

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

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

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

Temperature Units: eV

Density Units: cm-3

Metastable States

1S2	(1)S(0.0)
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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 :

Enable Hard Copy Replace

File Name : graph.ps

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

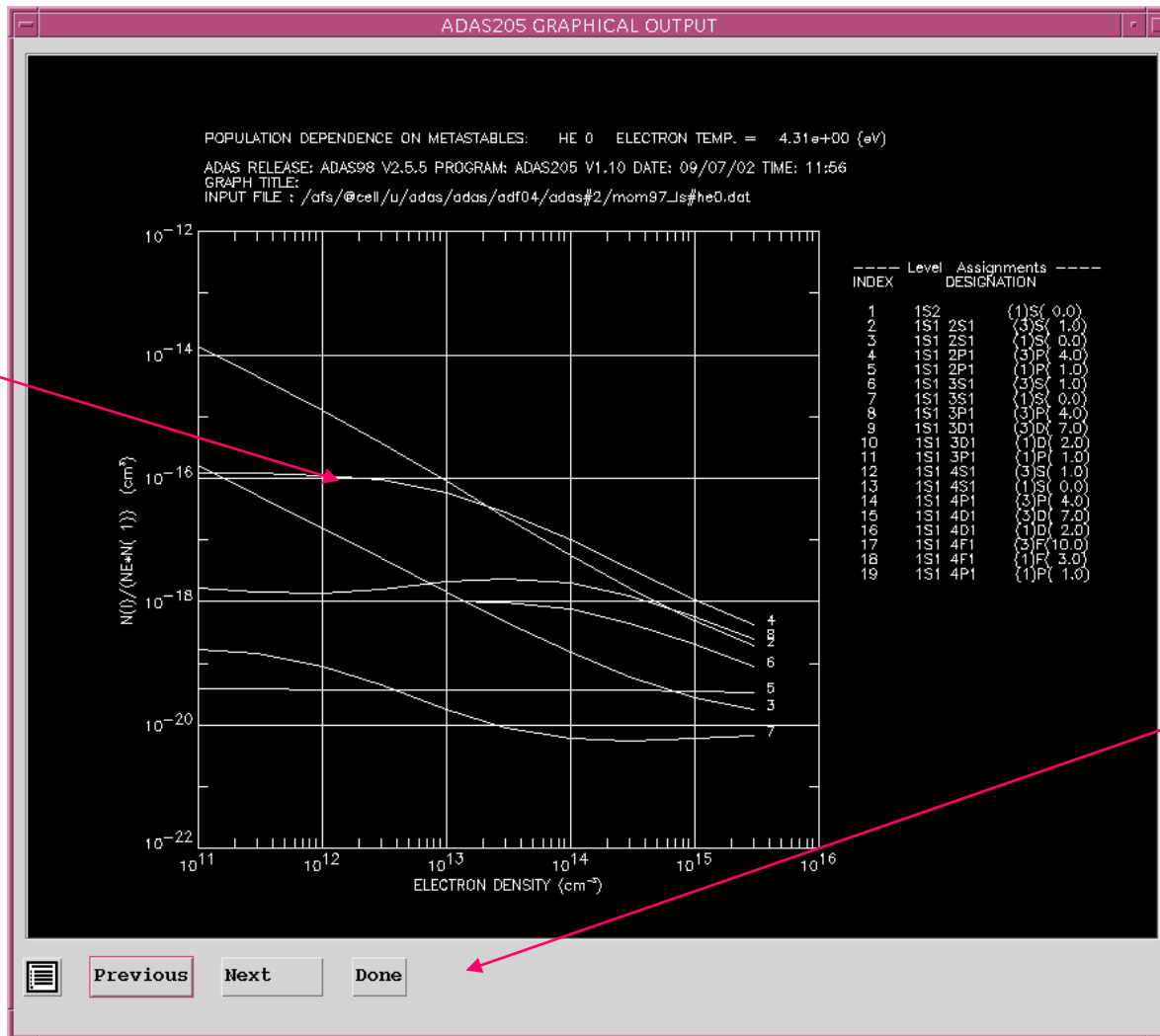
HP-GL

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

ADAS207 line assembly

Lines for First Composite Assembly

┌	1	2	1S2	2S1	2P1	(3)P(4.0)	1M	1S2	2S2	(1)S(0.0)	┌	66	5	1S2	2P2	(1)D(2.0)	3	1S2	2S1	2P1	(1)P(1.0)	┌	175	37	1S2	2S1	5P1	(1)P(1.0)	
✓	2	3	1S2	2S1	2P1	(1)P(1.0)	1M	1S2	2S2	(1)S(0.0)	┌	67	6	1S2	2P2	(1)S(0.0)	3	1S2	2S1	2P1	(1)P(1.0)	┌	183	9	1S2	2S1	3P1	(1)P(1.0)	
┌	5	9	1S2	2S1	3P1	(1)P(1.0)	1M	1S2	2S2	(1)S(0.0)	┌	69	8	1S2	2S1	3S1	(1)S(0.0)	3	1S2	2S1	2P1	(1)P(1.0)	┌	188	14	1S2	2P1	3S1	(1)P(1.0)
┌	6	10	1S2	2S1	3P1	(3)P(4.0)	1M	1S2	2S2	(1)S(0.0)	┌	73	12	1S2	2S1	3D1	(1)D(2.0)	3	1S2	2S1	2P1	(1)P(1.0)	┌	194	26	1S2	2P1	3D1	(1)P(1.0)
┌	10	14	1S2	2P1	3S1	(1)P(1.0)	1M	1S2	2S2	(1)S(0.0)	┌	76	15	1S2	2P1	3P1	(1)P(1.0)	3	1S2	2S1	2P1	(1)P(1.0)	┌	196	30	1S2	2S1	4P1	(1)P(1.0)
┌	16	26	1S2	2P1	3D1	(1)P(1.0)	1M	1S2	2S2	(1)S(0.0)	┌	78	17	1S2	2P1	3P1	(3)S(1.0)	3	1S2	2S1	2P1	(1)P(1.0)	┌	204	10	1S2	2S1	3P1	(3)P(1.0)
┌	18	30	1S2	2S1	4P1	(1)P(1.0)	1M	1S2	2S2	(1)S(0.0)	┌	82	21	1S2	2P1	3P1	(1)D(2.0)	3	1S2	2S1	2P1	(1)P(1.0)	┌	220	29	1S2	2S1	4P1	(3)P(1.0)
┌	21	37	1S2	2S1	5P1	(1)P(1.0)	1M	1S2	2S2	(1)S(0.0)	┌	89	28	1S2	2S1	4S1	(1)S(0.0)	3	1S2	2S1	2P1	(1)P(1.0)	┌	226	38	1S2	2S1	5P1	(3)P(1.0)
┌	26	4	1S2	2P2	(3)P(4.0)	2	1S2	2S1	2P1	(3)P(4.0)	┌	97	36	1S2	2S1	5S1	(1)S(0.0)	3	1S2	2S1	2P1	(1)P(1.0)	┌	235	14	1S2	2P1	3S1	(1)P(1.0)
┌	27	5	1S2	2P2	(1)D(2.0)	2	1S2	2S1	2P1	(3)P(4.0)	┌	109	10	1S2	2S1	3P1	(3)P(4.0)	4	1S2	2P2	(3)P(4.0)	┌	243	30	1S2	2S1	4P1	(1)P(1.0)	
┌	29	7	1S2	2S1	3S1	(3)S(1.0)	2	1S2	2S1	2P1	(3)P(4.0)	┌	121	22	1S2	2P1	3D1	(3)D(7.0)	4	1S2	2P2	(3)P(4.0)	┌	246	37	1S2	2S1	5P1	(1)P(1.0)
┌	30	8	1S2	2S1	3S1	(1)S(0.0)	2	1S2	2S1	2P1	(3)P(4.0)	┌	123	24	1S2	2P1	3D1	(3)P(4.0)	4	1S2	2P2	(3)P(4.0)	┌	261	21	1S2	2P1	3P1	(1)D(2.0)
┌	33	11	1S2	2S1	3D1	(3)D(7.0)	2	1S2	2S1	2P1	(3)P(4.0)	┌	128	29	1S2	2S1	4P1	(3)P(4.0)	4	1S2	2P2	(3)P(4.0)	┌	268	28	1S2	2S1	4S1	(1)S(0.0)
┌	38	16	1S2	2P1	3P1	(3)D(7.0)	2	1S2	2S1	2P1	(3)P(4.0)	┌	146	8	1S2	2S1	3S1	(1)S(0.0)	5	1S2	2P2	(1)D(2.0)	┌	276	36	1S2	2S1	5S1	(1)S(0.0)
┌	39	17	1S2	2P1	3P1	(3)S(1.0)	2	1S2	2S1	2P1	(3)P(4.0)	┌	147	9	1S2	2S1	3P1	(1)P(1.0)	5	1S2	2P2	(1)D(2.0)	┌	289	17	1S2	2P1	3P1	(3)S(1.0)
┌	40	18	1S2	2P1	3P1	(3)P(4.0)	2	1S2	2S1	2P1	(3)P(4.0)	┌	152	14	1S2	2P1	3S1	(1)P(1.0)	5	1S2	2P2	(1)D(2.0)	┌	299	27	1S2	2S1	4S1	(3)S(1.0)
┌	49	27	1S2	2S1	4S1	(3)S(1.0)	2	1S2	2S1	2P1	(3)P(4.0)	┌	158	20	1S2	2P1	3D1	(1)D(2.0)	5	1S2	2P2	(1)D(2.0)	┌	303	31	1S2	2S1	4D1	(3)D(7.0)
┌	53	31	1S2	2S1	4D1	(3)D(7.0)	2	1S2	2S1	2P1	(3)P(4.0)	┌	163	25	1S2	2P1	3D1	(1)F(3.0)	5	1S2	2P2	(1)D(2.0)	┌	307	35	1S2	2S1	5S1	(3)S(1.0)
┌	57	35	1S2	2S1	5S1	(3)S(1.0)	2	1S2	2S1	2P1	(3)P(4.0)	┌	164	26	1S2	2P1	3D1	(1)P(1.0)	5	1S2	2P2	(1)D(2.0)	┌	333	29	1S2	2S1	4P1	(3)P(1.0)
┌	65	4	1S2	2P2	(3)P(4.0)	3	1S2	2S1	2P1	(1)P(1.0)	┌	172	34	1S2	2S1	4F1	(1)F(3.0)	5	1S2	2P2	(1)D(2.0)	┌	337	33	1S2	2S1	4F1	(3)F(3.0)	

activate for lines to be included

Make a maximum of 20 selections

Cancel Done

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

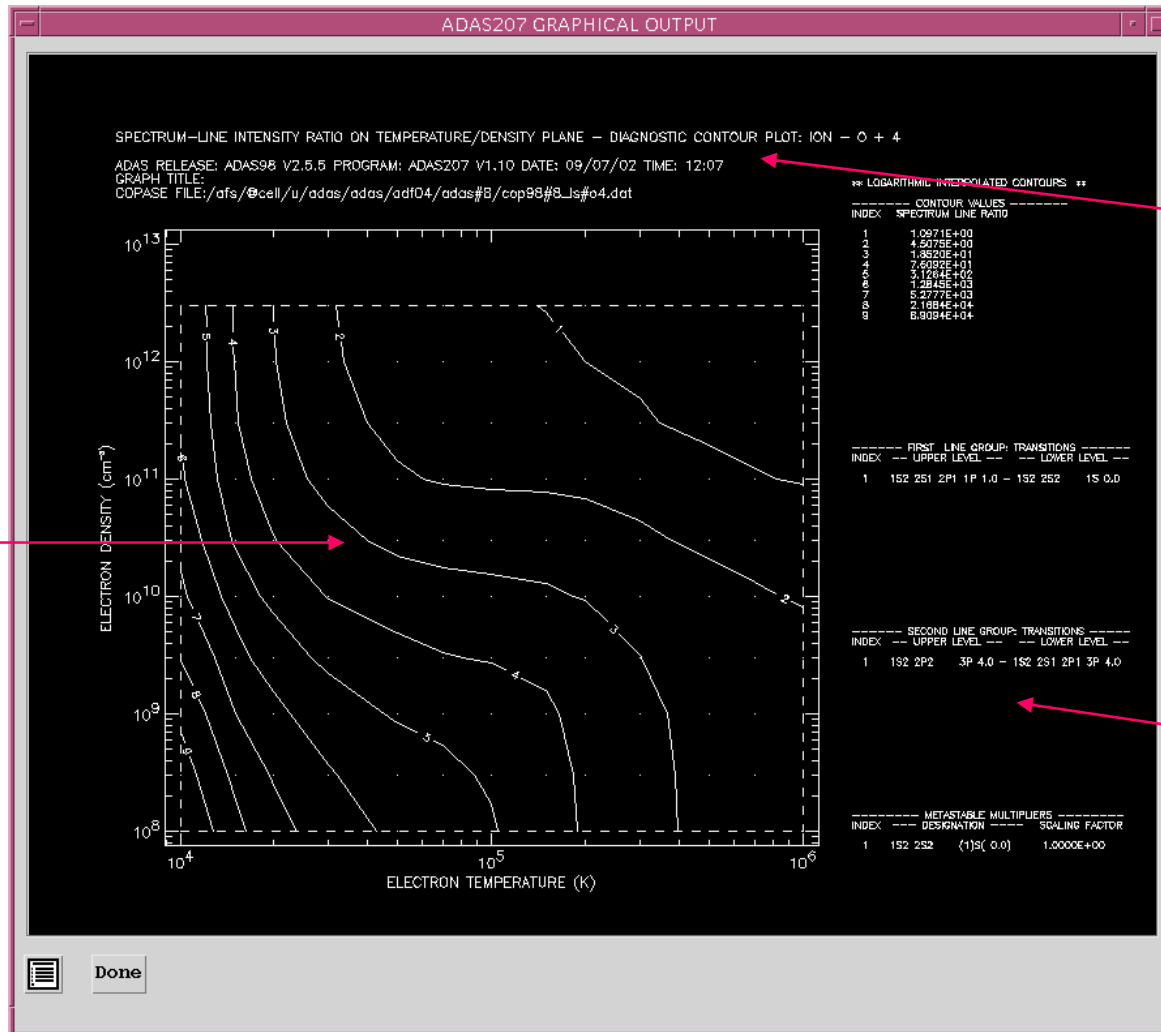
File Name:

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