

## 2a. The interactive system - working with adf04 datasets

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- 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     $\Omega_{ij}$       with independent variable

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

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

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.)

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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.

# The basic adf04 file

element	ion charge	nuclear charge	Ion charge+1	Ionisation Potential (cm-1)
H+	0	1	109679.	
	1 1S		(2)0( 0.5)	
	2 2S		(2)0( 0.5)	
	3 2P		(2)1( 2.5)	
	.	.	.	
	14 5F		(2)3( 6.5)	105348.
	15 5G		(2)4( 8.5)	105348.
	-1	.	.	
	1.00 3	5.80+03	1.16+04 3.48+04 5.80+04 1.16+05 1.74+05 2.32+05 2.90+05	
	2 1 0.00+00	2.60-01	2.96-01 3.26-01 3.39-01 3.73-01 4.06-01 4.36-01 4.61-01	
	3 1 6.27+08	4.29-01	5.29-01 8.53-01 1.15+00 1.81+00 2.35+00 2.81+00 3.20+00	
	4 1 0.00+00	6.51-02	6.96-02 7.76-02 8.13-02 8.70-02 9.21-02 9.66-02 1.01-01	
	5 1 1.67+08	1.12-01	1.26-01 1.86-01 2.43-01 3.54-01 4.38-01 5.07-01 5.66-01	
	.	.	.	
	12 10 0.00+00	3.48+01	4.05+01 3.97+01 3.70+01 3.32+01 3.11+01 2.98+01 2.89+01	
	13 10 5.05+04	7.51+01	1.03+02 1.32+02 1.32+02 1.26+02 1.22+02 1.22+02 1.22+02	
	14 10 0.00+00	1.67+02	2.71+02 5.28+02 6.50+02 7.64+02 8.01+02 8.15+02 8.21+02	
	15 10 4.26+06	3.87+02	7.33+02 1.76+03 2.46+03 3.64+03 4.48+03 5.14+03 5.69+03	
	-1	.	.	
	-1 -1			
Indexed levels				(2S+1)L(J)
Configuration				Energy (cm-1)
Transition level pairs				
A-values (s-1)				
Te (K) row vector				
Upsilon row vector				

# 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

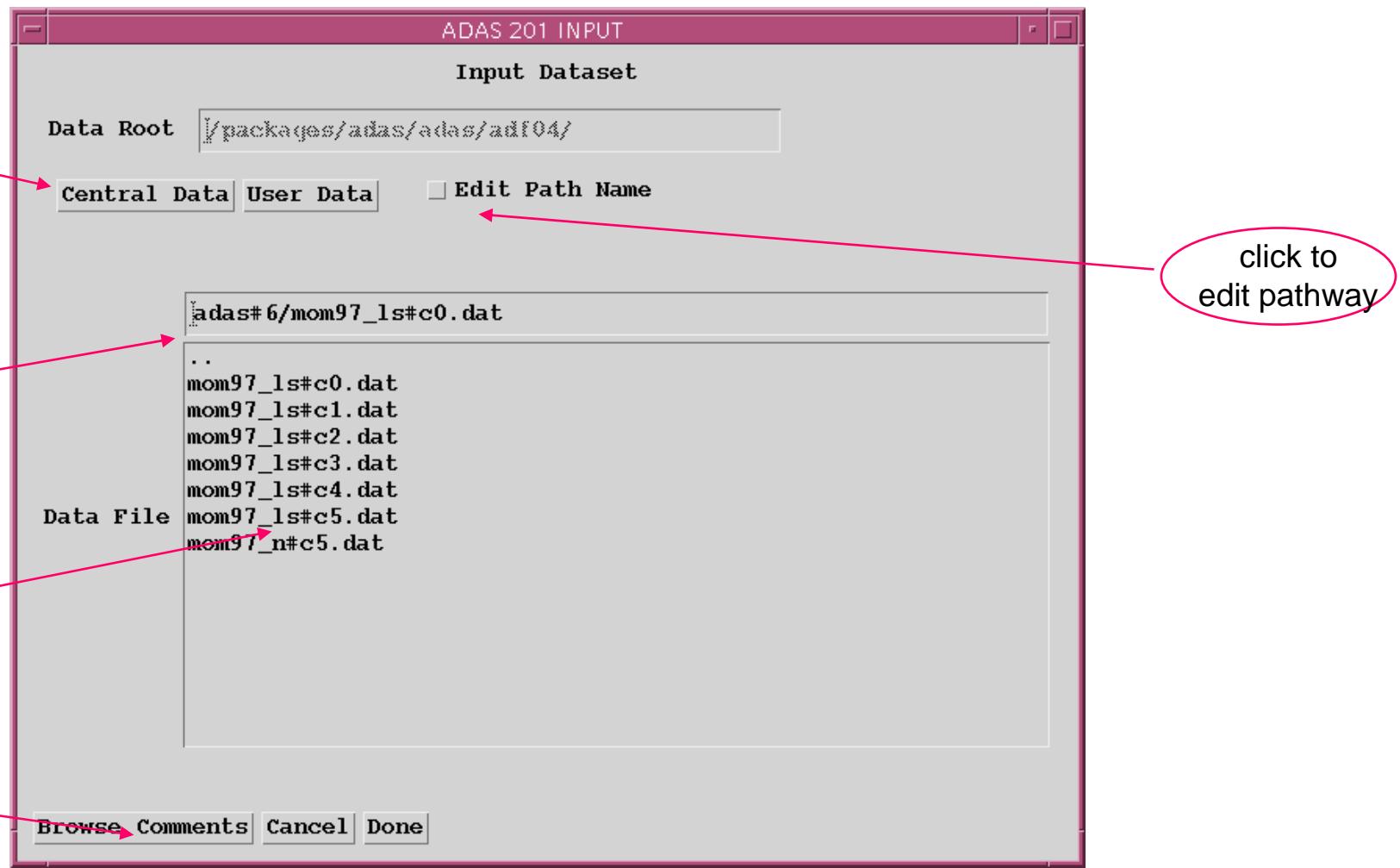
# The basic adf04 file

Standard form for  
configuration  
 $= 21512$   
in Eissner form

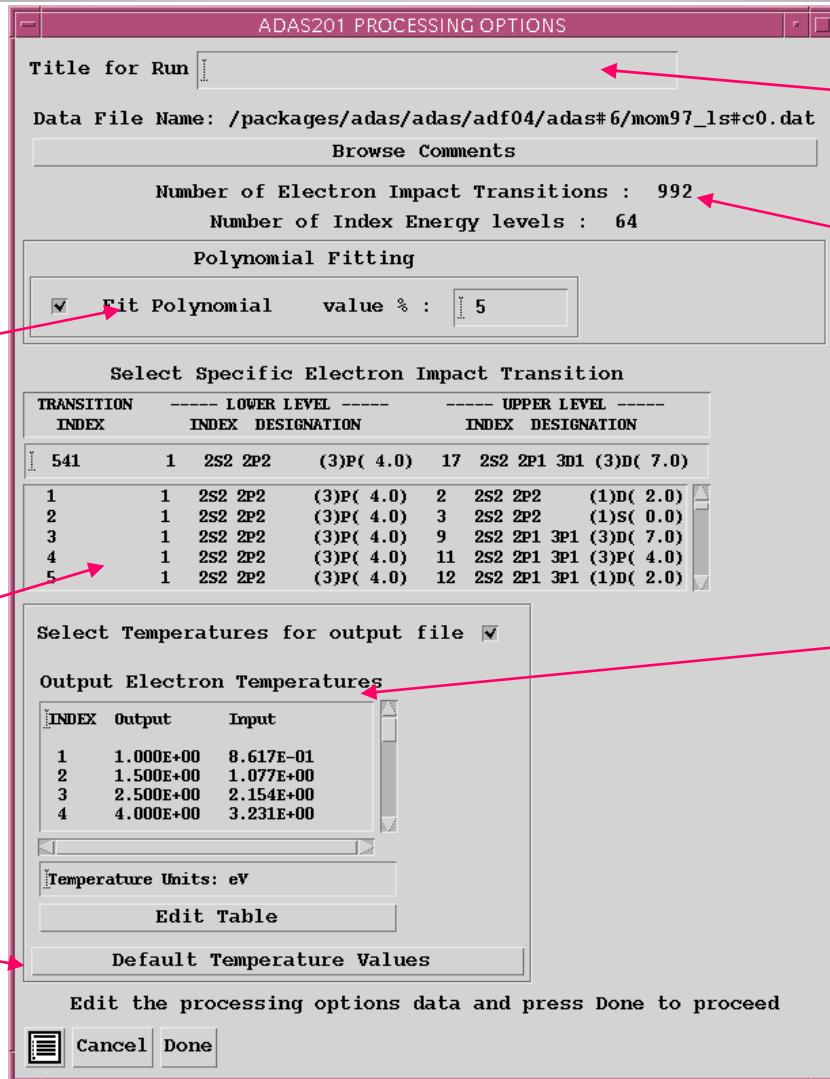
Eissner form for  
configuration  
 $= 1s2 4f1$   
in Standard form

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



# ADAS201 Processing



make polynomial fit to data

select transition for analysis

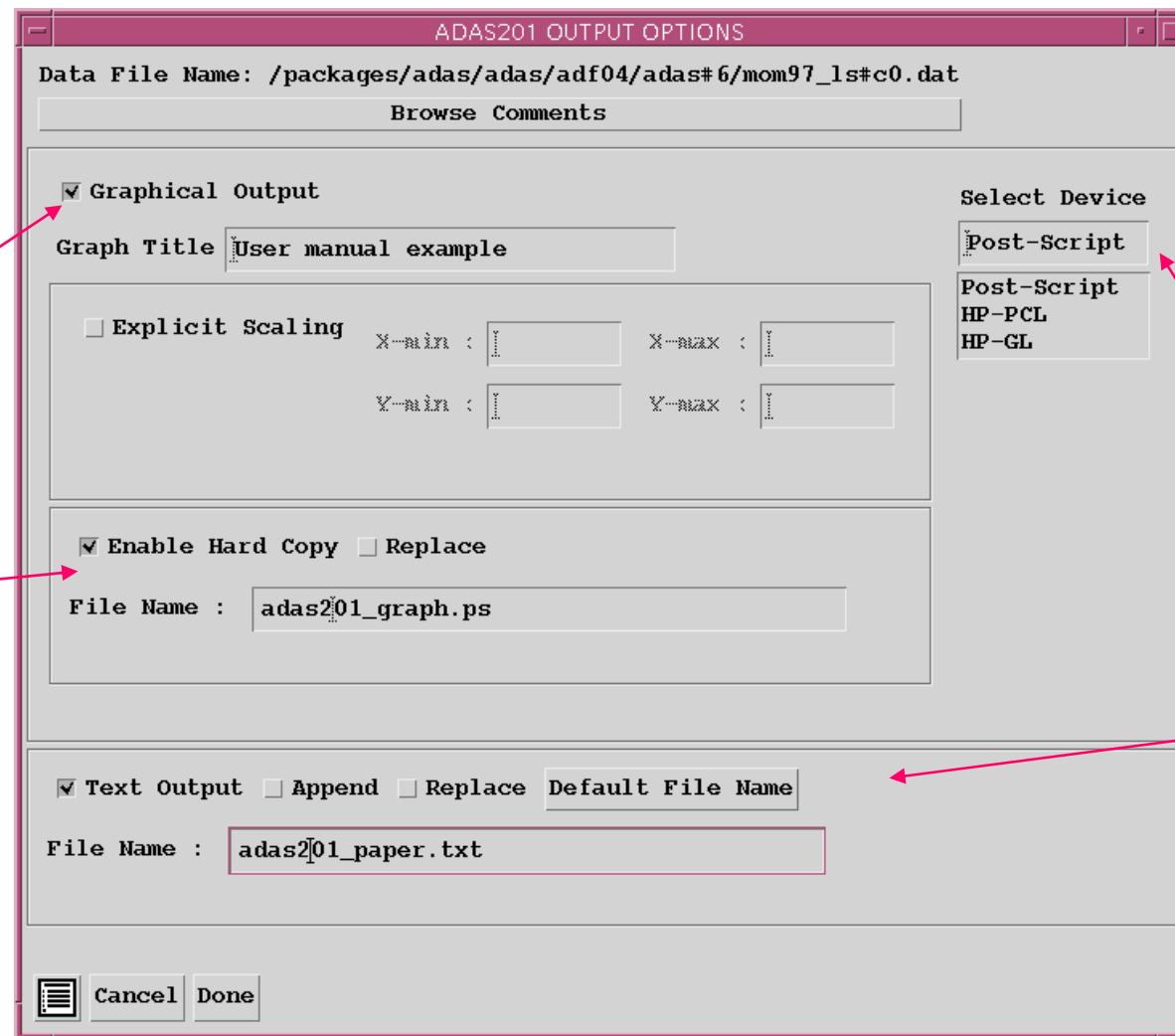
set default output values

your title to appear on graphs & tables

number of transitions and levels

Select & enter Te values for output

# ADAS201 Output



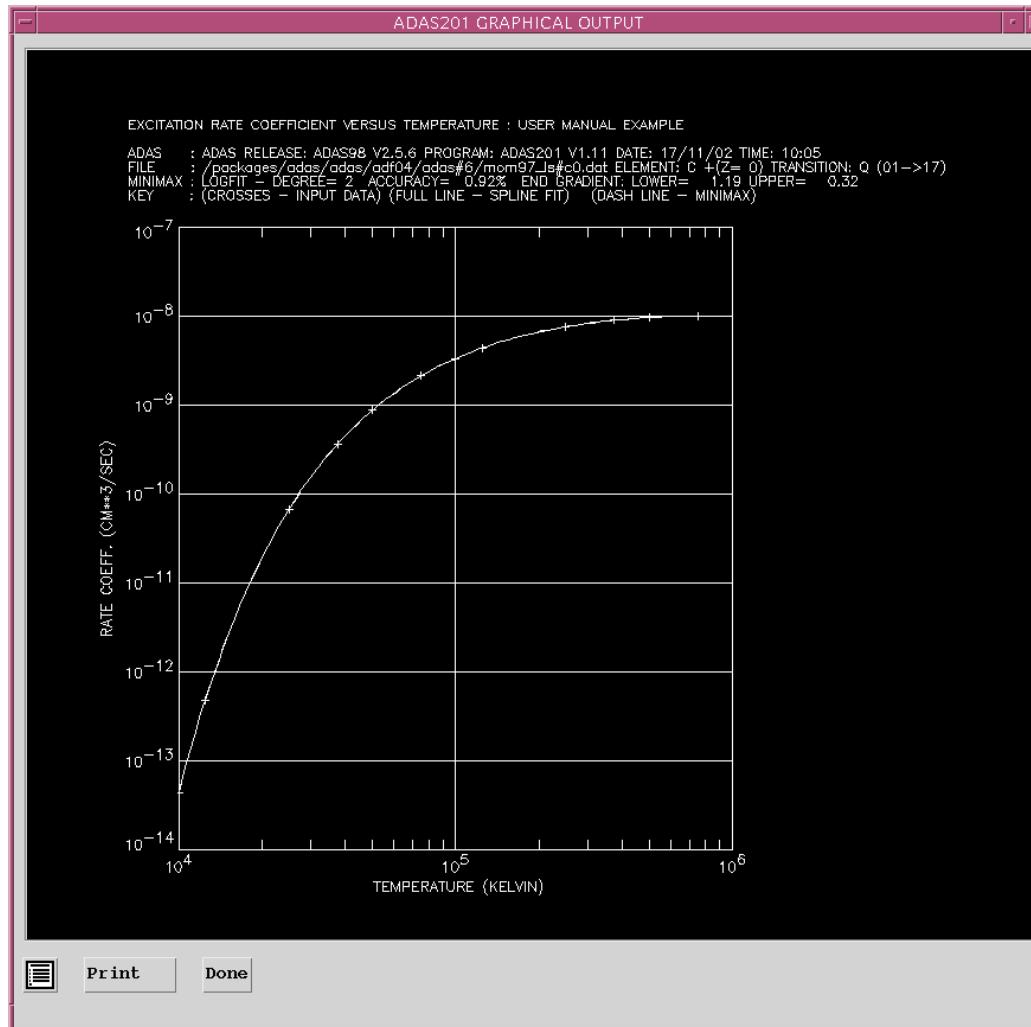
provide  
graphical  
output

allow  
graphical  
hard copy

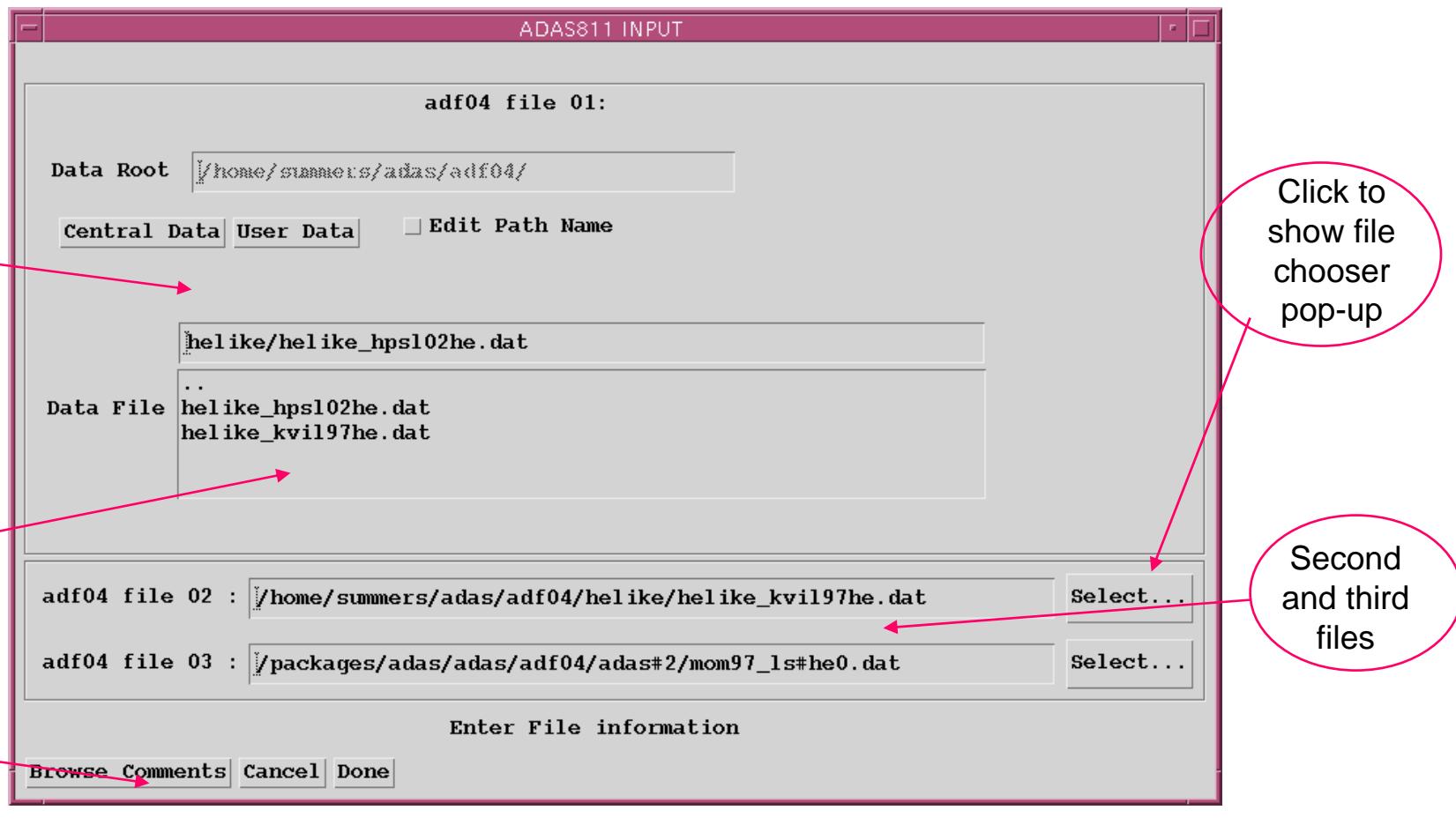
graphical  
output  
file coding

tabular  
output of  
results

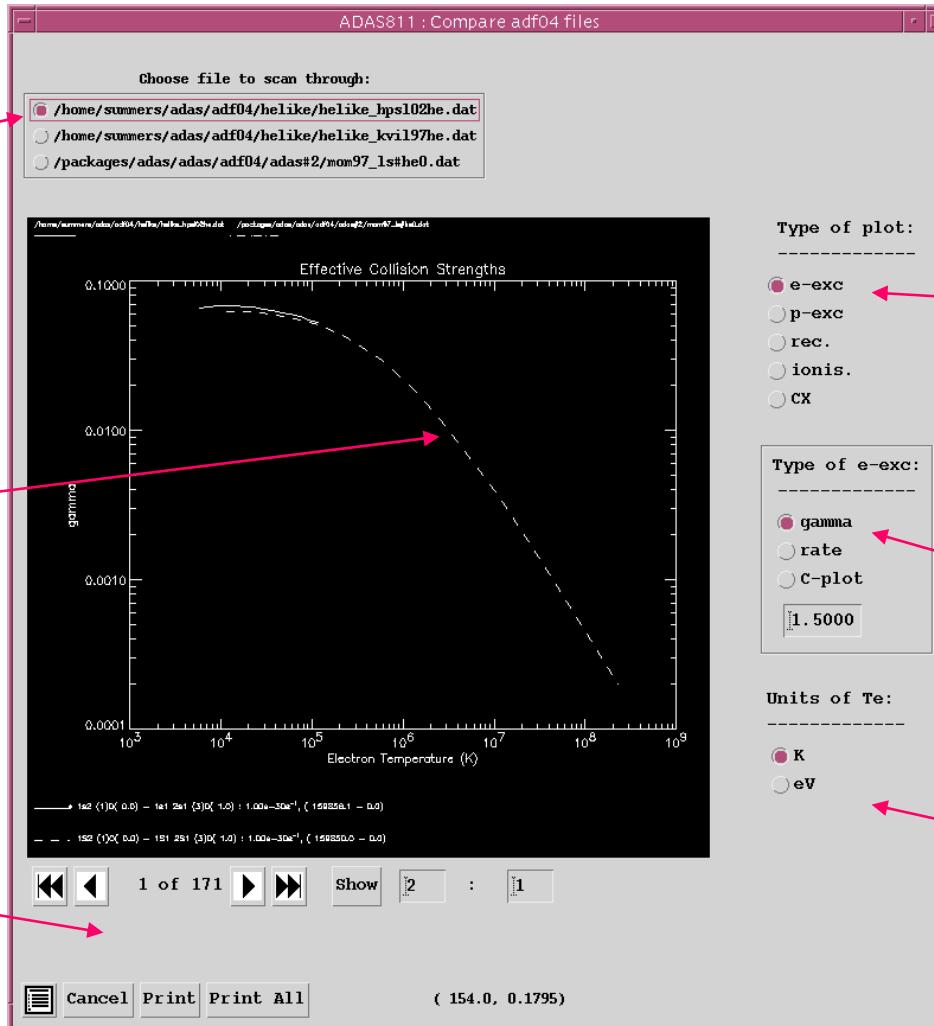
# ADAS201 Graph



# ADAS811 input



# ADAS811 Processing



select file  
to cycle  
through

comparative  
graph for  
matched  
transitions

tape  
recorder  
keys

select  
type  
e-exc

select  
type of  
e-exc  
display

select  
Te units