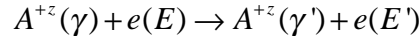# ADAS804: Calculate cross-sections & rate coefficients

The code calculates electron impact excitation cross-sections in a one electron distorted wave Born approximation using an optimised Slater type screening potential and observed level energies.

Background theory:

For a free electron colliding with a z times ionised ion A^{+z} in the state γ

$$A^{+z}(\gamma) + e(E) \rightarrow A^{+z}(\gamma') + e(E')$$
9.4.1

E and E' are the initial and final electron energies with $E > E'$ and $\Delta E = E - E'$ is the transition energy. The Born collision strength takes the form

$$\Omega_{\gamma,\gamma'}(E,E') = \omega_\gamma 8 \frac{\sqrt{EE'}}{I_H} \sum_\lambda Q_{\gamma,\gamma'}^{(\lambda)} R^{(\lambda)}(E,E') \qquad 9.4.2$$

where the sum is over the various multipoles λ. $Q_{\gamma,\gamma'}^{(\lambda)}$ comprises the angular factors and $R^{(\lambda)}(E,E')$ the momentum and radial integrals. The Ochkur extension allows the application tto spin change transitions, but with different $Q_{\gamma,\gamma'}^{(\lambda)}$ and $R^{(\lambda)}(E,E')$.

No spin change: $\gamma \equiv (S_p L_p) n l S L$; $\gamma' \equiv (S_p L_p) n' l' S L'$.

$$Q_{\gamma,\gamma'}^{(\lambda)} = (2l+1)(2l'+1)(2l'+1)(2\lambda+1) \begin{Bmatrix} l & L & L_p \\ L' & l' & \lambda \end{Bmatrix}^2 \begin{pmatrix} l & l' & \lambda \\ 0 & 0 & 0 \end{pmatrix}^2$$

$$R^{(\lambda)}(E,E') = \int_{-1}^{1} \frac{\left| \langle nl | j_\lambda(qr) | n'l' \rangle \right|^2}{a_0^4 q^4} d(\cos\theta) \qquad 9.4.3$$

Spin change: $\gamma \equiv (S_p L_p) n l S L$; $\gamma' \equiv (S_p L_p) n' l' S' L'$.

$$Q_{\gamma,\gamma'}^{(\lambda)} = (2l+1)(2l'+1)(2l'+1)(2\lambda+1).$$

$$\frac{(2S'+1)}{2(2S_p+1)} \begin{Bmatrix} l & L & L_p \\ L' & l' & \lambda \end{Bmatrix}^2 \begin{pmatrix} l & l' & \lambda \\ 0 & 0 & 0 \end{pmatrix}^2$$

$$R^{(\lambda)}(E,E') = \int_{-1}^{1} \frac{\left| \langle nl | j_\lambda(qr) | n'l' \rangle \right|^2}{a_0^4 q^4} \left(\frac{q}{k} \right)^4 d(\cos\theta) \qquad 9.4.4$$

q is the momentum transfer at scattering angle q and q is the initial momentum. Other notation is conventional. The radial integrals are evaluated from numerical wave functions as follows.

    Effective potential non-hydrogenic radial integrals: Let z_0 be the nuclear charge of ions A^{+z} and write $z_1 = z + 1$. A parameterized effective central potential is adopted here as the basis for calculating these wave functions. The central potential is established by defining an effective screening configuration

$$n_1 l_1^{q_1} n_2 l_2^{q_2} .... n_s l_s^{q_s} \quad \text{such that } q_1 + q_2 + ... + q_s = z_0 - z_1. \qquad 9.4.5$$

The electron in shell i is supposed to be screened from the nucleus by the electrons in shells $< i$ and partially screened by the other electrons in shell i itself. So the effective charge for the ith shell electron is

$$z_i = z_0 - \sum_{j=1}^{i-1} q_j - \tfrac{1}{2} q_i. \qquad 9.4.6$$

The adopted (Slater type) potential is then

$$V(r) = \frac{z_0}{r} - \sum_{i=1}^{s} \frac{q_i}{r} \exp(-\alpha_i z_i r / n_i) \left(\sum_{k=0}^{n_i} a_{ik} r^{-k} \right) \qquad 9.4.7$$

The α_i are adjustable parameters chosen so that the one electron wave function satisfies the one electron Schrodinger equation with potential $V(r)$ and the observed eigenenergy ε and quantum defect μ. In practice, we set $\alpha_i = \overline{\alpha_i} \alpha$ with $\overline{\alpha_i}$ specified so that only the overall scaling parameter α is varied to match the observed quantum defect. The radial integrals are evaluated by numerical quadratures.

Program steps:

These are summarised in figure 9.04.

Figure 9.04
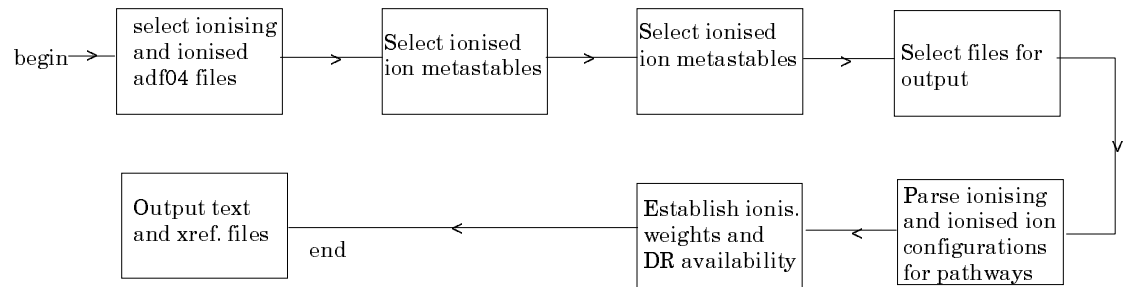
Interactive parameter comments:

The **archive selection window** appears first. It is slightly different in operation than the usual file selection window.

1. The recommended root path for user archiving for ADAS804 analysis   is

    .../uid/adas/arch804/

    which may be edited in the usual manner.

2. Click the appropriate button for opening an old archive file, starting a new archive file or ignoring archiving. In the first case, the usual file display window shows existing archive files from which selection may be made. The selected file is displayed in the selection window. In the second case, the file display window is the same, but the selection window is editable for entry of a new archive file name. **Remember to press the *return* key on the keyboard to record an entered value**.

3. The capability is given for reworking or re-displaying the results of an earlier analysis stored in an archive file. Click on the *Refresh from archive* button. Then give the *Archive index number*. The selected data will be used as the default data in the subsequent processing and output windows. Archiving is strictly sequential. A new analysis is simply appended at the end of the archive file and the index updated. These is no data replacement or substitution.

4. Clicking on the *Browse Index* button displays the index list for the selected archive file. The possibility of browsing the index appears in the subsequent main window also.

5. Clicking the *Done* button moves you forward to the next window. Clicking the *Cancel* button takes you back to the previous window
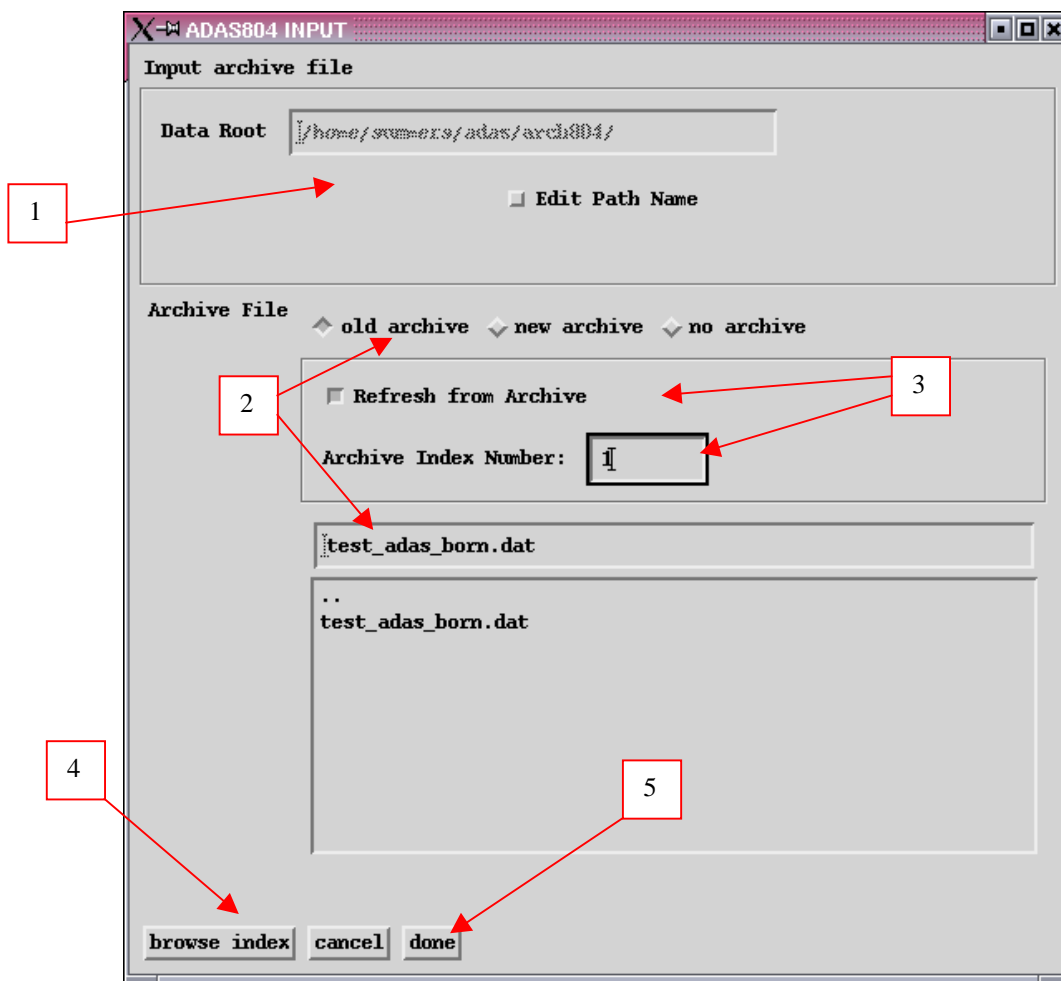
The **processing options window** appearance is shown below

1. An arbitrary title for the run may be set. If an archive is in use, then its name is given. Also the index of the archive can be browsed.
2. The nuclear and ionic charges should be specified along with Zeff, the effective ion charge. Normally, Zeff is set equal to the ion charge+1.
3. Specify the parent term or level. Note that the code can deal with LS-coupled terms or levels and with J-resolved parents in j-j coupling. If the parent is a term, leave the Jp field bank.
4. Specify the details of the lower and upper levels of the transition. For a transition between terms, leave the fields JT1 and JT2 blank. Note that the number of equivalent electrons are required for the initial and final shell of the active electron together with fractional paranetages associated with the identified parent. The binding energy is the energy (rydbergs) required to remove the active electron leaving the residual ion in the identified parent state.
5. Select required energies at which the collision strength should be calculated and temperatures at which the Upsilons should be calculated. The table is editable and there are default buttons for both the energies and temperatures. The default values are the standard ADAS sets.
6. At the present time, only the effective potential Born calculation is provided. The option for an impact parameter calculation (of dipole allowed transitions only) will be provided in the future.

7. A choice of Slater and Jucys forms for the effective potential is provided. The current trend of our work is to prefer the Slate form. At this time only internal (calculation) of wavefunctions is permitted. The option of reading in numerical radial wavefunctions may nbe made available at a later stage. Adjustable (alpha) parameters in the potential may be varied so that the wavefunction eigenenergy corresponds to the input energy. There is another option, whereby the potential parameters are locked and the eigenenergy sought. This is a less useful option in the present context.

8. The potential form is established by specification of a 'screening configuration'. Typically this is the distribution of the electrons amongst their various nl-shells in the initial state, excluding the active electron (that is the parent ion). Also, initial values of the adjustable parameters may be set. Usually both are set to 1.0 initially.
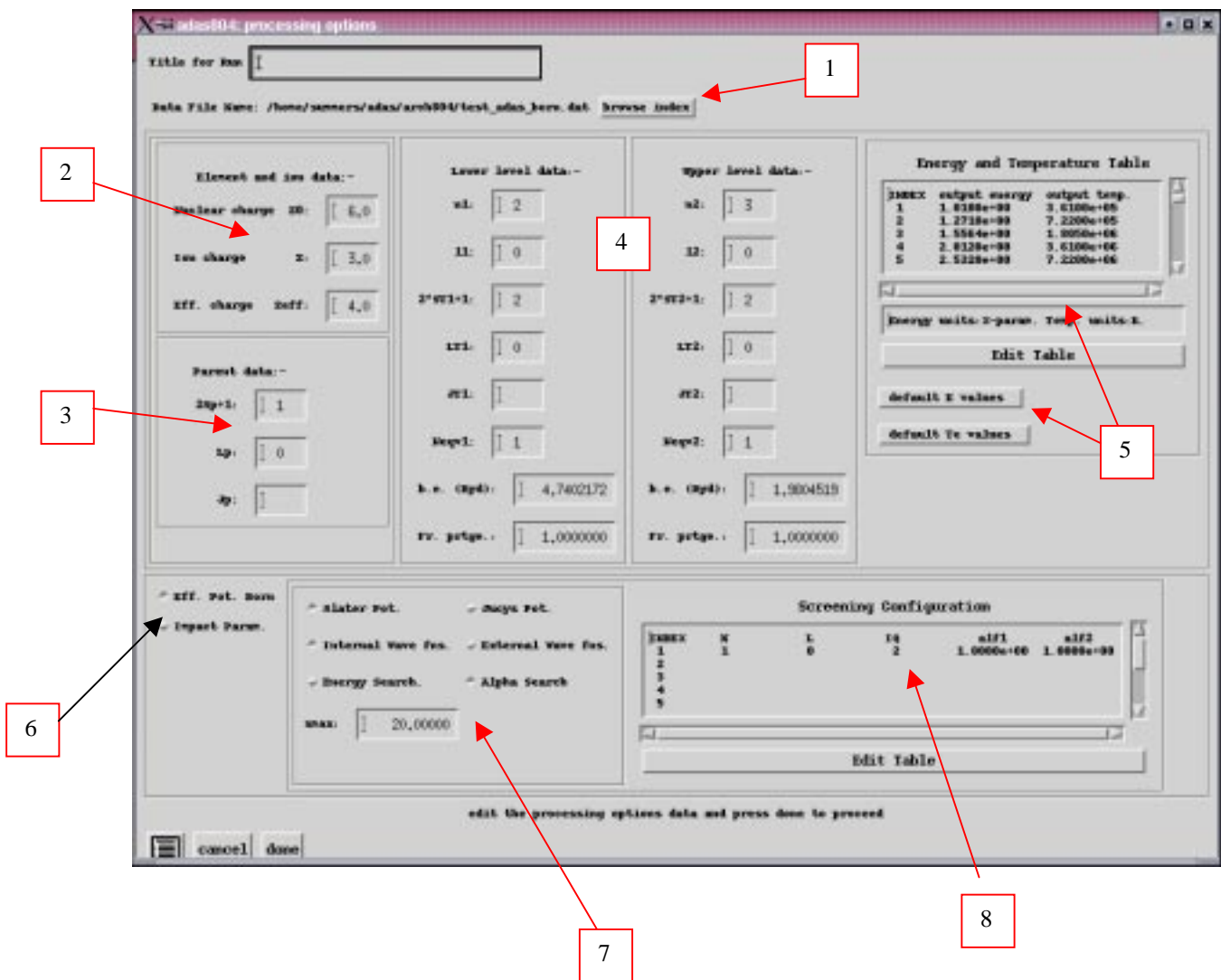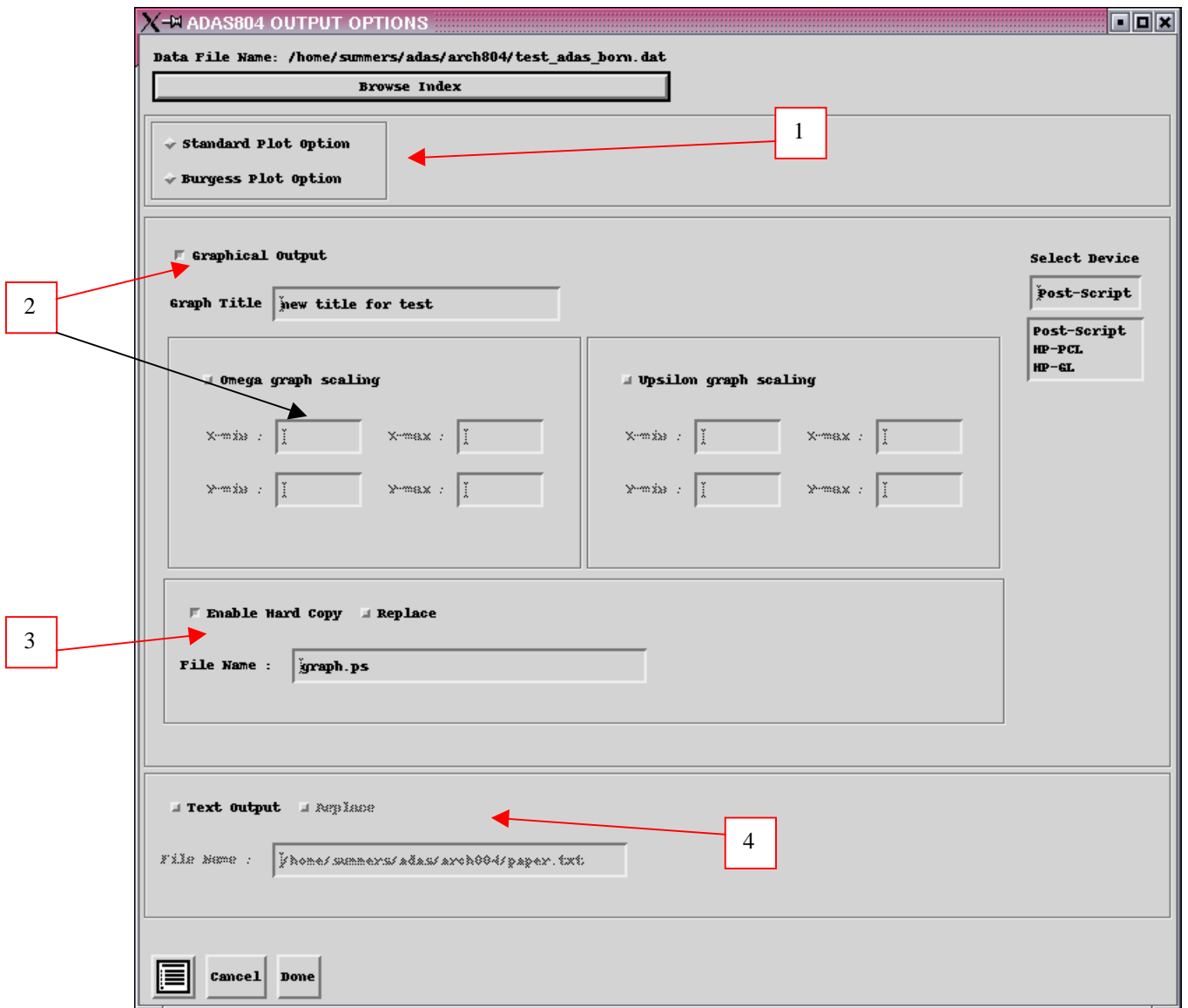

The **output options window** appearance is shown below

1. There is a choice of method for examination and display of the results data. Click either the *Standard Plot Option* of the *Burgess Plot Option*. The sub-window varies depending on this choice.

2. Graphical display is activated by the *Graphical Output* button. This will cause the graphs to be displayed following completion of this window. When graphical display is active, an arbitrary title may be entered which

appears on the top line of the displayed graph. By default, graph scaling is adjusted to match the required outputs. Press the *Explicit Scaling* button to allow separate explicit minima and maxima for the graph axes of the omega and Upsilon plots to be inserted.

3. Hard copy is activated by the *Enable Hard Copy* button . The File name box then becomes editable. If the output graphic file already exits and the *Replace* button has not been activated, a 'pop-up' window issues a warning. A choice of output graph plotting devices is given in the Device list window. Clicking on the required device selects it. It appears in the selection window above the Device list window.

4. The *Text Output* button activates writing to a text output file. The file name may be entered in the editable File name box when *Text Output* is on. The default file name 'paper.txt'may be set by pressing the button *Default file name*. A 'pop-up' window issues a warning if the file already exists and the *Replace* button has not been activated.

Notes: