

CAnELA

by Julio Rodríguez-García

INTRODUCTION

CAnELA

Código para el **Análisis Espectroscópico de Líneas Atómicas**
Version 1.0 (September 2012).

Julio Rodríguez-García, Manuel Rodríguez-Pascual, Rafael Mayo-García
CIEMAT – SPAIN

Contact: sci-track@ciemat.es

CAnELA is based on the code *Linefit*, developed by J. Campos, F. S. Ferrero and R. Mayo-García at Universidad Complutense de Madrid.

CAnELA is a PC program to fit spectral lines to a Voigt profile in order to make easy and accurate the measurements of some line parameters as relative intensity, height, width (Width at Half Maximum), etc. It allows user to save these parameters, set important lines for their study, load data from other sessions and make analysis for obtaining physical parameters such as transition probabilities.

The program front-out is a graphical interface. All options are activated with mouse.

CITATION

Might you use this software, please cite M. Ortiz, C. Aragón, J.A. Aguilera, J. Rodríguez-García, and R. Mayo-García. Experimental transition probabilities for spectral lines of Re II. *J. Phys. B: At. Mol. Opt. Phys.* **46**, 185702 (2013)

VERSION

This program was written with MATLAB[®], version 7.0.4.365 (R14) Service Pack 2 (January, 29, 2005). It should also work in later versions.

SUPPORTED FILES

CAnELA works with different extension files. Data are imported from *.m01* files, which are actually *csv* files, and from the *rangos_espectrales.csv* file. Both files are obtained when using the program *Espectro1*. Although users could create those files by themselves, it is highly recommended to use *Espectro1*, this way *CAnELA* will be for sure working with the appropriate data.

CAnELA exports some data to two excel files (*.xls*) and may import data from them, so it is highly recommended not to modify the original files.

1. CHOOSING IMPORTANT LINES.

A name should be written in the text box above, which will be used to name some files (for example, *ReII*).

Line values panel allows user to set some lines and their characteristics:

- Wavelength.
- Upper level energy.
- Lower level energy.
- Upper level multiplicity.
- Lower level multiplicity.
- Transition probability.

When all the parameters for one line are written, clicking on *Next* button will save them, clear the text boxes and get ready for a new line. The number at top indicates the number of the currently setting line.

The screenshot shows a 'Parameters' dialog box. At the top, there is a text input field labeled 'Enter file name: ion + ionization state (ie: ReII,ZnIV):'. Below this is a 'Line Values' panel for line 1. It contains several input fields: 'Wavelength (A):' with value 0.0, 'Upper level energy (cm-1):' with value 0.0, 'Lower level energy (cm-1):' with value 0.0, 'Upper level multiplicity (2J+1):' with value 0, 'Lower level multiplicity (2J+1):' with value 0, and 'Transition probability (s-1):' with value 0.0. At the bottom of the panel are buttons for 'Load', 'Next', and 'Done'. A 'Skip' button is located below the entire dialog box. Arrows from the text on the left point to the file name field and the 'Next' button.

When this step is finished, clicking on *Done* button will save all the parameters in an *excel* file with the name chosen plus the suffix '*_lineas*' as indicator (for example, *ReII_lineas.xls*). Then it will advance to next screen (*Fitting*).

It is also possible to load a previous parameters file by clicking on *Load* button. A dialog box will be open to choose the parameter file (**_lineas.xls*), and then will advance to next screen (*Fitting*).

Lines cannot be added to an existing file.

Warning: Loading data could take some time depending on file size.

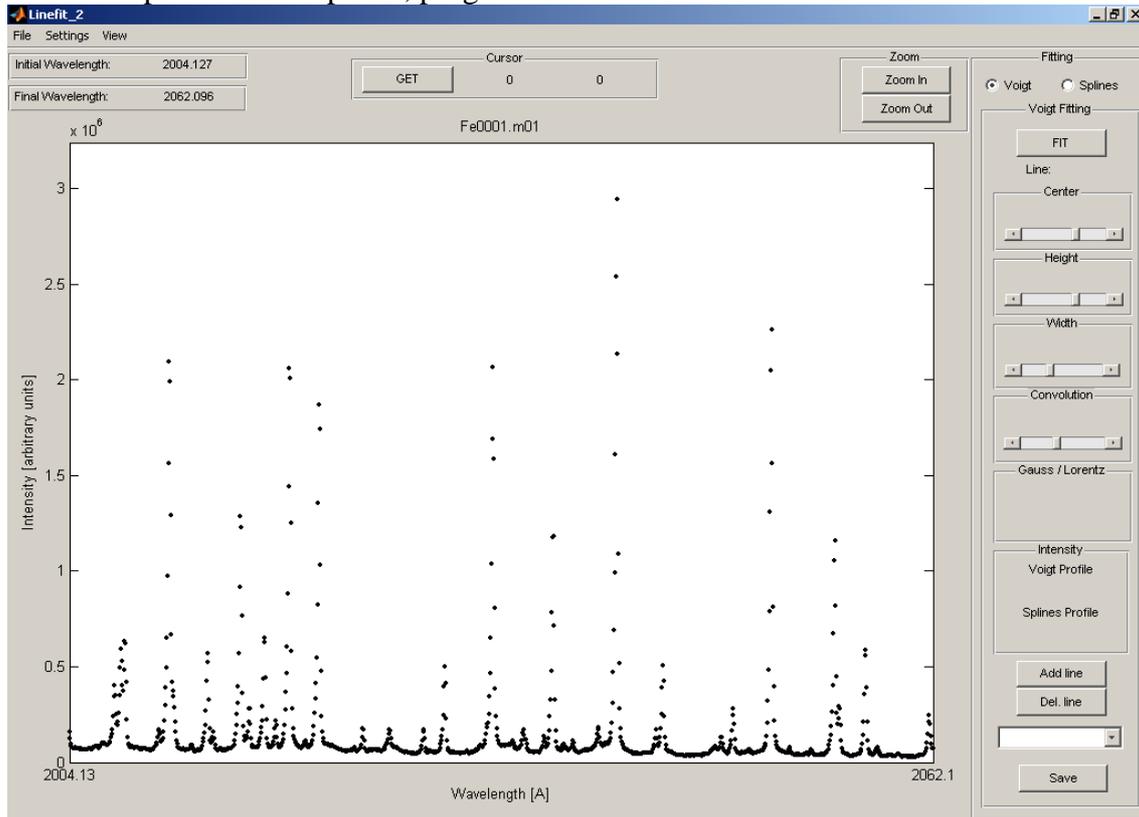
It is also possible to advance to *fitting screen* without saving or loading any data, by clicking on *Skip* button. Saving measurements will not be possible in this case. Calculus window will not be available either.

2. FITTING.

When fitting screen first appears, the only thing to do is open a file (*File>Open*), or go back to initial screen (*File>Restart*).

CANELA opens *.m01* files only, which should be CSV (comma-separated values) files, with just one column containing intensity values. In the same folder, there must be a file containing corresponding wavelength range called *rangos_espectrales.csv*. *CANELA* looks for that file automatically. If file *rangos_espectrales.csv* is not found, *CANELA* will ask user to open it.

Once the spectra file is opened, program window should look like this:



Interface.

CANELA shows, at upper-left corner, the wavelength range being displayed at the moment. It is the same as in *OX* axis, but usually with more decimals. It changes when focusing in and out.

CANELA shows the name of the opened file just above the graphic.

Cursor will indicate the coordinates of the point you click on.

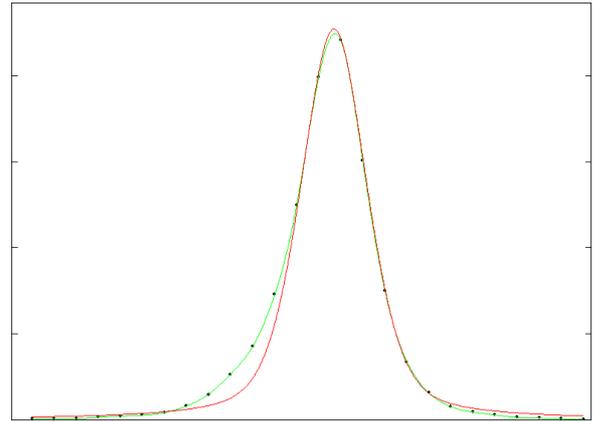
Zoom in and *zoom out* buttons will zoom in and out the figure.

- *Zoom in* waits for a click on two points to zoom (horizontally) between. *CANELA* only reads *X* coordinate, as vertical zoom is automatic.
- *Zoom out* goes back to initial range.

Fitting panel.

Fitting panel contains actually two panels inside, *Voigt* and *Splines*, but only one can be displayed at the same time. Radio buttons at top alternate between them.

It is highly recommended to zoom in the line of interest before using *FIT* button, as it will fit all data within the wavelength range on screen.



- Voigt panel:

Voigt panel fits the data to a *Voigt profile* (red line).

It also shows a **non-modifiable spline fitting** (green line), just as help. The slide bars in the panel allow modifying the Voigt profile parameters, so it best fits to the data.

FIT button starts the fitting routine, and creates a first approximation choosing the highest point as maximum and calculating the width. The fitting can be restarted by clicking on *FIT* button again.

The number just under the *FIT* button indicates the selected/active line.

The four slide bars modify the corresponding parameters of the selected line.

Gauss/Lorentz box shows the contribution of each of the profiles to the *Voigt profile*. It changes when *convolution* value is modified.

Intensity box shows the intensity (integral under the curve).

Splines profile intensity shows the total intensity corresponding to *splines* (green) curve.

Voigt profile intensity shows the intensity of the selected line. It is NOT the total intensity.

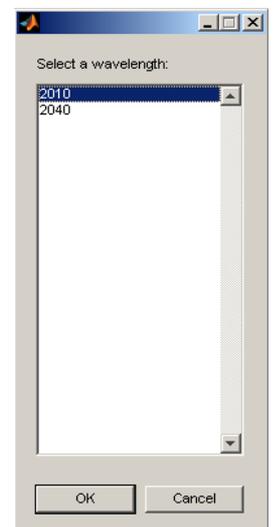
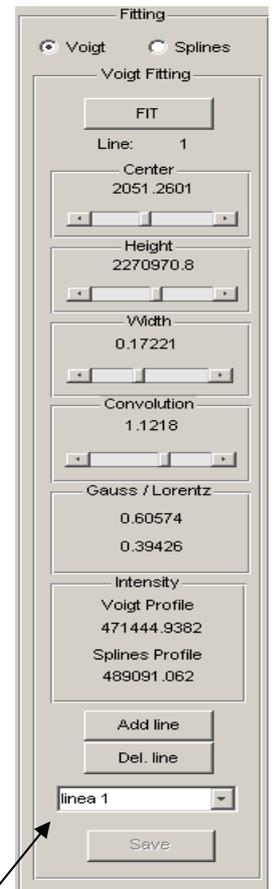
Add line button adds another line to the fitting, asking for a point to establish the maximum. The *Voigt profile* (red line) fitting will be the sum of each line added. As many lines as needed can be added.

Del. line deletes selected line. This operation cannot be undone.

Del. line should not be used to delete *line 1*. Instead, *FIT* button should be used: so fitting starts again.

Pop-up menu allows choosing the line you want to work with.

Save button will save some of the parameters of selected line: *Wavelength*, *Intensity*, *Width*, *Gauss and Lorentz fractions* and *Height*. These parameters will be saved in an excel file called with the name chosen in first screen plus the suffix *_medidas* (for example, *ReII_medicadas.xls*). First, it is necessary to choose the real wavelength from the ones listed on the pop-up window, corresponding to the ones indicated on first screen.



- Spline panel:

Spline panel fits the data to a *cubic spline interpolant*.

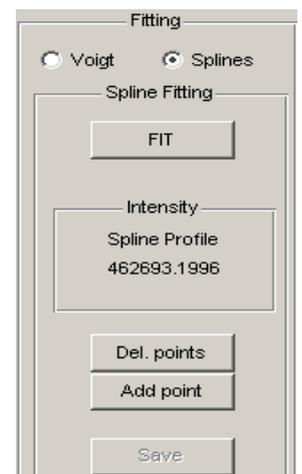
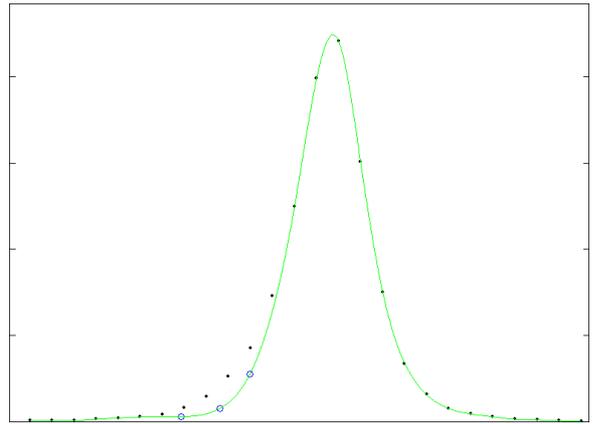
FIT button works as *FIT* button in *Voigt profile* panel.

Intensity box shows the total intensity of the *spline profile*.

Del. points button deletes all the points within a horizontal segment chosen with two mouse clicks. The points will still be visible, but the *spline profile* will not fit to them.

Add point button adds a point by clicking on the plot, so the *spline profile* fits to it too. As many points as needed can be added. The added points will have a small blue circle around them, so they can be distinguished. These points can also be deleted with *Del. points* button.

Save button works as the one on *Voigt profile* panel, but this time the only parameters saved are *Wavelength and Intensity*. Again, it is necessary to choose the real wavelength from the ones listed on the pop-up window.



Menu bar.

- *File:*

Open opens a new spectra file.

Reset undo any change done in the opened file.

Restart gets *CANELA* back to initial screen.

- *Settings:*

Background allows subtracting background noise from your data.

Set defines the background line by choosing two points.

On and *Off* options turn on and off the background correction.

Peaks finds every peak on the spectra.

On and *Off* options turn on and off the peaks.

Correction introduces a correction to the data: $Intensity \cdot C^{factor}$. The value *C* is a constant defined by user (when asked), and *factor* is different for each wavelength. *CANELA* will ask for the file containing the correction data.

Set imports the data.

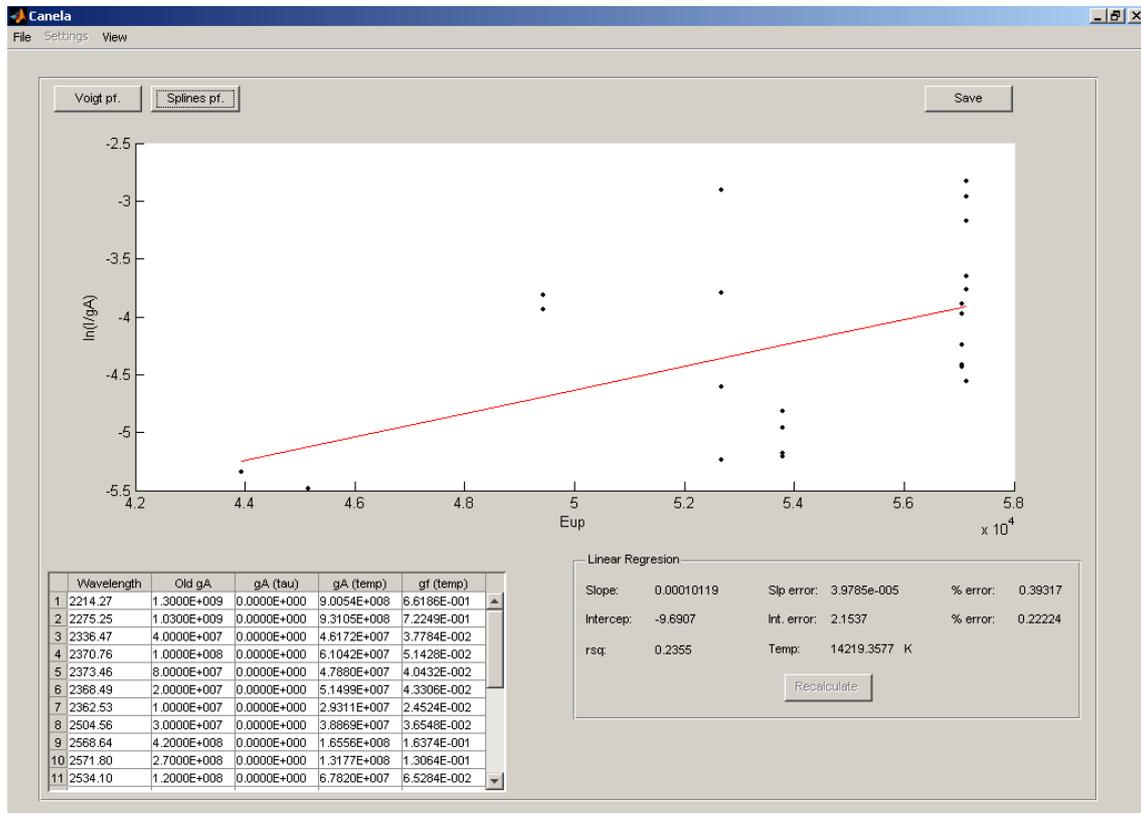
On and *Off* options turn on and off the correction.

- *View:*

On *View* menu it is possible to alternate through program windows: *Fitting* or *Calculus*.

3. CALCULATING NEW PARAMETERS.

This screen calculates *transition probability*, *oscillator strength* and *temperature*, from measurements obtained with either *Voigt* or *Splines* fitting method.



CANELA will ask then if all lines should be used, or just a number of them, chosen by user. Obviously gA parameter is needed, but not for every line: only lines with non zero values of gA are used.

When calculating gA (τ), the same process is followed: if any line has a zero value for τ , its gA (τ) will not be calculated.

If gA (τ) values are calculated, it is possible to recalculate the slope using these values instead of old gA values, clicking on *recalculate* button, inside *linear regression* box.

Both gA table and *linear regression* values can be saved in **_medidas.xls* file, in a new sheet called gA , by clicking on *save* button on upper-right corner.

When changing to *calculus* screen, CANELA will load data from corresponding file **_medidas.xls*, which should be on same folder than **_lineas.xls*. In case the file is not found, an error message will be shown, and no further actions will be taken.