

# ADAS604: Dielectronic satellite line profile fitting

The code fits multi-Gaussian line profiles, a background and optionally one detailed dielectronic satellite line group and associated resonance line compound feature to an observed spectral segment. It uses a maximum likelihood method together with statistical analysis to calculate the integrated counts under the features along with their estimated standard errors and 95% confidence limits of the fitting parameters. The multi-Gaussian fitting part of the code is due to Jim Lang and David Brooks and operates in a similar manner to ADAS602. The dielectronic part is due to Alan Whiteford and has been integrated by Ricky Martin as an ADAS code with an IDL user interface. It has been designed to interface easily with Yokhoh satellite and JET Joint Undertaking data organisations although a simple interface is also provided.

## Background theory:

This is a new code in preparation. The theory and interactive windows described here are designs only.

In the fitting of observed spectra for diagnostic analysis, it is generally the relative intensities of a set of connected spectrum lines which allow inference of underlying plasma parameters. From a spectral analysis point of view, connected spectrum lines which are close together in a fairly small wavelength segment are least influenced by calibration errors and so most useful. Such connected spectrum lines are properly called *feature primitives*, *features* or *super-features* depending upon whether the connections are via pure branching ratios, via an excited level population balance or via and ionisation balance. Ionisation balance in this context may include transport and /or transient influences. The generic name *feature* is used for all three types of connection. In spectral measurements on real plasmas, additional unconnected spectrum lines, called *ordinary lines*, from different ions or elements may lie in the observed spectral segment possibly overlaying the connected group. Special spectral feature fitting distinguishes the ordinary lines and background, and a special feature and conducts a non-linear search for the parameters of both simultaneously.

**The ordinary lines and background:** The representation is as a constant, linear or quadratic background together with several Gaussian shaped lines, that is

$$I_k^O = b_0 + b_1 x_k + b_2 x_k^2 + \sum_{i=1}^L h_i \exp[-((x_k - x_{oi}) / w_i)^2] \quad 7.4.1$$

$L$  is the number of ordinary lines in the spectrum to be fitted with  $x_{oi}$  the pixel position of the centre of the line  $i$  and  $w_i$  is its half width.

**The dielectronic satellite line special feature:** The name is used here to describe the connected set of spectrum lines as follow (i) dielectronic recombination stabilisation photons  $\lambda_{\sigma',nlJ'-\sigma''nlJ''}$  occurring in the recombination of an ion  $X_{\sigma'}^{+z}$  via the parent excited state  $X_{\sigma''}^{+z}$  with different spectators  $nl$ , (ii) photons  $\lambda_{\sigma',nlJ'-\sigma''nlJ''}$  associated with the radiative decay of resonances  $X_{\sigma'',nlJ''}^{+z-1}$  formed by inner shell excitation of an ion  $X_{\rho}^{+z-1}$ , (iii) the manifold of photons  $\lambda_{\sigma',J'-\sigma''J''}$  associated with transitions between the  $X_{\sigma'}^{+z}$  and  $X_{\sigma''}^{+z}$  complexes induced by electron impact excitation or recombination of the ion  $X_{\tau}^{+z+1}$ . The population of the level  $X_{\sigma'',nlJ''}^{+z-1}$  may be written as

$$N_{\sigma'',nlJ''}^{+z-1} = F_{\sigma'',nlJ'';\rho}^{(exc)} N_e N_{\rho}^{+z-1} + F_{\sigma'',nlJ'';\sigma'}^{(dr)} N_e N_{\sigma'}^{+z} \quad 7.4.2$$

and that of the level  $X_{\sigma''}^{+z}$  may be written as

$$N_{\sigma''}^{+z} = F_{\sigma'';\sigma'}^{(exc)} N_e N_{\sigma'}^{+z} + F_{\sigma'';\tau}^{(rec)} N_e N_{\tau}^{+z+1} \quad 7.4.3$$

where the factors  $F_{\sigma'',nIJ'';\rho}^{(exc)}$ ,  $F_{\sigma'',nIJ'';\sigma'}^{(dr)}$  are the contributions from inner shell excitation and dielectronic recombination for the  $z - 1$  times ionised ion and

the factors  $F_{\sigma'';\sigma'}^{(exc)}$ ,  $F_{\sigma'';\tau'}^{(rec)}$  are the contributions from excitation and recombination for the  $z$  times ionised ion.

The emissivity function of a satellite may be written as

$$\begin{aligned} \frac{I_{\sigma''nIJ''\rightarrow\sigma'nIJ'}}{N_e N_{\sigma'}^{+z}} &= [A_{\sigma''nIJ''\rightarrow\sigma'nIJ'} F_{\sigma''nIJ'';\rho}^{(exc)}] \frac{N_{\rho}^{+z-1}}{N_{\sigma'}^{+z}} + [A_{\sigma''nIJ''\rightarrow\sigma'nIJ'} F_{\sigma''nIJ'';\sigma'}^{(dr)}] \\ &= R_1 E_{\sigma''nIJ''\rightarrow\sigma'nIJ'}^{(exc)}(T_e, N_e) A_{\rho,\sigma'}^{(z-1,z)}(T_e, N_e) + E_{\sigma''nIJ''\rightarrow\sigma'nIJ'}^{(dr)}(T_e, N_e) \end{aligned}$$

where  $E_{\sigma''nIJ''\rightarrow\sigma'nIJ'}^{(exc)}(T_e, N_e)$  is the excitation emissivity coefficient,  $E_{\sigma''nIJ''\rightarrow\sigma'nIJ'}^{(dr)}(T_e, N_e)$  is the dielectronic recombination emissivity coefficient,

$$A_{\rho,\sigma'}^{(z-1,z)}(T_e, N_e) = \left. \frac{N_{\rho}^{+z-1}}{N_{\sigma'}^{+z}} \right|_{eq} \text{ measures the ionisation equilibrium relative metastable}$$

abundances and  $R_1$  measures the dis-equilibrium in the ionisation balance. Evidently the emissivity function is a function of the three parameters  $R_1$ ,  $T_e$  and  $N_e$ .

In like manner the emissivity function of an associated line of the recombining ion may be written as

$$\begin{aligned} \frac{I_{\sigma''\rightarrow\sigma'}}{N_e N_{\sigma'}^{+z}} &= [A_{\sigma''\rightarrow\sigma'} F_{\sigma'';\sigma'}^{(exc)}] + [A_{\sigma''\rightarrow\sigma'} F_{\sigma'';\tau'}^{(rr)}] \frac{N_{\tau}^{+z+1}}{N_{\sigma'}^{+z}} \\ &= E_{\sigma''\rightarrow\sigma'}^{(exc)}(T_e, N_e) + R_2 E_{\sigma''\rightarrow\sigma'}^{(rr)}(T_e, N_e) A_{\tau,\sigma'}^{(z+1,z)}(T_e, N_e) \end{aligned}$$

where  $E_{\sigma''\rightarrow\sigma'}^{(exc)}(T_e, N_e)$  is the excitation emissivity coefficient,  $E_{\sigma''\rightarrow\sigma'}^{(rr)}(T_e, N_e)$  is the radiative recombination emissivity coefficient,  $A_{\tau,\sigma'}^{(z+1,z)}(T_e, N_e) = \left. \frac{N_{\tau}^{+z+1}}{N_{\sigma'}^{+z}} \right|_{eq}$  measures the

ionisation equilibrium relative metastable abundances and  $R_2$  measures the disequilibrium in the ionisation balance. Evidently the emissivity function is a function of the three parameters  $R_2$ ,  $T_e$  and  $N_e$ . Thus the theoretical local emissivity of the combined satellite lines and associated resonance line feature is functionally dependent on four parameters,  $R_1$ ,  $R_2$ ,  $T_e$  and  $N_e$ . The functional dependence is specified numerically in rapid look-up tables called the compound feature.

Introduce a spectral profile for each line of the compound feature, indexed by  $c$  of natural wavelength,  $\lambda_c$ , of the form  $\psi_{\lambda-\lambda_c-\Delta\lambda}(T_i, b)$ .  $T_i$  is the ion temperature and  $b$  is a second parameter of the profile shape.  $\Delta\lambda$  is a further parameter which is displacement of lines driven from the lithium-like ground state from those driven from the helium-like ground state. Thus  $\Delta\lambda$  is zero for lines driven from the helium-like stage ground state.

Thus the theoretical count rate at detector pixel position  $x_k$  is

$$I_k^F = h \sum_c E_c(R_1, R_2, T_e, N_e) \psi_{\lambda_k-\lambda_c-\Delta\lambda}(T_i, b)$$

where  $E$  denotes a generic emissivity functional from the equations above.

**Profile functions:** Four profile forms are used to represent the combined influence of thermal Doppler broadening in the plasma and the instrumental profile, namely, single Doppler, Doppler/Lorentz, Voigt and double Doppler. For each of these the second parameter  $b$  is

fixed relative to Doppler broadening width from the ion temperature  $T_i$ , The specifications are as follow:

**The fitting algorithms:** The observed data are fitted to the equation

$$I_k = I_k^O + I_k^F \quad 7.4.1$$

where  $I_k$  is the observed count rate at a particular detector pixel position  $x_k$  and  $I_k^O$ ,  $I_k^F$  represent the ordinary line + background and the special feature parts respectively.

Statistical variation in  $I_k$  is assumed to have the normal form. With variance proportional to the mean value of  $I_k$ . Hence

$$\sigma_k^2 = \text{Var } I_k = \sigma^2 E(I_k) \quad k = 1, 2, \dots, P \quad 7.4.2$$

where  $\sigma^2$  is an unknown constant of proportionality,  $P$  is the number of pixel positions and  $E$  denotes the expected value. Under these conditions, the likelihood function can be formed and values which maximise it also maximise its (natural) logarithm. Thus to maximise the log likelihood to estimate the  $N$  variables  $b_0, b_1, b_2, h_i, x_{o_i}, w_i$  the need is to minimise the function

$$\sum_{k=1}^P \left[ \frac{I_k}{\sigma_k} - \frac{1}{\sigma_k} (b_0 + b_1 x_k + b_2 x_k^2 + \sum_{i=1}^L h_i \exp[-((x_k - x_{o_i}) / w_i)^2]) \right]^2 \quad 7.4.3$$

The  $\sigma_k^2$  are unknown. Assuming however that the counts per sampling interval follow the Poisson distribution, the  $\sigma_k^2$  are equal to the true unknown mean count per sampling interval divided by the number of sampling intervals. If the unknown mean count rate is estimated by  $I_k$ , then an estimate of  $\sigma_k^2$  follows, namely  $I_k$  divided by the number of intervals where the number of intervals is the dwell time in seconds. A standard numerical routine will find the unconstrained minimum of the function 7.4.4, i.e. minimise

$$F(x) = \sum_{i=1}^P [f_i(x)]^2 \quad 7.4.4$$

The functions  $f_i(x)$  (the residuals), their first derivatives and a starting point must be supplied. The starting point was obtained from the observed spectrum by indicating the number of lines to be fitted and estimating their peak positions and full-width half-maxima. The background was also obtained from the spectrum and estimates of  $b_0, b_1, b_2$  made. Once estimates of  $b_0, b_1, \dots$  (denoted by  $\hat{b}_0, \hat{b}_1, \dots$ ) have been found a second routine is used to find the diagonal elements of the variance-covariance matrix  $C$ . This routine depends on the use of the standard result of maximum likelihood theory which states that the variance-covariance matrix of the estimates is approximately given by the negative of the inverse of the expected value of the matrix of second derivatives of the logarithm of the likelihood. In the routine it is assumed that the Hessian (i.e. matrix of second partial derivatives) of  $F(x)$  at the solution can be approximated adequately by  $2J^T J$  where  $J$  is the Jacobian (i.e. matrix of first partial derivatives) of  $F(x)$  at the solution.  $C$  is then given by

$$C = \hat{\sigma}^2 (J^T J)^{-1} \quad J^T J \text{ on-singular} \quad 7.4.5$$

where  $\hat{\sigma}^2$  is the estimated variance of the residual at the solution ( $\hat{x} = \hat{b}_0, \hat{b}_1, \dots$ ) and is given by

$$\hat{\sigma}^2 = F(\hat{x}) / (P - N) \quad 7.4.6$$

The square root of the diagonal elements of  $C$  give the estimated standard errors of the corresponding elements of  $\hat{x}$ . A 95% confidence interval for each of the elements of  $\hat{x}$  is

obtained using  $\hat{x}_j \pm t_{P-N;97.5} (C_{jj})^{1/2}$  where  $t_{P-N;97.5}$  denotes the upper 97.5% point of the Student's  $t$  distribution with  $P - N$  degrees of freedom. Note that the approximation of the Hessian by  $2J^T J$  is justified as follows: the Hessian matrix  $G(x)$  is of the form

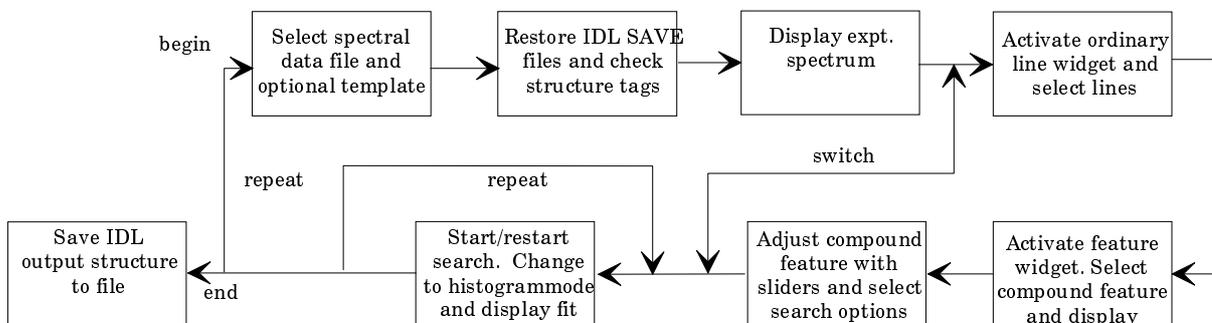
$$G(x) = 2[J^T(x)J(x) + \sum_{i=1}^P f_i(x)G_i(x)] \quad 7.4.7$$

where  $G_i(x)$  is the Hessian matrix of  $F(x)$ . In the neighbourhood of the solution  $\|f(x)\|$  is often small compared to  $\|J^T(x)J(x)\|$ , for example when  $f_i(x)$  represents the goodness of fit of a non-linear model to observed data. In such cases  $2J^T(x)J(x)$  may be an adequate approximation to  $G(x)$ . This avoids the need to compute or approximate second derivatives of the  $f_i(x)$ .

## Program steps:

These are summarised in the figure below.

Figure 2.8



## Interactive parameter comments:

Move to the directory in which you wish any ADAS created files to appear. These include the output text file produced after executing any ADAS program (*paper.txt* is the default) and the graphic file if saved (e.g. *graph.ps* if a postscript file)

The **file selection window** has the appearance shown below

1. The form of the primary input spectral data is selected at a). Input data sets are expected to be in the form of IDL 'SAVE' files. Forms allowed are as follow:

- a) The form *Standard* comprises a single array and a 'header' defined as

*spectrum* : *dblarr()*

*header* : " or *structure (ie.={a:a, b:b,...})*

*spectrum* contains the spectral counts as a function of pixel position. The array length must be  $\leq 1024$ . The array may be two-dimensional in which case the first index is the pixel number in the dispersion direction and the second the pixel number in the spatial (or other) direction. This latter case allows the cycling option described in section 5.2.

*header* is an optional string of the user's choice or may be a structure

- b) The form *Processed* is that of the output structure from ADAS603 itself. This form allows re-entry of output data for re-analysis. The input file contains a structure *lstr* defined as:

<i>lstr.b0</i>	: 0.0	<i>lstr.eseb0</i>	: 0.0
<i>lstr.eclb0</i>	: 0.0	<i>lstr.b1</i>	: 0.0
<i>lstr.eseb1</i>	: 0.0	<i>lstr.eclb1</i>	: 0.0
<i>lstr.b2</i>	: 0.0	<i>lstr.eseb2</i>	: 0.0
<i>lstr.eclb2</i>	: 0.0	<i>lstr.w</i>	: <i>dblarr</i> (10)
<i>lstr.esew1</i>	: 0.0	<i>lstr.eclw1</i>	: 0.0
<i>lstr.x0</i>	: <i>dblarr</i> (10)	<i>lstr.esexo</i>	: <i>dblarr</i> (10)
<i>lstr.eclx0</i>	: <i>dblarr</i> (10)	<i>lstr.h</i>	: <i>dblarr</i> (10)
<i>lstr.eseh</i>	: <i>dblarr</i> (10)	<i>lstr.eclh</i>	: <i>dblarr</i> (10)
<i>lstr.esewv</i>	: <i>dblarr</i> (10)	<i>lstr.eclwv</i>	: <i>dblarr</i> (10)
<i>lstr.flux</i>	: <i>dblarr</i> (10)	<i>lstr.esef</i>	: <i>dblarr</i> (10)
<i>lstr.eclf</i>	: <i>dblarr</i> (10)	<i>lstr.getfit</i>	: <i>intarr</i> (6)
<i>lstr.exptime</i>	: 0.0	<i>lstr.info</i>	: 0
<i>lstr.header</i>	: ‘	<i>lstr.xmin</i>	: 0
<i>lstr.xmax</i>	: 0	<i>lstr.x</i>	: <i>indgen</i> ()
<i>lstr.y</i>	: <i>dblarr</i> ()	<i>lstr.ya</i>	: <i>dblarr</i> ()
<i>lstr.nsize</i>	: 0.0	<i>lstr.numline</i>	: 0
<i>lstr.nfxl</i>	: 0	<i>lstr.bchl</i>	: 0.0
<i>lstr.bchr</i>	: 0.0	<i>lstr.lineid</i>	: <i>strarr</i> (10)
<i>lstr.getxp</i>	: <i>intarr</i> (6)	<i>lstr.lineidxp</i>	: ‘
<i>lstr.bfxp</i>	: 0.0	<i>lstr.esebfxp</i>	: 0.0
<i>lstr.eclbfxp</i>	: 0.0	<i>lstr.tixp</i>	: 0.0
<i>lstr.esetixp</i>	: 0.0	<i>lstr.ecltixp</i>	: 0.0
<i>lstr.iwxp</i>	: 0.0	<i>lstr.esewxp</i>	: 0.0
<i>lstr.ecliwxp</i>	: 0.0	<i>lstr.angxp</i>	: 0.0

with the meaning of the variables as follow:

<i>b0</i>	fitted constant part of the background
<i>eseb0</i>	estimated standard error in <i>b0</i>
<i>eclb0</i>	estimated 95% confidence limit in <i>b0</i>
<i>b1</i>	fitted linear part of the background
<i>eseb1</i>	estimated standard error in <i>b1</i>
<i>eclb1</i>	estimated 95% confidence limit in <i>b1</i>
<i>b2</i>	fitted quadratic part of the background
<i>eseb2</i>	estimated standard error in <i>b2</i>
<i>eclb2</i>	estimated 95% confidence limit in <i>b2</i>
<i>w</i>	fitted line widths
<i>esewl</i>	estimated standard error in <i>w</i> (fixed)
<i>eclwl</i>	estimated 95% confidence limit in <i>w</i> (fixed)
<i>x0</i>	fitted line centroid positions
<i>esexo</i>	estimated standard error in <i>x0</i>
<i>eclx0</i>	estimated 95% confidence limit in <i>x0</i>
<i>h</i>	fitted line heights at centroid
<i>eseh</i>	estimated standard error in <i>h</i>
<i>eclh</i>	estimated 95% confidence limit in <i>h</i>
<i>esewv</i>	estimated standard error in <i>w</i> (variable)
<i>eclwv</i>	estimated 95% confidence limit in <i>w</i> (variable)

*flux* fitted line flux (counts under profile)  
*esef* estimated standard error in *flux*  
*eclf* estimated 95% confidence limit in *flux*  
*getfit* options selected (see code)  
*exptime* the exposure time (1.0 if expval not set)  
*info* error from MINPACK routine (see XXDER1)  
*header* comment  
*xmin* minimum pixel for fitting range  
*xmax* maximum pixel for fitting range  
*x* pixel values  
*y* spectral data  
*ya* fit to data  
*nsiz*e spectral range width  
*numline* number of fitted lines  
*nfxl* number of fitted lines with fixed positions  
*bchl* initial estimate of background  
*bchr* inisial estimate of background  
*lineid* preliminary line identification labels  
*getxp* options selcted for Xpaschen (see code)  
*lineidxp* Xpaschen multiplet name from list  
*bfxp* fitted magnetic field strength  
*esebfxp* estimated standard error in *bfxp*  
*eclbfxp* estimated 95% confidence limit in *bfxp*  
*tixp*: fitted ion temperature (eV)  
*esetixp* estimated standard error in *tixp*  
*ecltixp* estimated 95% confidence limit in *tixp*  
*iwxp* fitted instrumental width (A).  
*eseiwxp* estimated standard error in *iwxp*  
*ecliwxp* estimated 95% confidence limit in *iwxp*  
*angxp*: specified observation angle

- c) The form *Other* is not yet implemented and we are open to suggestions for it (eg. an ascii tabulated version of *lstr* as *spectrum/header*?)
2. Data root b) shows the full pathway to the appropriate data subdirectories. Click the *Central Data* button to insert the default central ADAS pathway to *././adas/adas/arch603*. Note that there are only some sample data in this subdirectory (viz. a standard data set '*...clean*' and a processed data set '*fit...*') as there is no formal central ADAS data of archive type. Click the *User Data* button to insert the pathway to your own archived data for ADAS603.

3. The Data root can be edited directly. Click the *Edit Path Name* button first to permit editing. Available sub-directories are shown in the large file display window b). Scroll bars appear if the number of entries exceed the file display window size.
4. Click on a name to select it. The selected name appears in the smaller selection window c) above the file display window. Then its sub-directories in turn are displayed in the file display window. Ultimately the individual datafiles are presented for selection.
5. Clicking on the *Browse Comments* button displays the information header associated with the selected datafile.
6. A second data set may be selected at d), e) and f). Such a data set must be in the form of a processed output data from ADAS603. Its purpose is to provide initial selection values for analysing the new data set. This facility is important for repetitive analysis of data from the same spectral region where the same set of lines is being picked out. Note that the default pathway is to the *../adas/pass* directory in this case. Note also that if a processed file is selected **it will be used** to fit the new data.
7. Once a primary data file is selected, the buttons at the bottom of the main window become active.
8. Clicking the *Done* button moves you forward to the next window. Clicking the *Cancel* button takes you back to the previous window

B. The **processing options window** has the appearance shown below

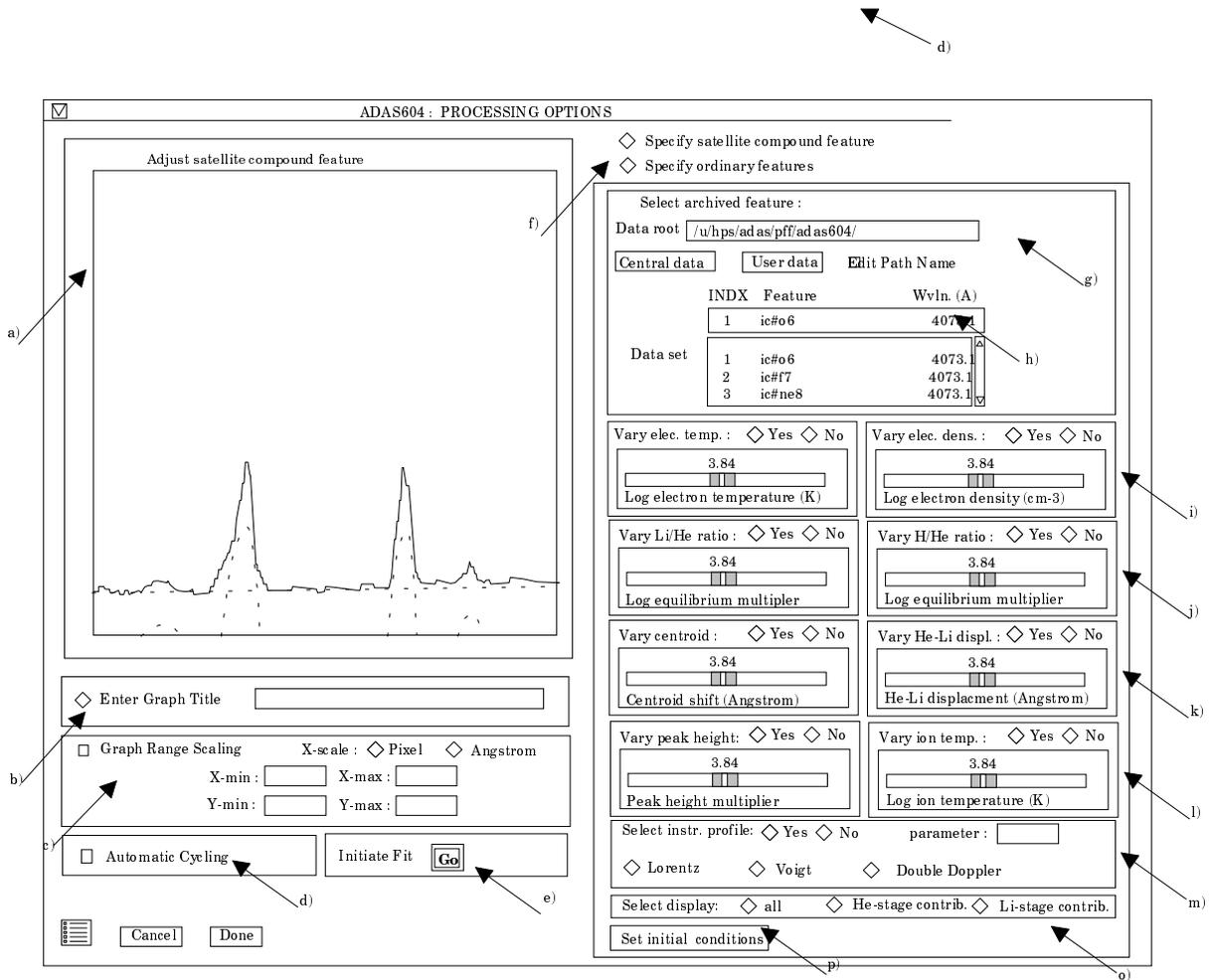
1. The spectrum (counts vs pixel number or wavelength) is displayed at a) and a title for the hard copy of the graph may be entered at b).
2. In general, one wishes to select only a segment of the spectrum for fitting and to adjust the y-scale. This is done by entering appropriate values at c) in the X-min, X-

max, Y-min and Y-max boxes. Note that the entries have effect immediately so the graph can be adjusted rapidly to requirements. The x-scale of the graph may be pixels or wavelength. Select the required choice at c).

3. There are two parts to the theoretical spectrum, a conventional set of ordinary line features and a satellite line compound feature including helium-like and lithium-like ion parts. The initial conditions for the two parts are set up in turn by activating the appropriate button at f). These are exclusive buttons and the associated sub-widget is displayed immediately below the buttons. The choice shown in the main figure is the Xpaschen sub-widget. The conventional line fitting sub-widget is shown separately in the subsequent figure.

4. **Specifying the satellite line compound feature:**

- a) The special features have been calculated for a large number of cases and archived for selection. The available choice may be scrolled through in the multiplet selection widget at h) Click on a feature to select it. The selected feature is shown in the window at g).



5. **Specifying ordinary features:**

- a) At g') select the number of line features you wish to fit to the spectrum. A maximum of ten is allowed. At h'), select the exposure time if the data are in counts. Omit this if they are in counts/sec.
- b) It is possible to constrain the position of any of the line features in the fitting procedure. To do so, click the *Fix Line Positions* button at i') and enter the pixel positions at which you wish the features locked. It need not be all of the features.
- c) A facility is also present to attach a name to a line feature which is helpful for known lines. These names are carried through to the output data

structure. Click the *Identify Lines* button at j') and enter the names in the appropriate fields below.

- d) Control of line widths is provided at k'). Select first of all whether you wish the line widths to be permitted to vary from the initial values during the fitting or not. If not is selected, a common line width must be entered. Then chose if you wish all the lines to have the same ( but varying) width or if each line width can vary separately.
- e) At l') select the form of background shape you wish to allow. Note that if you prepare the data with no background then the fitting to no background is allowed by deactivating the *Background Options* button
- f) The way the experimental pixel count data is weighted during the fit optimisation may be chosen at m'). The *Weighted Fit* button weights a count with the square root of the count. The *Equal Weighted Fit* button imposes the same weight on the data at each pixel position.

The image shows a software control panel for line fitting. It contains several sections:

- Enter No. of Lines to Fit :** A text box containing the number '4'.
- Enter Exposure Time :** An empty text box.
- Fix Line Positions / Identify Lines:** Two checkboxes. Below them are two columns of input fields numbered 1 through 10.
- Allow Variable Line Widths :** Radio buttons for 'Yes' and 'No'.
- Fit Different Widths :** Radio buttons for 'Yes' and 'No'.
- Background Options:** A checkbox followed by radio buttons for 'Constant', 'Linear', and 'Quadratic'.
- Weighted Fit / Equal Weighted Fit:** Radio buttons for 'Weighted Fit' and 'Equal Weighted Fit'.
- Set initial conditions:** A large button at the bottom.

Arrows labeled g) through n) point to specific elements: g) to the exposure time box, h) to the 'Identify Lines' checkbox, i) to the 'Fix Line Positions' checkbox, j) to the 'Identify Lines' button, k) to the 'Fit Different Widths' radio buttons, l) to the 'Background Options' radio buttons, m) to the 'Equal Weighted Fit' radio button, and n) to the 'Set initial conditions' button.

- g) To start the setting up of the initial conditions of line positions and widths, click the large button at n'). The displayed graph changes at this point to histogram mode. The mouse cursor position on the graph screen becomes meaningful and the left and right mouse buttons active. Advisory information of the action currently expected is given above the graph depending on the processing options chosen. In general one clicks to mark the peak, left half width position and right half width position for each feature in turn. A small square marks each selected position. Finally one marks the lowest and highest levels of the background. Clicking the right button can restart the process from the beginning. After completing the required marking, the fitting optimisation takes place.
6. If there are multiple spectra in the input data set, then the fitting procedure can be made to cycle automatically through each data set in turn using the initial settings from the first fit. Activate the *Automatic Cycling* button at d)
7. Finally click the button 'Go' at e) to initiate the fitting process.
8. The figure is redisplayed with the fitted ordinary line Gaussians, the background and the satellite line compound feature superimposed in dotted outline.

9. At the base of the window, the icon for *Exit to Menu* is present. This quits the program and returns you to the ADAS series 6 menu. Remember that *Done* takes you forward to the next screen while *Cancel* takes you back to the previous screen.

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

1. As in the previous window, the full pathway to the file being analysed is shown for information. Also the *Browse comments* button is available.
2. A graph hard copy is available by activation of the *Graphical Output* button a). The File name box then becomes editable. If the output graphic file already exists and the *Replace* button has not been activated, a 'pop-up' window issues a warning.
3. A choice of output graph plotting devices is given in the Device list window at d). 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.
5. At e) output of the processing and analysis may be saved by clicking the *Passing File* button. The *Default file name* sends the output file to your *././adas/pass* directory as *adas603.pass*. Note that the output file is an IDL SAVE file structured in the manner described in section 5.1.1.2. Note that defaults are updated after each run.

ADAS604 OUTPUT OPTIONS

Data file name : /u/hps/jet\_ks1/sep\_98/avg10/ p12468\_ar16\_4580\_clean10

Browse Comments

Graphical Output Default Device

HP-GL

Enable Hard Copy  Replace

File name :

Post-script

HP-PCL

HP-GL

Text Output  Replace Default File Name

File name :

Passing File  Replace Default File Name

File name :

6. At the base of the window, the icon for *Exit to Menu* is present. This quits the program and returns you to the ADAS series 6 menu. Remember that *Done* takes you forward to the next screen while *Cancel* takes you back to the previous screen.

## Illustration

## Notes