

# The ionisation state of ions in a plasma

## part 1

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- Effective ionisation and recombination coefficients
  - » 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

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- 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 coefficients give stage to stage connections. In GCR modelling, the coefficients 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 coefficients.

# Collisional-radiative theory

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Then the quasi-equilibrium statistical balance is

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

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.)

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

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

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

# Collisional-radiative theory (generalised)

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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

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Mnemonic	Class	Type
ACD	Coll.-diel. recom. coefft.	R & U
SCD	Coll.-diel. ionis. coefft.	R & U
CCD	Coll.-rad. charge exch. coefft.	R & U
PRB	Coll.-diel. recom./brems. power coefft.	R & U
PRC	Coll.-rad. charge exch. recom. power coefft.	R & U
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
PLS	Coll.-rad. specific line excit. power coefft.	R & U

# ADF11 iso-nuclear master file layout of the unresolved type

nuclear charge		LogNe (cm <sup>-3</sup> )		Log(Te) (eV)		Ion Charge+1		Log(ACD) (cm <sup>3</sup> s <sup>-1</sup> )	
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 of the resolved type

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
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
1.60015	1.70015	1.80015	1.90015	2.00015	2.20015	2.40015	2.60015	2.80015	3.00015
4.40015	4.60015	4.70015	3.40015	3.60015	3.80015	4.00015	4.20015	4.40015	4.60015
-----/ 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
-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
-7.13895	-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	-74.00000	-74.00000	-74.00000	-74.00000
-74.00000	-74.00000								

Connection vector

Metastable

Parent metastable



# ADF11 and date mnemonics

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- 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 ('85'), 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/		
Element	Classes	Datasets	Comments	Resolution	Quality
Hydrogen	sof, sof, ood, pch, pre, plh, plh	/class089/class089h.dat	JET base line	unresolved	low
Hydrogen	sof, sof, qod, xod, pch, plh	/class093e/class093e_h.dat	ADAS208, c-e	resolved	high
Hydrogen	sof, sof, ood, pch, plh, pre	/class095/class095_h.dat	ADAS208, c-e	unresolved	high
Helium	sof, sof	/class074/class074_h.dat	Sturman, c-e	unresolved	medium
Helium	sof, sof	/class085/class085_h.dat	Arnold & Rothenflig *HPS c-e	unresolved	medium
Helium	sof, sof, ood, pch, pre, plh, plh	/class089/class089_h.dat	JET base line	unresolved	low
Helium	sof, sof, qod, xod, pch, plh	/class093e/class093e_h.dat	ADAS208, c-e	resolved	high
Helium	sof, sof, ood, pch, plh, pre	/class095/class095_h.dat	ADAS208, c-e	unresolved	high
Helium	sof, sof, ood, qod, xod, pch, plh, pre	/class096/class096_h.dat	ADAS208, c-e	resolved	high
Lithium	sof, sof, ood, pch, pre, plh, plh	/class089/class089_l.dat	JET base line	unresolved	low
Lithium	sof, sof, ood, pch, plh, pre	/class095/class095_l.dat	ADAS208, c-e	unresolved	high
Lithium	sof, sof, ood, qod, xod, pch, plh, pre	/class096/class096_l.dat	ADAS208, c-e	resolved	high
Beryllium	sof, sof, ood, pch, pre, plh, plh	/class089/class089_b.dat	JET base line	unresolved	low
Beryllium	sof, sof, qod, xod, pch, plh	/class093e/class093e_b.dat	ADAS208, c-e	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 :  Standard  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

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The following files match the given parameters:-

Filename
./packages/adas/adas/adf11/acd96/acd96_n.dat
/packages/adas/adas/adf11/acd96/acd96_n.dat
/packages/adas/adas/adf11/acd96/acd96_n.dat
/packages/adas/adas/adf11/acd96/acd96_n.dat
/packages/adas/adas/adf11/acd89/acd89_n.dat

Cancel Select

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

INDEX	Temperature		Density	
	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<sup>-3</sup>

Edit Table

Default Temperature/Density Values

Approximate density to be extracted:  
1.00000 cm<sup>-3</sup>  
(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

Specify Te/Ne pair values

Polynomial fit

# ADAS402 Output

ADAS402 OUTPUT OPTIONS

Data File Name: /packages/adas/adas/adf11/acd89/acd89\_n.dat

Browse Comments

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

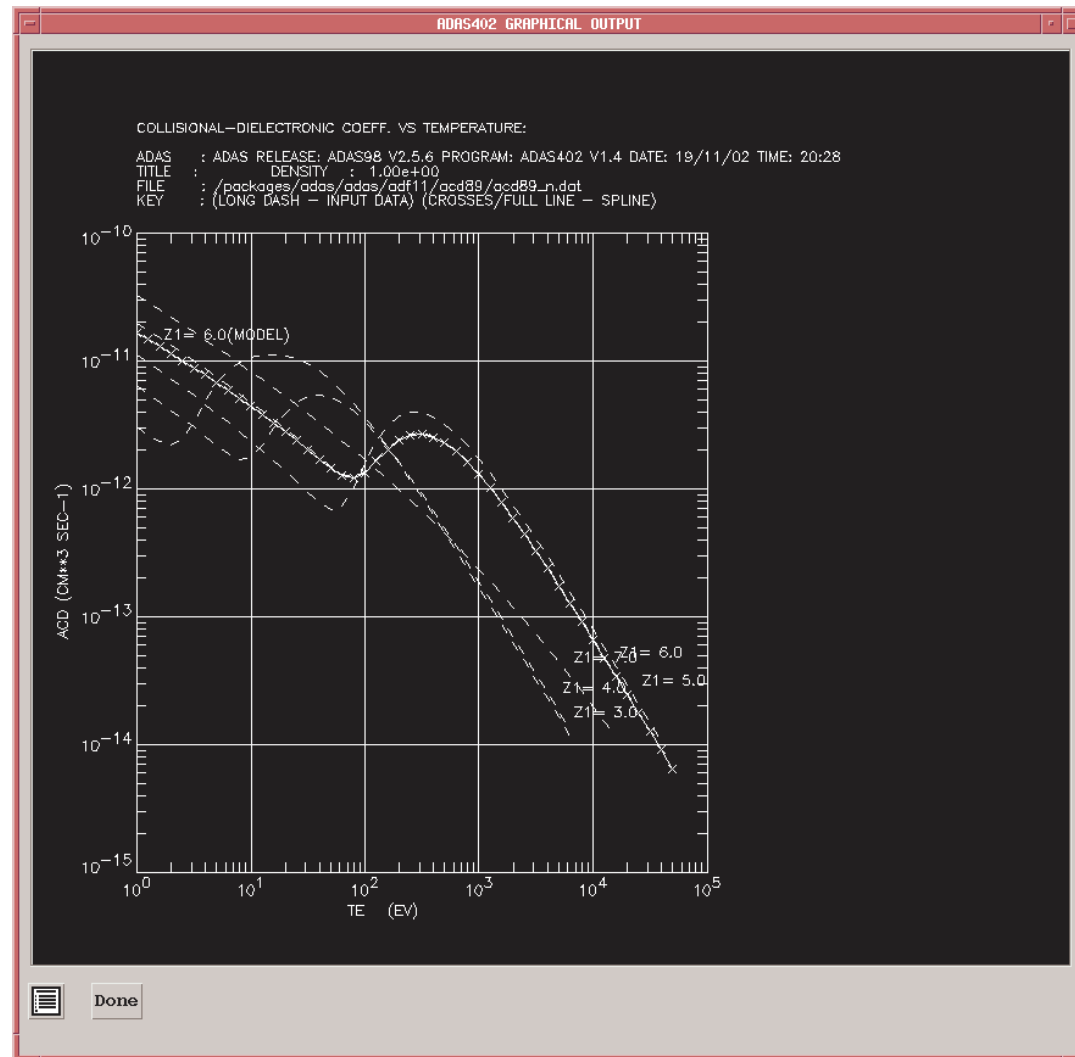
File Name :

Text Output  Replace

File Name :

 Cancel Done

# ADAS402 Graph



# Equilibrium ionisation balance

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- 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  $G(T_e, N_e)$  functions



# ADAS405 Input

The screenshot shows the ADAS 405 INPUT dialog box with the following fields and annotations:

- Select iso-nuclear master collisional-dielectronic classes**:  (Annotation: Select data classes required)
- Radiated power filter (blank for none)**:
- Member prefix (blank for none)**:
- Select directory branch**:  (Annotation: Central data)
- Year of data**:  (Annotation: Default year)
- Default year (if required)**:
- Isonuclear element symbol**:  (Annotation: Select by element and year)
- Type of master files**:  **Specify partial type code**:  (Annotation: Resolution level of data)
- Display data set availability**:
- Input Line and Analysis Selection File:-**
  - Data Root**:
  - Edit Path Name**
  - Data File**:  (Annotation: NULL script)
  - (Annotation: Resolution level of data)
  - (Annotation: Resolution level of data)
  - (Annotation: Resolution level of data)
  - (Annotation: Resolution level of data)
  - (Annotation: Resolution level of data)
- Buttons**:

# Availability of ADF11 data

ADAS405 INPUT

Class selection and file availability:-

Class	Year	Element	Member Power		USER DATA		DEFAULT DATA (96)		
			Prefix	Filter	Type	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<sup>-3</sup>

ADF11 classes selected

No script file present-  
no lines for selection

Set element parameters

Select Te and Ne pairs

# ADAS405 Output

Choice of graphs

No GCF output since no script

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

File Name:

Select Device  
Post-Script  
HP-PCL  
HP-GL

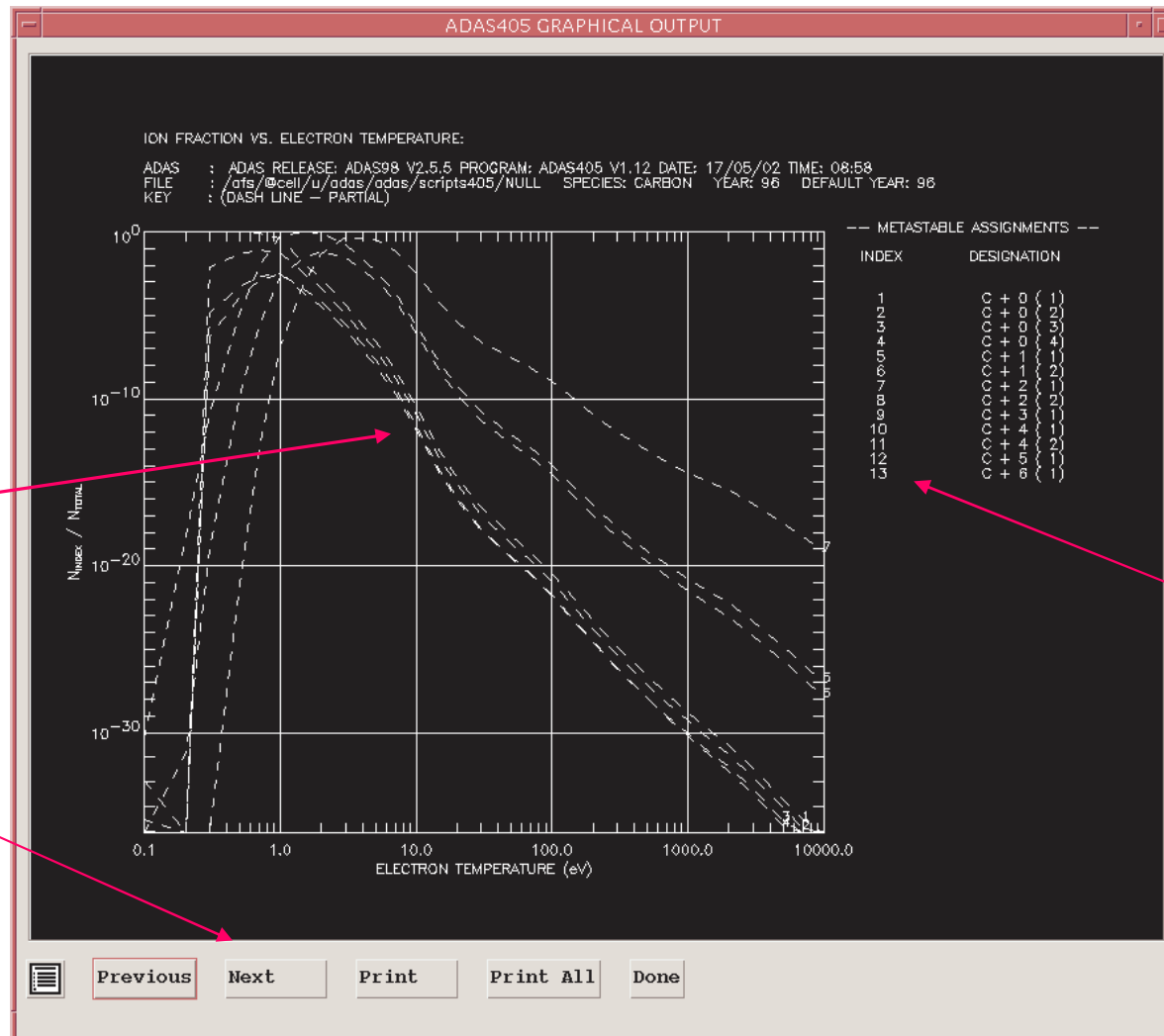
Text Output  Replace [Default File Name](#)

File Name:

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

File Name:

# ADAS405 fractional abundance graph

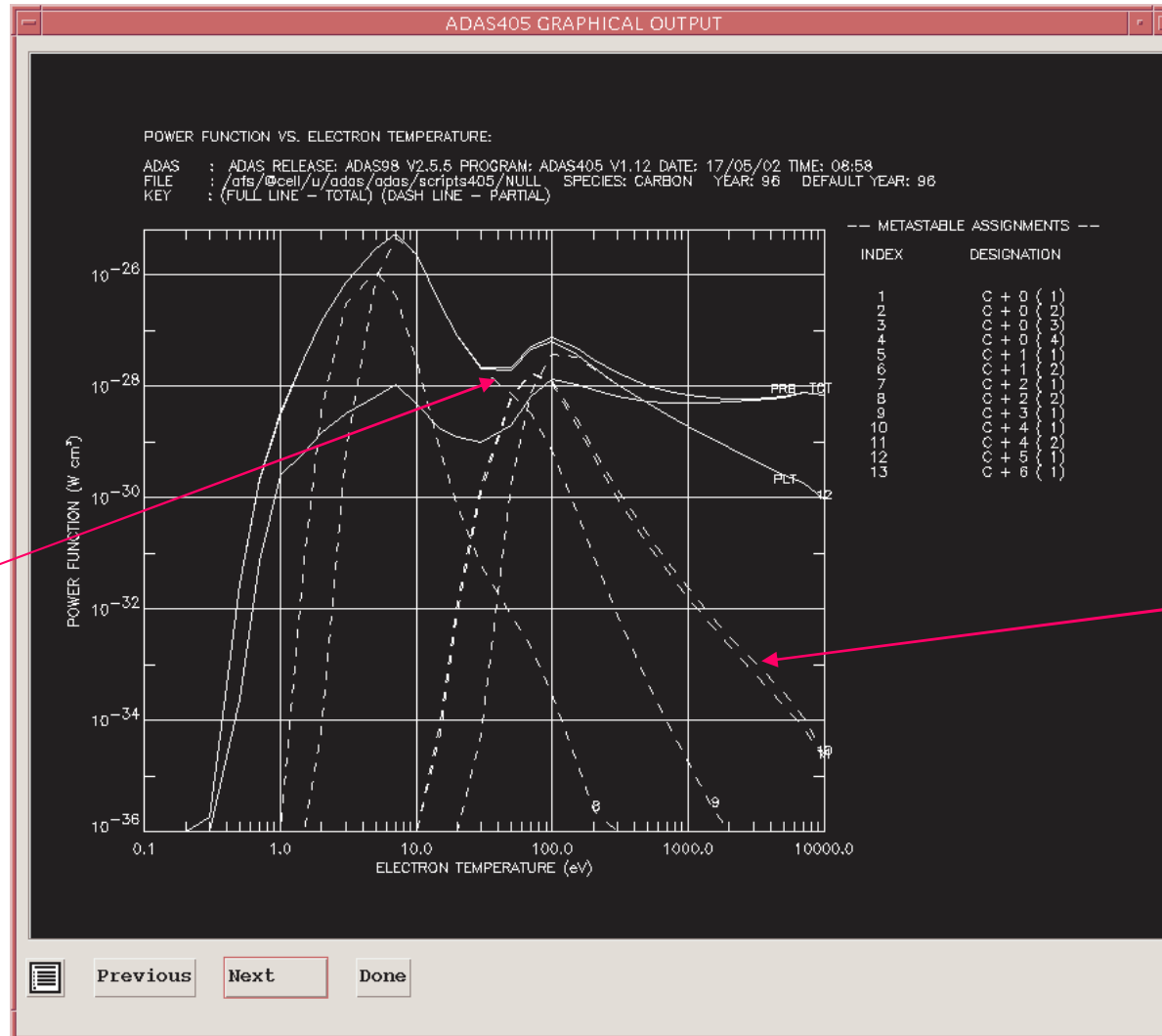


Fractional abundances - seven curves / screen

Page through graphs

Index - note metastable resolved case

# ADAS405 power graph



Total power and components

Metastable contributions to total