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# ADAS605: Molecular band profile fitting

This is s new code in development.

## Background theory:

## Program steps:

These are summarised in the figure below.

Figure 7.5

## 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:

```
lstr.b0 :      0.0          lstr.eseb0:      0.0
lstr.eclb0 :   0.0          lstr.b1:          0.0
lstr.eseb1 :   0.0          lstr.eclb1:      0.0
lstr.b2 :      0.0          lstr.eseb2:      0.0
lstr.eclb2 :   0.0          lstr.w:          dblarr(10)
lstr.esew1 :   0.0          lstr.eclw1      0.0
lstr.xo :      dblarr(10)   lstr.esexo:     dblarr(10)
lstr.eclxo :   dblarr(10)   lstr.h:         dblarr(10)
lstr.eseh :    dblarr(10)   lstr.eclh:      dblarr(10)
lstr.esewv :   dblarr(10)   lstr.eclwv:     dblarr(10)
lstr.flux :    dblarr(10)   lstr.esef:      dblarr(10)
lstr.eclf :    dblarr(10)   lstr.getfit:    intarr(6)
lstr.exptime : 0.0          lstr.info:      0
lstr.header :  "          lstr.xmin:      0
lstr.xmax :    0           lstr.x:         indgen()
lstr.y :      dblarr()     lstr.ya:        dblarr()
lstr.nsize :   0.0          lstr.numline:   0
lstr.nfxl :    0           lstr.bchl:      0.0
lstr.bchr :    0.0          lstr.lineid:    strarr(10)
lstr.getxp :   intarr(6)    lstr.lineidxp:  "
lstr.bfxp :    0.0          lstr.esebfxp :  0.0

lstr.eclbfxp : 0.0          lstr.tixp:      0.0
lstr.esetixp : 0.0          lstr.ecltixp :  0.0
```

<i>lstr.iwxp</i> :	0.0	<i>lstr.eseiwxp</i> :	0.0
<i>lstr.ecliwxp</i> :	0.0	<i>lstr.angxp</i> :	0.0

with the meaning of the variables as follow:

*b0* fitted constant part of the background  
*eseb0* estimated standard error in *b0*  
*eclb0* estimated 95% confidence limit in *b0*  
*b1* fitted linear part of the background  
*eseb1* estimated standard error in *b1*  
*eclb1* estimated 95% confidence limit in *b1*  
*b2* fitted quadratic part of the background  
*eseb2* estimated standard error in *b2*  
*eclb2* estimated 95% confidence limit in *b2*  
*w* fitted line widths  
*esewl* estimated standard error in *w* (fixed)  
*eclwl* estimated 95% confidence limit in *w* (fixed)  
*x0* fitted line centroid positions  
*esexo* estimated standard error in *x0*  
*eclxo* estimated 95% confidence limit in *x0*  
*h* fitted line heights at centroid  
*eseh* estimated standard error in *h*  
*eclh* estimated 95% confidence limit in *h*  
*esewv* estimated standard error in *w* (variable)  
*eclwv* estimated 95% confidence limit in *w* (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* initial estimate of background  
*lineid* preliminary line identification labels  
*getxp* options selected for Xpaschen (see code)  
*lineidxp* Xpaschen multiplet name from list  
*bfxp* fitted magnetic field strength  
*esbfxp* 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 (Å).  
*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*?)

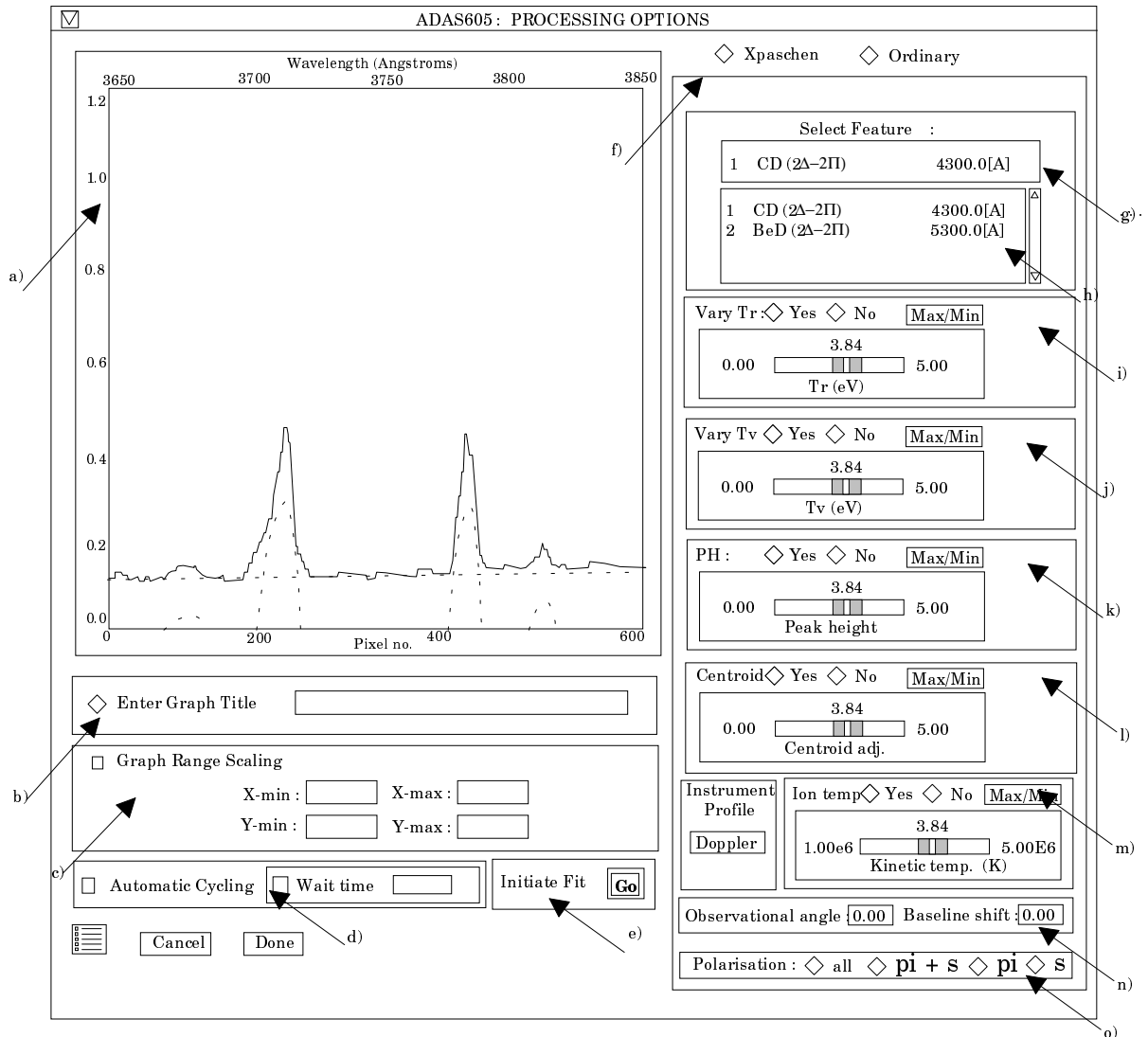
2. Data root b) shows the full pathway to the appropriate data subdirectories. Click the *Central Data* button to insert the default central ADAS pathway to *././adas/adas/arch605*. Note that there are only some sample data in this subdirectory (viz. a standard data set *'...clean'* and a processed data 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 ADAS605.

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 Zeeman/Paschen-Back feature primitive for an identified multiplet. 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 molecular feature primitive:**
  - a) The magnetic field effects have been calculated for a large number of multiplets and archived for selection. The available choice may be scrolled through in the multiplet selection widget at h) Click on a multiplet to select it. The selected multiplet is shown in the window at g).
  - b) At i), choose if the magnetic field is to be treated as a variable search parameter in the final spectrum fitting.
  - c) At j), choose if the ion temperature (eV) is to be treated as a variable search parameter in the final spectrum fitting. This parameter determines the thermal Doppler width of the components of the Zeeman/Paschen-Back multiplet.
  - d) At k), choose if the instrumental width (Angstrom) is to be treated as a variable search parameter in the final spectrum fitting. This parameter determines the Lorentzian width of the components of the Zeeman/Paschen-Back multiplet or contributes to the Voigt profile if a Doppler part is also present.
  - e) At l), choose if the multiplet centroid position (Angstrom) is to be treated as a variable search parameter in the final spectrum fitting.
  - f) At m), choose if the peak height for the multiple is to be treated as a variable search parameter in the final spectrum fitting.

- g) At n), enter the observation angle (degrees) relative to the magnetic field direction. This is not a variable parameter.
- h) In setting up the initial conditions, you can choose whether to display the whole theoretical multiplet or the component of a particular polarisation. Activate the appropriate button at o)
- i) To start the setting up of the initial conditions of line positions and widths, click the large button at p). 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. The theoretical multiplet is displayed in solid outline on the graph and the various sliders on the right at i), j), k), l), m) and n) become active. Adjust the sliders to set up your initial conditions.



### 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 consists of several stacked sections:

- Top section:** A label "Enter No. of Lines to Fit" followed by a text input field containing the number "4". An arrow labeled "g)" points to this field.
- Second section:** A label "Enter Exposure Time" followed by an empty text input field. An arrow labeled "h)" points to this field.
- Third section:** Two checkboxes: "Fix Line Positions" and "Identify Lines". Below them are two columns of input fields for line positions, numbered 1 through 10. An arrow labeled "i)" points to the "Fix Line Positions" checkbox, and an arrow labeled "j)" points to the "Identify Lines" checkbox.
- Fourth section:** A label "Allow Variable Line Widths" followed by two radio buttons: "Yes" and "No". Below it is another label "Fit Different Widths" followed by two radio buttons: "Yes" and "No". An arrow labeled "k'" points to the "No" radio button under "Fit Different Widths".
- Fifth section:** A checkbox "Background Options". Below it are three radio buttons: "Constant", "Linear", and "Quadratic". An arrow labeled "l'" points to the "Background Options" checkbox.
- Sixth section:** Two radio buttons: "Weighted Fit" and "Equal Weighted Fit". An arrow labeled "m'" points to the "Equal Weighted Fit" radio 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 Zeeman/Paschen-Back multiplet 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.

ADAS605 OUTPUT OPTIONS

Data file name /u/adas/adas/arch605/jet\_test.dat

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

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.
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**