

2a. The interactive system - working with adf04 datasets

- Preliminaries
 - » Electron impact cross-sections and rate coefficients
 - » The ADF04 file format
 - » Interrogating adf04 collisional excitation data using ADAS201 and ADAS811

Electron impact cross-sections and rates

The excitation reaction $X_i^{+z}(E_i) + e(\varepsilon_i) \rightarrow X_j^{+z}(E_j) + e(\varepsilon_j)$

is described by an excitation cross-section $\sigma_{i \rightarrow j}(\varepsilon_i)$

More useful for tabulation is the collision strength Ω_{ij} with independent variable

$$X = \varepsilon_i / \Delta E_{ij} \quad \text{with} \quad X \in [1, \infty]$$

$$\Omega_{ij} = \omega_i(E_i / I_H) (\sigma_{i \rightarrow j}(\varepsilon_i) / \pi a_0^2) = \omega_j(E_j / I_H) (\sigma_{j \rightarrow i}(\varepsilon_j) / \pi a_0^2)$$

ADAS principally deals with Maxwell averaged rate coefficients $q_{i \rightarrow j}(T_e)$

$$Y_{ij} \quad Y_{ij} = \int_0^{\infty} \Omega_{ij}(\varepsilon_j) \exp(-\varepsilon_j / kT_e) d(\varepsilon_j / kT_e)$$

Electron impact cross-sections and rates (contd.)

More useful for tabulation is the Maxwell averaged collision strength $Y_{ij}(T_e)$

$$Y_{ij} = \int_0^{\infty} \Omega_{ij}(\varepsilon_j) \exp(-\varepsilon_j/kT_e) d(\varepsilon_j/kT_e)$$

$$q_{j \rightarrow i}(T_e) = \frac{\omega_i}{\omega_j} \exp(\Delta E_{ij}/kT_e) q_{i \rightarrow j}(T_e) = 2\sqrt{\pi} \alpha c a_0^2 \frac{1}{\omega_j} [I_H/kT_e]^{1/2} Y_{ij}$$

The ADAS adf04 format is used to archive sets of energy level lists, A-values and Maxwell averaged collision strengths for an ion sufficient to allow a population calculation.

Configuration specification

$$\Gamma = n_1 l_1^{q_1} n_2 l_2^{q_2} \dots n_m l_m^{q_m}$$

where $q_i > 0$ for $i = 1, \dots, m$ and $\sum_{i=1}^m q_i = N$

ADAS prefers Standard and Eissner configuration representations in ADF04 files for automatic processing and matching of levels between different data sets.

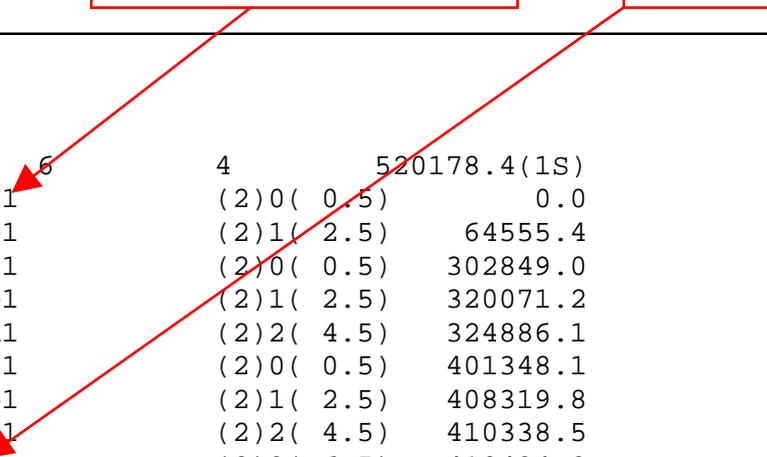
Configuration	Standard form	Eissner form
$1s^2 2s^2 2p^4$	1s2 2s2 2p4	21522543
$1s^2 2s^2 2p^6 6f^{11}$	1s2 2s2 2p6 6fb	2152254361J

The basic adf04 file

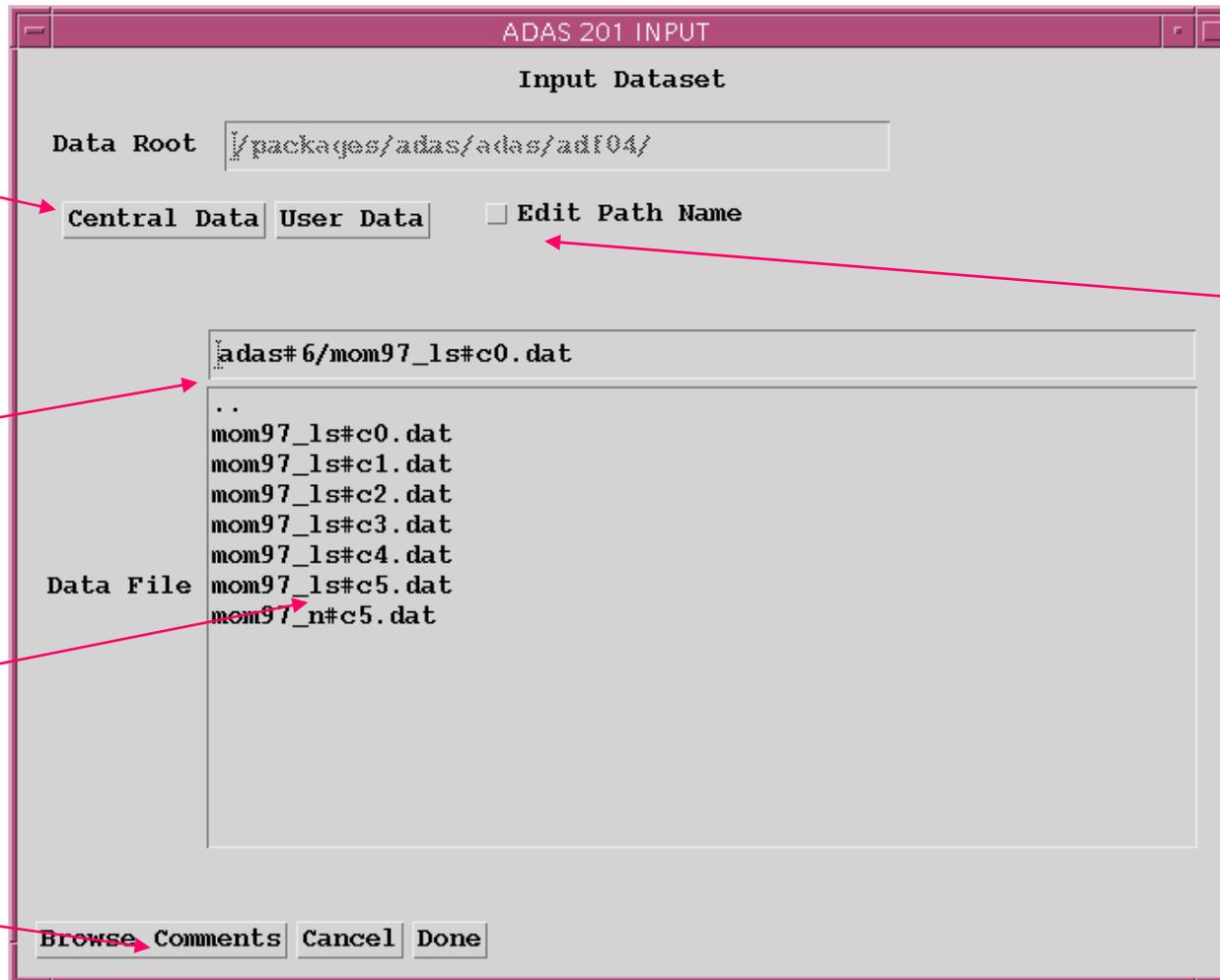
Standard form for
configuration
= 21512
in Eissner form

Eissner form for
configuration
= 1s2 4f1
in Standard form

```
C + 3      6      4      520178.4(1S)
 1 1s2 2s1 (2)0( 0.5)      0.0
 2 1s2 2p1 (2)1( 2.5)     64555.4
 3 1s2 3s1 (2)0( 0.5)    302849.0
 4 1s2 3p1 (2)1( 2.5)    320071.2
 5 1s2 3d1 (2)2( 4.5)    324886.1
 6 1s2 4s1 (2)0( 0.5)    401348.1
 7 1s2 4p1 (2)1( 2.5)    408319.8
 8 1s2 4d1 (2)2( 4.5)    410338.5
 9 2151A   (2)3( 6.5)    410434.2
10 1s2 5s1 (2)0( 0.5)    445368.5
11 1s2 5p1 (2)1( 2.5)    448860.5
12 1s2 5d1 (2)2( 4.5)    449889.2
13 1s2 5f1 (2)3( 6.5)    449939.8
14 1s2 5g1 (2)4( 8.5)    449948.4
-1
```



ADAS201 input



click to use central ADAS data

selected file for processing

ADF04 data file list

browse comments from selected data set

click to edit pathway

ADAS201 Processing

ADAS201 PROCESSING OPTIONS

Title for Run

Data File Name: /packages/adas/adas/adf04/adas#6/mom97_1s#c0.dat

Number of Electron Impact Transitions : 992
Number of Index Energy levels : 64

Polynomial Fitting

Fit Polynomial value % :

Select Specific Electron Impact Transition

TRANSITION INDEX	---	LOWER LEVEL INDEX	---	DESIGNATION	---	UPPER LEVEL INDEX	---	DESIGNATION
541	1	2S2 2P2	(3)P(4.0)	17	2S2 2P1 3D1	(3)D(7.0)		
1	1	2S2 2P2	(3)P(4.0)	2	2S2 2P2	(1)D(2.0)		
2	1	2S2 2P2	(3)P(4.0)	3	2S2 2P2	(1)S(0.0)		
3	1	2S2 2P2	(3)P(4.0)	9	2S2 2P1 3P1	(3)D(7.0)		
4	1	2S2 2P2	(3)P(4.0)	11	2S2 2P1 3P1	(3)P(4.0)		
5	1	2S2 2P2	(3)P(4.0)	12	2S2 2P1 3P1	(1)D(2.0)		

Select Temperatures for output file

Output Electron Temperatures

INDEX	Output	Input
1	1.000E+00	8.617E-01
2	1.500E+00	1.077E+00
3	2.500E+00	2.154E+00
4	4.000E+00	3.231E+00

Temperature Units: eV

Edit the processing options data and press Done to proceed

your title to appear on graphs & tables

number of transitions and levels

make polynomial fit to data

select transition for analysis

Select & enter Te values for output

set default output values

ADAS201 Output

ADAS201 OUTPUT OPTIONS

Data File Name: /packages/adas/adas/adf04/adas#6/mom97_ls#c0.dat

Browse Comments

Graphical Output

Graph Title: User manual example

Select Device: Post-Script

Post-Script
HP-PCL
HP-GL

Explicit Scaling X-min: X-max: Y-min: Y-max:

Enable Hard Copy Replace

File Name: adas201_graph.ps

Text Output Append Replace Default File Name

File Name: adas201_paper.txt

Cancel Done

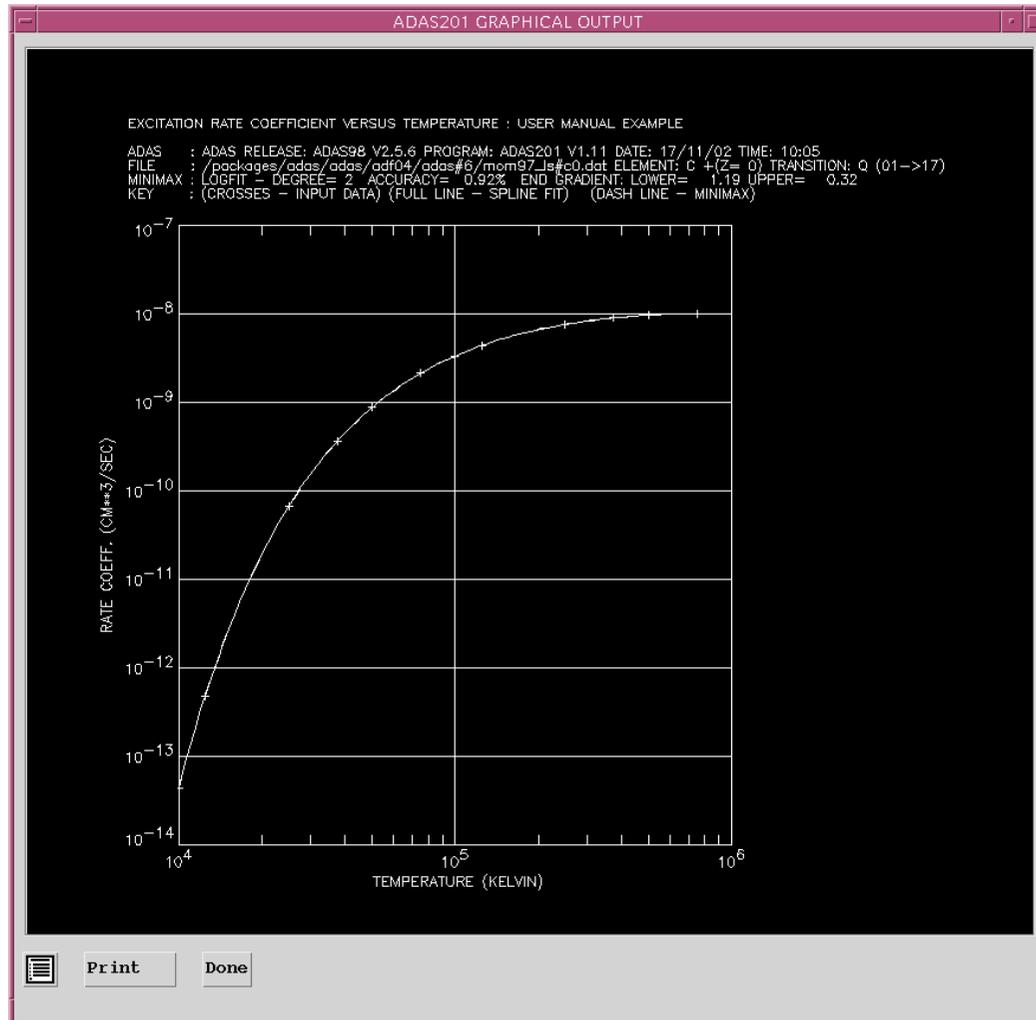
provide graphical output

allow graphical hard copy

graphical output file coding

tabular output of results

ADAS201 Graph



ADAS811 input

ADAS811 INPUT

adf04 file 01:

Data Root

Edit Path Name

Data File

- helike_hps102he.dat
- helike_kv1197he.dat

adf04 file 02 :

adf04 file 03 :

Enter File information

Select first file

Click to show file chooser pop-up

ADF04 data file list

Second and third files

browse comments from first data set

ADAS811 Processing

The screenshot displays the ADAS811 software interface for comparing adf04 files. The window title is "ADAS811 : Compare adf04 files".

File Selection: A dialog box titled "Choose file to scan through:" contains three radio button options:

- /home/summers/adas/adf04/helike/helike_hps102he.dat
- /home/summers/adas/adf04/helike/helike_kv1197he.dat
- /packages/adas/adas/adf04/adas#2/mom97_1s#he0.dat

Graph: A plot titled "Effective Collision Strengths" shows the relationship between Electron Temperature (K) on the x-axis (log scale from 10^3 to 10^9) and gamma on the y-axis (log scale from 0.0001 to 0.1000). Two curves are shown: a solid line and a dashed line, representing different data sets.

Plot Controls:

- Type of plot:** Radio buttons for e-exc (selected), p-exc, rec., ionis., and CX.
- Type of e-exc:** Radio buttons for gamma (selected), rate, and C-plot. A text box below contains the value "1.5000".
- Units of Te:** Radio buttons for K (selected) and eV.

Navigation and Output:

- Navigation keys: left arrow, right arrow, and "1 of 171".
- Buttons: "Show", "2", "1".
- Bottom buttons: "Cancel", "Print", "Print All".
- Status bar: "(154.0, 0.1795)".

Callouts:

- "select file to cycle through" points to the file selection dialog.
- "comparative graph for matched transitions" points to the Effective Collision Strengths plot.
- "select type e-exc" points to the "Type of plot:" section.
- "select type of e-exc display" points to the "Type of e-exc:" section.
- "select Te units" points to the "Units of Te:" section.
- "tape recorder keys" points to the navigation and control buttons at the bottom.

2b. The interactive system – working with excited population structure

- Datasets of class ADF04 contain all the information necessary to evaluate excited populations of an ion. It is called a ‘specific ion file’.
- Code ADAS205 computes the populations at temperatures and densities of your choice.
- The input, data set selection, screen is very similar to that for ADAS201

Populations calculation (contd.)

Distinguish metastable levels X_{ρ}^{+z} indexed by Greek letters
and ordinary levels X_i^{+z} indexed by Roman letters

Write the quasi-static equations for the ordinary levels populations in terms of the metastable populations as:

$$\sum_{j=1}^O C_{ij} N_j = - \sum_{\sigma=1}^M C_{i\sigma} N_{\sigma} + N_e N_1^+ r_i + N_e N_H q_i^{(CX)} \quad i = 1, 2, \dots$$

$$C_{ij} = -A_{j \rightarrow i} - N_e q_{j \rightarrow i}^{(e)} - N_p q_{j \rightarrow i}^{(p)} \quad i \neq j$$

$$C_{ii} = \sum_{j < i} A_{i \rightarrow j} + N_e \sum_{j \neq i} q_{i \rightarrow j}^{(e)} + N_p \sum_{j \neq i} q_{i \rightarrow j}^{(p)} + N_e q_i^{(I)}$$

Populations calculation (contd.)

Solution for the ordinary populations is

$$\begin{aligned} N_j &= -\sum_{i=1}^O C_{ji}^{-1} \sum_{\sigma=1}^M C_{i\sigma} N_\sigma + \sum_{i=1}^O C_{ji}^{-1} r_i N_e N_1^+ \\ &\quad + \sum_{i=1}^O C_{ji}^{-1} q_i^{(CX)} N_H N_1^+ \\ &\equiv \sum_{\sigma=1}^M F_{j\sigma}^{(exc)} N_e N_\sigma + F_{j1}^{(rec)} N_e N_1^+ + F_{j1}^{(CX)} N_H N_1^+ \end{aligned}$$

Populations calculation (contd.)

Spectrum line emissivities are

$$\mathcal{E}_{j \rightarrow k} = A_{j \rightarrow k} \left(\sum_{\sigma=1}^M F_{j\sigma}^{(exc)} N_e N_{\sigma} \right) + \sum_{\nu'=1}^{M_{z+1}} F_{j\nu'}^{(rec)} N_e N_{\nu'}^+ + \sum_{\nu'=1}^{M_{z+1}} F_{j\nu'}^{(CX)} N_H N_{\nu'}^+ + \sum_{\mu'=1}^{M_{z-1}} F_{j\mu'}^{(ion)} N_e N_{\mu'}^-$$

Identify excitation and recombination photon emissivity coefficients as

$$\text{PEC}_{\sigma, j \rightarrow k}^{(exc)} = A_{j \rightarrow k} F_{j\sigma}^{(exc)}$$

$$\text{PEC}_{\nu', j \rightarrow k}^{(rec)} = A_{j \rightarrow k} F_{j\nu'}^{(rec)}$$

ADAS205 processing

ADAS205 PROCESSING OPTIONS

Title for Run []

Data File Name: /afs/@cell/u/adas/adas/adf04/adas#2/mom97_ls#he0.dat

Browse Comments []

Nuclear Charge: 2 Ion Charge: 0

Temperatures

INDEX	Electron	Ion	Neutral Hydrogen	Input Value
1	2.000E+00	5.000E+02	5.000E+02	9.995E-01
2	3.000E+00	1.000E+03	1.000E+03	1.999E+00
3	5.000E+00	2.000E+03	2.000E+03	4.998E+00
4	7.000E+00	5.000E+03	5.000E+03	9.995E+00
5	1.000E+01	1.000E+04	1.000E+04	1.999E+01

Temperature Units: eV

Edit Table

Default Temperatures

Densities

INDEX	Electron Densities	Ion Densities	NH/NE Ratio	N(Z1)/N(Z)
1	1.000E+08	0.000E+00	0.000E+00	0.000E+00
2	1.000E+09	0.000E+00	0.000E+00	0.000E+00
3	1.000E+10	0.000E+00	0.000E+00	0.000E+00
4	1.000E+11	0.000E+00	0.000E+00	0.000E+00
5	1.000E+12	0.000E+00	0.000E+00	0.000E+00

Density Units: cm-3

Edit Table

Default Densities

Metastable States

1S2 (1)S (0.0)

Selections

Reaction Selection

Proton Impact Collisions

Scale Proton Impact for Zeff

Enter Z-Effective for Collisions []

Ionisation Rates

Neutral H Charge Exchange

Free Electron Recombination

Edit the processing options data and press Done to proceed

Cancel Done

Te grid specification

Ne grid specification

Designated metastables

activate to select metastables

advanced process control

Populations and line ratio studies (contd.)

- Output options

- » Graphical display of the $F_{j\sigma}^{(exc)}$ as a function of density is allowed.
- » An output file of the $F_{j\sigma}^{(exc)}$, called the 'contour' pass file, can be generated. This file must be created to allow the next step of looking a line ratios.

ADAS205 output - text

ADAS205 OUTPUT OPTIONS

Data File Name: /afs/@cell/u/adas/adas/adf04/adas#2/mom97_ls#he0.dat

Browse Comments

Select output option settings for display: Graphics Text

Text Output Replace Default File Name

File Name : paper1.txt

Contour File Replace Default File Name

File Name : /afs/ipp/home/u/ugs/adas/pass/contour.pa

METPOP File Replace Default File Name

File Name : /afs/ipp/home/u/ugs/adas/pass/metpop.pas

Cancel Done

ADF11 classes selected

output file required for ratio studies

graph of results

show text output choices

ADAS205 output - graphics

ADAS205 OUTPUT OPTIONS

Data File Name: /afs/@cell/u/adas/adas/adf04/adas#2/mom97_ls#he0.dat

Browse Comments

Select output option settings for display: Graphics Text

Graphical Output

Graph Title

Explicit Scaling

X-min : X-max :

Y-min : Y-max :

Graph Temperature

7.000E+00 eV

2.000E+00 eV

3.000E+00 eV

5.000E+00 eV

7.000E+00 eV

Select Device

Post-Script

Post-Script

HP-PCL

HP-GL

Enable Hard Copy Replace

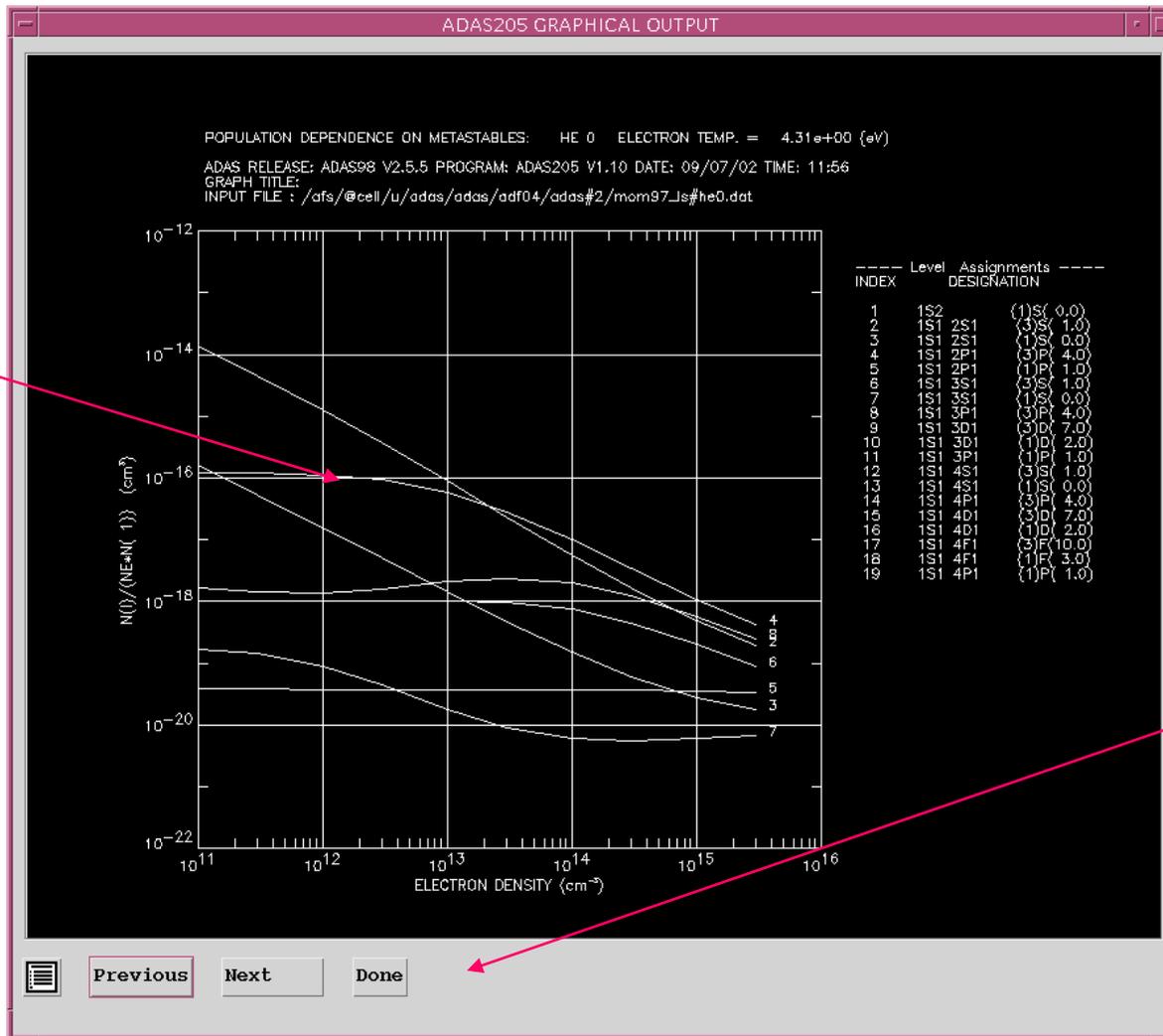
File Name : graph.ps

Cancel Done

show graphic output choices

graphs may be shown at one Te only

ADAS205 graph



excited population graph

Print button is present if graphic file chosen

Setting up lines

- Code ADAS207 is the diagnostic analysis program which allows study of line ratios.
- It needs the 'contour' pass file of populations. It also fetches the specific ion file, of type ADF04, which was used in the population calculation.

Setting up lines (contd.)

The program in deals with two line assemblies which from the numerator and denominator of the line ratio.

The composite emissivity for a line assembly is written as

$$\begin{aligned}\mathcal{E}_G &= \sum_{j \in J_G, i \in I_G} \mathcal{E}_{j \rightarrow i} = \sum_{j \in J_G, i \in I_G} A_{j \rightarrow i} N_j \\ &= \sum_{j \in J_G, i \in I_G} A_{j \rightarrow i} \left(\sum_{\sigma=1}^M F_{j\sigma}^{(exc)} N_e N_\sigma + F_{j1}^{(rec)} N_e N_1^+ + F_{j1}^{(CX)} N_H N_1^+ \right) \\ &= N_e N_1 \sum_{j \in J_G, i \in I_G} A_{j \rightarrow i} \left(\sum_{\sigma=1}^M F_{j\sigma}^{(exc)} \frac{N_\sigma}{N_1} + F_{j1}^{(rec)} \frac{N_1^+}{N_1} + F_{j1}^{(CX)} \frac{N_H}{N_e} \frac{N_1^+}{N_1} \right)\end{aligned}$$

Diagnostic line ratio modelling deals with $\mathcal{E}_{G_1} / \mathcal{E}_{G_2}$

ADAS207 processing

ADAS207 PROCESSING OPTIONS

Contour Passing File Name: /afs/ipp/home/u/ugs/adas/pass/contour.pass

Data File Name: /afs/@cell/u/adas/adas/adf04/adas#2/mom97_1s#he0.dat

ION: HE+ 0 Nuclear Charge: 2 Ionisation Potential: 1.9830D+05 (cm-1)

Transient Conditions		Metastable Levels				Enter ratio for each density:-		
Equilibrium	Met. Level	Index	Index	Designation	Scaling	INDEX	Electron Dens. (cm-3)	-Ratios N+/N(1)
Non-Equilibrium						1	1.000E+08	
Equilibrium		1	1	1S2	{1}S(0.0)	2	1.000E+09	

Lower Wavelength (A): Upper Wavelength (A): Emissivity lower bound (cm3 s-1):

No. of Electron Impact Transitions: 9 No. of Index Energy Levels: 19

Lines for First Composite Assembly					Lines for Second Composite Assembly											
1	5	1S1	2P1	(1)P(1.0)	1M	1S2	(1)S(0.0)	8	8	1S1	3P1	(3)P(4.0)	2	1S1	2S1	(3)S(1.0)

Edit the processing options data and press Done to proceed

advanced use with metastables

advanced use for recombination

restrict the choice of lines

lines in numerator of ratio

lines in denominator of ratio

show line selection list

Displaying line ratios

- Output options
 - » The type of display of the ratio of line assemblies may be chosen.
 - » The contour form on the Te/Ne plane seems to be the favourite.
 - » Crosses on the graph mark the tabular points at which the populations were explicitly evaluated.
 - » The extensive range of controls on the plot scales and contour lines should be used to refine the diagnostic plot.

ADAS207 output

ADAS207 OUTPUT OPTIONS

Contour Passing File Name: /afs/ipp/home/u/ugs/adas/pass/contour.pass
Data File Name: /afs/cell/u/adas/adas/adf04/adas#2/mom97_ls#he0.dat

Spectrum Line Intensity Ratio range: 1.4321D+00 - 2.5429D+01

Graphical Output: Diagnostic Contour Plot of spectrum line ratios on Temp/Density Plane

Diagnostic Contour Plot Title:

Default Contour Scaling

Contour Spacing	Contour Values	Contour Interpolation
<input type="button" value="Logarithmic"/>	<input type="text" value="INDEX"/>	<input type="button" value="Logarithmic"/>
<input type="button" value="Linear"/>	1 0.00E+00	<input type="button" value="Linear"/>
<input type="button" value="Logarithmic"/>	2	<input type="button" value="Logarithmic"/>

Enable Hard Copy Replace

File Name:

Select Device

Text Output Append Replace Default File Name

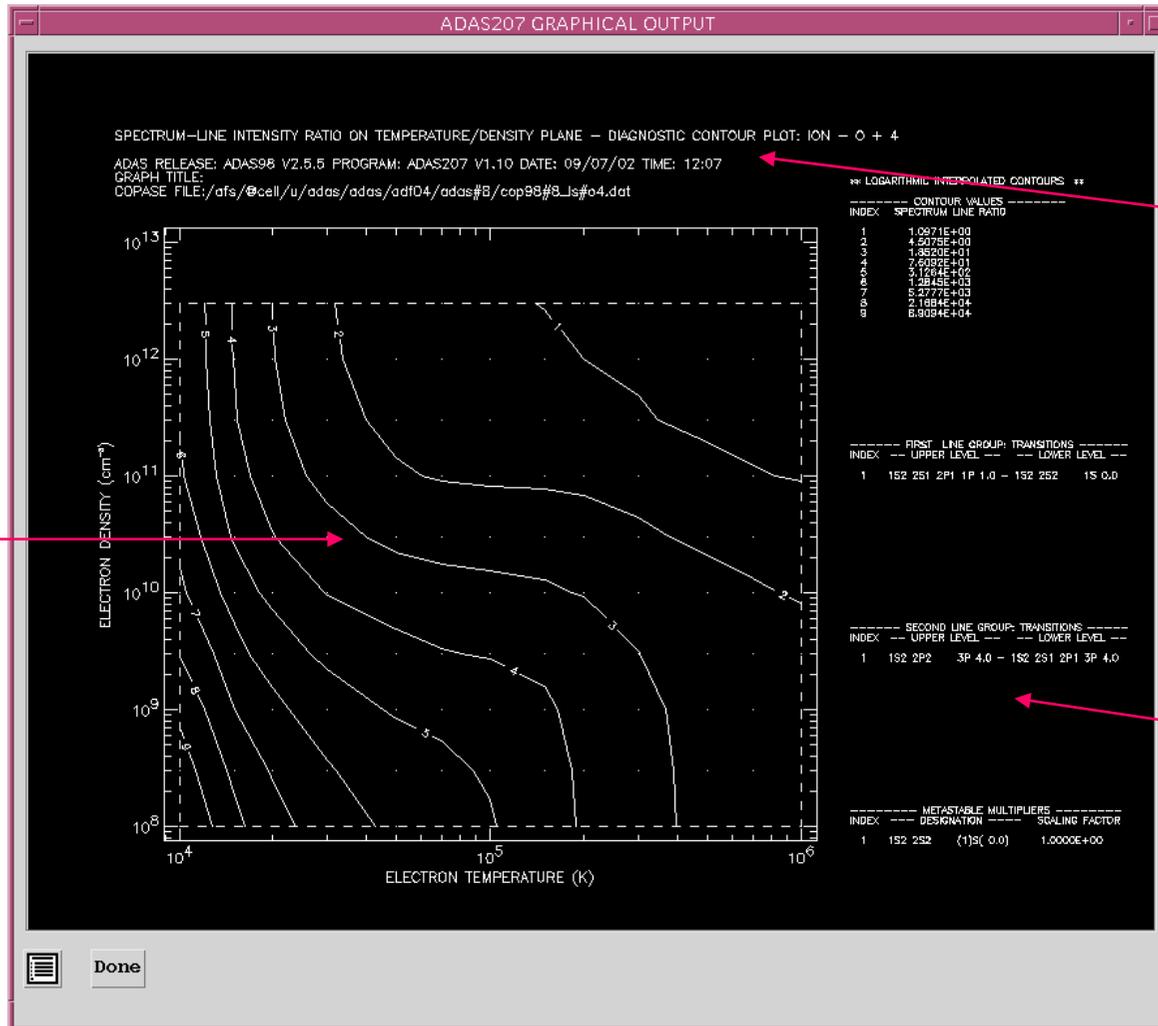
File Name:

controls on contour plotting

select type of plot

usual graph and text output choices

ADAS207 graph



final line ratio contours

unique record of case studied

details of graph presented