

# MODULE 1

## Impurity atomic species in fusion plasma, their ionisation state and radiating characteristics - the ADAS approach.

### Demonstration script

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# 1 Demo (a) Finding about ADAS

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DEMO A: Finding about ADAS  
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PURPOSE: Look at the ADAS, ADAS-EU and OPEN-ADAS websites and their structure.

EXAMPLE: There are three main websites related to ADAS:

1. <http://www.adas.ac.uk>: this website contains all information about ADAS, its history, news. It includes the online manual, which gives an overview of the theory behind and detailed explanation of all ADAS series and data formats. All material related to dissemination (e.g. bulletins, publications, theses) is available in the website, together with information about past and future ADAS courses and workshops. Links to ADAS-EU and OPEN-ADAS are also present.
2. <http://www.adas-fusion.eu>: this website is strictly related to the ADAS-EU project in support of fusion laboratories in Europe and for ITER (Euratom Framework 7 Support Action). It provides all information about the work packages supporting fusion research and implemented by ADAS. It also gives details on ADAS-EU courses and links to ADAS and OPEN-ADAS websites.
3. <http://open.adas.ac.uk>: this website enables non members to download and use ADAS data. It allows one multiple research choice:
  - a freedom research (e.g. typing the name of the elements or ion or wavelength range of interest);
  - a research according to the wavelength of interest
  - a research based on ion selecting the element from the periodic table.

DEMO a1: The ADAS and ADAS-EU websites

ADAS website

1. Open an internet browser and type <http://www.adas.ac.uk>.
2. Click on "Manual"
3. Look at the different ADAS series (ADAS102, ADAS102, etc.)
4. Scrolling down, look at the different ADAS data formats (adf00, adf01, etc.)  
(Example files: demo\_a1\_adas\_web.png, demo\_a1\_adas\_web\_series.png, demo\_a1\_adas\_web\_adf.png)

ADAS-EU website

5. Click on "ADAS-EU" and, in the webpage which appears, click to the link <http://www.adas-fusion.eu>. Alternatively, type directly on the browser <http://www.adas-fusion.eu>.
6. Look at the ADAS-EU website.  
(Example files: demo\_a1\_adaseu\_web.png)

DEMO a2: OPEN-ADAS

1. Type on the browser <http://open.adas.ac.uk>.
2. Click on "Freedom" to look at the freedom research.
3. Then click on "Ion" and choose an element from the periodic table.  
(Example files: demo\_a2\_open\_adas\_search.png, demo\_a2\_open\_adas\_z.png)

## 1.1 Demo (a) Figures

### 1.1.1 Demo (a-1) demo\_a/demo\_a1\_adaseu\_web.png



Figure 1: ADAS-EU website - first page

### 1.1.2 Demo (a-1) demo\_a/demo\_a1\_adas\_web.png

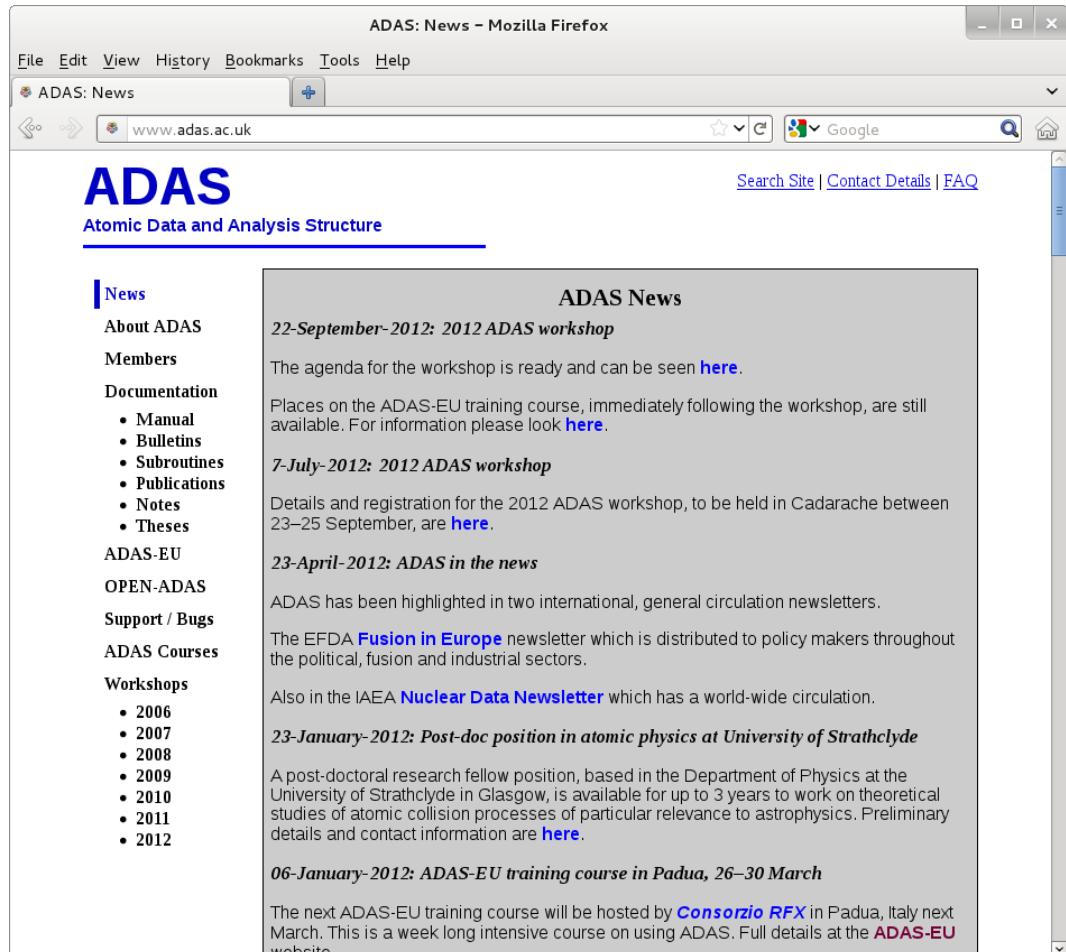


Figure 2: ADAS website - first page

### 1.1.3 Demo (a-1) demo\_a/demo\_a1\_adas\_web\_series.png

The screenshot shows a Mozilla Firefox window displaying the ADAS Documentation website at [www.adas.ac.uk/manual.php](http://www.adas.ac.uk/manual.php). The page title is "ADAS: Documentation - Mozilla Firefox". The left sidebar contains a navigation menu with links to News, About ADAS, Members, Documentation (with sub-links for Manual, Bulletins, Subroutines, Publications, Notes, and Theses), ADAS-EU, OPEN-ADAS, Support / Bugs, ADAS Courses, and Workshops (listing years from 2006 to 2012). The main content area is titled "ADAS Manual 2.6" and includes sections for "Introductory Material" (Table of Contents, Introduction), "ADAS Series 1 - Atomic Data Entry and Verification" (listing files ADAS101 through ADAS108), "ADAS Series 2 - General Z Data and Population Processing" (listing files ADAS201 through ADAS216), and "ADAS Series 3 - Charge Exchange Processing". A footer link at the bottom left points to <http://www.adas.ac.uk/man/chap2-04.pdf>.

Figure 3: ADAS - code series

#### 1.1.4 Demo (a-1) demo\_a/demo\_a1\_adas\_web.adf.png

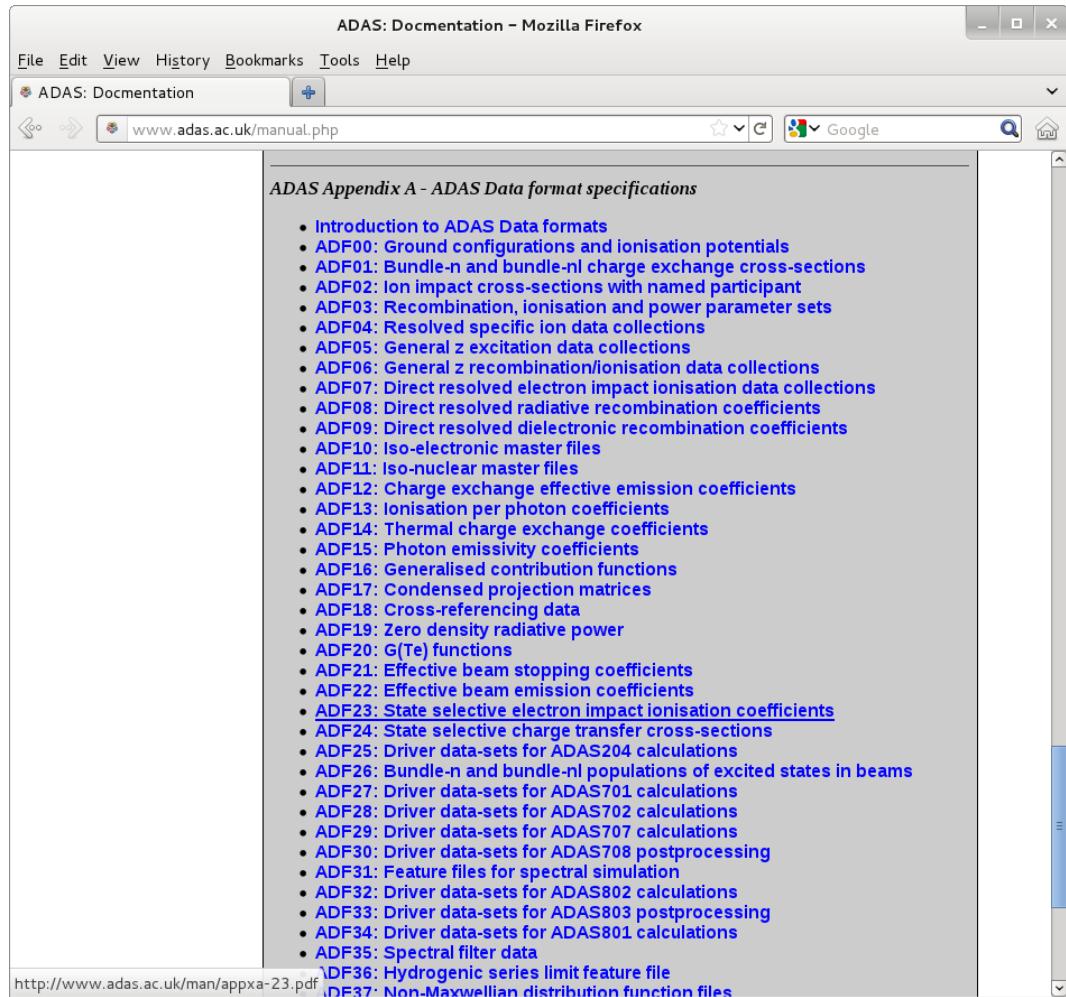


Figure 4: ADAS data formats

### 1.1.5 Demo (a-2 demo.a/demo.a2\_open\_adas\_search.png

The screenshot shows a Mozilla Firefox browser window displaying the OPEN-ADAS website at [open.adas.ac.uk](http://open.adas.ac.uk). The title bar reads "OPEN-ADAS - Mozilla Firefox". The main content area features the OPEN-ADAS logo and navigation links for About, Data classes, Tools, and Help. A search bar at the top right contains the text "[Fe I (5097Å)]". Below the search bar are three search options: "Freeform" (highlighted with a dashed orange border), "Wavelength", and "Ion". The "Freeform" section contains a search input field, a "Search" button, and a link to "Freeform search examples". Below this are three buttons: "Freeform search", "Search by wavelength", and "Search by ion". The "Data classes" section is divided into "FUNDAMENTAL CLASSES" and "DERIVED CLASSES". Under "FUNDAMENTAL CLASSES", there is a card for "Charge exchange cross sections" (ADF 01). Under "DERIVED CLASSES", there is a card for "Iso-nuclear master files" (ADF 11).

Figure 5: OPEN-ADAS - freeform search

### 1.1.6 Demo (a-2 demo.a/demo.a2\_open\_adas.z.png)

The screenshot shows the OPEN-ADAS website in Mozilla Firefox. The title bar reads "OPEN-ADAS - Mozilla Firefox". The menu bar includes File, Edit, View, History, Bookmarks, Tools, and Help. The address bar shows "open.adas.ac.uk". The main content area features the OPEN-ADAS logo and atomic data analysis structure information. A search bar at the top right allows searching by Freeform, Wavelength, or Ion. Below the search bar is a periodic table grid. To the right of the table is a search form with fields for Element (Atomic number or symbol) and Charge (Ion charge or iso-sequence symbol), separated by a plus sign. Below this are three search buttons: "Search", "Freeform search", "Search by wavelength", and "Search by ion".

Figure 6: OPEN-ADAS - search by ion

## 2 Demo (b) The code and data organisation

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DEMO B: The code and data organisation  
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PURPOSE: Overview of ADAS database and code organisation. This demo shows the interactive and non-interactive capabilities of ADAS. It also illustrates how to access the atomic and molecular database and look at the different libraries and codes (fortran,idl, etc.).

EXAMPLE: ADAS provides atomic data as well as sets of codes for modelling the radiating properties of ions and atoms in plasmas and for assisting in the interpretation and analysis of spectral measurements. It is addressed to a large variety of plasmas, ranging from astrophysical (from solar atmosphere to interstellar medium) to laboratory devices (from fusion to technological plasmas).

Documentations: The entire ADAS manual and related documentation are in the directory /home/adas/doc/

Components of ADAS structure:

1. an extensive database of fundamental and derived atomic data. They are collected in the directory /home/adas/adas/

```
adf00  adf06  adf12  adf18  adf24  adf34  adf48    arch103  arch603  scripts409
adf01  adf07  adf13  adf19  adf25  adf35  adf49    arch105  arch804  scripts416
adf02  adf08  adf14  adf20  adf26  adf38  adf54    arch106  mdf00
adf03  adf09  adf15  adf21  adf27  adf39  adf56    arch108  mdf02
adf04  adf10  adf16  adf22  adf28  adf40  arch101  arch601  scripts405
adf05  adf11  adf17  adf23  adf32  adf42  arch102  arch602  scripts406
```

adf is ADAS data file  
mdf is molecular data format  
arch are archives  
scripts are drivers

2. a large set of libraries, routines and utilities (including FORTRAN, C,C++, IDL and MATLAB) for accessing the database, delivering data, performing calculation of fundamental data and spectroscopic analysis (ADAS series, e.g. ADAS201).

Some of the most relevant directories are the following:

- /home/adas/fortran/  
which contains:

```
adas1xx  adas3xx  adas5xx  adas7xx  adas9xx
adas2xx  adas4xx  adas6xx  adas8xx  adaslib
```

-/home/adas/C/  
which contains:

adas5xx adas6xx adaslib

-/home/adas/idl/  
which contains:

adas1xx adas3xx adas5xx adas7xx adas9xx write\_adf  
adas2xx adas4xx adas6xx adas8xx adaslib read\_adf

The subdirectories adaslib, write\_adf and read\_adf include utility and reading routines.

Each of the subdirectories of the type adas1xx, adas2xx etc are related to the ADAS series: e.g. adas2xx is ADAS series 2 for the investigation of "General Z data and Population Processing". In turn this includes the directories:

adas201 adas203 adas205 adas207 adas209 adas211 adas213 adas215 adaslib  
adas202 adas204 adas206 adas208 adas210 adas212 adas214 adas216

for specific displaying or analysis purposes: e.g. adas201 contains a set of routines which allows one to graph and fit coefficients for specific Z excitation.

Capabilities of ADAS structure:

1. the interactive part, which provides immediate display of fundamental and derived data used in analysis and allow one to explore parameter dependencies and diagnostic predictions of atomic population and plasma models;
2. the non-interactive part, provides a set of subroutines than can be accessed from the users and embedded in their own codes.

COMMENTS: The use of ADAS and its full capabilities, as described by this demo, is reserved to the members. However, the database (fundamental and derived atomic data) and the fortran reading routines for the ADAS data files are available also in the OPEN-ADAS website (see demo a) and free from the restriction of ADAS membership..

DEMO b1: Language and library structure

1. Open the directory /home/adas/doc/ to look at the documentation.
2. Open the directory /home/adas/adas/ to look at the location of the atomic and molecular database.
3. Open the directory /home/adas/idl/ to look at the ADAS series.
4. Open the directory /home/adas/fortran/ to look at the ADAS series (as point 3.).

DEMO b2: ADAS data formats

1. Open the directory /home/adas/adas/adf04 to look at an example of ADAS data file.

DEMO b3: Interactive ADAS menus and starting code

1. Go into the directory /home/adas/pass/.
2. Run adas.

3. Click on series 2: "2 General Z Data and Population Processing".
4. Click on "ADAS201: Specific Z Excitation File - Graph and Fit Coefficient"
5. Select a data set, e.g. from /home/adas/adas/adf04/adas#6/mom97\_ls#c1.dat and start the program.

### 3 Demo (c) Fundamental data collections

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DEMO C: Fundamental data collections  
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PURPOSE: Look at the fundamental data collection.

EXAMPLE: This demo gives examples of how look at some of the fundamental data collected in the ADAS data files (adf).

Three samples are provided:

1. adf04: These ADAS data files are collections of energy levels (or terms or configuration arrays according to the resolution adopted), radiative transitions probabilities (A-values) and rate coefficients for specified low states of an ion. There are five types of adf04: a) Type 1: electron collision transition line Omega (collision strength) as a function of the threshold parameter X. X, with  $1 < X < \infty$ , is defined as  $e_i/(E_j - E_i)$ , where  $e_i$  is the incident electron energy,  $E_j$  the energy of the upper state of the transition and  $E_i$  the energy of the lower state (Note that  $e_i + E_i = e_j + E_j$ , where  $e_j$  is the energy of the scattered electron). b) Type 3: electron collision transition line Upsilon (effective collision strength) as a function of electron temperature. c) Type 4: electron collision transition line Upsilon and Downpsilon as a function of energy (see Bryans 2005 - [http://www.adas.ac.uk/theses/bryans\\_thesis.pdf](http://www.adas.ac.uk/theses/bryans_thesis.pdf)). d) Type 5: electron collision transition line Omega as a function of the final state energy (which is the energy of scattered electron  $e_j$ ). e) Type 6: electron collision transition line Omega\_l as a function of l.

For the demo a distorted wave adf04 for Be-like oxygen (0+4) has been chosen: /home/adas/adas/adf04/cophps#be/dw/ls#o4\_t5.dat

This is a type 5 adf04 in ls resolution. The term configurations are in the Eissner notation.

Three different transitions, which involve the ground term, have been chosen: 1) a dipole transition: 2s2 1S - 2s 3p 1P (corresponding to indices 1-9) 2) a spin change transition: 2s2 1S - 2s 3p 3P (corresponding to indices 1-10) 3) a monopole transition: 2s2 1S - 2p 3p 1S (corresponding to indices 1-24)

The three transitions show three characteristic behaviour (see viewgraphs).

2. adf08: This data file set contains the radiative recombination coefficients. For ionised H which recombines to neutral H, the adf08 is: /home/adas/adas/adf08/rrc98##/rrc98##\_h1.dat. This is in LS resolution. Consider the first three shells n=2,3,4. For n=2 shell the corresponding terms are 2s 2S and 2p 2P, with indices 2 and 3 respectively. For n=3 shell the corresponding terms are 3s 2S, 3p 2P and 3d 2D with indices 4, 5 and 6 respectively. Finally, for n=4 shell the corresponding terms are 4s 2S, 4p 2P, 4d 2D and 4f 2F with indices 7, 8, 9 and 10 respectively. The

contribution of radiative recombination to each shell is given by the sum of the term contributions.

3. adf09: This data file provides final state level-resolved dielectronic recombination rate coefficients into final terms (LS resolution) or levels (J-resolved). For Be-like  $\rightarrow$  B-like carbon ( $C^{+2} \rightarrow C^{+1}$ ), in LS resolution and considering the recombination from  $n=2$  shell of recombining ion into  $n=2$  shell of recombined ion, the adf09 is:

`/home/adas/adas/adf09/nrbjc00#be/nrb00#be_c2ls22.dat` The total contribution due to dielectronic recombination is calculated for each metastable of the recombining ion. In this case the recombining ion is  $C^{+2}$  and the metastable terms are  $2s2\ 1S$  and  $2s\ 2p\ 3P$  (see also MODULE 2 DEMO a: Identifying metastables).

COMMENTS: Note that an adf04 type 5 has been used in DEMO 1c instead of an adf04 type 1. Therefore the final energy  $e_j$  (energy of scattered electron) has been converted into the  $X$  parameter for each transitions, which is  $X = (e_j + \Delta E) / \Delta E$ , where  $\Delta E$  is the equals to  $E_j - E_i$ , that is the energy difference between level  $j$  and level  $i$  of the corresponding transition.

DEMO c1: Looking at adf04: understanding the cross sections

1. Look at the adf04 type 5 for  $O^{+4}$  and select three transitions: e.g. dipole, spin change and monopole.
2. Use `read_adf04.pro` to read the adf04 selected.
3. Convert type 5 in type 1 adf04 to show the behaviour of the collision strength of each transition as a function of the threshold parameter.
4. Plot the Omega for the three transitions.

Program: `demo_c_1.pro`

Sample of output file: `demo_c_1.ps`

DEMO c2: Looking at adf08: radiative recombination data.

1. Look at the adf08 for  $H$  to select the appropriate level indices.
2. Use `read_adf08.pro` to read the selected adf08.
3. Sum over the shell ( $n=2$ ,  $n=3$ ,  $n=4$ ).
4. Plot the radiative recombination coefficients into  $n=2$ ,  $n=3$  and  $n=4$  shells for  $H$  as a function of electron temperature.

Program: `demo_c_2.pro`

Sample of output file: `demo_c_2.ps`

DEMO c3: Looking at adf09: dielectronic recombination data

1. Use `xxdata_09.pro` to read adf09.
2. Plot the total contribution of dielectronic recombination from the two metastables of recombining ion.

Program: `demo_c_3.pro`

Sample of output file: `demo_c_3.ps`

### 3.1 Demo (c) Figures

#### 3.1.1 Demo (c-1) demo\_c/demo\_c\_1.pdf

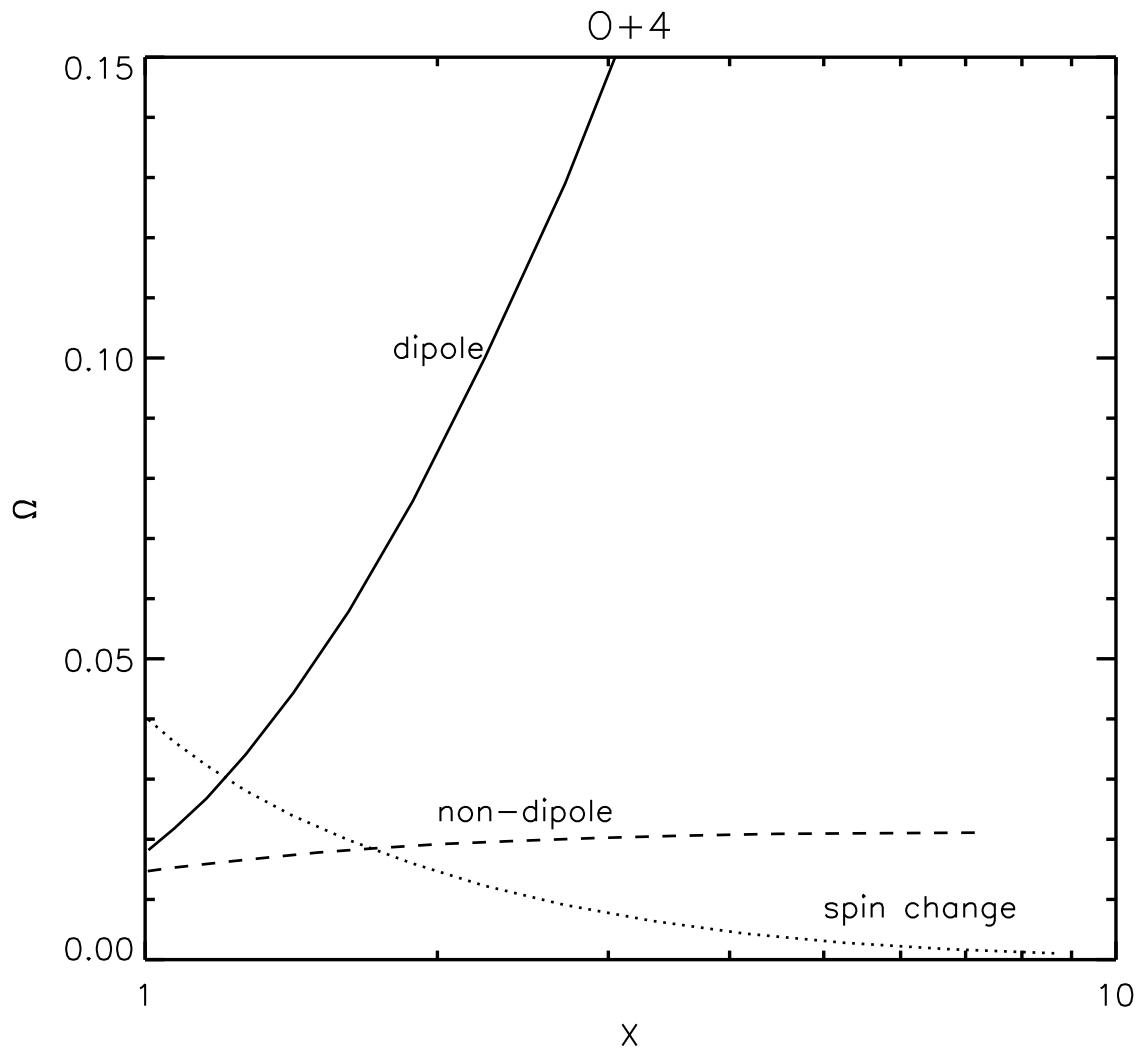


Figure 7:

### 3.1.2 Demo (c-2) demo\_c/demo\_c\_2.pdf

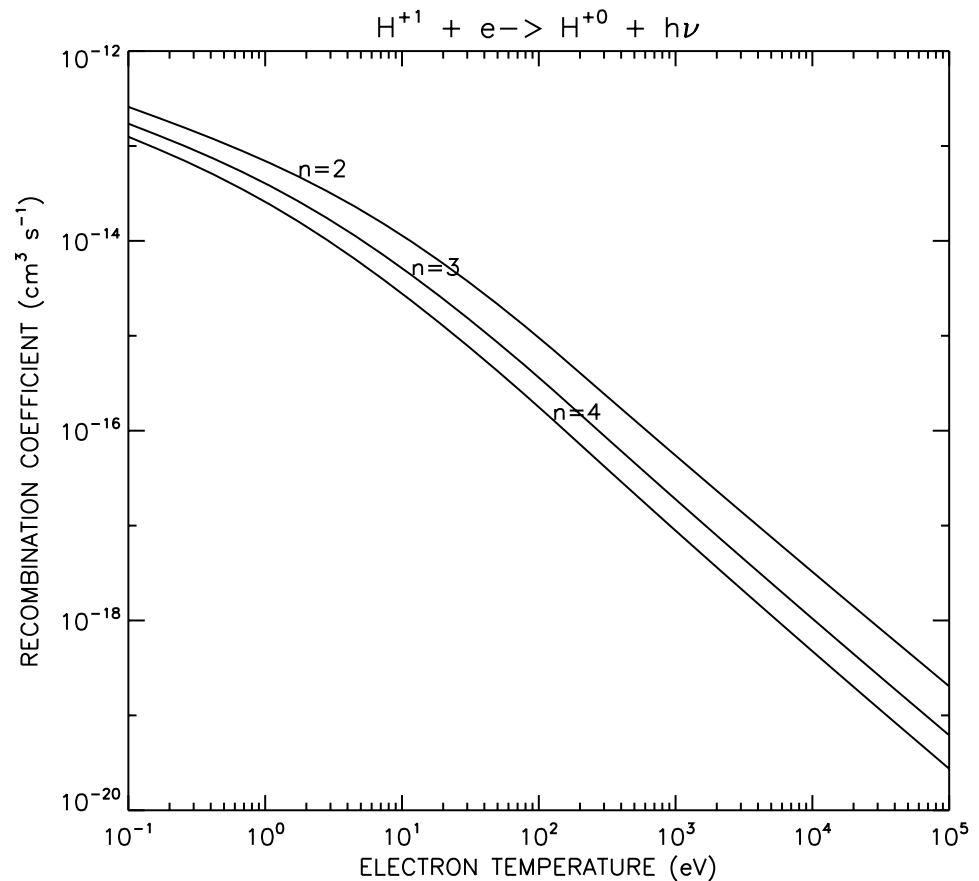


Figure 8:

### 3.1.3 Demo (c-3) demo\_c/demo\_c\_3.pdf

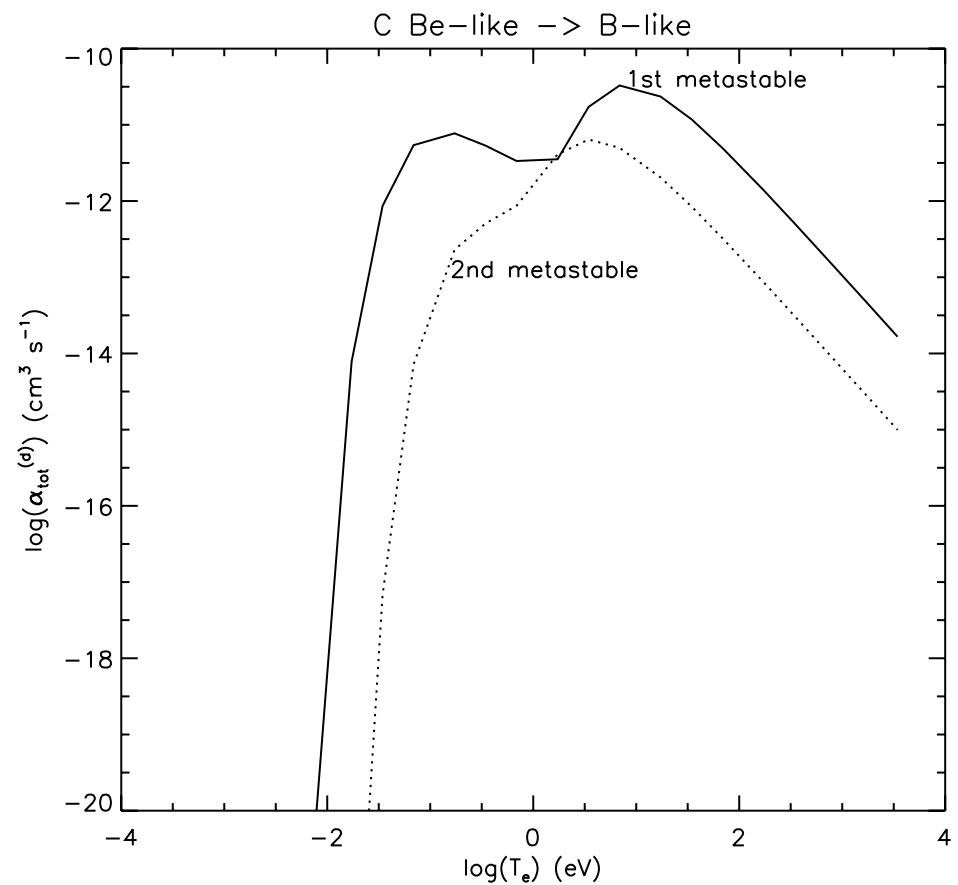


Figure 9:

## 3.2 Demo (c) Procedures

### 3.2.1 Demo (c-1) demo\_c/demo\_c\_1.pro

```
pro demo_c_1
;Use read_adf04.pro to read type 5 adf04 for 0+4 (Be-like)
;select three different transitions (e.g. dipole, spin change and monopole)
;plot the omega as a function of the threshold parameter [X=ei/(Ej-Ei)]

;adf04 type 5 in ls resolution
adf04='/home/agiunta/adas/adf04/cophps#be/dw/ls#o4_t5.dat'

;read the adf04 using read_adf04.pro
read_adf04,file=adf04,fulldata=data

;dipole transition: e.g. 2s2 1S - 2s 3p 1P
dd=where(data.lower eq 1 and data.upper eq 9)

;spin exchange transition: e.g. 2s2 1S - 2s 3p 3P
ee=where(data.lower eq 1 and data.upper eq 10)

;monopole transition: e.g. 2s2 1S - 2p 3p 1S
mm=where(data.lower eq 1 and data.upper eq 24);8)

ej=data.te

;Derive the X parameter for the three transitions

;1. Dipole transition
;identify the levels
d1=where(data.ia eq 1)
d2=where(data.ia eq 9)
;Values of energy in cm-1 corresponding to the previous levels
Ej_d=data.wa[d2]
Ei_d=data.wa[d1]
;calculate the delta_E for the dipole transition and convert to eV
delta_E_d=(Ej_d-Ei_d)/8066.0
;convert eV to Ryd
delta_E_d=delta_E_d/13.6
X_d=dblarr(n_elements(ej))
for i=0,n_elements(ej)-1 do X_d[i]=(ej[i]+delta_E_d)/delta_E_d

;2. Spin exchange transition
;identify the levels
s1=where(data.ia eq 1)
s2=where(data.ia eq 10)
;Values of energy in cm-1 corresponding to the previous levels
Ej_s=data.wa[s2]
Ei_s=data.wa[s1]
```

```

;calculate the delta_E for the dipole transition and convert to eV
delta_E_s=(Ej_s-Ei_s)/8066.0
;convert eV to Ryd
delta_E_s=delta_E_s/13.6
X_s=dblarr(n_elements(ej))
for i=0,n_elements(ej)-1 do X_s[i]=(ej[i]+delta_E_s)/delta_E_s

;3. Monopole transition
;identify the levels
m1=where(data.ia eq 1)
m2=where(data.ia eq 24)
;Values of energy in cm-1 corresponding to the previous levels
Ej_m=data.wa[m2]
Ei_m=data.wa[m1]
;calculate the delta_E for the dipole transition and convert to eV
delta_E_m=(Ej_m-Ei_m)/8066.0
;convert eV to Ryd
delta_E_m=delta_E_m/13.6
X_m=dblarr(n_elements(ej))
for i=0,n_elements(ej)-1 do X_m[i]=(ej[i]+delta_E_m)/delta_E_m

;plot Omega as a function of the threshold parameter X
set_plot,'ps'
device, /isolatin1, font_index=8
device, bits=8, filename='demo_c_1.ps', $
    font_size = 14, xsize=18.0, ysize=16.0, $
    yoffset=7.0, /color
device, /helvetica

;using a normalisation factor to show the behaviour of the three transitions
plot_oi,X_d,data.gamma[dd,*],xrange=[1.,10.],yrange=[0.,0.15],$
    title='0+4',xtitle='X',ytitle='!7X!3'
plots,X_s,data.gamma[ee,*],line=1
plots,X_m,data.gamma[mm,*],line=2

xyouts,1.8,0.1,'dipole'
xyouts,5.,0.007,'spin change'
xyouts,2.,0.023,'non-dipole'

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

end

3.2.2 Demo (c-2) demo_c/demo_c_2.pro
pro demo_c_2

```

```

;Use read_adf08 to read adf08 for H
;and extract and plot state selective radiative
;recombination coefficients for H into n=2, n=3 and n=4 shells

adf08='/home/adas/adas/adf08/rrc98##/rrc98##_h1.dat'
parent=1
;define the level indices looking at the adf08 selected
level=[2,3,4,5,6,7,8,9,10]
nlev=n_elements(level)

;define electron temperature (eV)
te=adas_vector(low=0.1,high=1.e5,num=30)
nte=n_elements(te)

rec=fltarr(nte,nlev)

;read the adf08 selected using read_adf08.pro
for i=0,nlev-1 do begin
  read_adf08,file=adf08,parent=parent,level=level[i],te=te,data=data
  rec[*,i]=data
endfor

;sum over the shell
;n=2: level=2 -> 2s 2S; level+3 -> 2p 2P
recn2=total(rec[*,0:1],2)

;n=3: level=4 -> 3s 2S;level=5 -> 3p 2P;level=6 -> 2d 2D
recn3=total(rec[*,2:4],2)

;n=4: level=7 -> 4s 2S;level=8 -> 4p 2P;level=9 -> 4d 2D; level=10 -> 4f 2F
recn4=total(rec[*,5:8],2)

;plot recombination coefficients to n=2, n=3 and n=4
set_plot,'ps'
device, /isolatin1, font_index=8
device, bits=8, filename='demo_c_2.ps', $
  font_size = 14, xsize=18.0, ysize=16.0, $
  yoffset=7.0, /color
device, /helvetica

plot_oo,te,recn2,title='H!u+1!n + e-> H!u+0!n + h!7m!3',$
  xtitle='ELECTRON TEMPERATURE (eV)', $
  ytitle='RECOMBINATION COEFFICIENT (cm!u3!n s!u-1!n)'

oplot,te,recn3
oplot,te,recn4

xyouts,te[nte/5],recn2(nte/5),'n=2'
xyouts,te[nte/3],recn3(nte/3),'n=3'

```

```

xyouts,te[ntr/2],recn4(ntr/2),'n=4'

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

end

3.2.3 Demo (c-3) demo_c/demo_c_3.pro

pro demo_c_3
;Use xxdata_09.pro to read adf09 for C Be-like -> B-like
;in ls resolution from n=2 -> n=2

adf09='/home/adas/adas/adf09/nrbjc00#be/nrb00#be_c2ls22.dat'

;read adf09 using use xxdata_09.pro
xxdata_09,file=adf09,fulldata=data

;convert electron temperature units from Kelvin to eV
te=data.tea/11604.5

;plot the total contribution of dielectronic recombination
;from the two metastables of recombining ion
set_plot,'ps'
device, /isolatin1, font_index=8
device, bits=8, filename='demo_c_3.ps',           $
    font_size = 14, xsize=18.0, ysize=16.0,      $
    yoffset=7.0, /color
device, /helvetica
plot,alog10(te),alog10(data.diel_tot[0,*]),          $
    yrange=[-20.,-10.],                           $
    title='C Be-like -> B-like',                 $
    xtitle='log(T!de!n) (eV)',                   $
    ytitle='log(!7a!3!dtot!n!u(d)!n) (cm!u3!n s!u-1!n)' $
oplot,alog10(te),alog10(data.diel_tot[1,*]),line=1

xyouts,0.9,-10.5,'1st metastable'
xyouts,-0.8,-13.0,'2nd metastable'

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

end

```

## 4 Demo (d) Executing population calculations

-----  
DEMO D: Executing population calculations  
-----

PURPOSE: Perform population calculations, look at the different coefficients and calculate ionisation balance and radiated power.

The population of excited levels is calculated by ADAS205 and ADAS208. The input dataset is a specific ion file in the adf04 format. ADAS208 is an extension of ADAS205 and includes in the population calculation: a) metastable parents; b) condensed influenced of very highly excited level populations; c) inner shell ionisation forming excited states; d) three body recombination.

Additionally, ADAS208 generates the Generalised Collisional-Radiative (GCR) coefficients:

- 1) adf15, which is the Photon Emissivity Coefficients, PEC;
- 2) adf11, which includes the following coefficients:

scd= ionisation coefficients  
acd= free electron recombination coefficients  
ccd= charge exchange recombination coefficients  
xcd= metastable cross-coupling coefficients  
qcd= parent metastable cross-coupling coefficients

plt= total excitation line power coefficients  
prb= free electron recombination cascade bremsstrahlung power coefficients  
prc= charge exchange power coefficients  
pls= specific line excitation power coefficients

ecd= effective ionisation potential  
zcd= effective superstage charge  
ycd= effective superstage square of effective charge

The units of first group are cm<sup>3</sup> s<sup>-1</sup>, while for the power coefficients the units are ergs cm<sup>3</sup> s<sup>-1</sup>. The last group is used for heavy species.

The adf11 data files are identified by year (e.g. 85, 89, 93, 96).  
96 -> full GCR (also 93 is GCR, however they are available only for a small set of elements)

Once all the GCR coefficients adf11 are available (metastable resolved and stage to stage), fractional abundances and radiated power may be calculated using ADAS405 at equilibrium and ADAS406 using a simple transient model.

EXAMPLE: For the population calculation, this demo provides an example of the use of ADAS205 applied to neutral helium. The population of excited levels is calculated with respect to the ground or metastable level population.

The behaviour of the ratio between excited level population and ground level population as a function of electron density helps to identify:

- 1) different plasma regimes: coronal, CR, LTE
- 2) metastable levels or terms (see also MODULE 2 DEMO a: Identifying metastables).

The adf04 selected for the demo is:  
`/home/adas/adas/adf04/adas#2/mom97_ls#he0.dat`

The temperature chosen is 8.6 eV.

Two outputs from the advanced calculation performed by ADAS208 are included in the demo:

- 1) adf15 for C+1 (excitation PEC):

`/home/adas/adas/adf15/pec96#c/pec96#c_pjr#c1.dat`  
 spectral line: 858.4 Ang. 2s2 2p 2P - 2s2 3s 2P  
 C+1 has two metastable terms: 2s2 2p 2P, which is the ground term, and 2s 2p2 4P.  
 The excitation PECs driven by the two metastables have been chosen for the demo.

- 2) adf11 for O+3 (free electron recombination coefficient, acd):

In central ADAS the data file is:

`/home/adas/adas/adf11/acd96r/acd96r_o.dat`

However, if one wants to investigate the behaviour at high density, it would be better to increase the electron density range at which the coefficient is calculated. This is done running ADAS404 interactively for oxygen and editing the electron temperature and density range. The output file used as example has been saved locally and named acd404\_o.pass.

O+4 has 2 metastable terms, 2s2 1S and 2s 2p 3P, as well as O+3 which has the 2 metastable terms 2s2 2p 2P and 2s 2p2 4P.

The recombination coefficient from the second metastable of O+4 (iprt=2) to the second metastable of O+3 (igrd=2) has been selected for this demo.

The adf11 data files are of two types: stage to stage or unresolved (also called standard type) and metastable resolved - e.g. the file `/home/adas/adas/adf11/acd96r/acd96r_o.dat`, mentioned above provides metastable resolved recombination coefficients, while the file `/home/adas/adas/adf11/acd96/acd96_o.dat` gives stage to stage recombination coefficients. Once the adf11 files (scd, acd, etc) are available for an element, it is possible to calculate the fractional abundances and the radiated power at equilibrium using ADAS405.

For oxygen the inputs are the following:

```
Element symbol= o
Year=96
Default year=96
Isonuclear master classes: scd, acd, prb, plt (for stage to stage)
                           scd, acd, qcd, xcd prb, plt (for metastable resolved)
```

**COMMENTS:** Note that the full GCR adf15 used for the demo is in LS resolution.

**DEMO d1:** Running ADAS205 for populations

1. Use ADAS205 with the interactive ADAS windows.  
(sample of output file: demo\_d1.ps)

**DEMO d2:** Looking at adf15 and adf11

1. Look at the adf15 selected to identify blocks corresponding to the line chosen (C II 858.4 Ang.).
2. Use read\_adf15.pro to read the metastable resolved PEC data file adf15
3. Plot a surface of the excitation PEC as a function of Te and Ne comparing the behaviour due to the two metastables of C+1.
3. Look at the adf11 year 96 resolved for oxygen. Look at the electron temperature and density range. If it is not appropriate, run the interactive ADAS404, with a wider range of Te and Ne, to produce a new adf11 for oxygen and save it locally.
4. Use read\_adf11.pro to read the selected adf11.
5. Plot a surface of ACD as a function of electron temperature and density.

Program: demo\_d\_2.pro

Output files: demo\_d\_2\_pec.ps, demo\_d\_2\_acd.ps

**DEMO d3:** Running ADAS405 interactively and offline

1. Using the input defined above run ADAS405 using the interactive windows:
  - a. Select -> Type of master files: Standard
  - b. Select -> Data file: NULL
  - c. Produce a fractional abundance plot and a power function plot  
(output files: demo\_d\_3\_intv\_ion\_unres.ps, demo\_d\_3\_intv\_power\_unres.ps)
  - d. Repeat a.- c. selecting Type of master files: Partial - Resolved  
(output files: demo\_d\_3\_intv\_ion\_res.ps, demo\_d\_3\_intv\_power\_res.ps)
2. Use run\_adas405.pro from the command line for oxygen.
3. Plot stage to stage fractional abundances as a function of electron temperature for a fixed electron density (e.g. dens=1.e10 cm<sup>-3</sup>).
4. Plot metastable resolved fractional abundances as a function of electron temperature for a fixed electron density (e.g. dens=1.e10 cm<sup>-3</sup>).
5. Plot metastable resolved radiated power (total, plt, prb and ion) as a function of electron temperature for a fixed electron density (e.g. dens=1.e10 cm<sup>-3</sup>).

Program: demo\_d\_3.pro

Output files: demo\_d\_3\_ion\_unres.ps, demo\_d\_3\_ion\_res.ps, demo\_d\_3\_power\_res.ps

## 4.1 Demo (d) Figures

### 4.1.1 Demo (d-1) demo\_d/demo\_d\_1.pdf

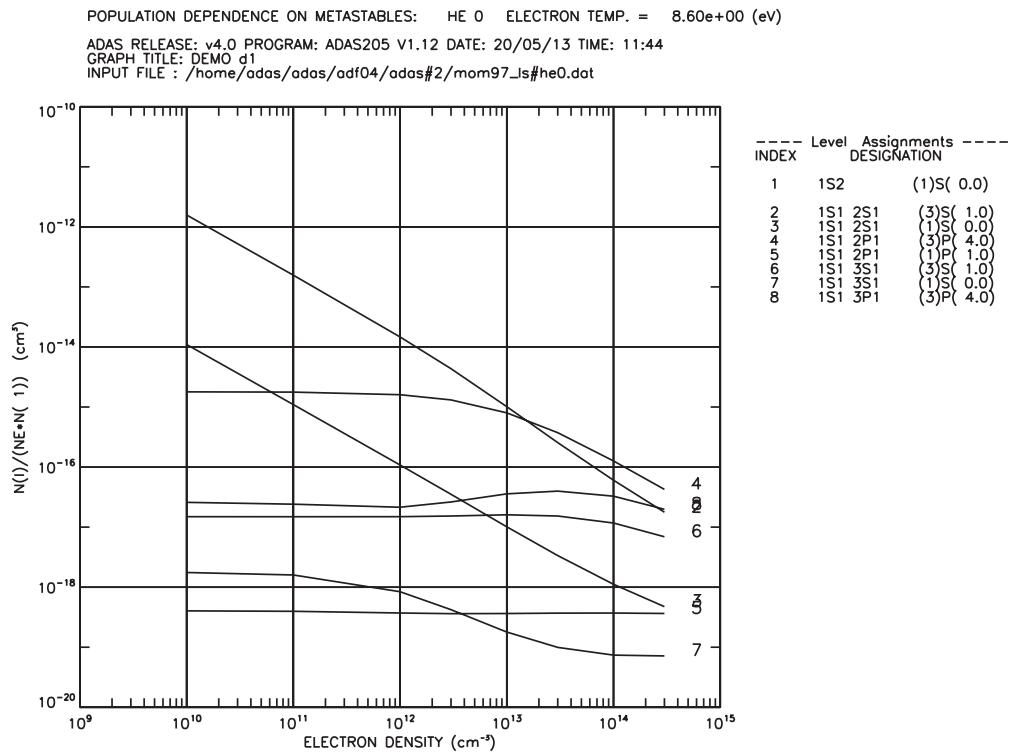


Figure 10:

#### 4.1.2 Demo (d-2) demo\_d/demo\_d\_2.acd.pdf

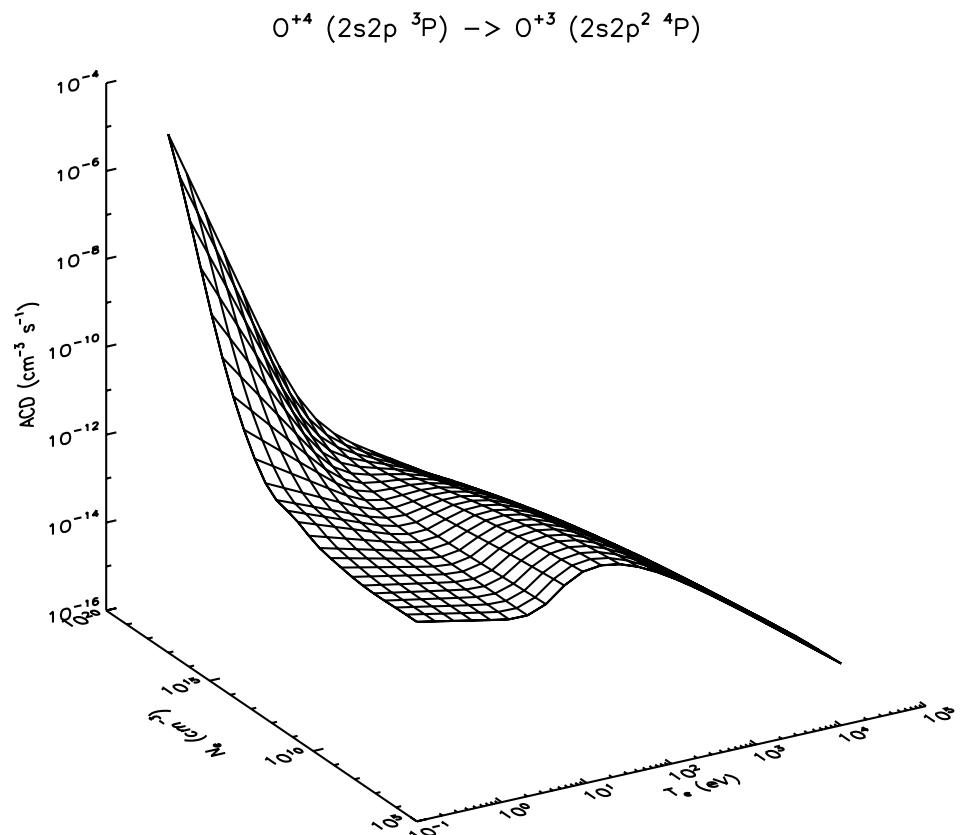


Figure 11:

#### 4.1.3 Demo (d-2) demo\_d/demo\_d\_2\_pec.pdf

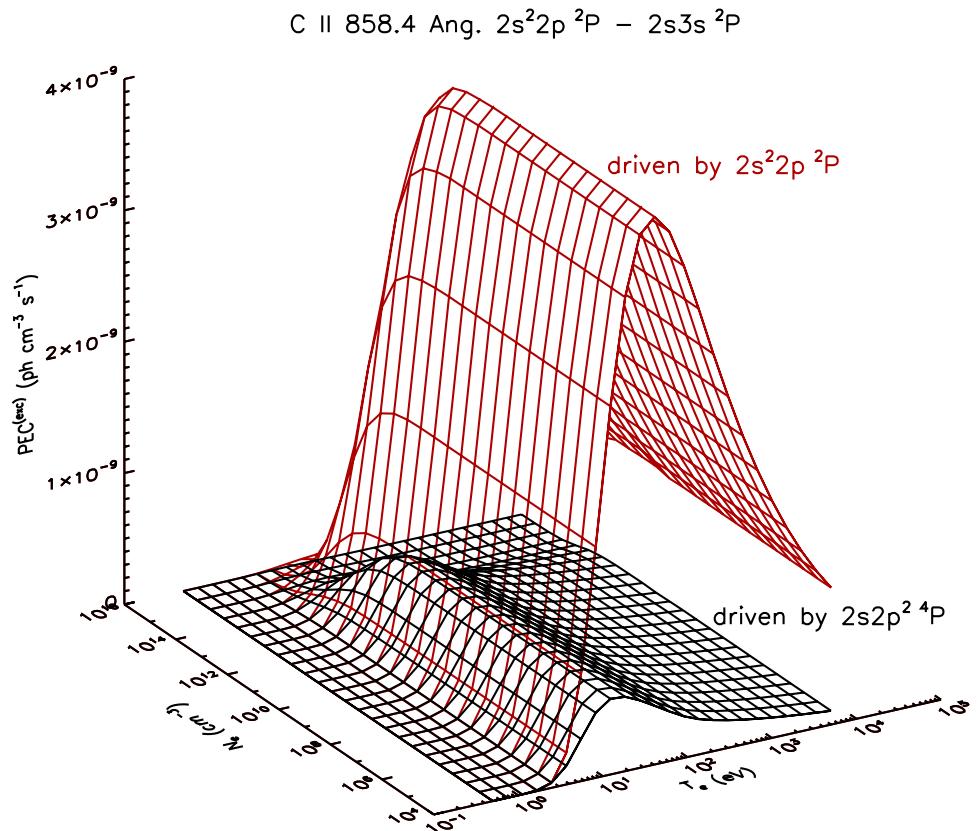


Figure 12:

#### 4.1.4 Demo (d-3) demo\_d/demo\_d\_3\_intv\_ion.res.pdf

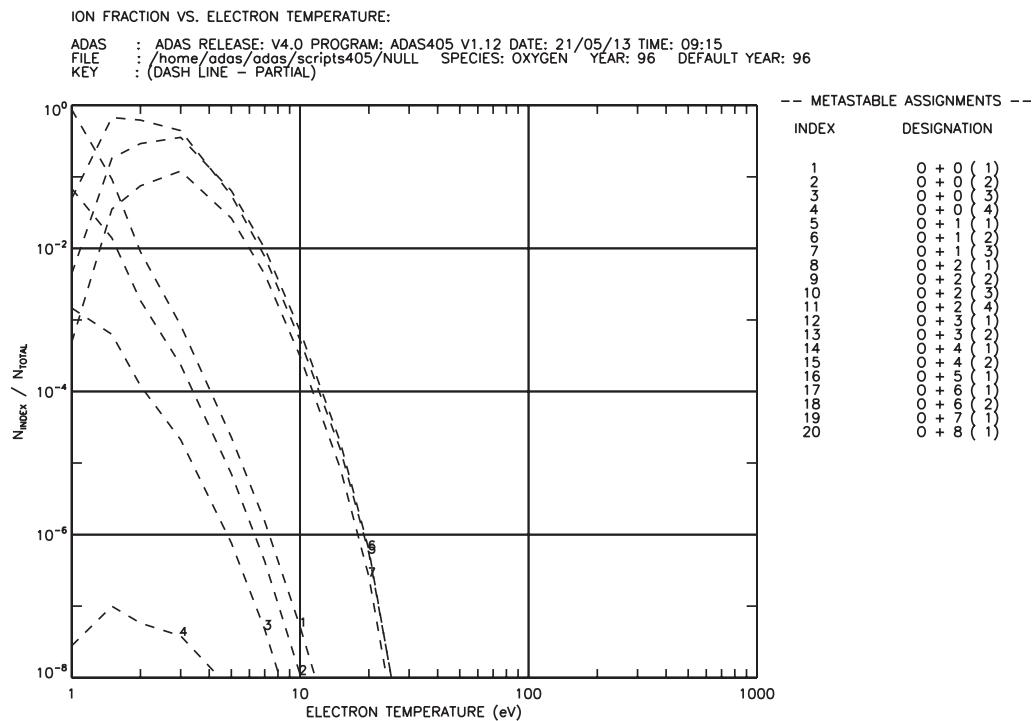


Figure 13:

#### 4.1.5 Demo (d-3) demo\_d/demo\_d\_3\_intv\_ion\_unres.pdf

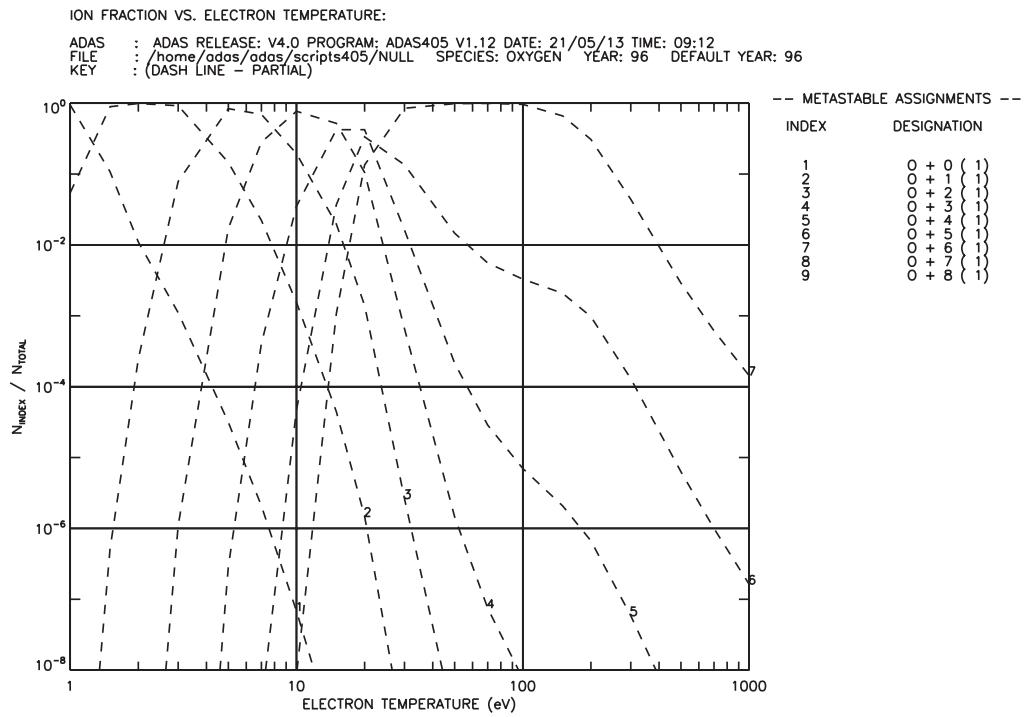


Figure 14:

#### 4.1.6 Demo (d-3) demo\_d/demo\_d\_3\_intv\_power\_res.pdf

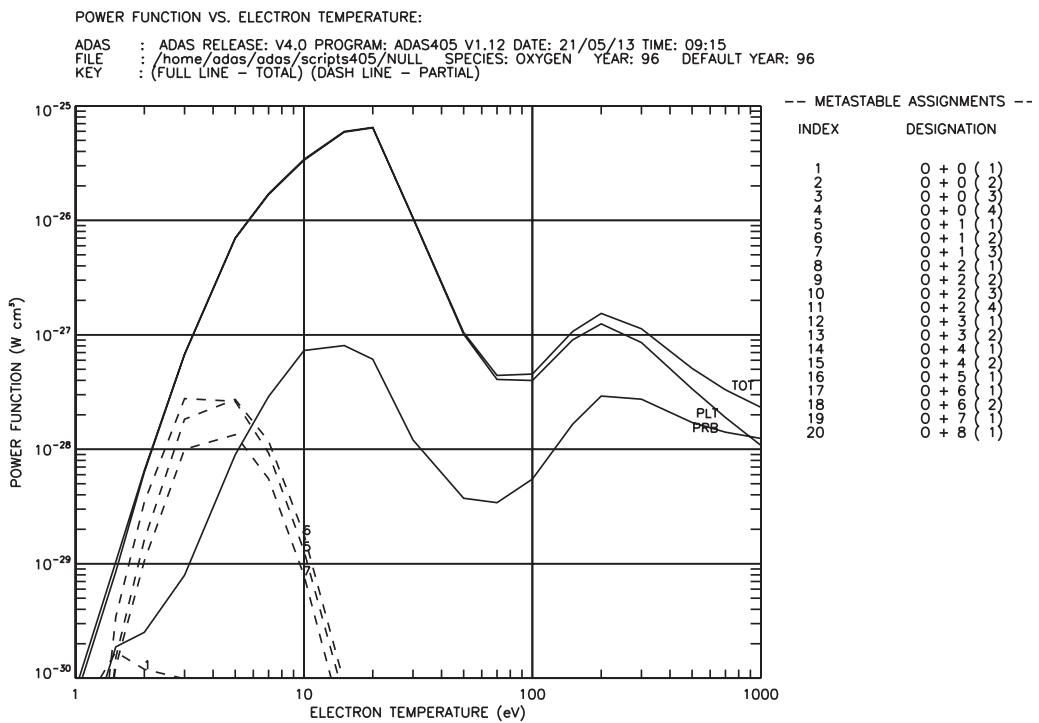


Figure 15:

#### 4.1.7 Demo (d-3) demo\_d/demo\_d\_3\_intv\_power\_unres.pdf

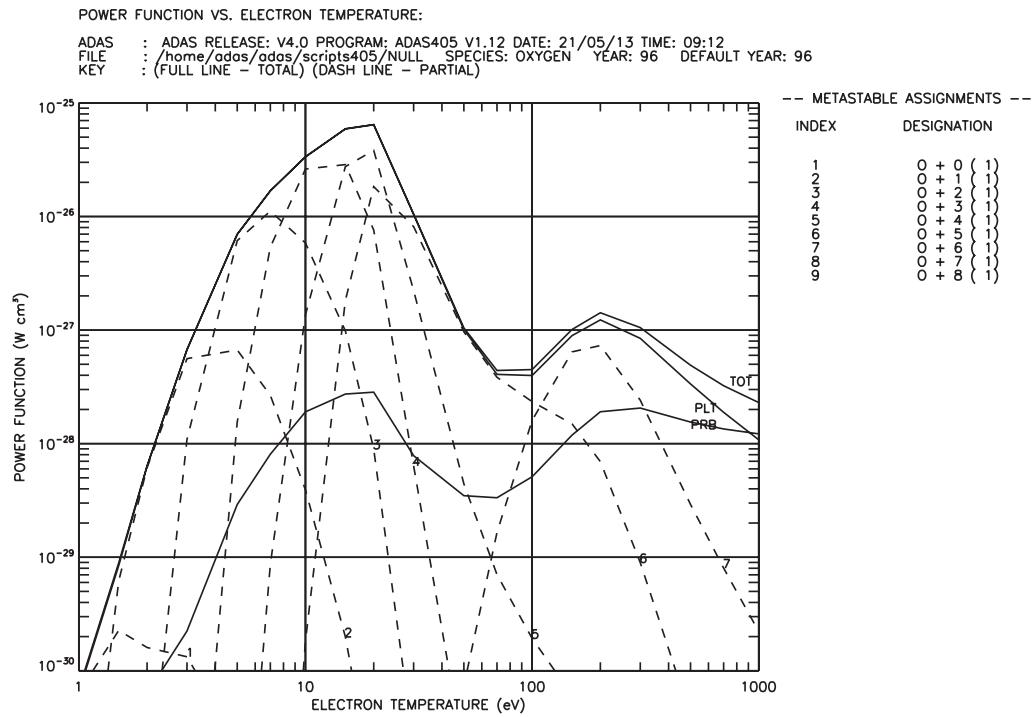


Figure 16:

#### 4.1.8 Demo (d-3) demo\_d/demo\_d\_3\_ion\_res.pdf

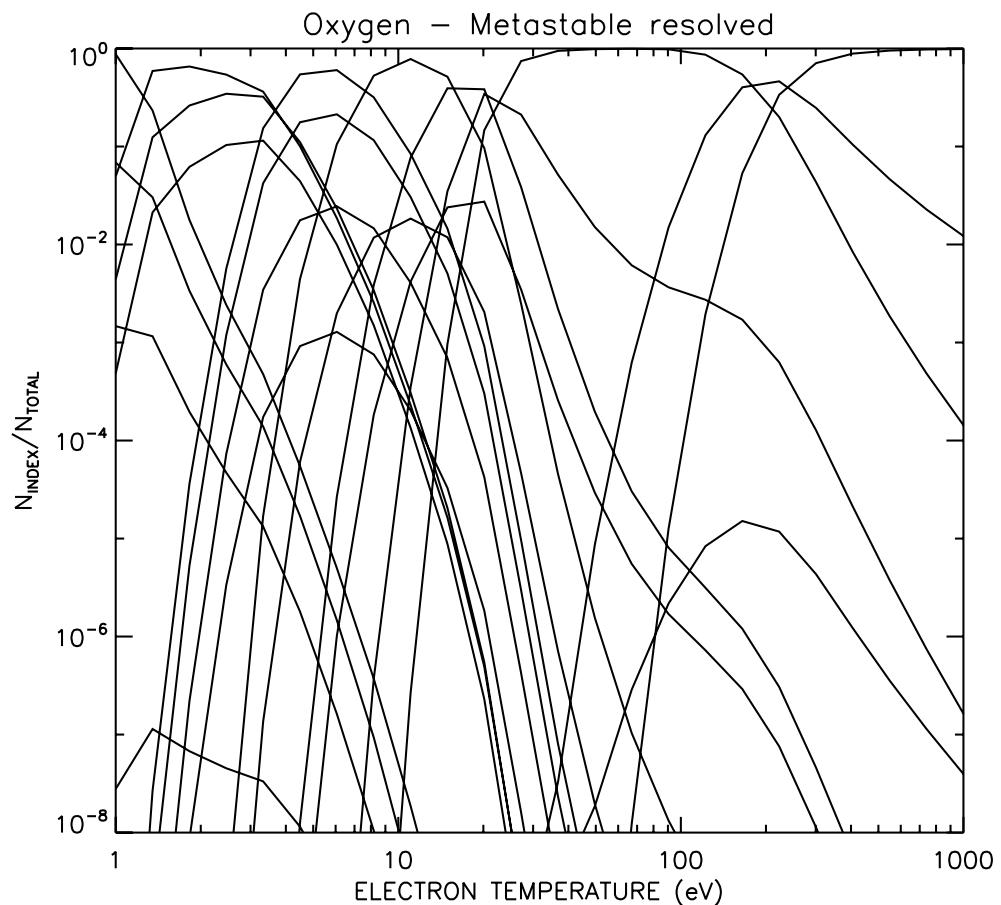


Figure 17:

#### 4.1.9 Demo (d-3) demo\_d/demo\_d\_3\_ion\_unres.pdf

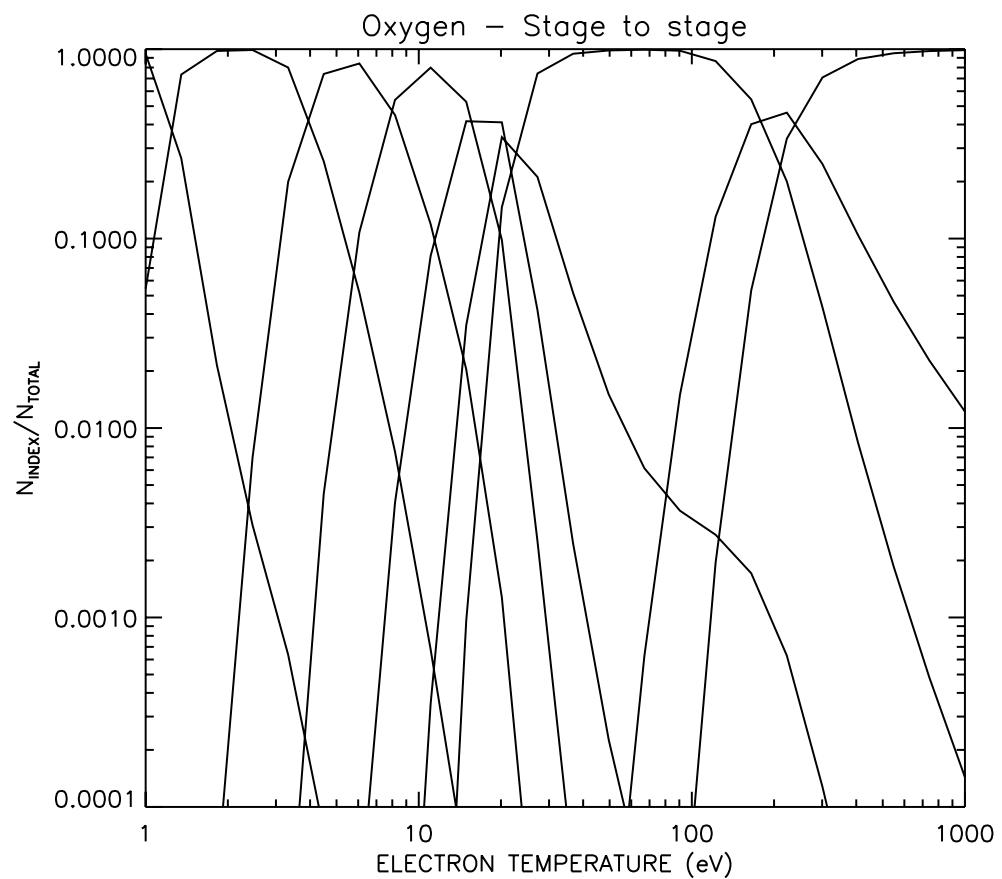


Figure 18:

#### 4.1.10 Demo (d-3) demo\_d/demo\_d\_3\_power\_res.pdf

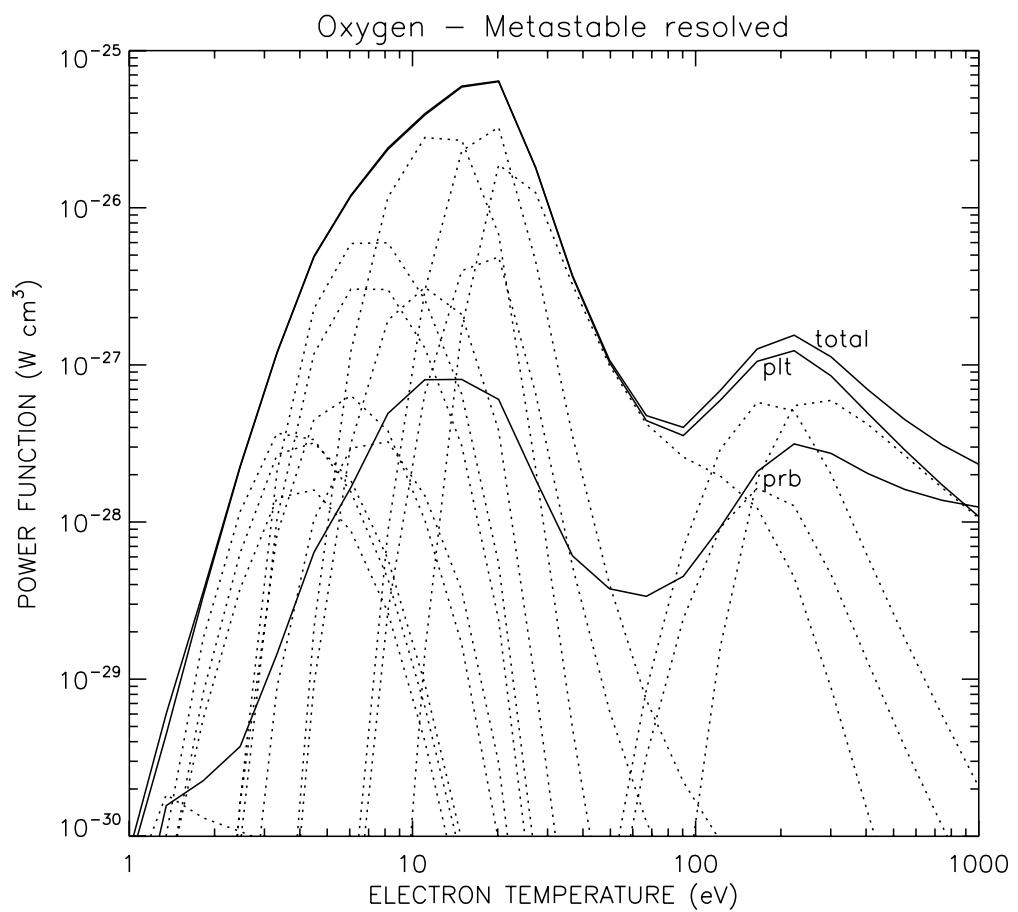


Figure 19:

## 4.2 Demo (d) Procedures

### 4.2.1 Demo (d-3) demo\_d/demo\_d\_3.pro

```
pro demo_d_3
;Use run_adas405.pro to produce stage to stage and metastable resolved
;fractional abundances and radiated power for oxygen

;Define electron temperature (eV) array
te=adas_vector(low=1.,high=1000.,num=24)

;Define a constant electron density (cm-3)
dens=1.e10

;Set up source (central ADAS or user directory),
;element, year and default year

uid='adas'
elem='o'
year=96
defyear=96

;Run run_adas405.pro to produce both fractional abundances and power
;in the unresolved or standard (stage to stage) case
run_adas405, uid=uid, year=year, defyear=defyear, elem=elem, te=te,$
dens=dens, frac=frac_unres, power=power_unres,/all

;Run run_adas405.pro to produce both fractional abundances and power
;in the metastable resolved case
run_adas405, uid=uid, year=year, defyear=defyear, elem=elem, te=te,$
dens=dens, partial=1, frac=frac_res, power=power_res,/all

;Plot oxygen fractional abundances for stage to stage case
set_plot,'ps'
device, /isolatin1, font_index=8
device, bits=8, filename='demo_d_3_ion_unres.ps',           $
font_size = 14, xsize=18.0, ysize=16.0, $ 
yoffset=7.0, /color
device, /helvetica

plot_oo,te,frac_unres.ion[0,*,0],xrange=[1.,1000.],yrange=[1.e-4,1.],$ 
title='Oxygen - Stage to stage',$
xtitle='ELECTRON TEMPERATURE (eV)',$
ytitle='N!dINDEX!n/N!dTOTAL!n' ,/nodata
for i=0,n_elements(frac_unres.stage)-1 do oplot,te,frac_unres.ion[0,*,i]

device, /close
set_plot,'X'
```

```

!p.font=-1

;Plot oxygen fractional abundances for metastable resolved case
set_plot,'ps'
device, /isolatein1, font_index=8
device, bits=8, filename='demo_d_3_ion_res.ps',           $
      font_size = 14, xsize=18.0, ysize=16.0,   $
      yoffset=7.0, /color
device, /helvetica

plot_oo,te,frac_res.ion[0,*,0],xrange=[1.,1000.],yrange=[1.e-8,1.],$
      title='Oxygen - Metastable resolved', $
      xtitle='ELECTRON TEMPERATURE (eV)', $
      ytitle='N!dINDEX!n/N!dTOTAL!n' ,/nodata
for i=0,n_elements(frac_res.stage)-1 do oplot, te,frac_res.ion[0,*,i]

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

;Plot oxygen radiated power for metastable resolved case
set_plot,'ps'
device, /isolatein1, font_index=8
device, bits=8, filename='demo_d_3_power_res.ps',           $
      font_size = 14, xsize=18.0, ysize=16.0,   $
      yoffset=7.0, /color
device, /helvetica

plot_oo,te,power_res.plt[0,*],xrange=[1.,1000.],yrange=[1.e-30,1.e-25],$
      title='Oxygen - Metastable resolved', $
      xtitle='ELECTRON TEMPERATURE (eV)', $
      ytitle='POWER FUNCTION (W cm!u3!n)'
oplot,te,power_res.prb[0,*]
oplot,te,power_res.total[0,*] ,thick=3
for i=0,n_elements(power_res.stage)-1 do oplot,te,power_res.ion[0,*,i],line=1

xyouts,0.8,0.63,'total',/normal
xyouts,0.75,0.6,'plt',/normal
xyouts,0.75,0.48,'prb',/normal

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

end

```