------------------
C-------------------
C  I made this!
C-------------------
```

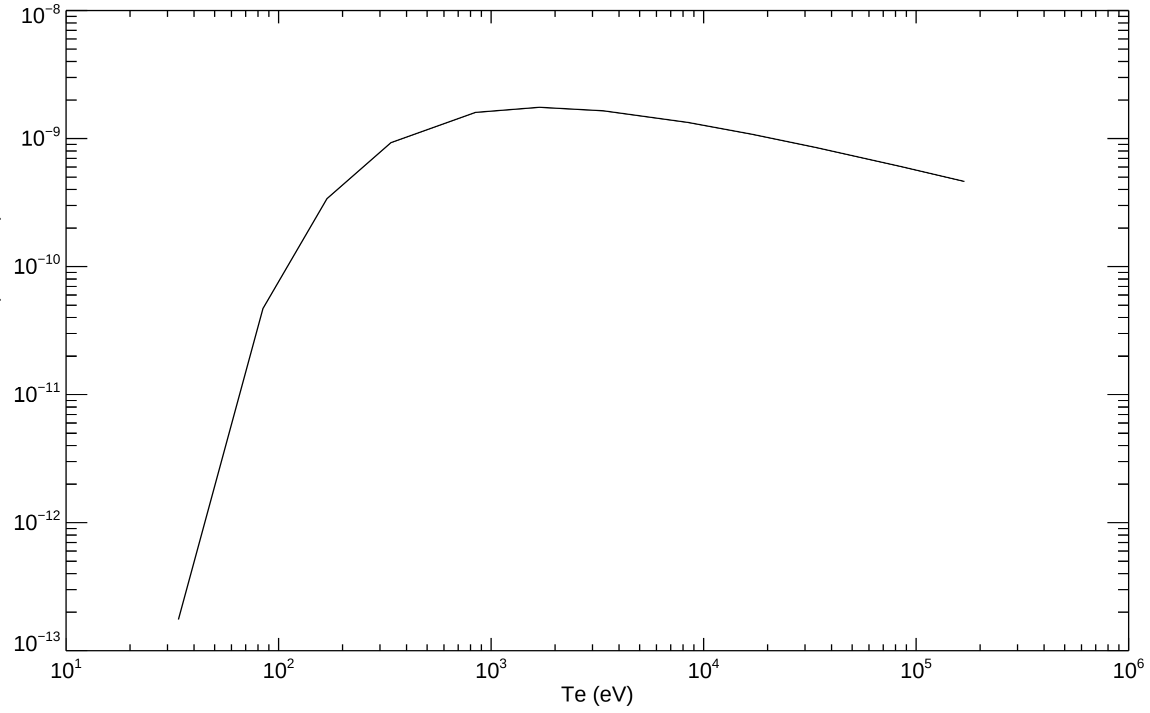
Next to the unix command line

```
 /u/adas/offline_adas/adas8#2/adas8#2.pl adf32_ca_sn13.dat adf23_ca_sn1
```

Return to IDL to inspect the results

```
read_adf23, file='adf23_ca_sn13.dat', fulldata=all, szd_total=szd

help, szd,/st

** Structure <a3e784c>, 7 tags, length=6576, data length=6576, refs=1:
   TE              DOUBLE    Array[12]
   Q_ION           DOUBLE    Array[1, 3, 12]
   IS_Q_ION        LONG      Array[1, 3, 12]
   Q_EXC           DOUBLE    Array[1, 41, 12]
   IS_Q_EXC        LONG      Array[1, 41, 12]
   QTOT            DOUBLE    Array[1, 1, 12]
   IS_QTOT         LONG      Array[1, 1, 12]
```

```
te  = reform(szd.te) / 11605.0
szd = reform(szd.qtot*10.0^szd.is_qtot) > 1.0e-36

plot_oo, te, szd,            $
         xtitle='Te (eV)', $
         ytitle = 'Ionisation rate (cm!u3!n s-1!n)
```



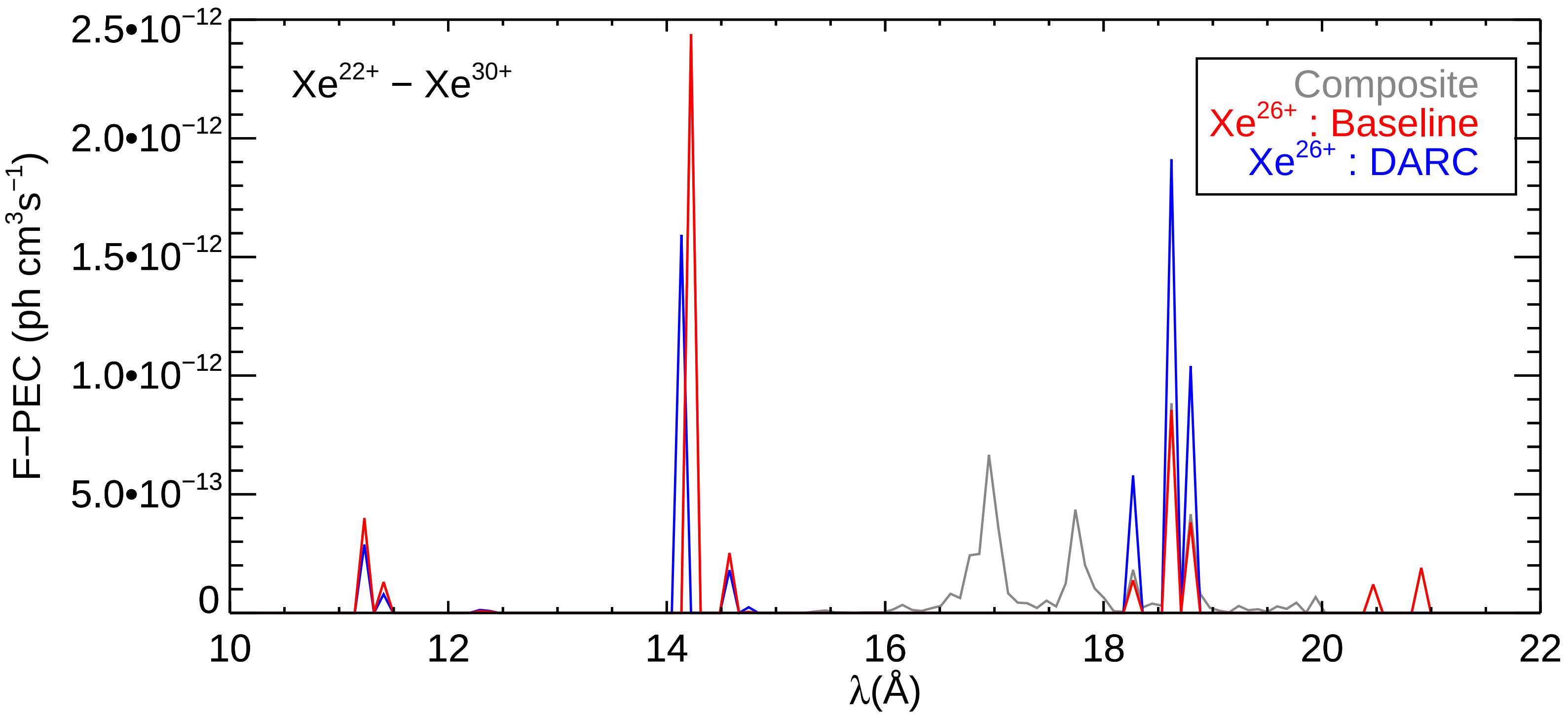
Recombination

- *adf55* rules are imminent.
- However, use ADAS407/ADAS408 for now.

Selectively uplift the quality of baseline

- With increasing atomic number relativistic effects assume a greater importance.
- Compare the baseline Born data to DARC to assess its validity.

Consider Ni-like Xe^{+26} with a 3d^{10} ground configuration:



Handling heavy species data

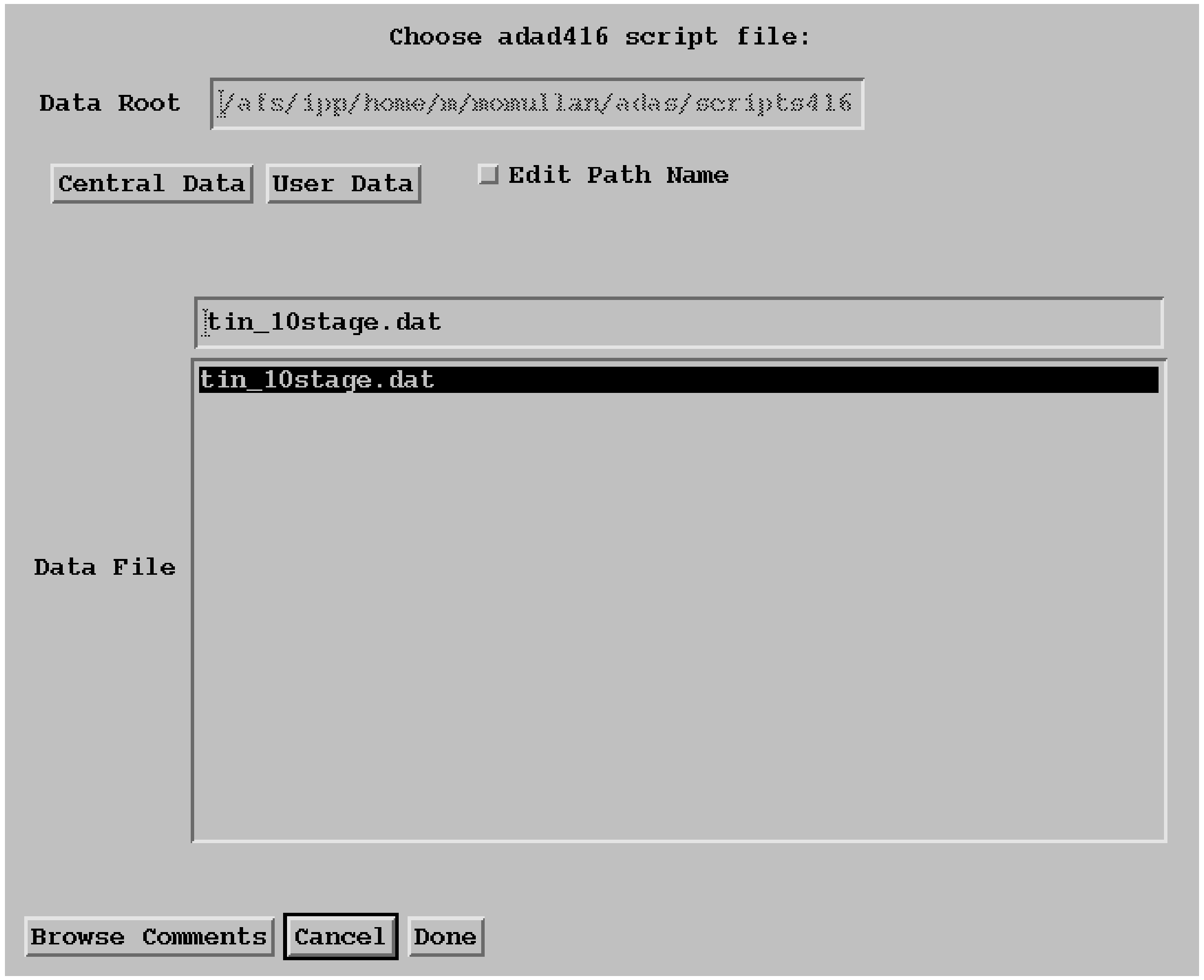
It may not always be necessary to consider all ionisation stages of an element.

Again, for tin, consider the partiton (extract from *scripts416* driver file:

```
//#02/p00/ 00/
      p01/ 01 02 03 04 05 06 07/
      p02/ 08/
      p03/ 09/
      p04/ 10/
      p05/ 11/
      p06/ 12/
      p07/ 13/
      p08/ 14/
      p09/ 15 16 17 18 19 20 21 22 23 24 25 26 27 28 29 30 31 32
      33 34 35 36 37 38 39 40 41 42 43 44 45 46 47 48 49/
      p10/ 50/
```

Generate partitioned *adf11* data

Process with ADAS416 : See `/u/mog/adas/scripts416/tin_10stage.dat`



Choose adad416 script file:

Data Root: /afs/ipp/home/m/momullan/adas/scripts416

[Central Data] [User Data] ☐ Edit Path Name

Data File: tin_10stage.dat

tin_10stage.dat

Note: *adf11* datasets in `/u/mog/ADAS-EU_course/`.

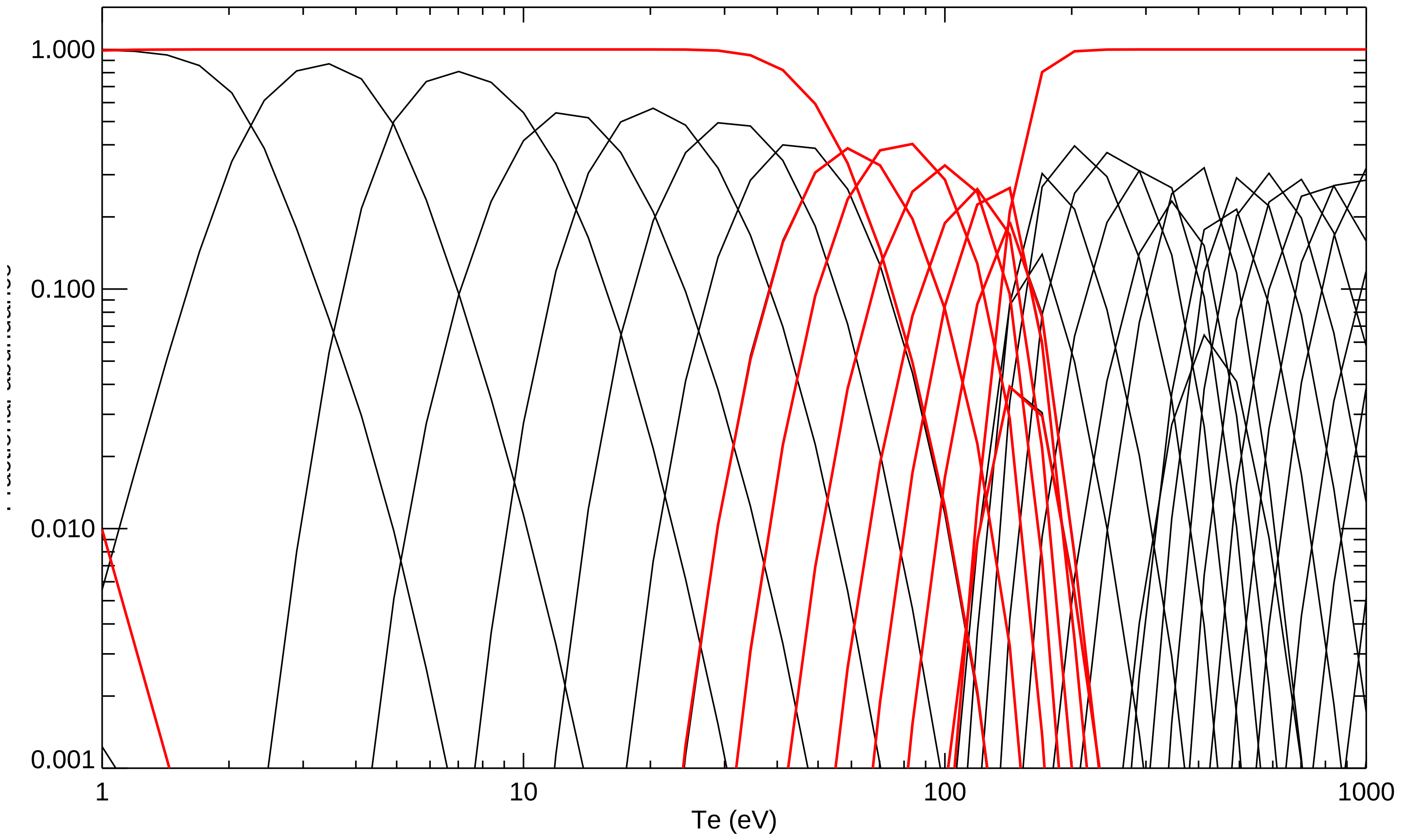
Compare ionisation equilibrium balance

At the IDL command line

```
te = adas_vector(low=1, high=1000, num=40)
dens = fltarr(40) + 1e12

; Explicity name adf11 files

files = {acd : 'acd66_sn#10stage.dat', $
         scd : 'scd66_sn#10stage.dat'  }

run_adas405, uid='adas', elem='sn', year=89, te=te, dens=dens, $
             files=files, frac=frac_par

files = {acd : 'acd89_sn.dat', $
         scd : 'scd89_sn.dat'  }

run_adas405, uid='adas', elem='sn', year=89, te=te, dens=dens, $
             files=files, frac=frac
```

```
xmin = min(te, max=xmax)
ymin = 0.001
ymax = 1.5

plot_oo, [xmin, xmax], [ymin, ymax], /nodata, ystyle=1, $
         xtitle = 'Te (eV)', ytitle = 'Fractional abundance'

for j = 0, n_elements(frac.stage)-1 do begin
   oplot, te, frac.ion[*,j]
endfor

for j = 0, n_elements(frac_par.stage)-1 do begin
   oplot, te, frac_par.ion[*,j], color=5, thick=5
endfor
```

We assume that we have no great interest ouside our chosen ions!


Te (eV)
Fractional abundance