

3a. The ionisation state of ions in a plasma – part 1

- Effective ionisation and recombination
 - » Data sets of class ADF11
 - » Interrogating ADF11 using ADAS402.
- Equilibrium ionisation balance
 - » Using adas405 to examine the temperature and density dependent equilibrium ionisation balance

Effective ionisation and recombination

- Collisional-radiative modelling
 - » Full modelling for the populations of an ion also gives the collisional-radiative ionisation and recombination coefficients.
 - » In basic CR modelling, the coeffs. give stage to stage connections. In GCR modelling, the coeffs. give connections between metastables within and across ionisation stages.
 - » The data format ADF11 is assigned to Maxwell averaged, T_e and N_e dependent CR and GCR coeffs.

Collisional-radiative theory

Then the quasi-equilibrium statistical balance is

$$\frac{d}{dt} N_1 = \sum_{j \neq 1} C_{1j} N_j + C_{11} N_1 + N_e N_+ r_1$$
$$0 = \sum_{j \neq 1} C_{ij} N_j + C_{i1} N_1 + N_e N_+ r_i \quad , \quad i = 2, \dots$$

In matrix form these become

$$\begin{bmatrix} \frac{d}{dt} N_1 \\ 0 \end{bmatrix} = \begin{bmatrix} C_{11} & C_{1j} \\ C_{i1} & C_{ij} \end{bmatrix} \begin{bmatrix} N_1 \\ N_j \end{bmatrix} + N_e N_+ \begin{bmatrix} r_1 \\ r_i \end{bmatrix}$$

The populations of the excited levels in quasi-equilibrium, N_j^{eq} are given by

$$N_j^{eq} = -N_e N_+ \sum_{i \neq 1} C_{ji}^{-1} r_i - \sum_{i \neq 1} C_{ji}^{-1} C_{i1} N_1$$

Collisional-radiative theory (contd.)

Collisional-dielectronic ionisation coefficient

$$S_{CD} = C_{11} - \sum_{j \neq 1} \sum_{i \neq 1} C_{1j} C_{ji}^{-1} C_{i1}$$

and collisional-dielectronic recombination coefficient

$$\alpha_{CD} = r_1 - \sum_{j \neq 1} \sum_{i \neq 1} C_{1j} C_{ji}^{-1} r_i$$

$$\frac{d}{dt} N_1 = -N_e S_{CD} N_1 + N_e \alpha_{CD} N_+$$

Collisional-radiative theory (generalised)

The ionisation coefficients

$$S_{CD,\sigma \rightarrow \nu} = (S_{\nu\sigma} - \sum_{j=1}^O S_{\nu j} \sum_{i=1}^O C_{ji}^{-1} C_{i\sigma})$$

the free electron recombination coefficients

$$\alpha_{CD,\nu' \rightarrow \rho} = (R_{\rho\nu'} + \sum_{j=1}^O C_{\rho j} \sum_{i=1}^O C_{ji}^{-1} R_{i\nu'})$$

the charge exchange recombination coefficients

$$C_{CD,\nu' \rightarrow \rho} = (Q_{\rho\nu'} + \sum_{j=1}^O C_{\rho j} \sum_{i=1}^O C_{ji}^{-1} Q_{i\nu'})$$

the metastable cross-coupling coefficients

$$X_{CD,\sigma \rightarrow \rho} = (C_{\rho\sigma} - \sum_{j=1}^O C_{\rho j} \sum_{i=1}^O C_{ji}^{-1} C_{i\sigma}) / N_e$$

and the parent metastable cross-coupling coefficients

$$Q_{CD,\nu' \rightarrow \nu} = \sum_{j=1}^O S_{\nu j} \sum_{i=1}^O C_{ji}^{-1} R_{i\nu'} \quad e$$

ADF11 iso-nuclear master file classes

Mnemonic	Class	Data prefix
ACD	Coll.-diel. recom. coefft.	R & U (or none)
SCD	Coll.-diel. ionis. coefft.	R & U (or none)
CCD	Coll.-rad. charge exch. coefft.	R & U (or none)
PRB	Coll.-diel. recom./brems. power coefft.	R & U (or none)
PRC	Coll.-rad. charge exch. recom. power coefft.	R & U (or none)
QCD	Coll.-rad. metastable cross coupling coefft.	R
XCD	Coll.-diel. parent meta. cross-coupling coefft.	R
PLT	Coll.-rad. excit. line power coefft.	R & U (or none)
PLS	Coll.-rad. specific line excit. power coefft.	R & U (or none)

ADF11 iso-nuclear master file layout (standard- unresolved)

The diagram illustrates the layout of the ADF11 iso-nuclear master file. Red boxes and arrows highlight key fields:

- nuclear charge**: Points to the first column of the data grid.
- Log Ne (cm-3)**: Points to the second column of the data grid.
- Log(Te) (eV)**: Points to the third column of the data grid.
- Ion Charge+1**: Points to the header line for the first ionization state (Z=1).
- Log(ACD) (cm3 s-1)**: Points to the final column of the data grid.

2	13	51	1	2	/HELIUM	/ ARNAUD-ROTHEN(NE SCALED)	9/11/90
4.00000	5.00000	6.00000	7.00000	8.00000	9.00000	10.00000	11.00000
12.00000	13.00000	14.00000	15.00000	16.00000			
-0.06466	0.03533	0.13534	0.23535	0.33534	0.43534	0.53534	0.63534
0.73534	0.83534	0.93534	1.03533	1.13534	1.23535	1.33534	1.43534
1.53534	1.63534	1.73534	1.83534	1.93534	2.03533	2.13534	2.23535
2.33534	2.43534	2.53534	2.63534	2.73534	2.83534	2.93534	3.03533
3.13534	3.23535	3.33534	3.43534	3.53534	3.63534	3.73534	3.83534
3.93534	4.03533	4.13534	4.23535	4.33534	4.43534	4.53534	4.63534
4.73534	4.83534	4.93534					
-----/ Z1= 1 / DATE= 09/11/90							
-21.02274	-21.02448	-21.01428	-20.98969	-20.97136	-20.98573	-21.03465	-21.02173
-20.82594	-20.37585	-19.79799	-19.26837	-18.92128			
.							
-8.26043	-8.26360	-8.25394	-8.22642	-8.19355	-8.17223	-8.17398	-8.18895
-8.20194	-8.20187	-8.19411	-8.18816	-8.19132			
-----/ Z1= 2 / DATE= 09/11/90							
-36.43890	-36.43925	-36.43584	-36.42578	-36.40593	-36.37265	-36.31938	-36.23863
-36.10640	-35.80753	-35.19548	-34.17990	-32.98088			
.							
-9.04721	-9.04720	-9.04707	-9.04648	-9.04495	-9.04234	-9.04021	-9.04073
-9.04481	-9.04660	-9.03791	-9.01206	-8.97073			

ADF11 iso-nuclear master file layout (partial- resolved)

4	26	35	1	4	/BERYLLIUM	/DICKSON ET AL 1992		
2	1	2	1	1				
10.00000	10.20003	10.40002	10.59999	10.80003	11.00000	11.20003	11.40002	
11.59999	11.80003	12.00000	12.20003	12.40002	12.59999	12.80003	13.00000	
13.20003	13.40002	13.59999	13.80003	14.00000	14.20003	14.40002	14.59999	
14.80003	15.00000							
0.00015	0.10016	0.20015	0.30015	0.40015	0.50015	0.60015	0.70015	
0.80015	0.90015	1.00015	1.10016	1.20015	1.30015	1.40015	1.50015	
1.60015	1.70015	1.80015	1.90015	2.00015	2.20015	2.40015	2.60015	
2.80015	3.00015	3.20015	3.40015	3.60015	3.80015	4.00015	4.20015	
4.40015	4.60015	4.70015						
/ IPRT= 1 / IGRD= 1 /-----/ Z1= 1 / DATE= 16/11/93								
-11.57681	-11.55926	-11.53861	-11.51437	-11.48604	-11.45315	-11.41518	-11.37166	
-11.32210	-11.26598	-11.20285	-11.13244	-11.05561	-10.97341	-10.88689	-10.79719	
-10.70532	-10.61241	-10.51952	-10.42769	-10.33806	-10.25165	-10.16957	-10.09290	
-10.02268	-9.96003							
.								
-7.20840	-7.21561	-7.22233	-7.22831	-7.23329	-7.23700	-7.23918	-7.23957	
-7.23791	-7.23394	-7.22740	-7.21811	-7.20627	-7.19216	-7.17605	-7.15822	
-7.13895	-7.11852	-7.09722	-7.07531	-7.05308	-7.03080	-7.00876	-6.98724	
-6.96650	-6.94684							
-6.85348	-6.85100							
.								
.								
.								
/ IPRT= 1 / IGRD= 1 /-----/ Z1= 4 / DATE= 16/11/93								
-74.00000	-74.00000	-74.00000	-74.00000	-74.00000	-74.00000	-74.00000	-74.00000	
-74.00000	-74.00000	-74.00000	-74.00000	-74.00000	-74.00000	-74.00000	-74.00000	
-74.00000	-74.00000	-74.00000	-74.00000	-74.00000	-74.00000	-74.00000	-74.00000	
-74.00000	-74.00000							

Connection vector

Metastable

Parent metastable

ADF11 (contd.)

- ADF11 year numbers
 - » baseline CR data are assigned the '89' year number. They are stage to stage data and available for very many elements.
 - » GCR data on the restricted Te/Ne grid are assigned the '93' year number. They are LS-coupled, metastable resolved data for selected light elements.
 - » GCR data on the extended Te/Ne grid are assigned the '96' year number. They are LS-coupled, metastable resolved data for selected light elements. CR data 'condensed' from the GCR data is also provided.
 - » Other approximations, eg. Arnaud/Rothenflug. are available but sub-categories are generally incomplete.

appxa-11.pdf

ADF11: iso-nuclear master files

Isomuclear master file data. Formatting conventions and variable storage are given below.

Utilising subroutines :

ADAS405 ADAS406

Formatted files to ADF11 specification :

Database Status	Date = March 17, 2005	Data type = isomuclear master file	Data root = /.../ada/ada/ADF11/		
<i>Element</i>	<i>Classes</i>	<i>Database</i>	<i>Comments</i>	<i>Resolution</i>	<i>Quality</i>
Hydrogen	sof, soe, cod, pch, pro, plh, plb	/class089/class089b.be.dat	JET base line	unresolved	low
Hydrogen	sof, soe, qcd, xcd, pch, plh	/class093/class093r.be.dat	ADAS208, o-r	resolved	high
Hydrogen	sof, soe, cod, pch, plh, pro	/class096/class096r.be.dat	ADAS208, o-r	unresolved	high
Helium	sof, soe	/class074/class074r.be.dat	Suzanne, o-r	unresolved	medium
Helium	sof, soe	/class085/class085r.be.dat	Arnold & Rothberg *HPS o-r	unresolved	medium
Helium	sof, soe, cod, pch, pro, plh, plb	/class089/class089r.be.dat	JET base line	unresolved	low
Helium	sof, soe, qcd, xcd, pch, plh	/class093/class093r.be.dat	ADAS208, o-r	resolved	high
Helium	sof, soe, cod, pch, plh, pro	/class096/class096r.be.dat	ADAS208, o-r	unresolved	high
Helium	sof, soe, cod, qcd, xcd, pch, plh, pro	/class096/class096r.be.dat	ADAS208, o-r	resolved	high
Lithium	sof, soe, cod, pch, pro, plh, plb	/class089/class089r.be.dat	JET base line	unresolved	low
Lithium	sof, soe, cod, pch, plh, pro	/class096/class096r.be.dat	ADAS208, o-r	unresolved	high
Lithium	sof, soe, cod, qcd, xcd, pch, plh, pro	/class096/class096r.be.dat	ADAS208, o-r	resolved	high
Beryllium	sof, soe, cod, pch, pro, plh, plb	/class089/class089r.be.dat	JET base line	unresolved	low
Beryllium	sof, soe, qcd, xcd, pch, plh	/class093/class093r.be.dat	ADAS208, o-r	resolved	high

ADAS402 Input

ADAS 402 INPUT

Data Root

Central Data User Data Edit Path Name

Data File

- ..
- acd89_ar.dat
- acd89_b.dat
- acd89_be.dat
- acd89_c.dat

Search for iso-nuclear master file from details:-

Select iso-nuclear master collisional-dielectronic class :

Radiated power filter (blank for none) :

Member prefix (blank for none) :

Year of data : Default year (if required) :

Isonuclear element symbol :

Type of master files : Specify partial type code :

Parent index Recombined ion index

Direct data set selection

Search method

Select year and default year

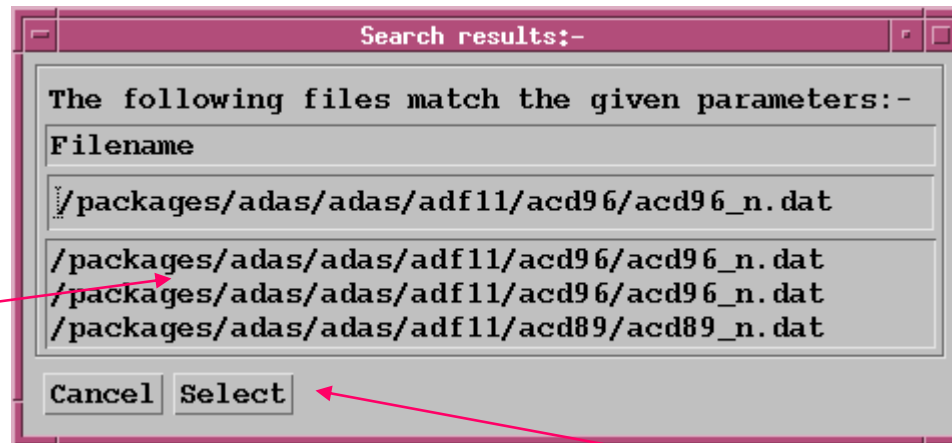
Standard or partial and resolution

Select data classes required

Select element

Search

ADAS402 Search



Choose
file

Select

ADAS402 Processing

ADAS402 PROCESSING OPTIONS

Title for Run []

Data File Name: /packages/adas/adas/adf11/acd89/acd89_n.dat

Browse Comments

Data file information:-

Class : ACD - Recombination coefficients
Year : 89
File type : Unknown

Please input the following charge information:-

Element nuclear charge Z0 : 7
Recombining ion charge Z1 : 5
Recombined ion charge Z : 5

Polynomial Fitting

Fit Polynomial Value % : 5

Select Output Temperature/Density pairs

Temperature & Density Values

	Temperature		Density	
INDEX	Output	Input	Output	Input
1	1.160E+04	1.160E+04	2.512E+13	1.000E+10
2	1.460E+04	1.460E+04	2.512E+13	1.585E+10
3	1.838E+04	1.838E+04	2.512E+13	2.512E+10
4	2.314E+04	2.314E+04	2.512E+13	3.981E+10

Temperature Units: Kelvin Density Units : cm⁻³

Edit Table

Default Temperature/Density Values

Approximate density to be extracted:

1.00000 cm⁻³

(Dataset closest to the above value will be selected)

Edit the processing options data and press Done to proceed

Cancel Done

ion required

Data class selected

Polynomial fit

Specify Te/Ne pair values

ADAS402 Output

ADAS402 OUTPUT OPTIONS

Data File Name: /packages/adas/adas/adf11/acd89/acd89_n.dat

Graphical Output

Graph Title

Explicit Scaling

X-min : X-max :

Y-min : Y-max :

Select Device

Post-Script
HP-PCL
HP-GL

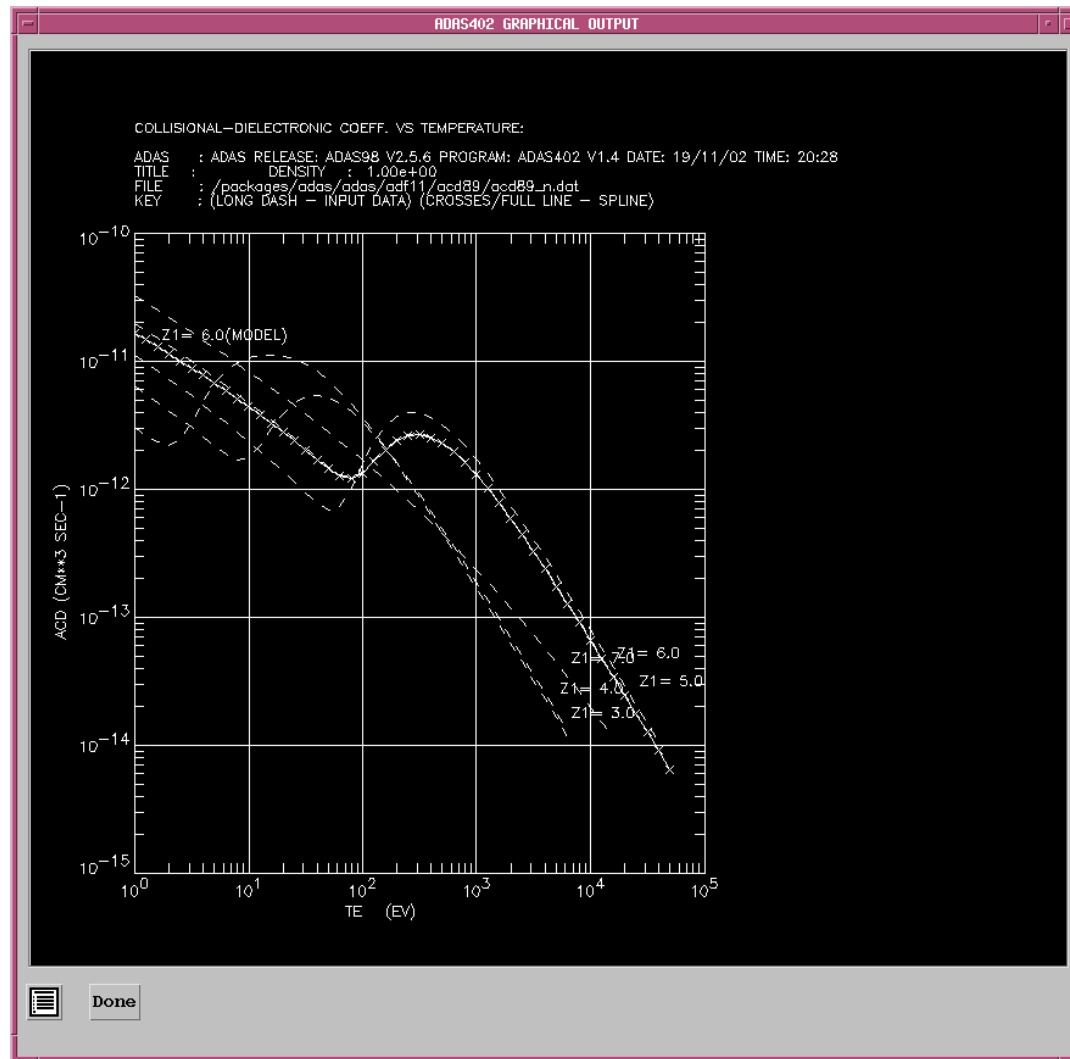
Enable Hard Copy Replace

File Name :

Text Output Replace

File Name :

ADAS402 Graph



Equilibrium ionisation balance

- The ionisation balance is often a weakness in the theoretical input.
- Code ADAS405 is provided for examining and contrasting ionisation balances as a function of T_e and N_e .
- It has also capability for examining radiated power and the ingredients of $G(T_e(h), N_e(h))$ functions

ADAS405 Input

ADAS 405 INPUT

Enter details of the iso-nuclear master files to be analysed:-

Select iso-nuclear master collisional-dielectronic classes :

Radiated power filter (blank for none) :

Member prefix (blank for none) :

Select directory branch :

Year of data : Default year (if required) :

Isonuclear element symbol :

Type of master files : Specify partial type code :

Input Line and Analysis Selection File:-

Data Root

Edit Path Name

Data File

-
-
-
-
-
-

Default year

Select data classes required

Central data

Select by element and year

NULL script

Resolution level of data

Availability of ADF11 data

ADAS405 INPUT

Class selection and file availability:-

Class	Year	Element	Member		Type	USER DATA		DEFAULT DATA (96)	
			Prefix	Filter		Selected	Available	Used	Available
acd	96	c			RPartial	YES	YES	no	YES
scd	96	c			RPartial	YES	YES	no	YES
ccd	96	c			RPartial	no	YES	no	YES
prb	96	c			RPartial	YES	YES	no	YES
prc	96	c			RPartial	no	YES	no	YES
qcd	96	c			RPartial	YES	YES	no	YES
xcd	96	c			RPartial	YES	YES	no	YES
plt	96	c			RPartial	YES	YES	no	YES

All requested files available from user data sets.

OK

Data set information

Data obtained from primary year

Data obtained from default year

ADAS405 processing

ADAS405 PROCESSING OPTIONS

Title for Run

Script file: /afs/@cell/u/adas/adas/scripts405/NULL

Data file information:-

Selected master file element: C

Selected master classes: ACD, SCD, PRB, QCD, XCD, PLT

Enter isotope information:-

Enter element isotope mass number (amu) :

Enter hydrogen isotope mass number (amu) :

Select spectral line for analysis:-

There is no selected script file.

Enter Output Temperature/Density data

INDEX	Temperatures		Densities	
	Electron Output values	Hydrogen Output values	Electron Output values	Hydrogen Output values
1	1.000E-01	1.000E-01	2.000E+13	1.000E+10
2	2.000E-01	2.000E-01	2.000E+13	1.000E+10
3	3.000E-01	3.000E-01	2.000E+13	1.000E+10
4	5.000E-01	5.000E-01	2.000E+13	1.000E+10

Temperature Units: eV Density Units : cm⁻³

ADF11 classes selected

No script file present - no lines for selection

Set element parameters

Select Te and Ne pairs

ADAS405 Output

ADAS405 OUTPUT OPTIONS

Script file: /afs/cell/u/adas/adas/scripts405/NULL [Browse](#) [Comments](#)

Graphical output

Graph Title:

Fractional abundance plot
 Power function plot
 Contribution function plot

Fractional abundance plot:-

Explicit scaling

X-min: X-max:
Y-min: Y-max:

Enable Hard Copy Replace

Select Device

File Name : [Post-Script](#)
[Post-Script](#)
HP-PCL
HP-GL

Text Output Replace [Default File Name](#)

File Name :

GCF : G(Te) Passing File Replace [Default File Name](#)

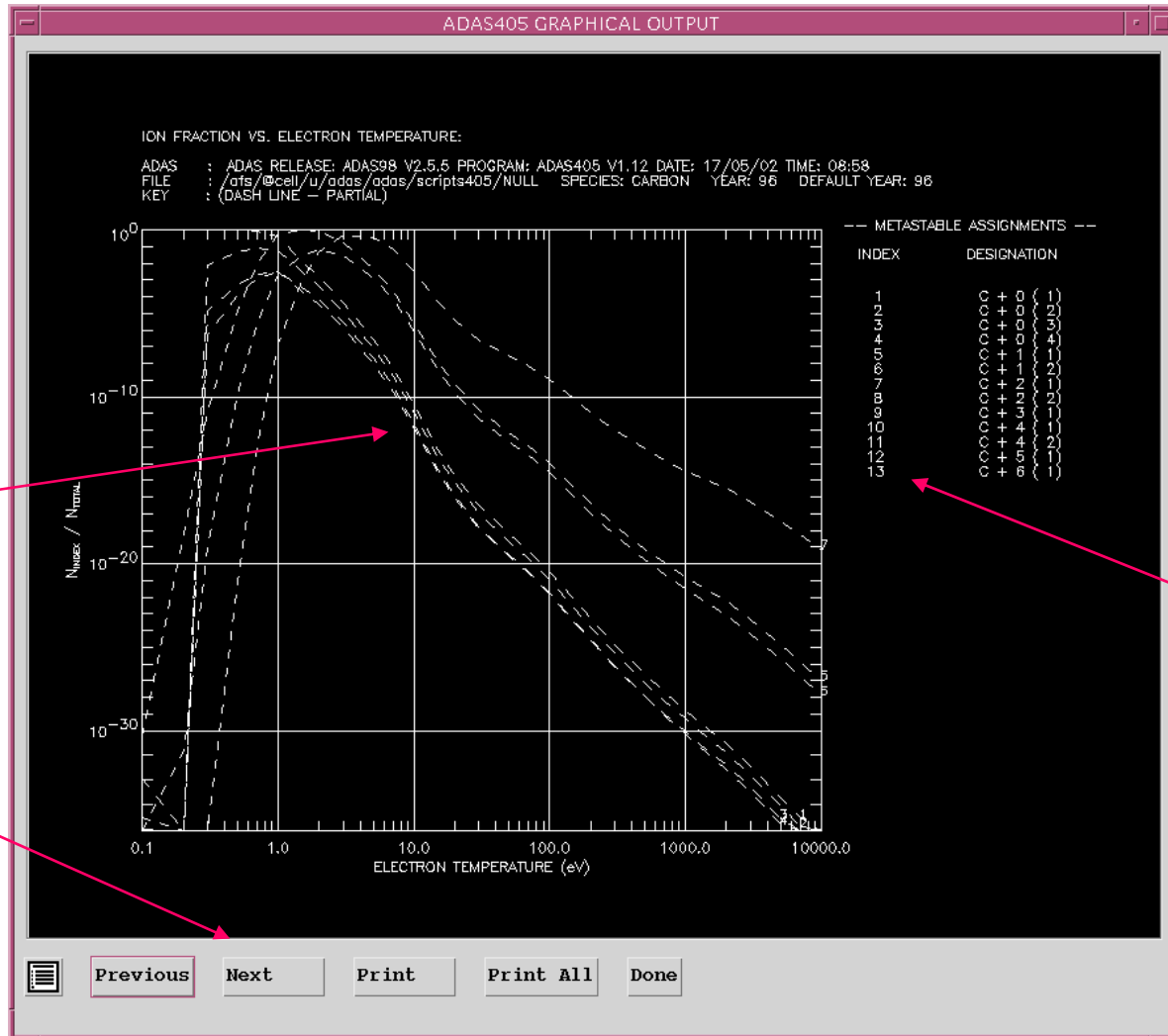
File Name :

[Cancel](#) [Done](#)

Choice of graphs

No GCF output since no script

ADAS405 fractional abundance graph

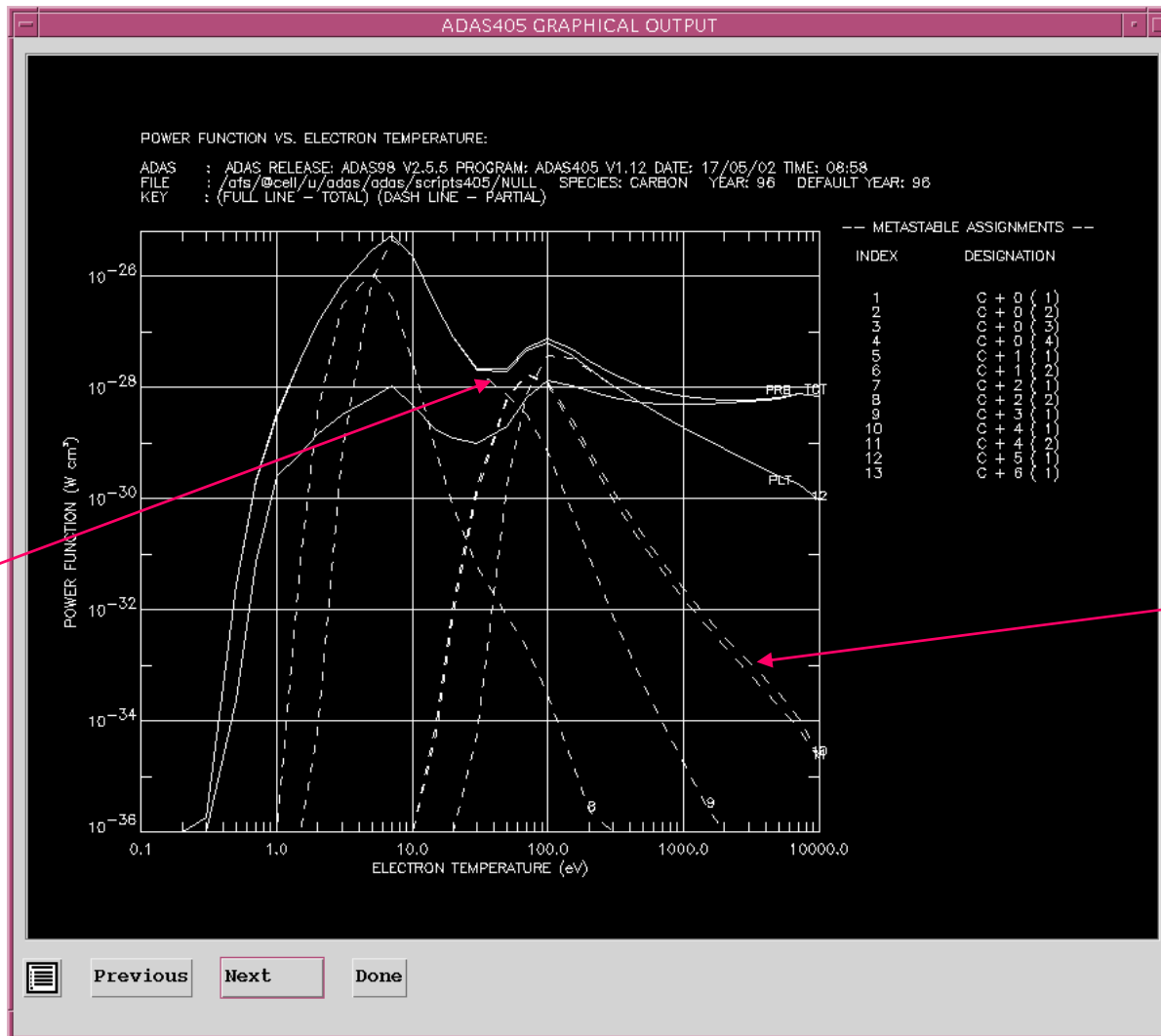


Fractional abundances - seven curves / screen

Page through graphs

Index - note metastable resolved case

ADAS405 power graph

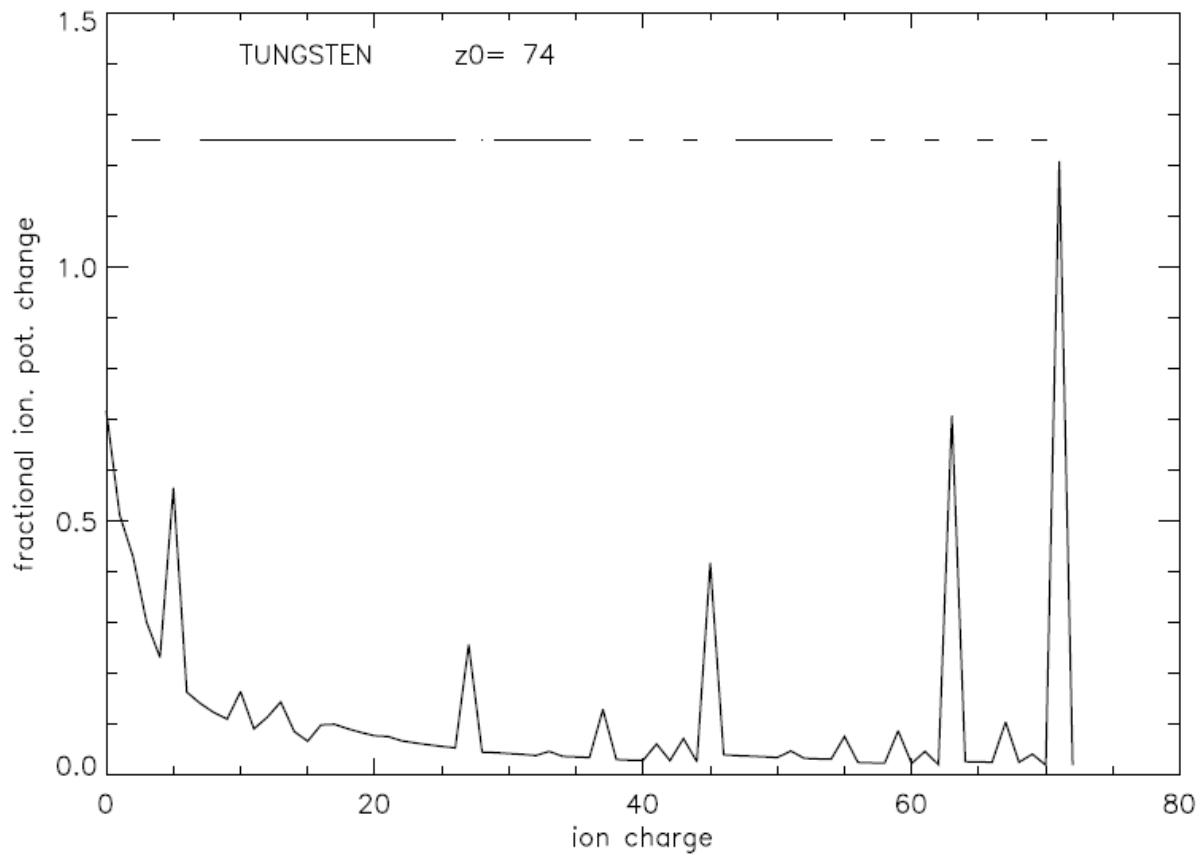


Total power and components

Metastable contributions to total

Superstages and partitions

- Another IDL procedure: [preview_natural_partition.pro](#)



Natural partition ionisation balance for tungsten

