

## 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)<br>row vector   |               |                |   |                             |
| Upsilon<br>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  |

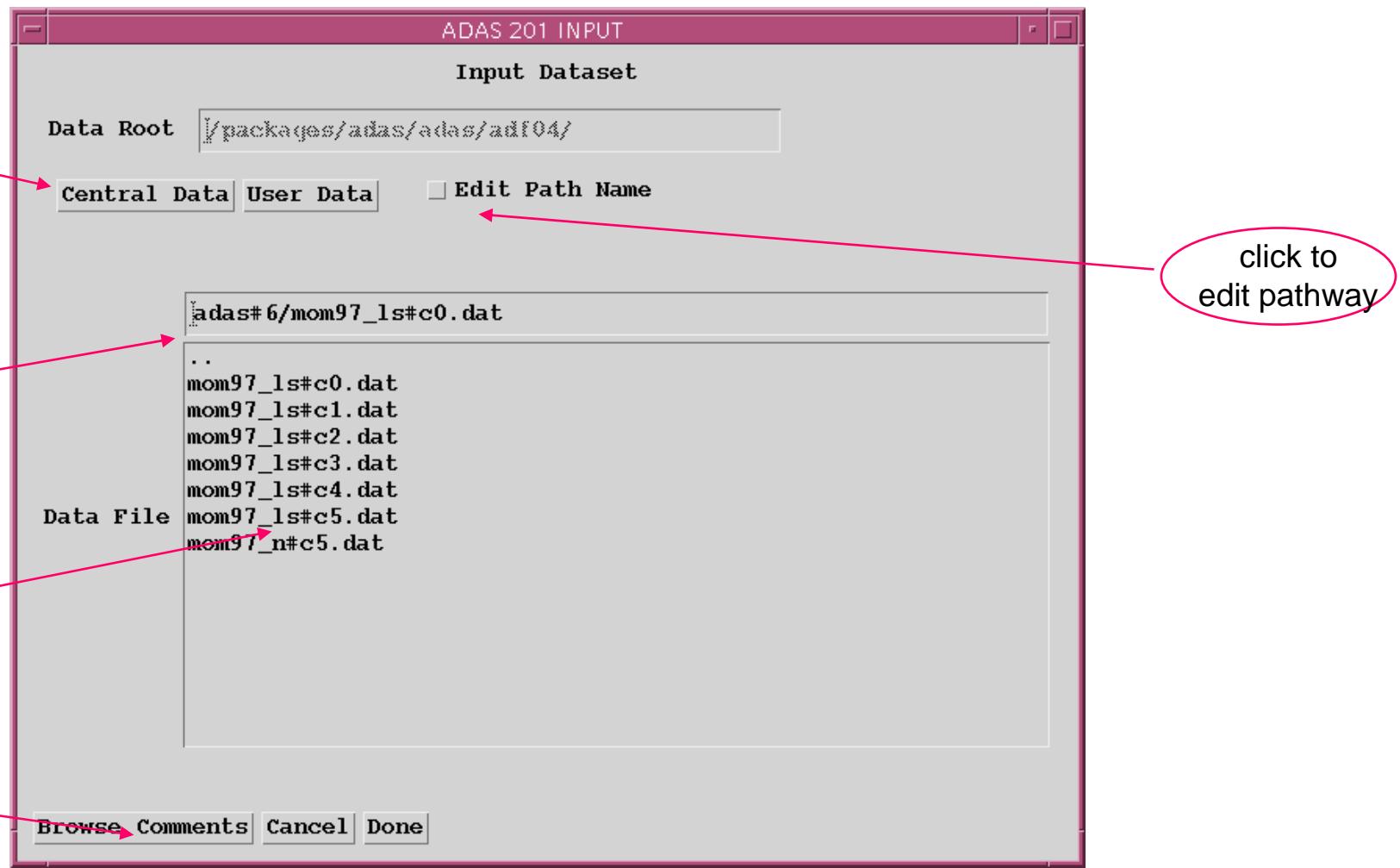
# The basic adf04 file

Standard form for  
configuration  
= 21512  
in Eissner form

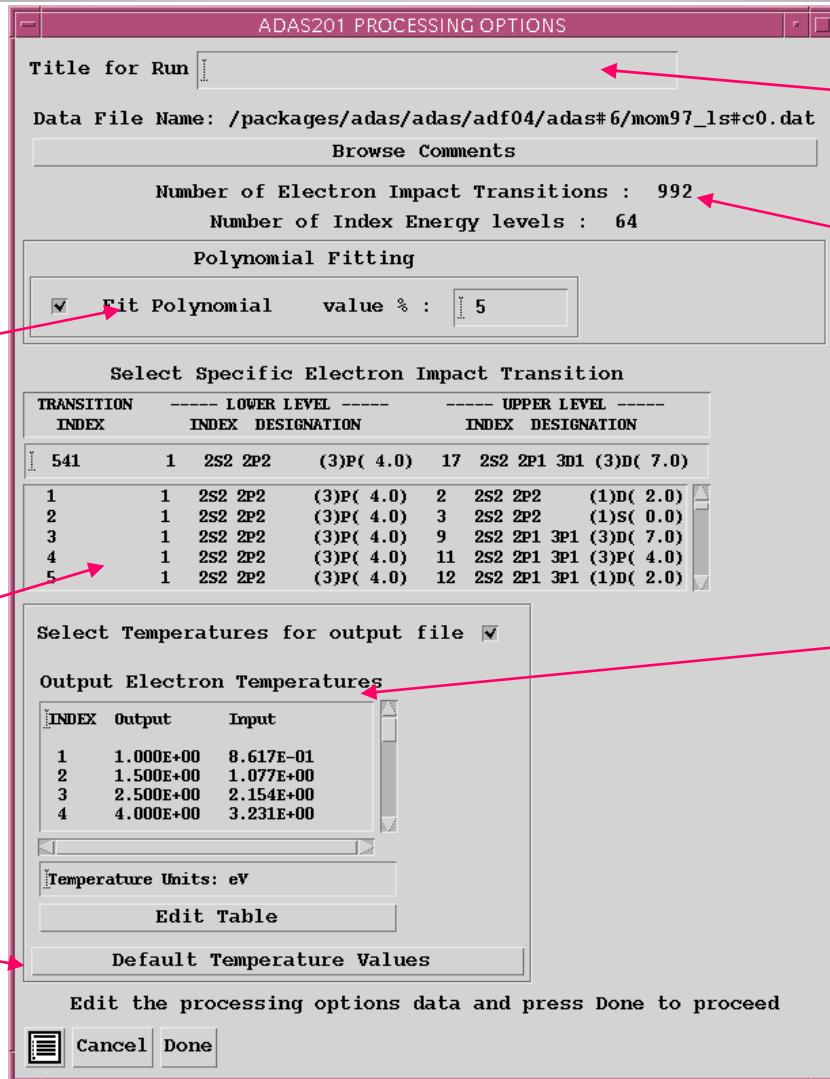
Eissner form for  
configuration  
= 1s2 4f1  
in Standard form

|            |   |            |              |
|------------|---|------------|--------------|
| 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

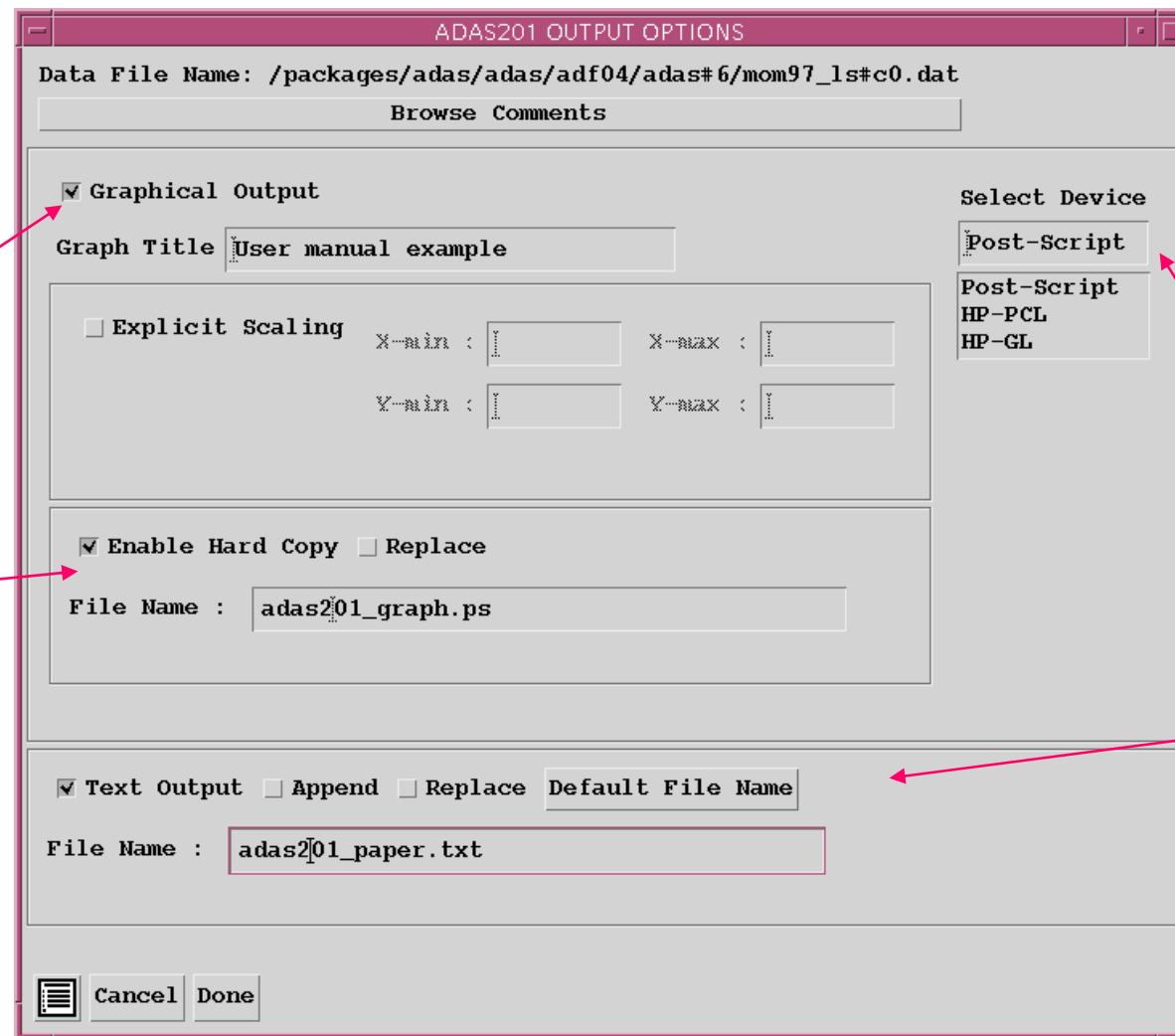
set default output values

your title to appear on graphs & tables

number of transitions and levels

Select & enter Te values for output

# ADAS201 Output



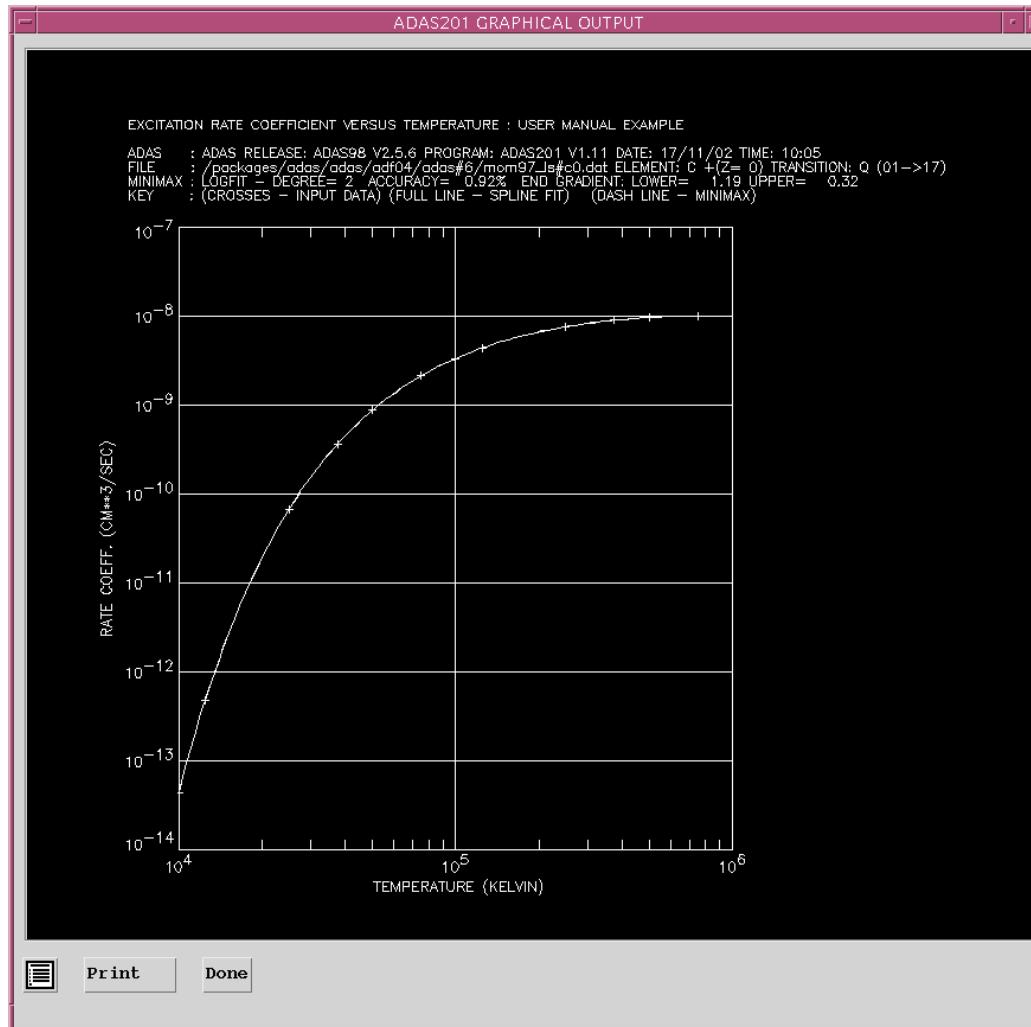
provide  
graphical  
output

allow  
graphical  
hard copy

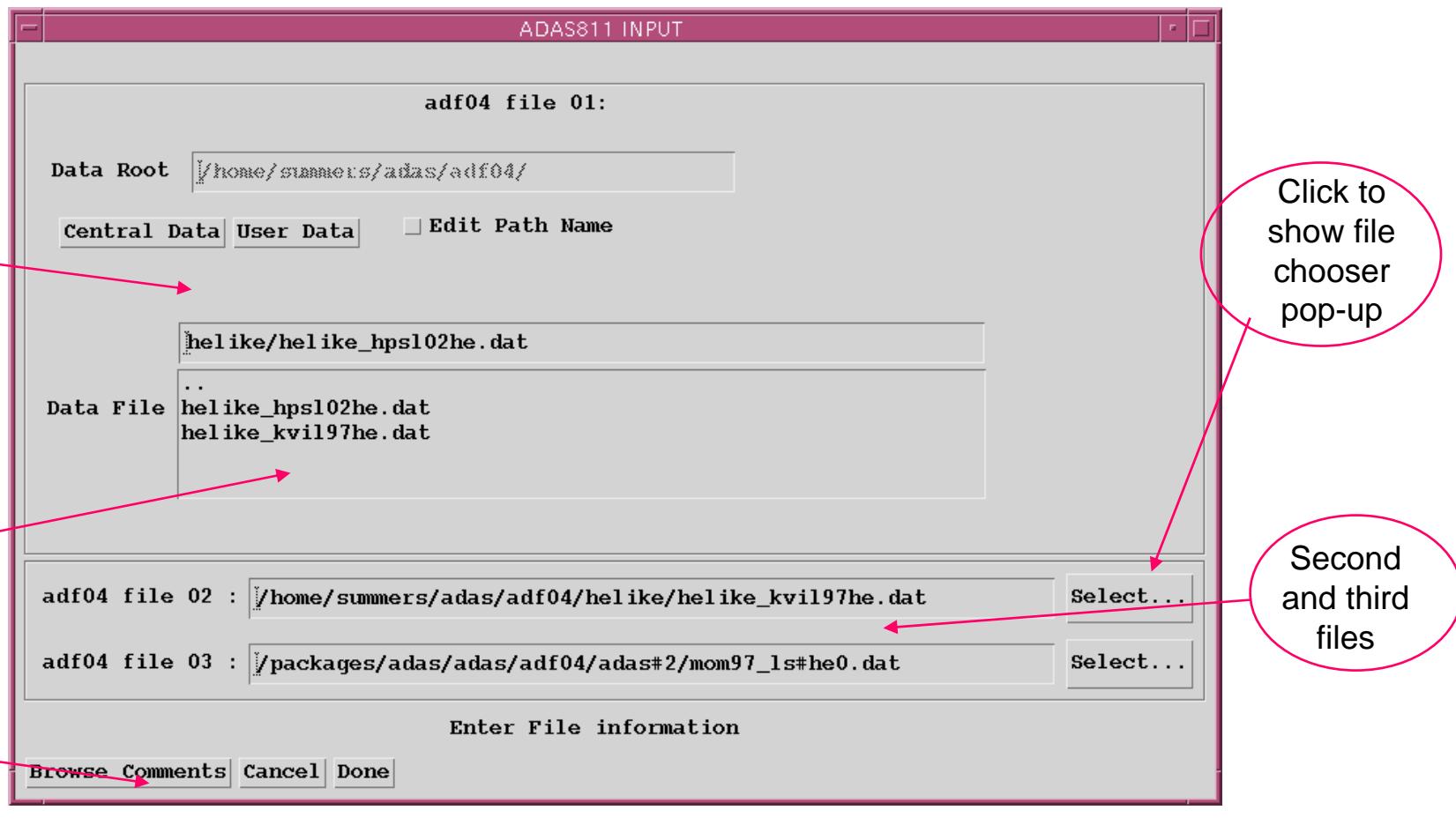
graphical  
output  
file coding

tabular  
output of  
results

# ADAS201 Graph



# ADAS811 input



# ADAS811 Processing

